ASSESSMENT OF DISCRIMINATION OF MAFIC ROCKS USING TRACE ELEMENT SYSTEMATICS WITH MACHINE LEARNING

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ABSTRACT

ASSESSMENT OF DISCRIMINATION OF MAFIC ROCKS USING TRACE ELEMENT SYSTEMATICS WITH MACHINE LEARNING

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Having an important role in the elucidation of the evolution of ancient oceans and related continental fragments, the determination of original tectonic settings of ancient igneous rocks is an essential part of the geodynamic inferences. Geochemical classification of mafic rocks is important for the tectono-magmatic discrimination of igneous rocks especially when geological information is insufficient as the link of the igneous rocks to their original tectonic setting had been erased due to large scale events.

Starting from 1960s, first traditional methods (functions of elements or element ratios, bivariate and ternary diagrams of elements or element ratios), and then, recently, modern methods such as decision trees, support vector machines, sparse multinomial regression and random forest have been applied to develop tectono-magmatic discrimination methods.

The purpose of this study is to assess new and better classification methods which are both statistically and geochemically rigorous using trace element systematics with decision tree learning, an effective machine learning method for classification. Dataset included a large number of samples well distributed through different tectonic settings (continental arcs, continental within-plates, mid-oceanic ridges, oceanic arcs, oceanic back-arc basins, oceanic islands and oceanic plateaus) as classes. Data is gathered from high quality articles which is known to follow accurate geochemical sampling procedures and have their samples analyzed in internationally accredited and trustworthy laboratories. Only element ratios have been used as features in order to increase the successful applicability of constructed decision trees to external datasets.

With this study, successful decision trees with their alternatives are proposed for the tectono-magmatic discrimination between (1) subduction and non-subduction settings, (2) arc-related and back-arc-related settings within subduction settings, (3) oceanic arcs and continental arcs within arc-related settings, (4) oceanic and continental settings within subduction settings, (5) oceanic arcs and oceanic back-arcs within subduction-related oceanic settings, (6) mid-oceanic ridges + oceanic plateaus and oceanic islands + continental within-plates within non-subduction settings, (7) mid-oceanic ridges and oceanic plateaus within non-subduction settings and (8) oceanic islands and continental within-plates within non-subduction settings.

Keywords: Decision trees, machine learning, tectonic discrimination, mafic rocks, trace elements

ÖZ

MAFİK KAYAÇLARIN AYIRDIMLANMASININ ESER ELEMENT SİSTEMATİĞİ KULLANILARAK MAKİNE ÖĞRENİMİ İLE DEĞERLENDİRİLMESİ

Öztürk, Mehmet Sinan
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Eski magmatik kayaçların original tektonik ortamlarının belirlenmesi, eski okyanusların ve ilgili kıta parçalarının evriminin aydınlatılmasında önemli bir rol oynamakla birlikte; jeodinamik çıkarımların yapılması açısından önemli bir konudur. Mafik kayaçların jeokimyasal sınıflandırması, özellikle kayaç ile original tektonik ortamı arasındaki bağlantının büyük ölçekli olayların etkisiyle silindiği ve yeterli jeolojik bilginin mevcut olmadığı durumlarda, magmatik kayaçların tektono-magmatik olarak ayırdımlanması için önemli hale gelmektedir.

1960'lı yıllardan başlayarak, tektono-magmatik ayırdımlama yöntemleri geliştirmek amacıyla, önce geleneksel yöntemler (element veya element oranlarının kullanıldığı fonksiyonlar, iki veya üç değişkenli diyagramlar) ve daha sonra ise, özellikle son zamanlarda karar ağaçları, destek vektör makineleri, seyrek multinomial regresyon ve rastgele orman gibi modern yöntemler kullanılmıştır.

Bu çalışmanın amacı, eser element sistematiği ile birlikte sınıflandırmalar için etkin bir makine öğrenimi yöntemi olan karar ağacı öğrenmesini kullanarak hem istatistiksel hem de jeokimyasal açıdan daha titiz, daha yeni ve daha iyi sınıflandırma yöntemleri önermektir. Çalışmada kullanılan verisetinde, sınıflar olarak farklı tektonik ortamlara (kıtasal yay, kıta içi tabakaları, okyanus ortası sırtları, oknayus yayları, okyanus yay

arkası havzaları, okyanus adaları ve okyanus platoları) ait iyi dağılım gösteren çok sayıda numune içermektedir. Veri, doğru jeokimyasal numuneleme prosedürleri takip edilerek örneklenen ve uluslararası akreditasyona sahip güvenilir laboratuvarlarda analiz edilmiş numunelerin kullanıldığı yüksek kaliteli makalelerden elde edilmiştir. Sınıflandırmada, oluşturulan karar ağaçlarının harici very setlerine de başarıyla uygulanabilmesi amacıyla, parameter olarak sadece element oranları kullanılmıştır.

Bu çalışma ile, (1) yitim zonlarında yer alan ve yer almayan tektonik ortamlar, (2) yitim zonlarında, yay içerisinde veya yay gerisinde bulunan tektonik ortamlar, (3) yay içerisinde yer alan okyanus yayları (OA) ve karasal yaylar (CA), (4) yitim zonlarında okyanusal ortama ait ve karasal ortama ait tektonik ortamlar, (5) okyanusal ortama ait yitim zonlarında yay içerisinde (OA) veya yay gerisinde (OBAB) yer alan tektonik ortamlar, (6) yitim zonlarında yer almayan tektonik ortamlar arasında okyanus ortası sırtı ve okyanus platosu (MOR ve OP) ile okyanus adası ve karasal kıta içi (OI ve CWP), (7) okyanus ortası sırtı (MOR) ve okyanus platosu (OP) ile (8) okyanus adası (OI) ve karasal kıta içi (CWP) tektonik ortamlarını birbirinden başarıyla ayırdımlamak amacıyla alternatifleri ile birlikte, karar ağaçları oluşturulmuş ve önerilmiştir.

Anahtar Kelimeler: Karar ağaçları, makine öğrenimi, tektonik ayırdımlama, mafik kayaçlar, eser elementler

To my wife, Evrim Öztürk;

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ABBREVIATIONS

AUC	Area Under ROC Curve
BAB	Back-Arc Basin
BABB	Back-Arc Basin Basalts
CA	Continental Arc
CL.ACC.	Classification Accuracy
CRB	Continental Rift Basalt
CWP	Continental Within-Plate
DF	Discriminant Function
DT	Decision Tree
E-MORB	Enriched Mid-Oceanic Ridge Basalts
FC	Fractional Crystallization
FN	False Negative
FP	False Positive
GEOROC	Geochemistry of Rocks of the Oceans and Continents
HFSE	High-Field Strength Elements
HREE	Heavy Rare-Earth Elements
IAB	Island-Arc Basalts
ICP-MS	Inductively-Coupled Plasma Mass Spectrometry
IGBA	Igneous Database

INAA	Instrumental Neutron Activation Analysis
LDA	Linear Discriminant Analysis
LKT	Low-K Tholeiites
LREE	Light Rare-Earth Elements
MOR	Mid-Ocean Ridge
NONSUB	Non-Subduction
N-MORB	Normal Mid-Oceanic Ridge Basalts
OA	Oceanic Arc
OBAB	Oceanic Back-Arc Basin
OI	Oceanic Island
OIB	Ocean Island Basalts
OP	Oceanic Plateau
QA/QC	Quality Assurance / Quality Control
PCB	Basalts of Post-Collisional Setting
PetDB	Petrological Database of the Ocean Floor
REE	Rare Earth Elements
ROC	Receiver Operating Characteristics
SCLM	Subcontinental Lithospheric Mantle
SMR	Sparse Multinomial Regression
SSZ	Supra-Subduction Zone
SUB	Subduction
SVM	Support Vector Machines

TN	True Negative
TP	True Positive
WPB	Within-Plate Basalts
XRF	X-ray Fluorescence Spectrometry

CHAPTER 1

INTRODUCTION

1.1. Purpose and Scope

The determination of original tectonic settings of ancient igneous rocks is an essential part of the geodynamic inferences since it plays an important role in the elucidation of the evolution of ancient oceans and related continental fragments. As a natural consequence of plate tectonics, the Earth's lithospheric plates go through the Wilson cycles, which ends up with the destruction of oceanic lithosphere, and eventually the collisional orogenesis. It is not surprising that these large-scale events may have totally erased the link of the igneous rocks to their original position/setting. The fragmentation and slicing are very effective in the orogenic systems so that most oceanic- and continent-derived pieces occur as tectonic slices or blocks within the subduction-accretion complexes and mélanges. Thus, tectono-magmatic discrimination of igneous rocks, especially within such occurrences has always been an important problem to solve when relevant geological information is insufficient. In this regard, the geochemical features of rocks are of critical importance (Pearce and Cann, 1973).

On the third phase of geochemistry, which begins with the development of new qualitative and quantitative geochemical methods; new definitions, such as abundance, accuracy, and precision, have been released and gained importance. The true representation of rocks by the sample became much more critical along with these definitions. Measurement of accuracy with the use of standard samples was probably the first steps of today's quality assurance and quality control (QA/QC) procedures. Shaw and Bankier (1954) emphasized the importance of statistics in geochemistry as the best technique for handling a large amount of geochemical data in the literature.

They applied several statistical evaluation methods such as F-test and modified t-test for the diabases from Ontario and stated that the application of statistical methods could be very important for geochemists, especially related to the distributions of observations in geochemistry.

The idea (Ahrens, 1954a, 1954b; Chayes, 1954) that deals with any connection between the nature and chemical composition of rocks initially focused on the distribution of elements within igneous rocks. Ahrens (1954a) examined the chemical composition of diabases and granites from different locations such as New England and Ontario with a wide range of chemical properties and evaluated the frequency distributions of thirteen elements (K, Rb, Cs, F, Sc, Zr, Cr, Co, La, Pb, Mo, Ga, and V). He stated that the concentration of these elements shows a log-normal distribution in a specific igneous rock; hence, they require log-transformation in order to compare the dispersion of different elements and make predictions about the nature of igneous rocks. Chayes (1954), on the other hand, suggested that log-normal distribution would only be possible for trace and minor elements but not for major elements in crystalline rocks. Ahrens (1954b) presented more examples for the distributions of elements in granites, diabases, and muscovites and emphasized three elements for granites: Ga (small dispersion), Zr (moderate dispersion) and Cr (extreme dispersion). Ahrens (1954b) evaluated the distribution of elemental ratios (K/Rb, Rb_2O/TiO_2 and Sr/Ca) for the first time and also examined the relationship between the arithmetic mean/geometric mean ratio and the magnitude of dispersion in order to support the similar findings with the previous study.

Discrimination methods have not only been applied in order to discriminate original tectonic settings of basalts and other volcanic rocks but for some other reasons such as rock classification (Kuno, 1960; Kushiro and Kuno, 1963; Streckeisen, 1967; Winchester and Floyd, 1977; Barker, 1983; Ewart, 1982; Le Bas et al., 1986), rock series discrimination based on various factors such as alkalinity (Chayes, 1966; Irvine and Baragar, 1971; Miyashiro, 1975; Miyashiro and Shido, 1975; Peccerillo and Taylor, 1976; Floyd and Winchester, 1975, Hastie et al., 2007), oceanic-continental separation (Ahrens, 1954a, 1954b, Chayes, 1964, 1965; Chayes and Velde, 1965), and nature of magma sources (Pearce and Stern, 2006). Apart from basic igneous rocks, tectonomagmatic discrimination methods have also been applied for other type of rocks such as intermediate or acidic rocks (Taylor and White, 1966; Arth, 1979; Bailey, 1981; Pearce et al., 1984; Whalen et al., 1987; Eby, 1992; Gorton and Schandl, 2000; Pandarinath, 2008; Verma et al., 2012; Verma and Verma, 2013; Verma and Oliveira, 2013; Verma et al., 2013; Verma et al., 2015), or sedimentary rocks (Roser and Korsch, 1986; Bhatia and Crook, 1986; Amstrong-Altrin and Verma, 2005; Verma and Altrin, 2013 and Verma and Altrin, 2016). Rocks have also been discriminated not only based on their geochemistry but on their mineralogy (Morimito, 1988).

Kuno (1960) classified basaltic rocks under three groups: tholeiites, high-alumina basalts, and alkali basalts. Kushiro and Kuno (1963), on the other hand, modified this classification using mantle norm calculations and major element chemistry of rocks. They plotted samples in binary diagrams of Na_2O+K_2O vs CaO+MgO and Na_2O+K_2O vs SiO_2 in order to discriminate different types of basalts from each other visually. They did not consider the tectonic discrimination of igneous rocks but using binary diagrams for the visual representation for classification of basalts guided other researchers to apply similar methods in tectonic discrimination of igneous rocks.

The idea that the magmas from different tectonic settings such as volcanic arcs, back-arcs, ocean floors or within-plates may be discriminated through the differences in their chemistry was first pioneered by Pearce and Cann (1971, 1973); but before them, Chayes and Velde (1965) had already attempted to distinguish two basalt types of island arcs and ocean islands from each other just by using discrimination functions of major elements (Verma, 2010).

The concept of tectono-magmatic discrimination is simply based on the comparison of previously determined element concentrations or ratios in the rocks of unknown tectonic setting with those of known tectonic setting (Pearce and Cann, 1973). Most of these tectono-magmatic discrimination methods have been designed for basic and ultrabasic rocks with $SiO_2 < 52\%$ (Rivera-Gómez and Verma, 2016). However, there are also fewer diagrams for intermediate or acidic rocks with $SiO_2 > 52\%$ or even sedimentary rocks (Bailey, 1981; Bhatia, 1983; Bhatia and Crook, 1986; Roser and Korsch, 1986; Gorton and Schandl, 2000; Dare et al., 2009).

From these methods, traditional tectono-magmatic discrimination diagrams (bivariate or ternary) are well-known and highly preferred by the researchers even today. Especially, ternary diagrams have the major advantage of visualizing three variables in two dimensions, providing visibility of relative proportions of all variables in a single diagram (Verma, 2017). Usually, traditional discrimination diagrams are easy to use; but, despite their advantage of visualizing capacity, they are considered to be fairly inaccurate (Vermeesch, 2006a). Based on the application of traditional diagrams to a variety of tectonic settings by several researchers (eg. Li, 2015), it was concluded that they are not functioning effectively as they do not provide high success rates (Verma, 2010), especially when used for tectono-magmatic discrimination of hydrothermally altered or highly weathered rocks or of older, complex or transitional settings (Rivera-Gómez and Verma, 2016). There are also some inconsistencies related to magma mixing, crustal contamination, degree of partial melting, and mantle versus crustal origin (Verma, 2017). Many discrimination diagrams are not statistically rigorous for several reasons such as their decision boundaries are drawn by eye (Vermeesch, 2006a). They violate the basic assumption of randomness and the normal distribution of the plotted variables (Verma, 2015). Another important defect of these diagrams is the use of a limited database for the construction of these diagrams (Verma, 2017). Diagrams are created using only a limited amount of samples of a certain sampling area, which limits users to classify only data from similar tectonic settings. They can also discriminate only a few (two or three) tectonic settings (Agrawal, 1999; Agrawal and Verma, 2007; Verma, 2010). The existence of overlapped regions with combinations of two or more tectonic settings in a single decision field prevents a complete classification. Unclassified regions in ternary diagrams are another problem, which returns no result for samples plotting on these regions. For traditional discrimination diagrams, closure (constant sum) is another problem (Chayes, 1960, 1971; Aitchison, 1983, 1984, 1986, Agrawal and Verma, 2007) and is not generally considered carefully (Chayes, 1971; Aitchison, 1986; Woronow and Love, 1990). Diagrams are also vulnerable to the existence of missing data as their success ratio falls drastically (Vermeesch, 2006a).

Discrimination diagrams are highly preferred as they do not require complicated discriminant methods. Since the first use of discrimination diagrams in order to classify different tectonic settings by Pearce and Cann (1973), a variety of discrimination diagrams have been proposed by different authors. For having the major advantage of their visualizing capacity in two dimensions, these diagrams have been frequently used by both petrologists and non-petrologist for many years (Verma, 2017). The researchers proposing the first tectonic discrimination diagrams in the early 1970s, had access only to a limited number of trace elements that could be analysed with analytical methods such as X-ray Fluorescence Spectrometry (XRF) and Instrumental Neutron Activation Analysis (INAA) with reasonable accuracy. Mobile elements such as Rb, Ba, and Sr restricted or eliminated the use of these diagrams for altered samples. However, with the development of inductively- coupled plasma mass spectrometry (ICP-MS) in 1970s, it became possible to analyse a wide spectrum of trace elements, with lower detection limits and higher analytical accuracy, allowing researchers such as Pearce, Wood and Shervais to choose elemental ratios/groups that best reflect the elemental fractionation for the crustal/mantle processes operating within diverse tectonic settings. It has been approved that magma compositions from different tectonic settings have a wide range of distributions. The number of analyses of basalts has increased drastically obtaining researchers to have access to a huge database of analytical data (Li, 2015).

Because of the continuous debate for the application of traditional discrimination methods as a result of low success ratios, researchers are encouraged to search for newer robust discrimination methods such as advance of new multi-dimensional discrimination diagrams, which is based on linear discriminant analysis (LDA) of log-transformed ratios of major elements and selected relatively immobile major and trace elements (eg. Agrawal et al., 2004 using major elements; Verma et al.,2006 using log-transformed ratios of major elements; Agrawal et al., 2008; Verma et al.,2011 using log-transformed ratios of relatively immobile trace elements) or machine learning methods such as decision trees (Vermeesch, 2006a), random forests, support vector machines (SVM) or sparse multinomial regression (SMR) (Ueki, 2017) or modification of existing traditional discrimination diagrams by application of linear discriminant analysis (LDA) (Vermeesch, 2006b).

For the development of multi-dimensional discrimination diagrams, compositional data have been handled by some studies (Aitchison, 1981, 1983, 1984, 1986; Egozcue, 2003). These studies suggested log-ratio transformation for the solution of problems arising from compositional data. Caution is required while handling compositional data through conventional statistical methods (eg. Pearson, 1897; Chayes, 1960; 1971; Aitchison, 1983, 1984; 1986; Rollinson, 1993, Egozcue et al., 2003; Pawlowsky-Glahn and Egozcue, 2006; Agrawal and Verma, 2007; Buccianti, 2013; Verma, 2015). For statistical handling of compositional data, Aitchison (1981, 1984, 1986) developed a solution in terms of log-transformation prior to the application of conventional statistical tools (Verma et al., 2016). Later, Egozcue et al. (2003) provided another type of log-ratio transformation (Verma, 2015). Data is normally distributed as long as multivariate discordant outliers are detected and eliminated (Verma, 2015). Additive log-ratio transformation of Aitchison (1981) was used by several researchers (Verma et al., 2006; Agrawal et al., 2008; Verma and Agrawal, 2011) for basic and ultrabasic igneous rocks. Development of multi-dimensional discrimination diagrams generally follows the order of construction of training databases, log-ratio transformations, discordant outlier detection and elimination, application of statistical tests for the choice of elements, application of multi-variate technique of linear discriminant analysis, and determination of probability-based tectonic field boundary equations. Probability values for individual samples were calculated using methods of Agrawal (1999) and Verma and Agrawal (2011) and used to decide the tectonic fields in which a given sample plots (Verma, 2017). One of the disadvantages of multi-dimensional discrimination diagrams is the use of complex equations that have to be solved for these probability calculations. The development of a computer program is necessary for an efficient, accurate and routine application of these diagrams (Verma et al., 2016).

Several discriminant-function based multi-dimensional discrimination diagrams (Agrawal et al., 2004, 2008; Verma et al., 2006; Verma and Agrawal, 2011) are proposed to identify tectonic settings. These diagrams generally focused on the discrimination of five tectonic settings: island arcs, continental arcs, continental rifts, oceanic islands, and continental collisions (Verma, 2017). In general, binary and ternary discrimination diagrams are found to be less useful than multi-dimensional diagrams (Verma, 2017; Gomez and Verma, 2016; Verma and Oliveira, 2015; Verma et al., 2015; Li, 2015, Pandarinath, 2014; Pandarinath and Verma, 2013, Verma et al., 2012; Verma, 2010; Sheth, 2008). Indeed, Verma (2010) concluded that newer methods such as the multidimensional diagrams worked satisfactorily with a high success rate as a result of his evaluation of all discrimination diagrams through an extensive database. The success rate of discrimination diagrams falls drastically when used with granitic or felsic rocks and sedimentary rocks (Rivera-Gómez and Verma, 2016).

Application of decision trees in the development of tectono-magmatic discrimination methods is limited to Vermeesch (2006a), which only discriminated three tectonic settings (island arcs, mid-ocean ridges and ocean islands). The use of mobile elements and isotope ratios for decision trees decreased their efficiency and applicability. Therefore, new decision tree alternatives are required using an extensive geochemical database in order to discriminate a variety of tectonic settings (more than six).

This study focuses on finding a more effective way for the tectono-magmatic discrimination methods of basic igneous rocks (basalts, trachybasalts, picrobasalts, foidites and tephrites/basanites). For this purpose, it is aimed first to assess the trace element systematics of the basic igneous rocks from different tectonic settings. This is followed by the integration of the decision tree algorithm on the selected geochemical features of these rocks. Although the main focus remains on the rocks of basic chemical composition, extensive external datasets of intermediate/acidic igneous rocks (basaltic andesites, basaltic trachyandesites, phonotephrites, andesites, trachyandesites, tephriphonolites, phonolites, trachytes/trachydacites, dacites and rhyolites along with basalts, trachybasalts, picrobasalts, foidites and tephrites/basanites) are also be used in order to evaluate the applicability of provided decision trees for the more evolved compositions.

1.2. Review of Tectono-Magmatic Discrimination Methods of Basic Igneous Rocks

In order to discriminate basalts and other basic igneous rocks based on their original tectono-magmatic settings, following the use of a single discriminating criteria of elements (such as Chayes, 1964; Chayes, 1965) or functions with the combination of elements (such as Chayes and Velde, 1965), the traditional discrimination diagrams (bivariate or ternary) have first been proposed by several researchers (bivariate: Pearce and Gale, 1977; Pearce and Norry, 1979; Shervais, 1982; Pearce, 1982; ternary: Pearce and Cann, 1973; Pearce et al., 1977; Wood, 1980; Mullen, 1983; Meschede, 1986; Cabanis and Lecolle, 1989). Discriminating functions with a combination of elements or element ratios have also been applied in traditional discrimination diagrams by several researchers (Pearce, 1976; Butler and Woronow, 1986).

Traditional discrimination diagrams are still in use for nearly four decades in order to classify different tectono-magmatic settings such as island arc, continental rift, ocean floor, ocean island and mid-oceanic ridge on the basis of their chemistry and their effectiveness is frequently tested and evaluated by many other researchers (Verma, 2010, 2016; Li, 2015; Gomes and Verma, 2016; Verma, 2017).

These diagrams have been followed by multi-dimensional discriminant function diagrams with the implementation of statistical methods such as log-ratio transformation and linear discriminant analysis (Agrawal et al., 2004; Verma et al., 2006; Agrawal et al., 2008) or with the implementation of machine learning methods such as decision tree learning (Vermeesch, 2006a) or support vector machines (SVM), random forest and sparse multinomial regression (SMR) approaches (Ueki et al., 2017).

1.2.1. Elements as Discriminating Criteria

Chayes (1964) and Chayes (1965) applied a single element's concentration (TiO_2) as a discriminating criterion.

Chayes (1964) searched through an extensive database of oceanic island basalts (Atlantic, Indian and Pacific) and circumoceanic basalts (Japan, South Pacific, South America, Central America, Mexico, Alaska and Aleutian Chain, Kamchatka and Kurile Chain and Indonesia) on the basis of their chemistry and included 834 analyses of oceanic and 1003 analyses of circumoceanic rocks.

He evaluated the sample distributions of Thornton-Tuttle index and proposed a classification based on TiO_2 content and the degree of alkalinity (relative to SiO_2 and Al_2O_3) and came up with a statement that oceanic basalts are normatively alkaline and contain more than 1.75% TiO_2 content in discrimination of oceanic and circumoceanic basalts from each other.

Chayes (1965) examined the distribution of elements for oceanic and circumoceanic basalts and determined that the average TiO_2 content of circumoceanic and ocean island basalts are 1.15% and 3.05% with respectively. Although there are similar differences through other oxides, they are highly overlapped.

He also stated that TiO_2 content of rocks along with alkalinity is a discriminating factor between oceanic and circumoceanic basalts with a discrimination value of

1.75%. Out of 360 circumoceanic basalts, 32 samples and out of 497 oceanic basalts, 29 samples have been misclassified based on TiO_2 content.

1.2.2. Traditional Bivariate Diagrams

Traditional bivariate diagrams are generally based on immobile or high field strength elements such as Ti, Zr, Nb, Y, and V, providing an advantage for these diagrams to be applied for discrimination of altered samples.

Pearce and Cann (1973) published a binary diagram in order to discriminate ocean-floor basalts, low-potassium tholeiites and calc-alkali basalts from island arcs using Ti and Zr. The Ti-Zr diagram (Figure 1.1) is applicable to the altered samples. Ocean-floor basalts (regions B and D), low-K tholeiites (regions A and B) and calc-alkali basalts (regions B and C) are discriminated with this diagram.

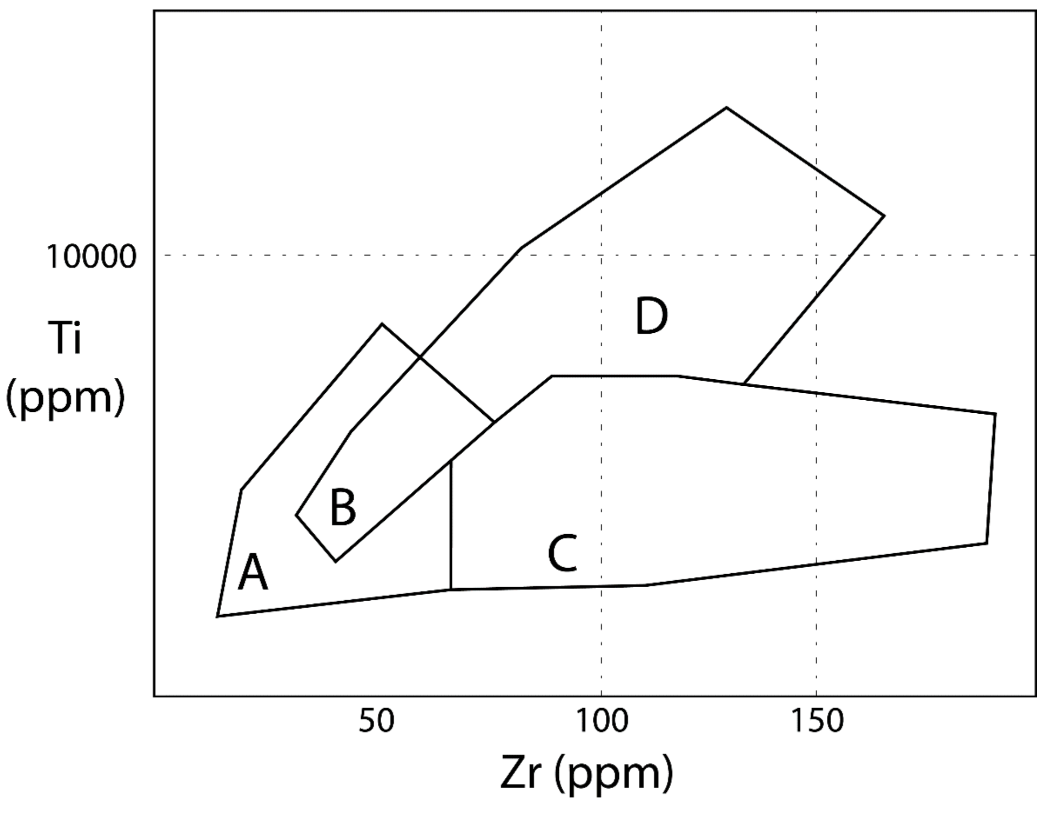

Figure 1.1. Bivariate diagram of Ti versus Zr by Pearce and Cann (1973)

Dilek and Furnes (2009) recently published another bivariate diagram of Ti versus Zr (Figure 1.2) in order to discriminate arc tholeiites, boninites, and mid-oceanic ridge basalts from each other.

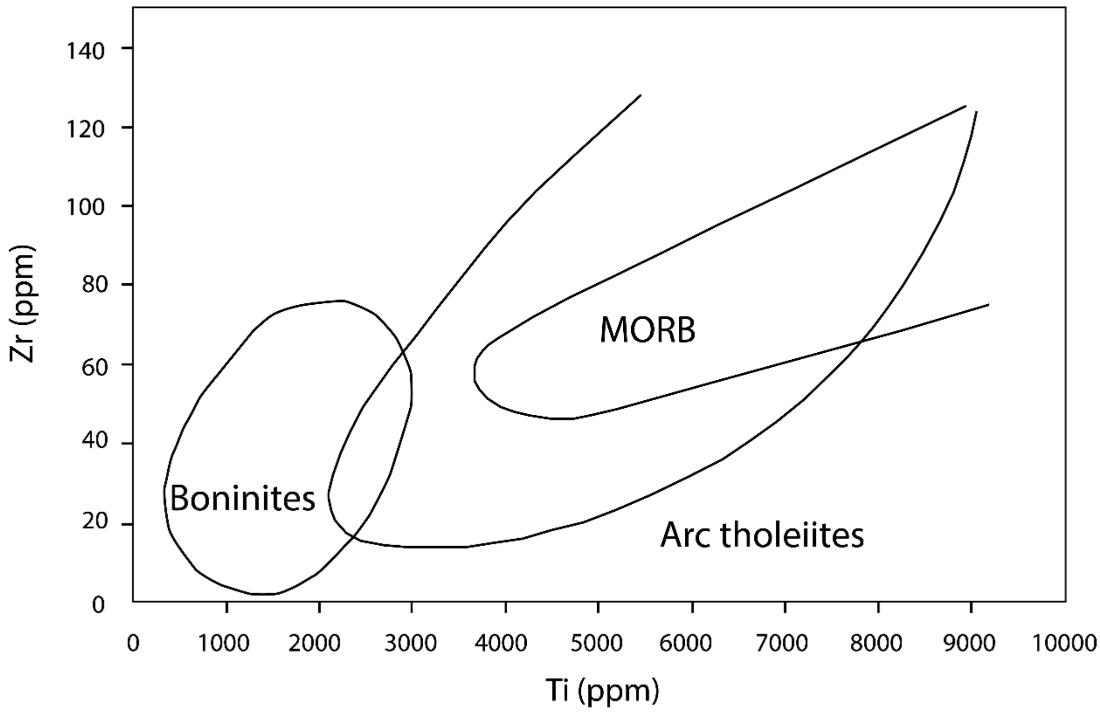

Figure 1.2. Bivariate diagram of Ti versus Zr by Dilek and Furnes (2009)

Pearce (1975) studied four suites of volcanic rocks in Cyprus to investigate their past tectonic environments. Pearce (1975) published a new tectonic discrimination diagram based on Cr along with Ti (Figure 1.3) as a modified version of Pearce and Cann (1973). He studied volcanic rocks of Cyprus to understand the tectonic history of the island. The Troodos Massif is an ophiolite complex with a sequence of, from bottom to top (Moores and Vine, 1971), a plutonic complex (Böttcher, 1969), sheeted intrusive complex, lower pillow lavas, upper pillow lavas and pelagic sediments (Robertson and Hudson, 1973). These rocks have features of both ocean-floor and island-arc. Pearce (1975) used 6 samples of lower pillow lavas, 13 samples of diabases and 9 samples of upper pillow lavas from Troodos Massif in Cyprus.

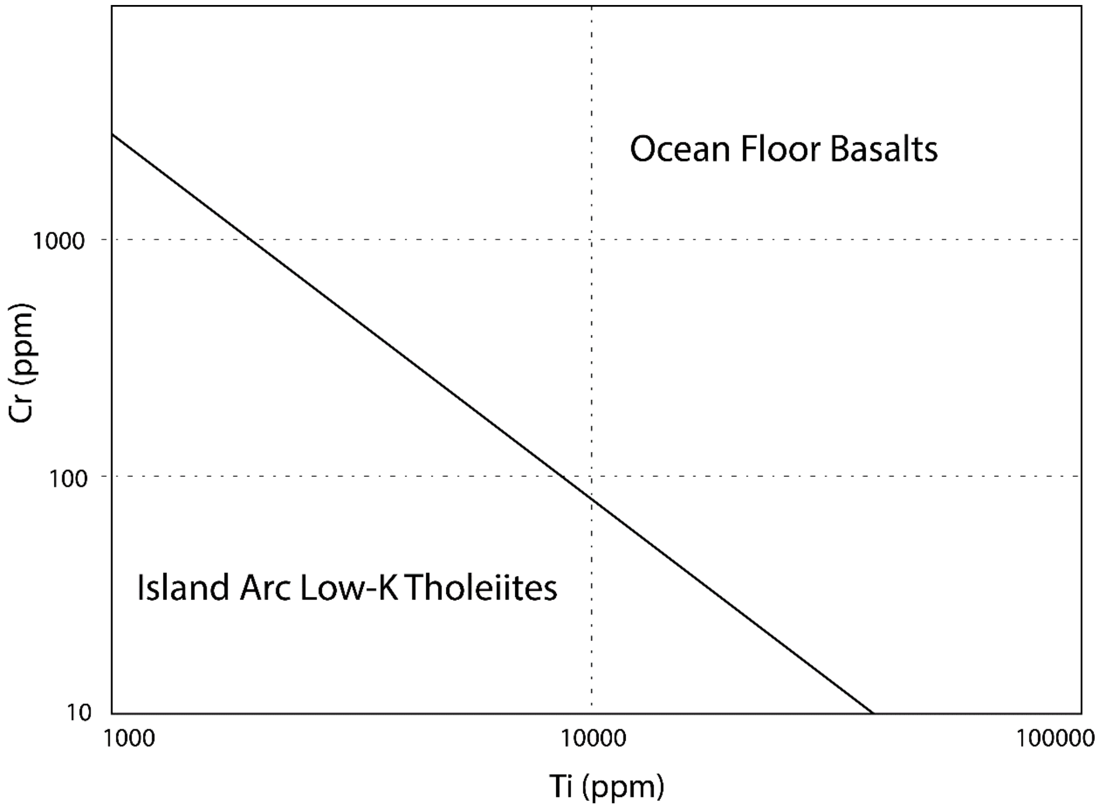

Figure 1.3. Bivariate diagram of Pearce (1975)

Pearce (1975) first applied Ti-Zr-Y and Ti-Zr diagrams (Pearce and Cann, 1971, 1973) in order to eliminate rock samples of within-plate origin. However, these diagrams are not satisfactory enough to distinguish between ocean-floor and volcanic arc settings. As elements Sr, Rb, and K are highly affected by alteration, Pearce (1975) carefully applied Ti-Zr-Sr diagram (Pearce and Cann, 1973). Most samples fall into ocean-floor basalts; Sr-enriched samples fall into island-arc field. Pearce (1975) developed a new discrimination diagram using elements Ti and Cr in order to distinguish ocean-floor and island-arc basalts. According to the Ti-Cr discrimination diagram, the lower pillow lavas and diabases of the Troodos Massif fall into both ocean-floor basalts and island arc tholeiites, whereas the upper pillow lavas have low Cr concentrations indicating an island-arc origin as previously defined by Miyashiro (1973). He used samples from Pearce and Cann (1973) to construct a bivariate diagram of Ti-Cr in order to discriminate ocean-floor basalts (OFB) and island arc low-K tholeiites (LKT). The importance of Ti is its relative insensitivity to secondary processes (Cann, 1970). Cr is also not largely affected by alteration (Bloxam and Levis, 1972) and a good discriminator between ocean floor and island-arc basalts (Figure 1.3).

Pearce and Gale (1977) studied the tectonic environments of formation of volcanogenic massive sulfide deposits and porphyry tin and copper deposits. They considered stable trace element geochemistry of meta-basalts in these deposits (especially Ti, Zr, Y, Nb, Cr and rare earth elements) and suggested a bivariate diagram of Ti/Y versus Zr/Y (Figure 1.4) in order to discriminate two grouped tectonic settings from each other using a dividing line; which are the combination of different tectonic settings: plate margins including island arcs and mid-ocean ridges (ocean-floor basalts) or within-plates including rifts and ocean island settings. This diagram is analogous to the Ti-Zr-Y diagram of Pearce and Cann (1973).

Pearce and Norry (1979) used analysis data of HFSE (High-Field Strength Elements) along with Ti, Zr, Y, and Nb from mafic and volcanic rocks. By the comparison of the results of these analyses, they published a new discrimination diagram using Zr/Y ratio and Zr (Figure 1.5). This element ratio to element diagram has a logarithmic scale in both axes and discriminated between island-arc, MOR and within-plate settings. On the diagram, Zr content increases from island-arc and mid-oceanic ridge towards within-plate basalts. Island-arc basalts, though some overlap exists, have lower Zr and Zr/Y ratio with respect to mid-ocean ridge basalts. Alkali basalts both in mid-ocean ridges and within-plate regimes have the highest Zr/Y ratios. This element ratio-ratio bivariate diagram is still widely applied for discrimination of these settings.

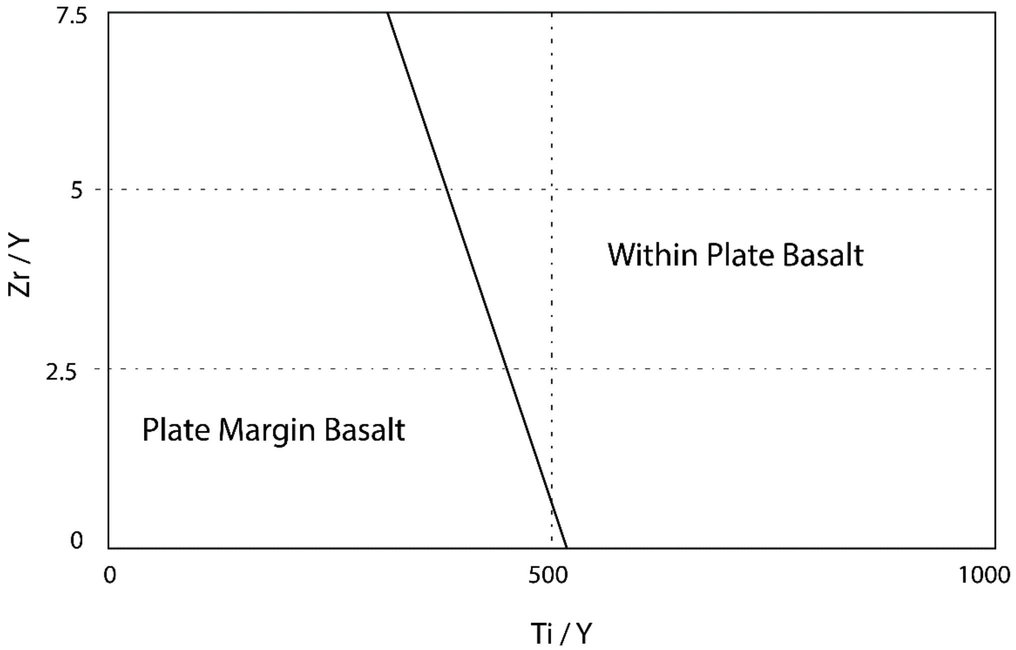

Figure 1.4. Bivariate diagram of Pearce and Gale (1977)

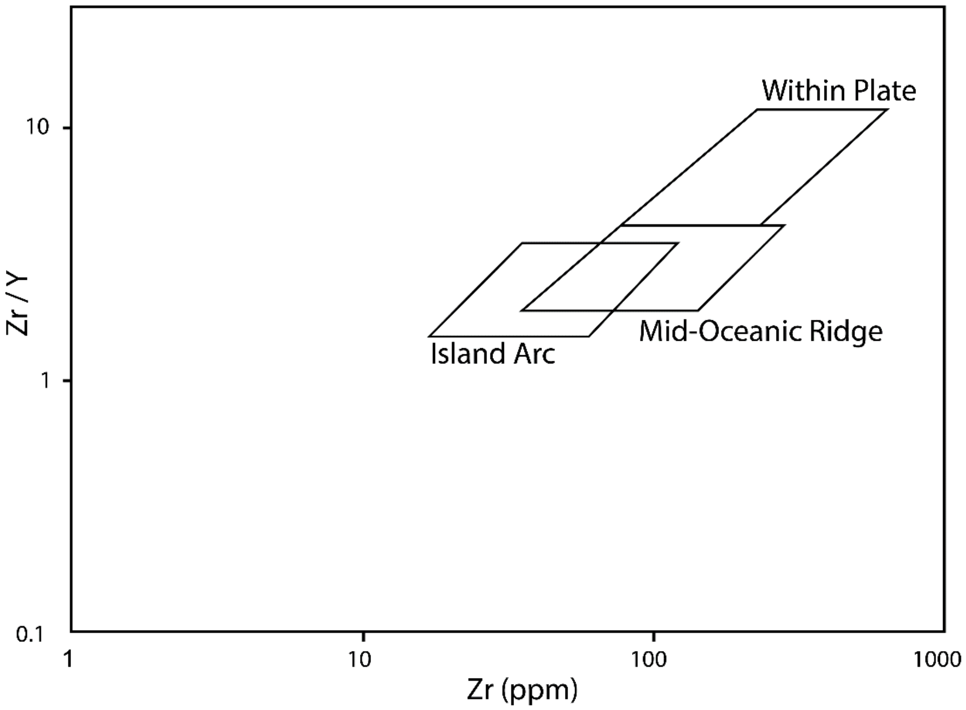

Figure 1.5. Bivariate diagram of Pearce and Norry (1979)

Pearce et al. (1981) introduced a Ti-Zr diagram (Figure 1.6) for the lavas of the Oman ophiolite, using lower back-arc spreading units and upper arc units. The diagram discriminates within-plate lavas, mid-ocean ridge basalts, and arc lavas from each other. Pearce et al. (1981) used samples of various sources as Pearce (1980) and Aldiss (1978). In the diagram, the field defined for mid-ocean ridge basalts is completely intersected with arc lavas and within-plate lavas.

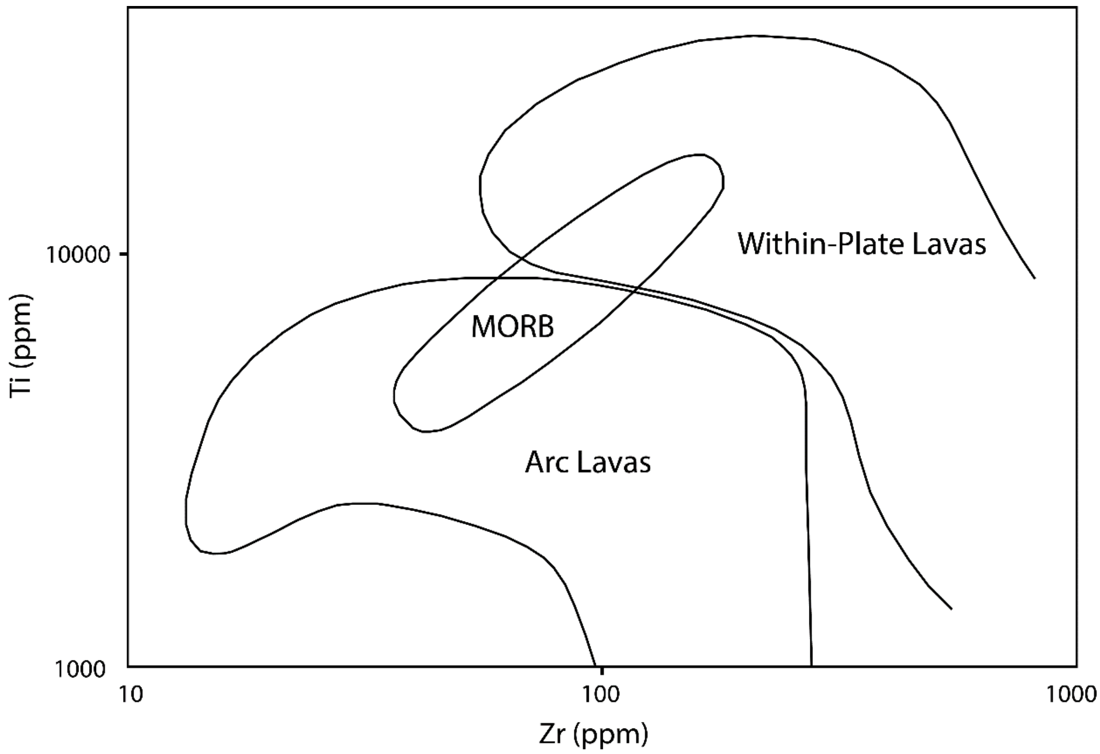

Figure 1.6. Bivariate diagram of Pearce et al. (1981)

Pearce (1982) published three diagrams: a binary diagram of Nb/Y versus Ti/Y ratios on a log-log scale (Figure 1.7), K_2O/Yb versus Ta/Yb ratios on a log-log scale (Figure 1.8), and Ce/Yb versus Ta/Yb ratios on a log-log scale (Figure 1.9).

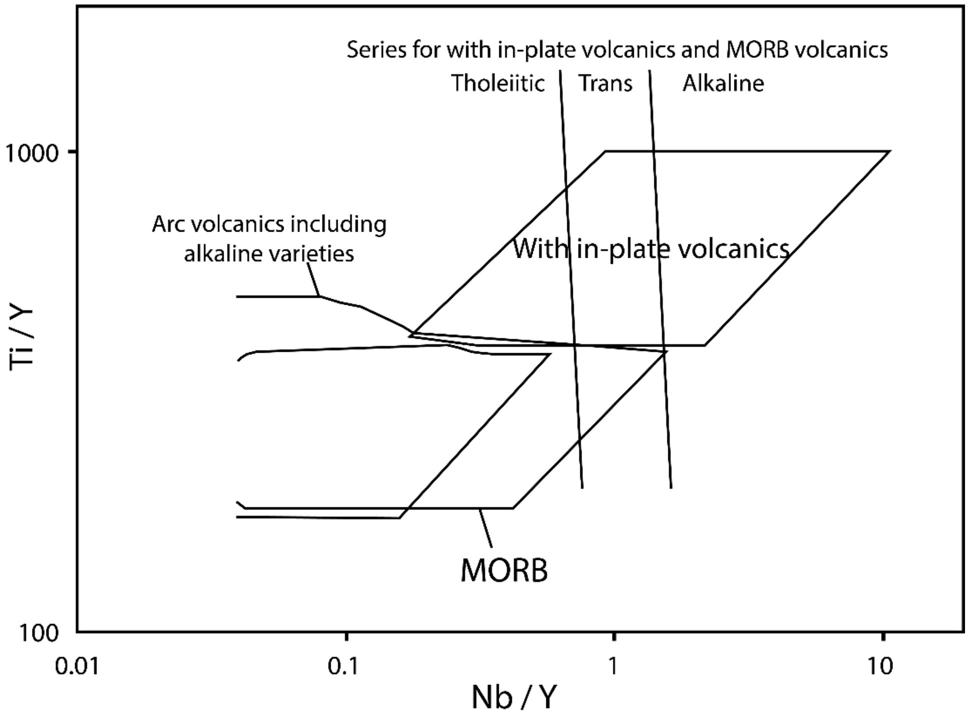

Figure 1.7. Bivariate diagrams of Peace (1982) using Ti/Y versus Nb/Y

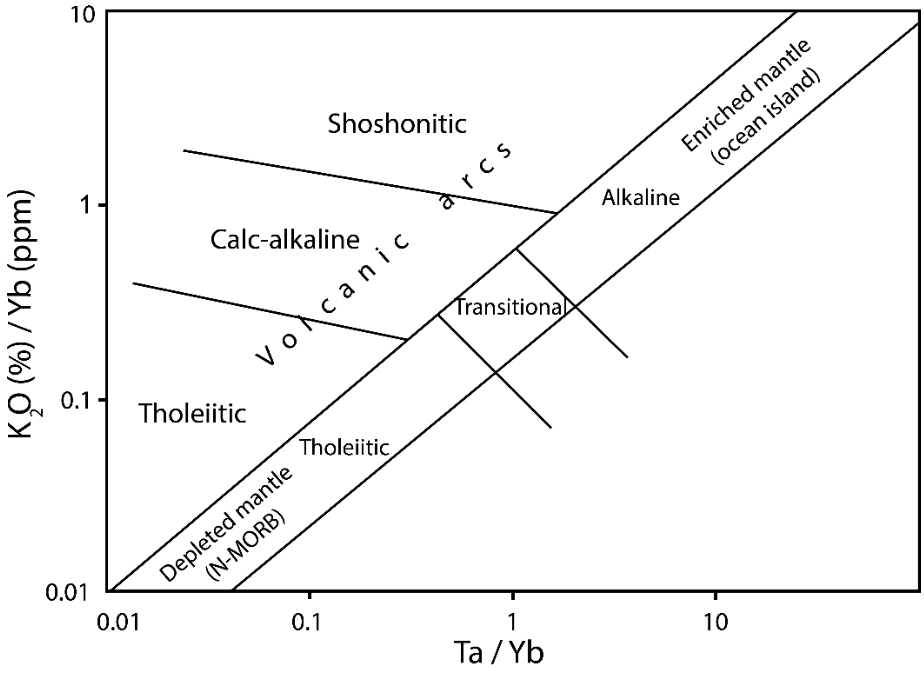

Figure 1.8. Bivariate diagrams of Peace (1982) using K_2O/Yb versus Ta/Yb

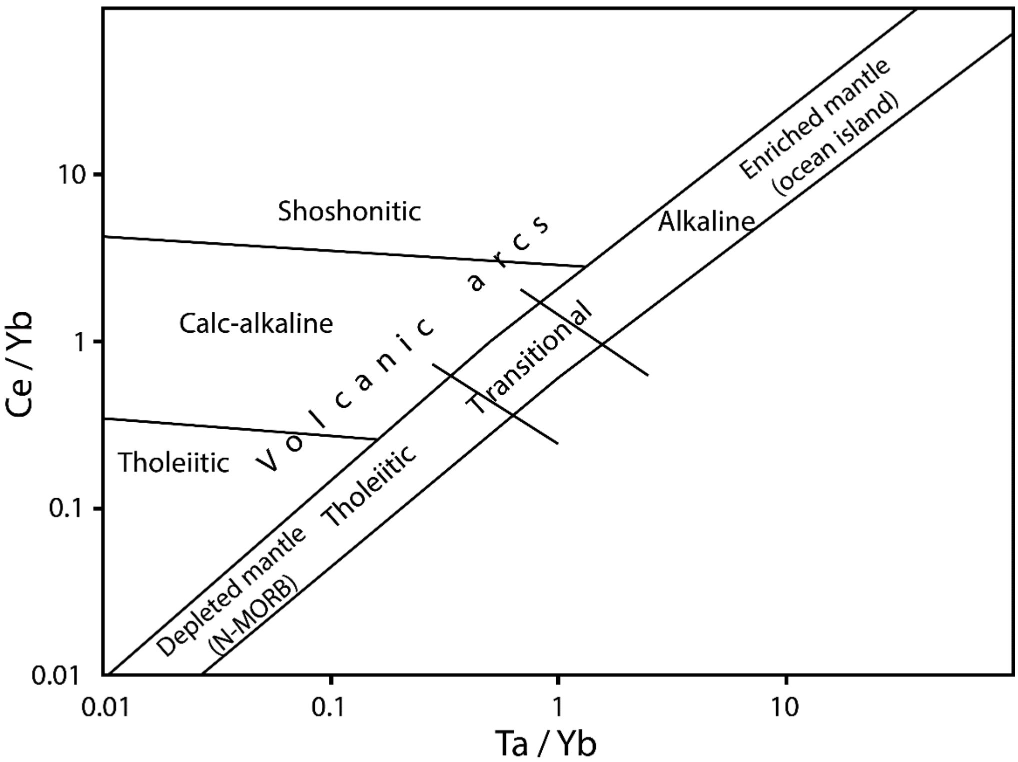

Figure 1.9. Bivariate diagrams of Peace (1982) using Ce/Yb versus Ta/Yb

Shervais (1982) used analyses of Ti and V to construct a new bivariate diagram that can discriminate four tectonic settings within both modern and ophiolitic lavas: ocean basins, island arcs, back-arc basins, and continental interiors. Shervais (1982) stated that MORB has a uniform distribution of Ti/V without difference between N-MORB and E-MORB, and also tholeiitic flood basalts can be discriminated from MORB despite their similarity. Tholeiitic and alkali basalts plot in distinct fields with minimum overlap, reflecting several factors such as mantle sources, degree of partial melting, and volatiles. Volcanic rocks from island arc-related settings may be divided into three groups based on their alkalinity, and they show broad variations of Ti and V. Basalts in back-arc basins show overlaps with MOR and island arc volcanic rocks. These settings were discriminated by the Ti versus V diagram of Shervais (1982), using equi-Ti/V boundaries drawn by eye (Figure 1.10).

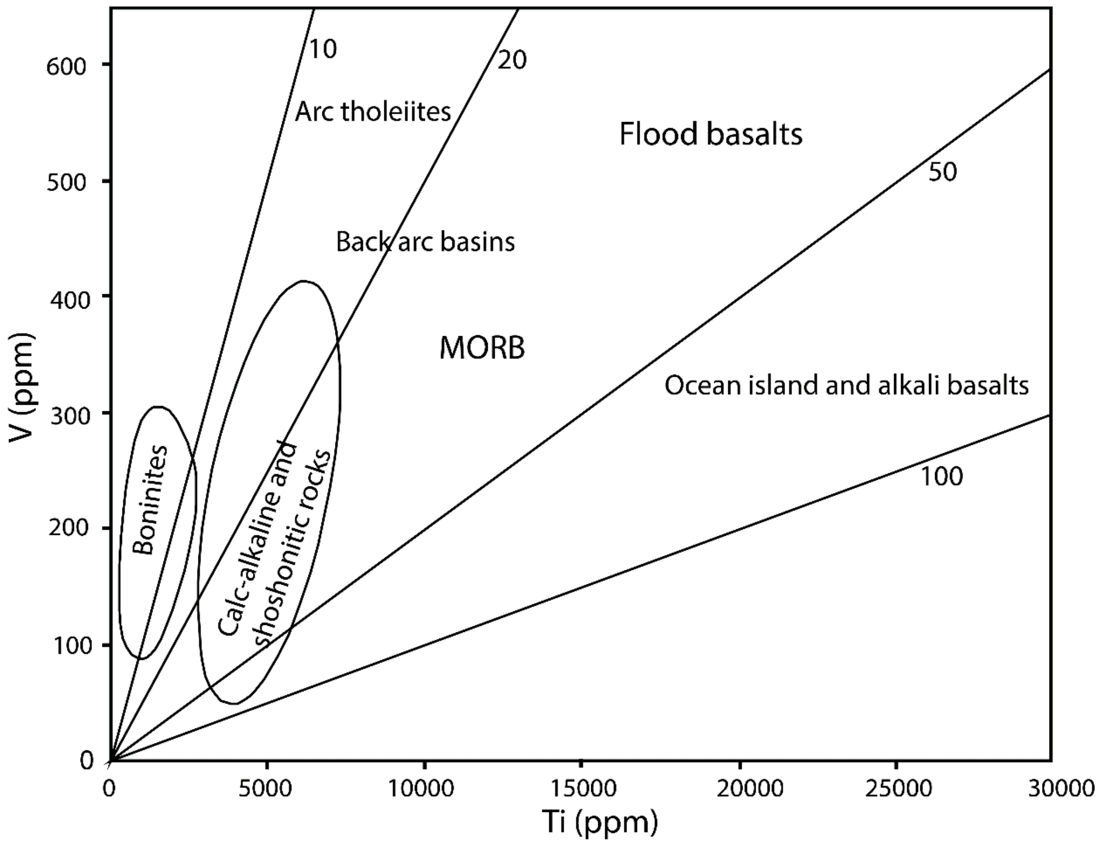

Figure 1.10. Bivariate diagram of Shervais (1982)

Pearce (1983) published two diagrams: a bivariate diagram of Ta/Yb versus Th/Yb (Figure 1.11) and a bivariate diagram of Zr versus Zr/Y (Figure 1.12). The first diagram is quite similar to diagrams of Pearce et al. (1981), discriminating arc-related basalts from within-plate and mid-oceanic ridge basalts, using a similar structure of enclosed regions. A somewhat similar version, but including Nb (instead of Ta) was proposed by Pearce and Peate (1995). The second diagram, on the other hand, simply discriminates continental arcs from oceanic arcs using a single line. Pearce (1983) stated that continental arcs have a higher ratio of Zr/Y compared to oceanic arcs, regardless of their Zr content.

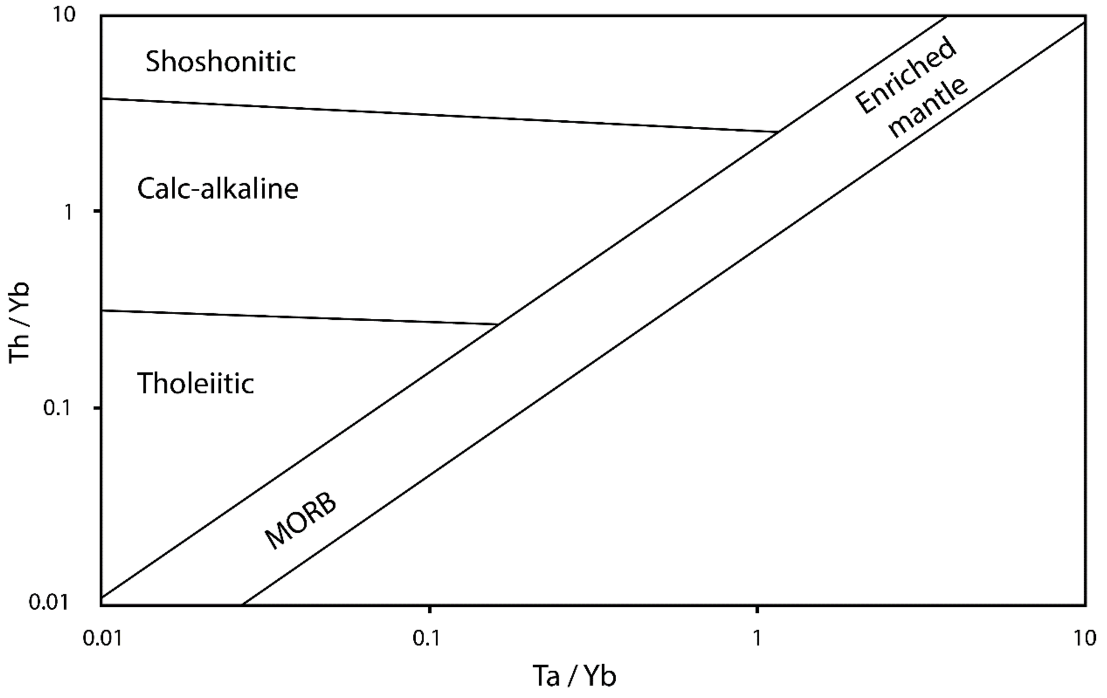

Figure 1.11. Bivariate diagrams by Pearce (1983) using Ta/Yb versus Th/Nb

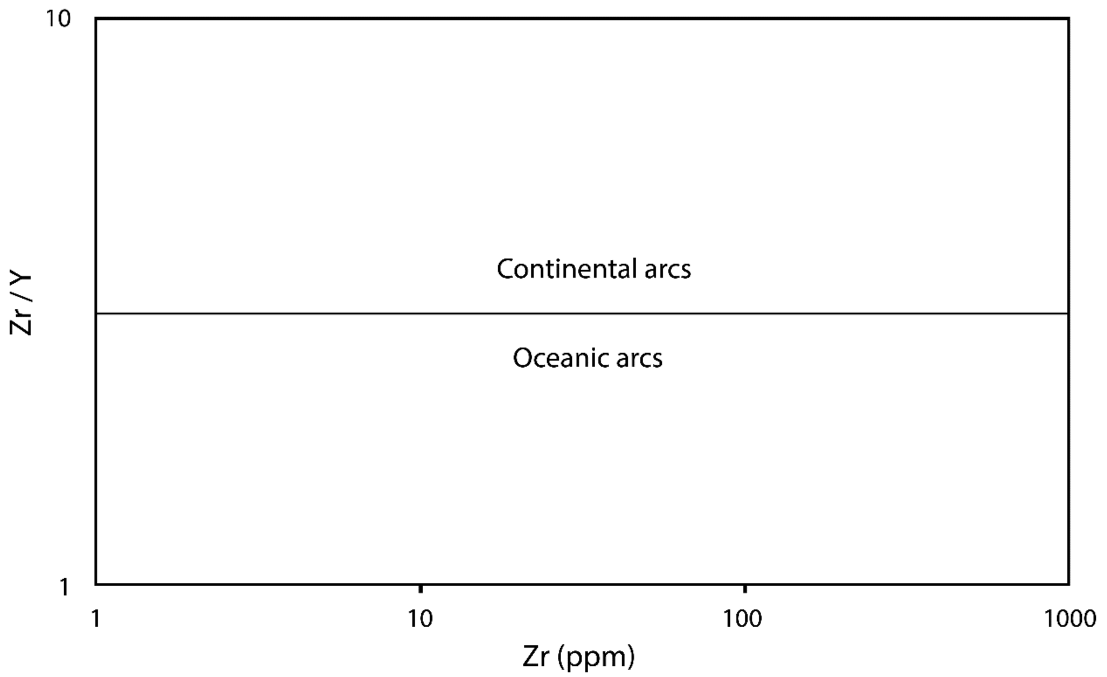

Figure 1.12. Bivariate diagrams by Pearce (1983) using Zr versus Zr/Y

Pearce et al. (1984) published a bivariate diagram of Cr vs TiO_2 (Figure 1.13) in order to discriminate SSZ (supra-subduction zone) ophiolites from MOR ophiolites. The SSZ ophiolite mantle is generally more residual than that of MOR ophiolites. They are derived by higher degrees of melting of a similar source or by similar degrees of melting of a less fertile source.

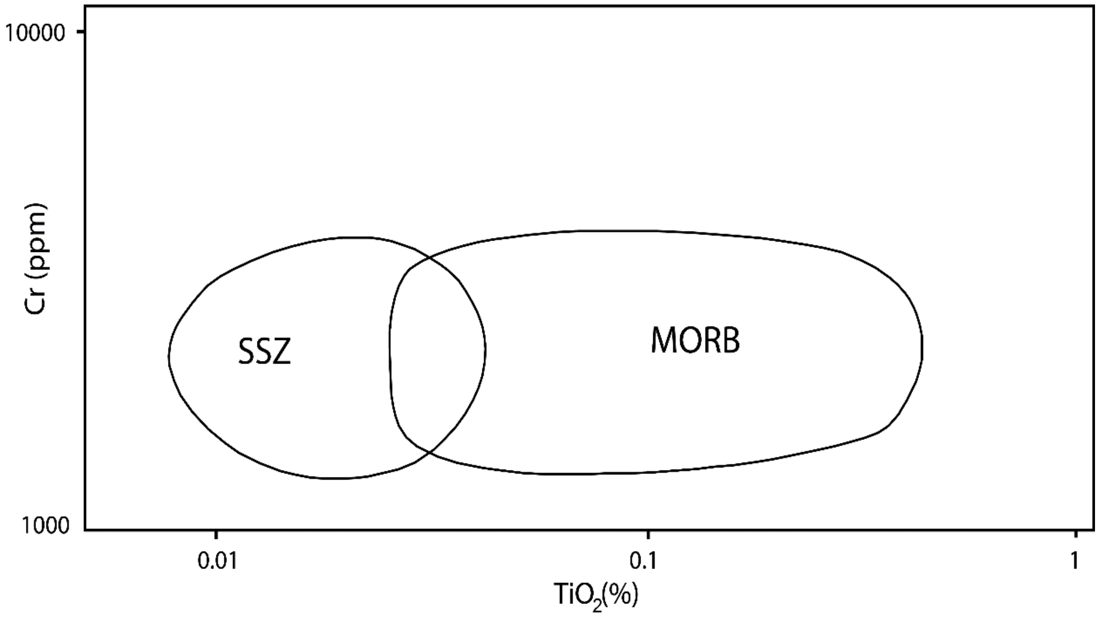

Figure 1.13. Bivariate diagram of TiO_2 versus Cr by Pearce et al. (1984)

Dilek et al. (2007), on the other hand, modified this diagram and published another bivariate diagram of Y versus Cr as this diagram (Figure 1.14) in order to discriminate between boninites, arc tholeiites and mid-ocean ridge basalts from each other. Dilek et al. (2007) used magmas of Western-type ophiolites in order to define regions of MORB and lavas and dikes of the Eastern-type ophiolites in order to define regions of island arc tholeiites and boninites.

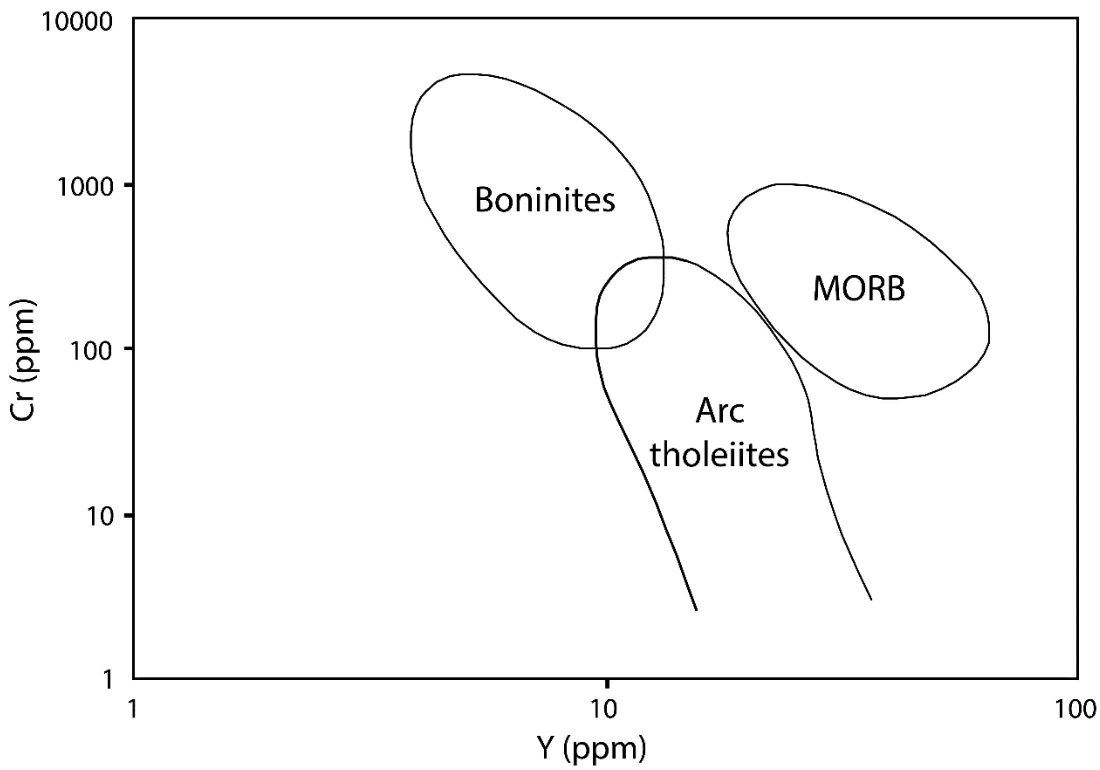

Figure 1.14. Bivariate diagram of Y versus Cr by Dilek et al. (2007)

Hollocher et al. (2012) published two bivariate diagrams (Figure 1.15 and Figure 1.16) in order to discriminate mid-oceanic ridge basalts, ocean islands and a variety of arc-type basalts from each other. Hollocher et al. (2012) used the analysis results of the samples from the Upper Allochthon metamorphosed igneous rocks of the Scandinavian Caledonides in Norway over a large region with well-defined but discontinuous units, for which analysis data were taken from PetDB. Data were filtered in order to include only volcanic glass with a SiO_2 range of 45-55%. Element conversion using a conversion factor was applied in order to increase the number of samples plotted in diagrams. The filtered dataset included 1.586 mid-oceanic ridge basalts, 518 oceanic-arc and 1.793 continental arc, 1.021 alkaline arc, 958 back-arc basin, and 2.438 ocean island samples. Discriminant lines were drawn by eye with wide overlapping fields.

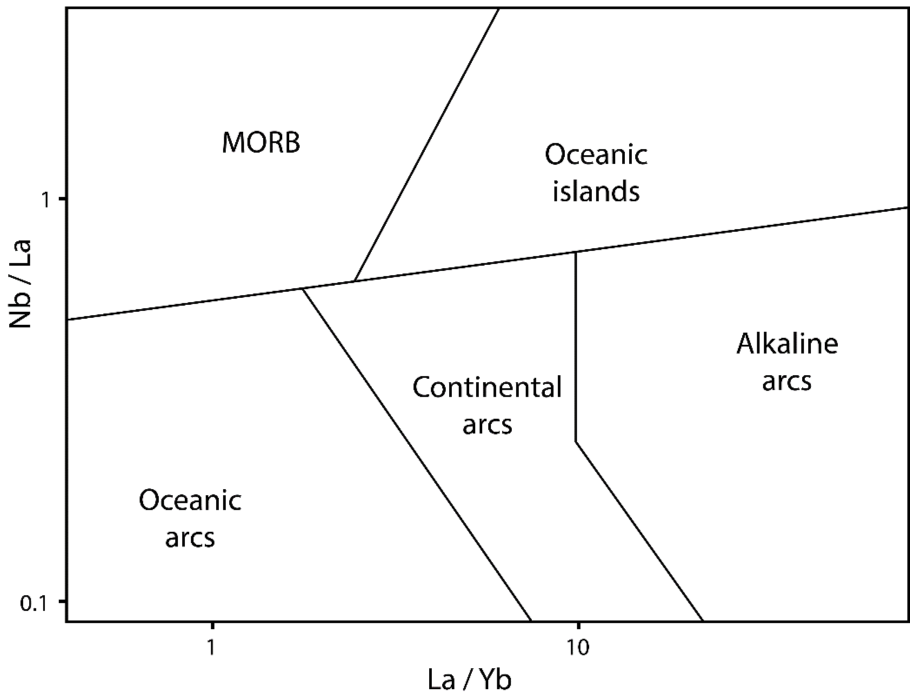

Figure 1.15. Bivariate diagrams of Hollocher (2012) using La/Yb vs Nb/La

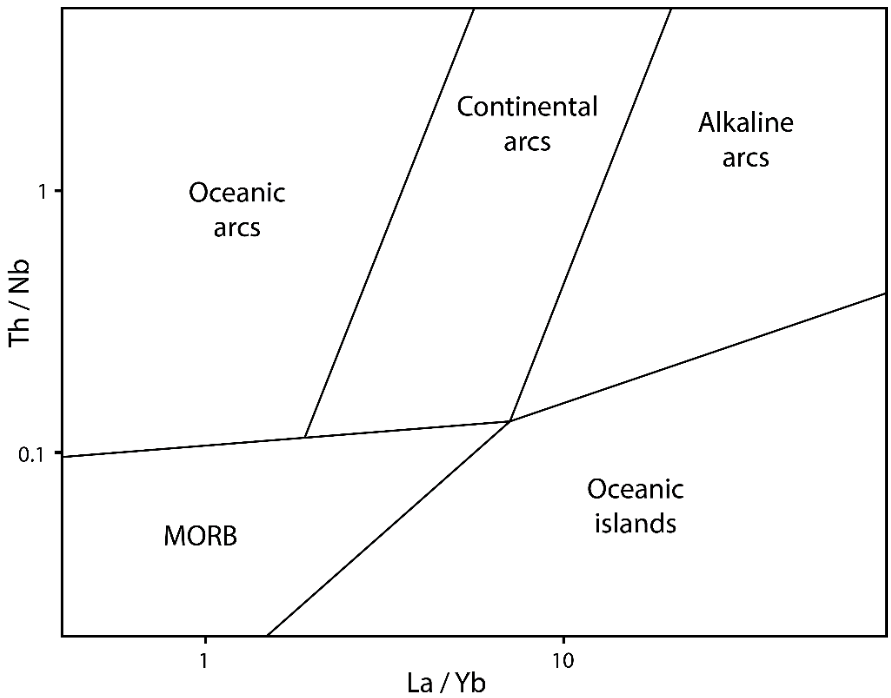

Figure 1.16. Bivariate diagrams of Hollocher (2012) using La/Yb vs Th/Nb

Saccani (2015) published a new bivariate tectonomagmatic discrimination diagram using N-MORB-normalized values of Th and Nb for the tectonomagmatic discrimination of different ophiolitic basalts (Figure 1.17). More than 2000 ophiolitic basalts from ten different basalt localities were used in order to obtain this diagram. The diagram is used for discrimination of convergent and divergent plate settings from each other and also discrimination of back-arcs, subduction unrelated settings and rifted margins, fore-arcs, intra-arcs, island arcs and volcanic arcs.

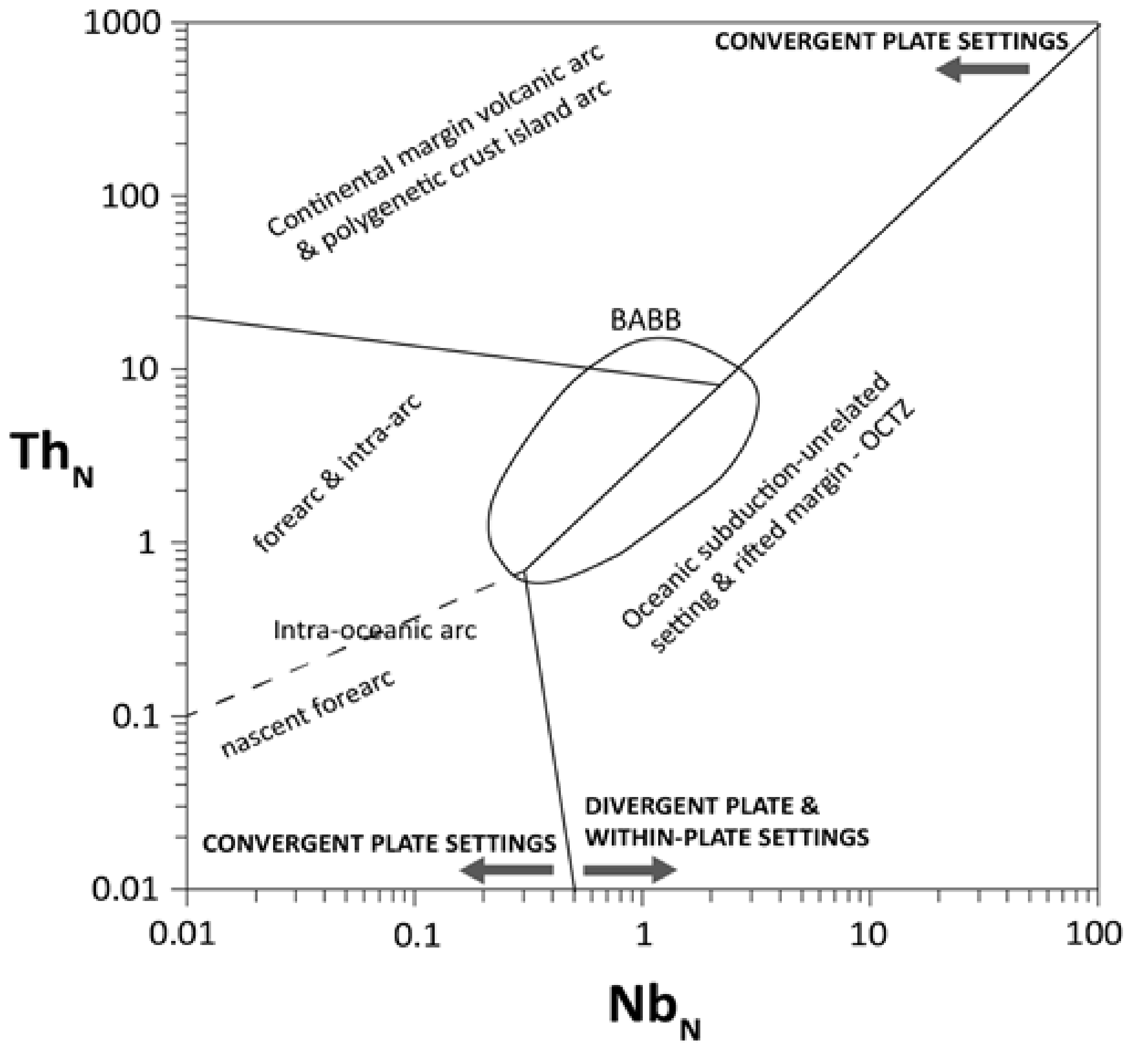

Figure 1.17. Bivariate diagrams of Saccani (2015) using normalized values of Th versus Nb

1.2.3. Traditional Ternary Diagrams

Traditional ternary diagrams, as in the bivariate diagrams, are also based on relatively immobile elements such as Ti, P, Zr, Hf, Nb, Y, and V. The use of these elements in discrimination diagrams is an advantage for the application of diagram for altered samples and especially from older terrains (Verma, 2010). Ternary diagrams can also be replaced by natural log-ratio bivariate diagrams (Verma and Agrawal, 2010).

Pearce and Cann (1973) used analyses for Ti, Zr, Y, Nb, and Sr in basaltic rocks from different tectonic settings to construct their discrimination diagrams. The distinctions between different tectonic settings in the discrimination diagram were obtained by selected elements as axes instead of discrimination functions, used by Pearce and Cann (1971). Present-day volcanic rocks are classified based on tectonic settings associated with their eruption. They defined four major groups: ocean-floor basalts as diverging plate margins, volcanic arc basalts as converging plate margins, ocean-island basalts and continental basalts as within-plate regimes. Pearce and Cann (1973) selected randomly distributed rock samples from known tectonic settings in a statistically sufficient quantity. Samples were fresh, yet a small number was altered. Altered samples were not involved in diagrams of Sr. The results of analyses from the literature were also used when acceptable. A compositional limit of 20% > CaO+MgO > 12% were used to select rock samples. Pearce and Cann (1973) used 72 samples of ocean floor basalts from ocean ridges, 46 samples of low-K tholeiites, 60 samples of calc-alkali basalts and 9 samples of shoshonites from volcanic arcs, 78 samples of ocean island basalts from ocean islands and 35 samples of continental basalts from continental settings for the construction of discrimination diagrams. Elements to be used for discrimination were selected as (1) they have great variation in concentration, (2) they are insensitive to secondary processes such as weathering and/or metamorphism, (3) their analyses are reproducible. Ti-Zr-Y diagram (Figure 1.18) is first used to discriminate basalts erupted in both oceanic and continental plates. Within-plate basalts (region A), calc-alkaline basalts (region B and C), ocean floor basalts (region C) and low-K arc tholeiites (region C and D) are discriminated through this diagram. For the rock samples not classified as "within-plate basalt" by discrimination by the Ti-Zr-Y diagram, Pearce and Cann (1973) established another ternary diagram using Ti-Zr-Sr (Figure 1.19). Tectonic discrimination diagrams are much more efficient when constructed based on stable elements as they are not easily affected by secondary processes such as weathering and metamorphism (Pearce, 1975). The discrimination diagrams of Pearce and Cann (1971, 1973) are highly efficient for distinguishing magma types as they use stable elements Ti, Zr, Y, and Nb. Cr is another fairly stable element which is resistant to alteration (Bloxam and Levis, 1972).

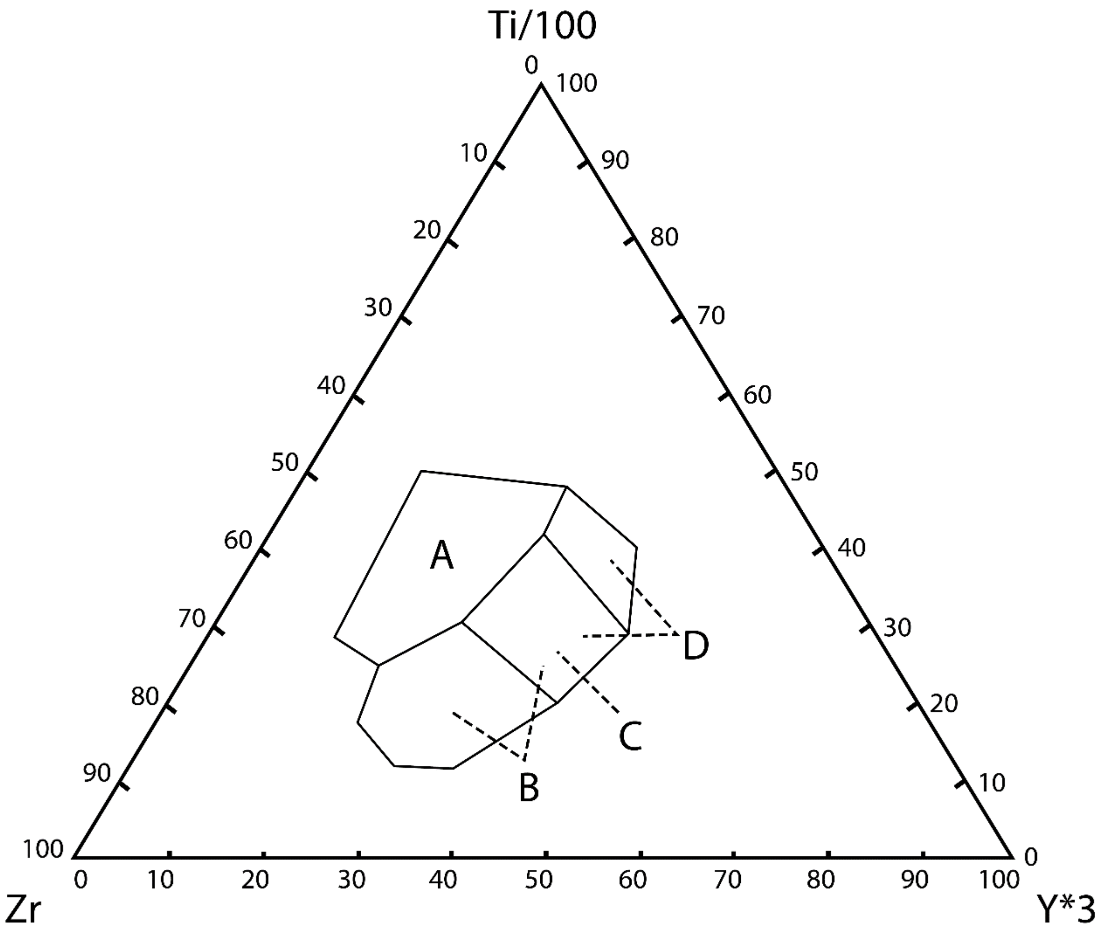

Figure 1.18. Discrimination diagrams of Pearce and Cann (1973) using Ti/100-Zr-Y*3

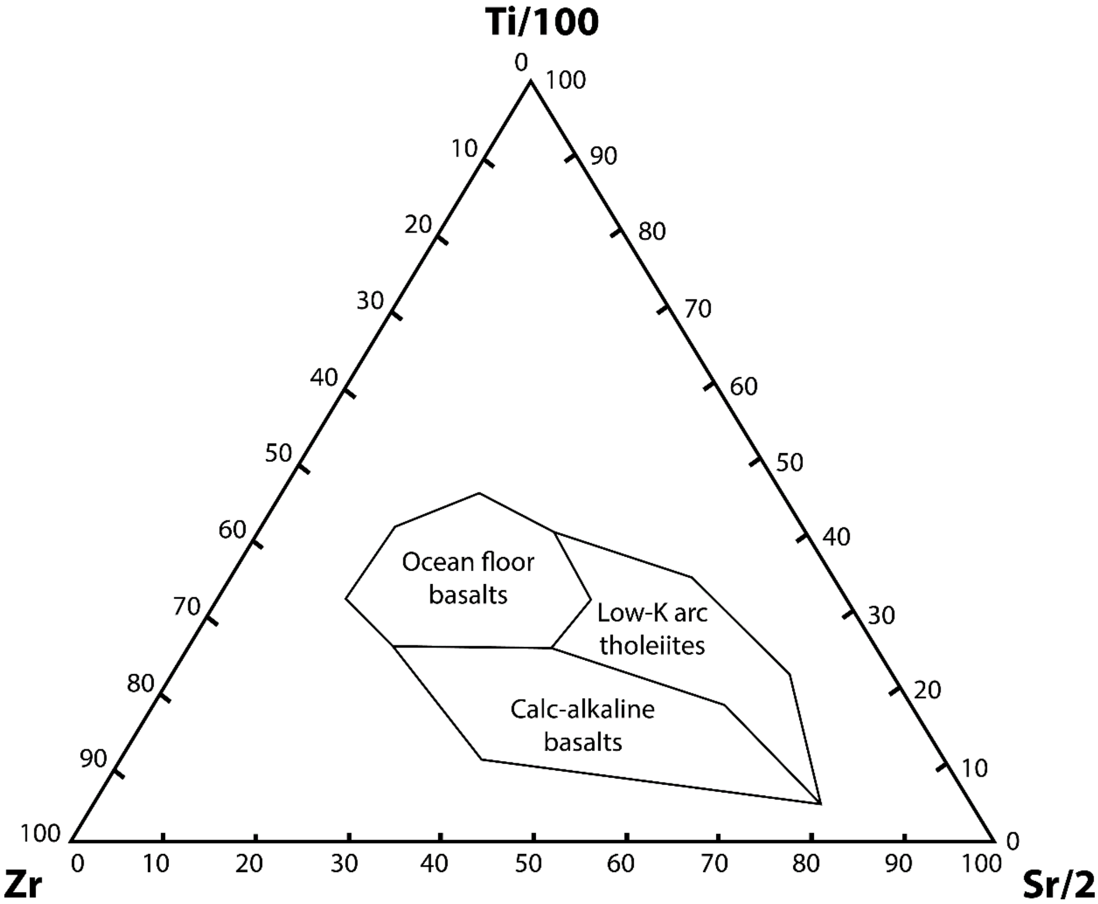

Figure 1.19. Discrimination diagrams of Pearce and Cann (1973) using Ti/100-Zr-Sr/2

Wood et al. (1979) stated that discrimination using Zr-Ti-Y is problematic for magma types erupted at tectonically anomalous ridge segments with respect to those erupted at normal ridge segments. They also stated that these discrimination diagrams: (1) fail at the discrimination of tectonically different mid-ocean ridge segments, and (2) are restricted to a certain number of immobile trace elements detected by X-ray fluorescence (XRF). Wood et al. (1979) developed a new discrimination diagram using different elements (Th, Ta, Hf) which can be efficiently detected by instrumental neutral activation analysis (INAA). Wood et al. (1980) reconsidered the Hf/3-Th-Ta diagram (Wood et al., 1979) by using additional data (Figure 1.20). By the addition of new data, Wood et al. (1980) modified the previous diagram so that it is possible to discriminate calc-alkaline lavas from island arc tholeiites. Wood et al. (1980) enlarged some fields and modified boundaries.

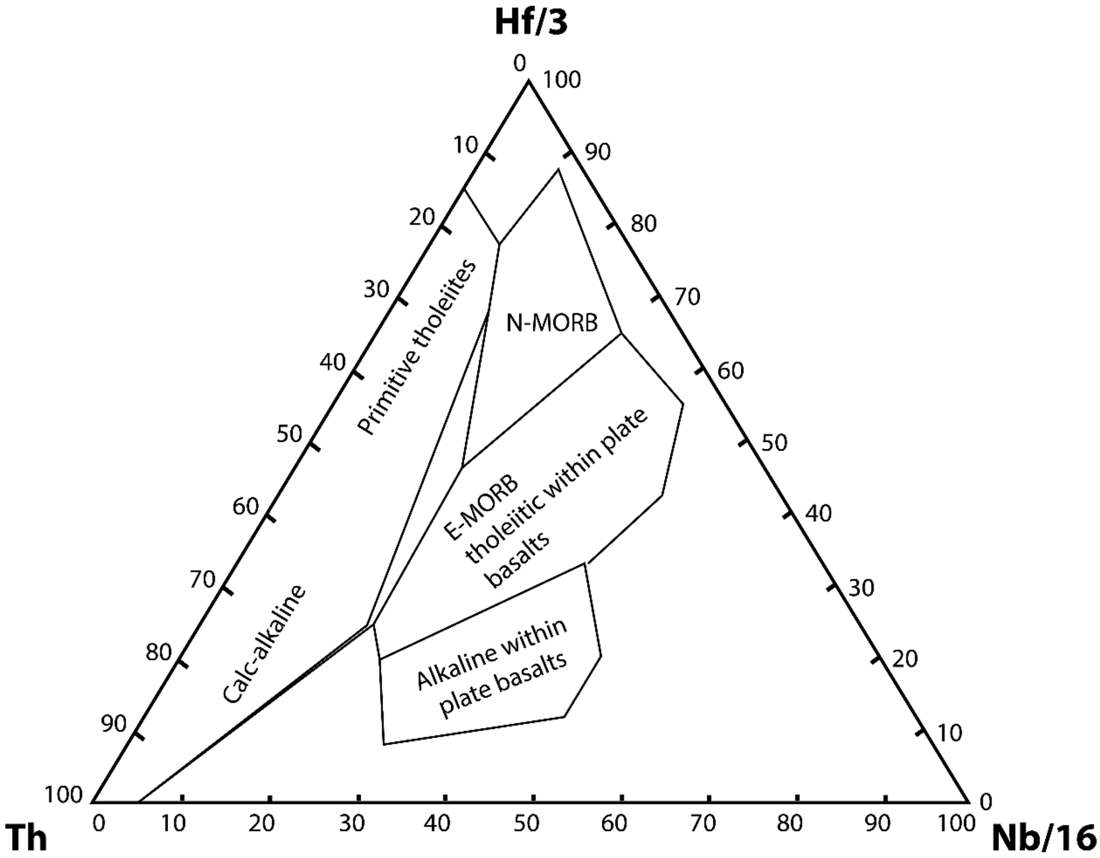

Figure 1.20. Discrimination diagram of Wood (1980), modified after Wood et al. (1979) using Hf/3, Th and Nb/16

Mullen (1983) divided the entire ternary field into six regions: ocean-island tholeiites (region A), mid-oceanic ridge basalts (region B), island arc tholeiites (region C), boninites (region D), calc-alkaline basalts (region E) and ocean-island alkali basalts (region F) using basic and ultrabasic rocks from different oceanic tectonic settings (Figure 1.21). Boninites and calc-alkaline basalt fields are not divided from each other by a solid line. Since the diagram uses Mn, which is a relatively mobile element, it is especially applicable for fresh samples.

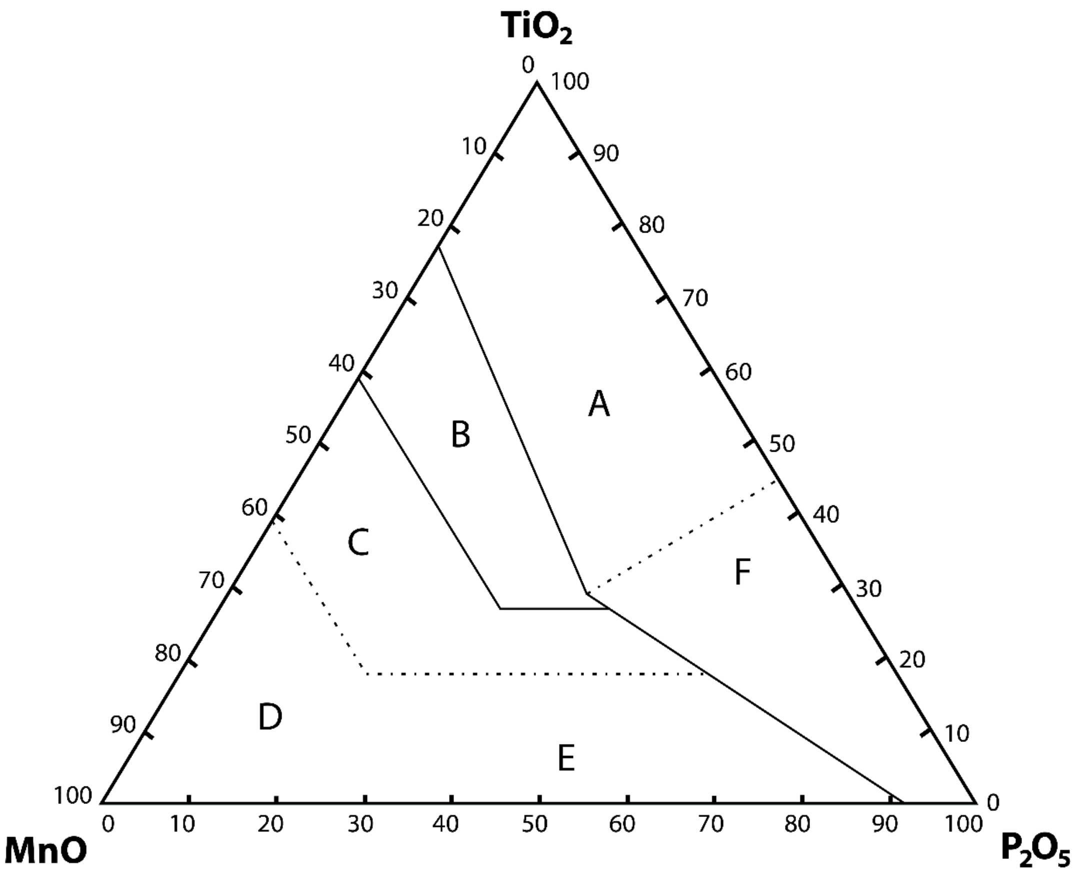

Figure 1.21. Discrimination diagram of Mullen (1983) using TiO_2, MnO*10, P_2O_5*10

Meschede (1986) published the Zr-Nb-Y diagram (Figure 1.22) with a suggestion for two different types of ocean-floor basalt as N-MORB and E-MORB (also known as P-MORB) and their discrimination from each other using immobile trace element Nb. N-MORBs are depleted in incompatible trace elements, yet E-MORBs are generally enriched. Meschede (1986) used a ternary diagram of Zr/4, Nb*2, and Y in order to discriminate four tectonic settings for basaltic rocks. Within-plate alkali basalts (region A and B), within-plate tholeiites (region B and D), E-MORB (region C) and

N-MORB (region E) are discriminated through this diagram. The fields for these settings were defined on the basis of 1800 analyses of modern basalts with a compositional range between 12 and 20 for CaO + MgO. The fields are within-plate alkali basalts, within-plate tholeiites, E-MORB, N-MORB, and volcanic arc basalts.

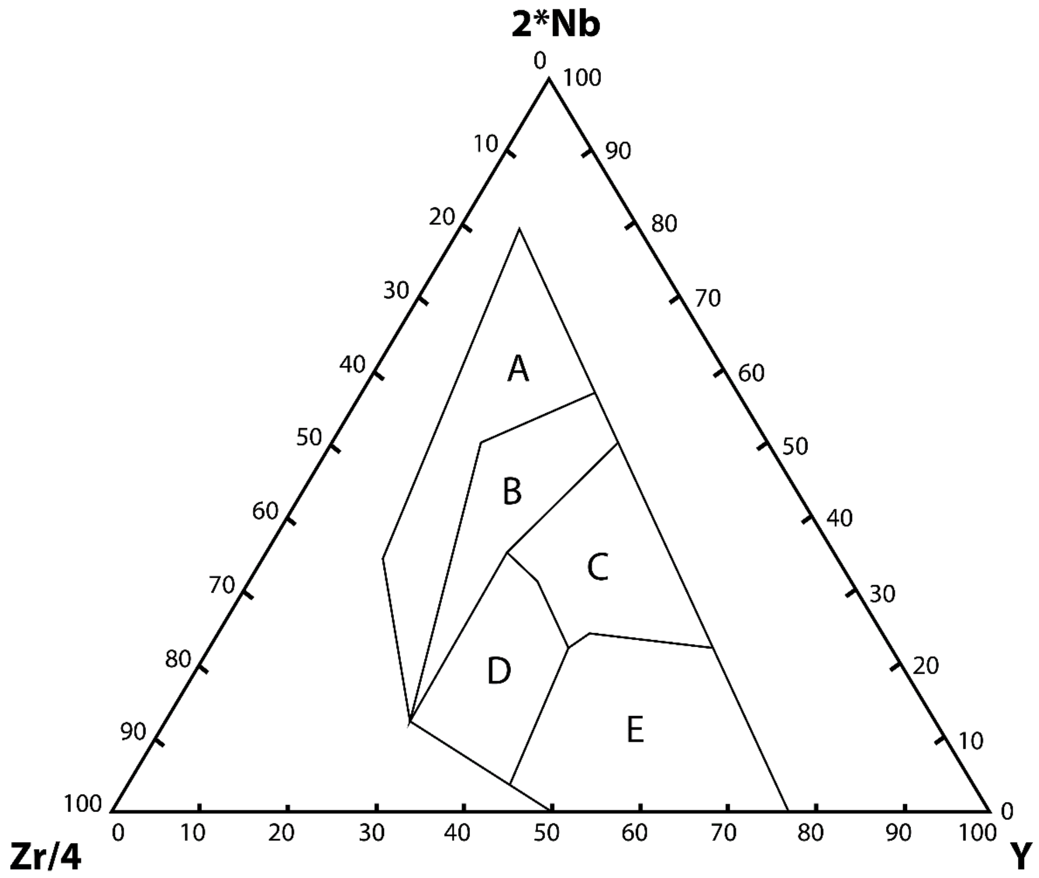

Figure 1.22. Discrimination diagram of Meschede (1986) using 2*Nb, Zr/4 and Y

Cabanis and Lecolle (1989) used a comparatively small number of samples in order to publish a tectonic discrimination diagram on a ternary plot of La-Y-Nb concentrations (Figure 1.23). The diagram is used for the discrimination between volcanic arc basalts, continental basalts, and oceanic basalts. Volcanic arc basalts are subdivided into two groups: calc-alkali basalts and island-arc tholeiites. The settings are defined in enclosed regions and there are regions where no tectonic setting is provided.

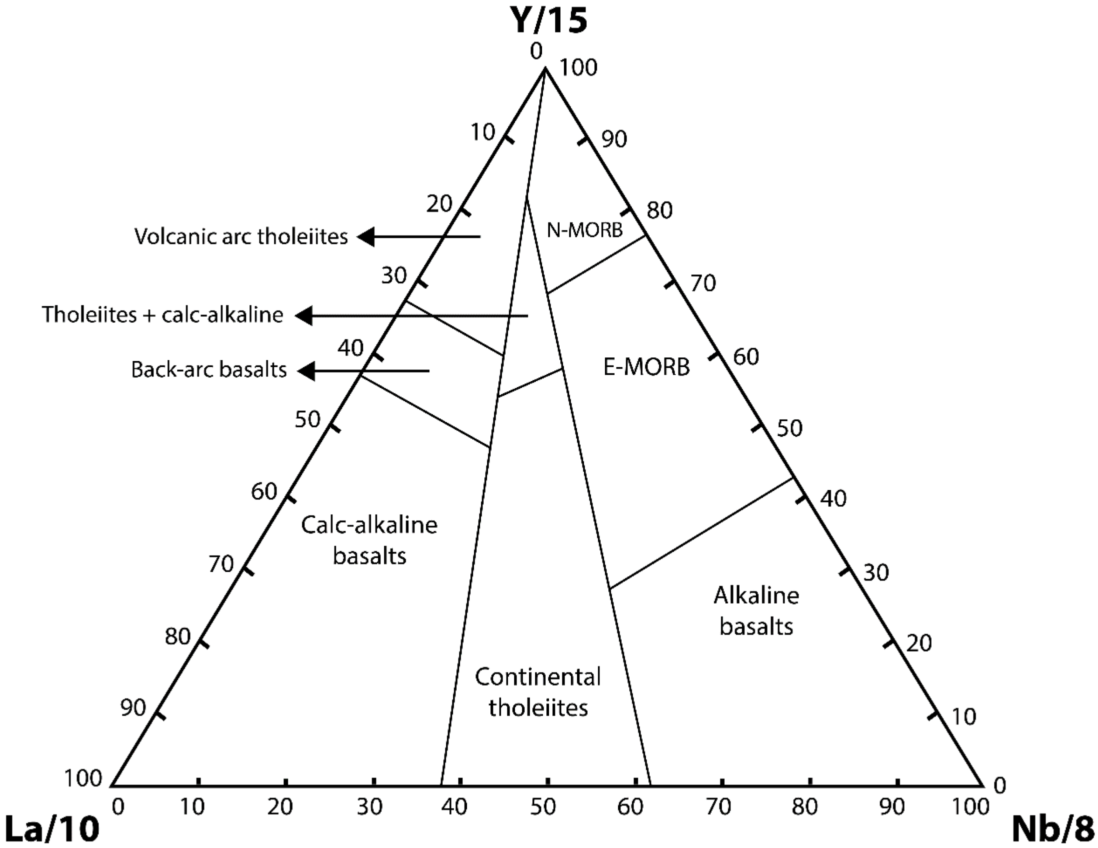

Figure 1.23. Discrimination diagram of Cabanis and Lecolle (1989) using Y/15, La/10 and Nb/8

1.2.4. Traditional Diagrams with Discriminating Functions

Pearce (1976) performed linear discriminant analysis for major element oxides in order to discriminate six tectonic settings from each other: ocean floor basalts, island arc tholeiites, calc-alkali basalts, shoshonites, ocean-island basalts, continental basalts. A maximum number of 75 samples for each tectonic setting is selected from different localities. Only analyses where CaO+MgO are between 12 and 20% are selected. Only fresh samples were used. He published five discriminant functions

(Table 1.1). based on major element oxides (DF1, DF2, DF3, DF4, and DF5) and presented two discrimination diagrams based on DF1-DF2 DF3 (Figure 1.24) and DF1-DF3 (Figure 1.25).

Table 1.1. Discrimination functions used in diagrams of Pearce (1976)

Discrimination Functions	
DF1	$+0.0088SiO_2-0.0774TiO_2+0.0102Al_2O_3+0.0066FeO-0.0017MgO-0.0143CaO-0.0155Na_2O-0.0007K_2O$
DF2	$-0.0130SiO_2-0.0185TiO_2-0.0129Al_2O_3-0.0134FeO-0.0300MgO-0.0204CaO-0.0481Na_2O+0.0715K_2O$
DF3	$-0.221SiO_2-0.0532TiO_2-0.0361Al_2O_3-0.0016FeO-0.0310MgO-0.0237CaO-0.0614Na_2O-0.0289K_2O$

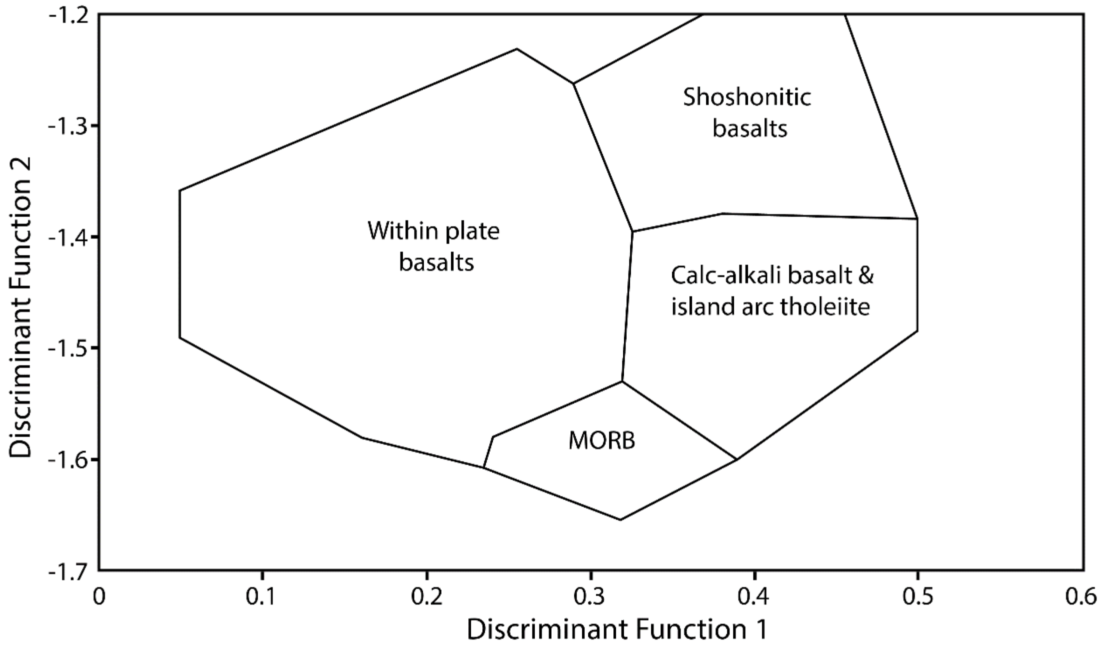

Figure 1.24. Discrimination diagrams of Pearce (1976) using DF1 and DF2

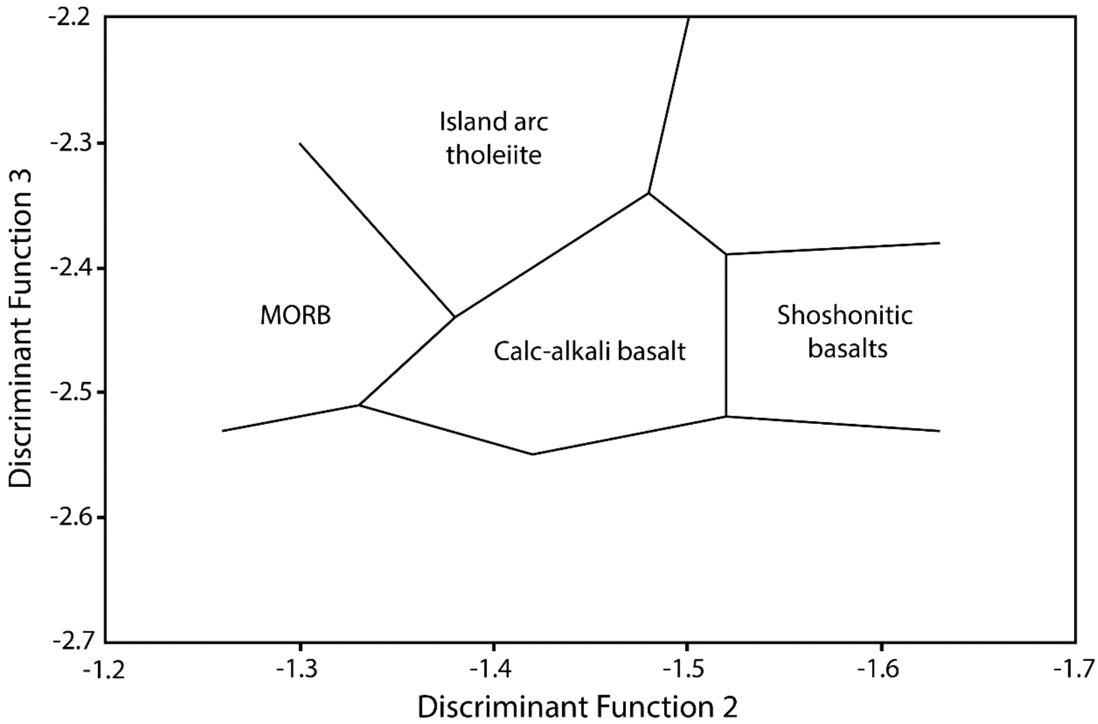

Figure 1.25. Discrimination diagrams of Pearce (1976) using DF2 and DF3

Butler and Woronow (1986) proposed an alternative approach to the tectonic discrimination of igneous rocks by using principal component analysis. They created a bivariate graph which uses two principal components (Table 1.2) in the form of functions of Ti, Zr, Y, and Sr (Figure 1.26). The settings discriminated in this graph are similar to Pearce and Cann (1973), yet this graph is accepted to be more mathematical with respect to the original Ti-Zr-Y diagram.

Table 1.2. Discrimination functions used in diagrams of Butler and Woronow (1986)

Discrimination Functions	
Score 1	0.3707Ti-0.0668Zr-0.398Y+0.8362Sr
Score 2	-0.3376Ti-0.5602Zr+0.7397Y +0.1582Sr

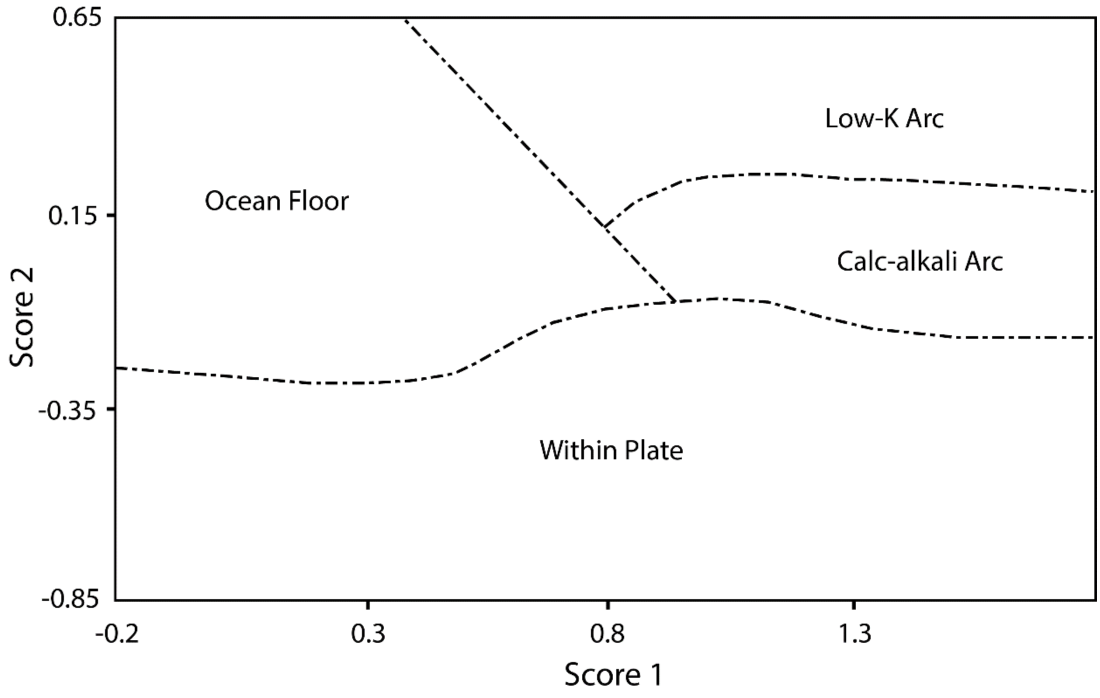

Figure 1.26. Discrimination diagrams of Pearce (1976) using DF1 and DF2

Velikonslavinsky and Kykrylov (2014) published new tectono-magmatic discrimination diagrams (Figure 1.27) for basalts from tectonic settings of island-arcs, within-plates, mid-ocean ridges, and post-collisional settings using discrimination functions (Table 1.3). They used a database from global geochemical datasets such as GEOROC, PetDB, IGBA, RidgeDB. They used a two-stage discrimination. At first stage, they discriminate WPB, IAB and MOR creating discriminating functions with combinations of elements including major oxides (SiO_2, TiO_2, Al_2O_3, FeO* (total iron in form of FeO), MgO, CaO, Na_2O, K_2O, P_2O_5, Rb, Sr, Y, Zr, Nb, La, Ce, Nd, Sm, Eu, and Yb). At the second stage, PCB (basalts of post-collisional setting) is separated with discriminating functions by a combination of major oxides and minor elements (Rb, Sr, Y, Zr, and Nb).

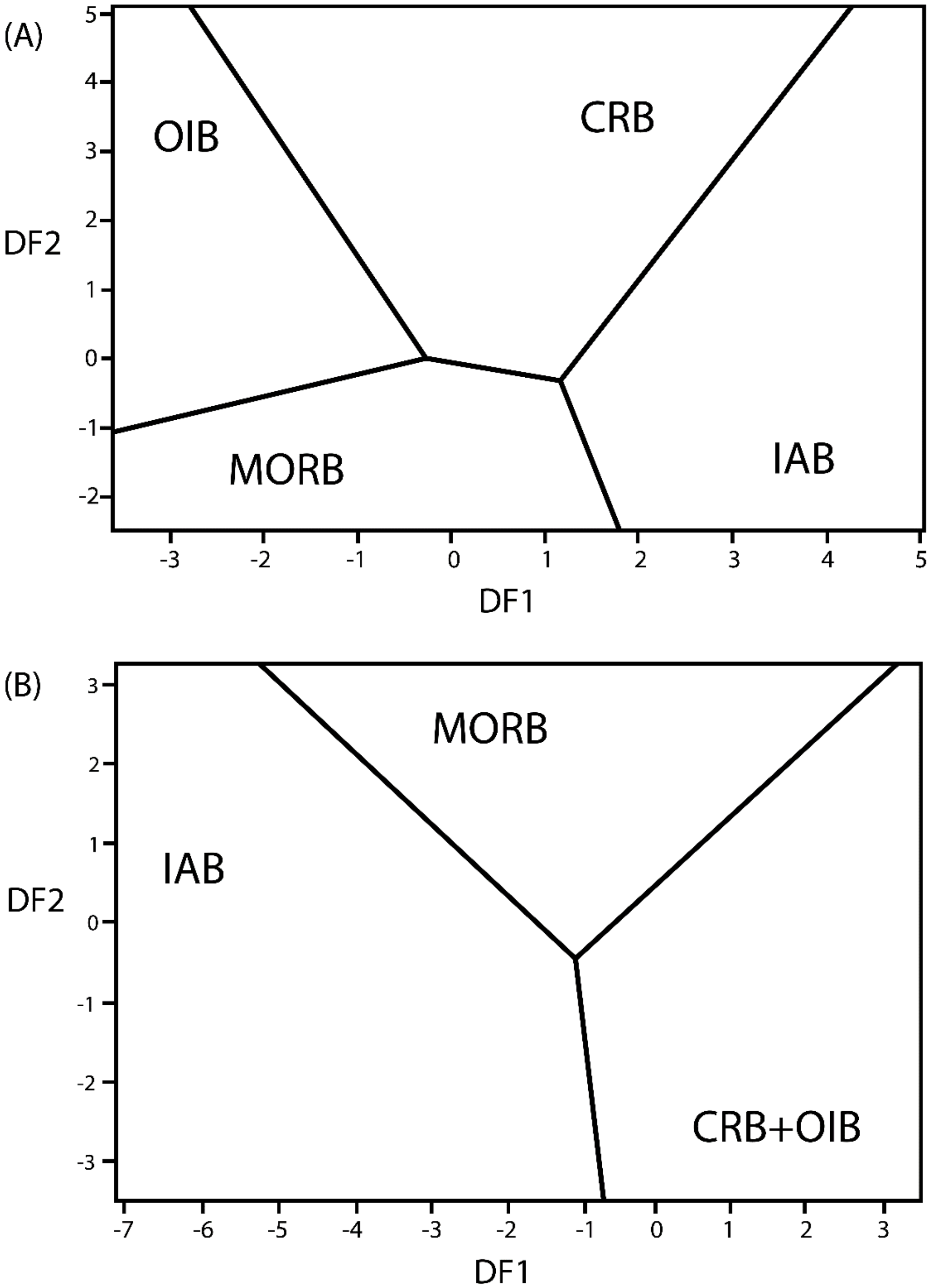

Figure 1.27. Discrimination diagrams of Velikoslavinsky and Kykrylov (2014) using discrimination functions of (A) by major element contents, (B) by inert minor element contents

Table 1.3. Discrimination functions used in diagrams of Velikoslavinsky and Kykrylov (2014)

Discrimination Functions by major element contents	
DF1	$-4.6761ln(TiO_2/SiO_2)+2.5330ln(Al_2O_3/SiO_2)-0.3884ln(Fe_2O_3/SiO_2)+3.9688ln(FeO/SiO_2)+0.8980ln(MnO/SiO_2)-0.5832ln(MgO/SiO_2)-0.2896ln(CaO/SiO_2)-0.2704ln(Na_2O/SiO_2)+1.0810ln(K_2O/SiO_2)+0.1845ln(P_2O_5/SiO_2)+1.5445$
DF2	$+0.6751ln(TiO_2/SiO_2)+4.5895ln(Al_2O_3/SiO_2)-2.0897ln(Fe_2O_3/SiO_2)+0.8514ln(FeO/SiO_2)+0.4334ln(MnO/SiO_2)-1.4832ln(MgO/SiO_2)-2.3627ln(CaO/SiO_2)-1.6558ln(Na_2O/SiO_2)+0.6757ln(K_2O/SiO_2)+0.4130ln(P_2O_5/SiO_2)+13.1639$
Discrimination Functions by inert minor element contents	
DF1	$0.3518ln(La/Th)+0.6013ln(Sm/Th)-1.3450ln(Yb/Th)+2.1056ln(Nb/Th)-5.4763$
DF2	$-0.305ln(La/Th)-1.1801ln(Sm/Th)+1.6189ln(Yb/Th)+1.226ln(Nb/Th)-0.9944$

1.2.5. New Multi-Dimensional Diagrams with Discriminating Functions

Agrawal et al. (2004) applied linear discriminant analysis in order to discriminate Pliocene to recent basic rocks on the basis of their major element chemistry (Figure 1.28). Four tectonic settings were discriminated: island arc, continental rift, ocean island, and mid-oceanic ridge. 1159 samples with SiO_2 content less than 52% were selected for discriminant analysis. Field boundaries were derived by computing probability functions. Multi-dimensional discrimination diagram of discriminant functions DF1 and DF2 (Table 1.4) obtained a success ratio of 76% to 96%.

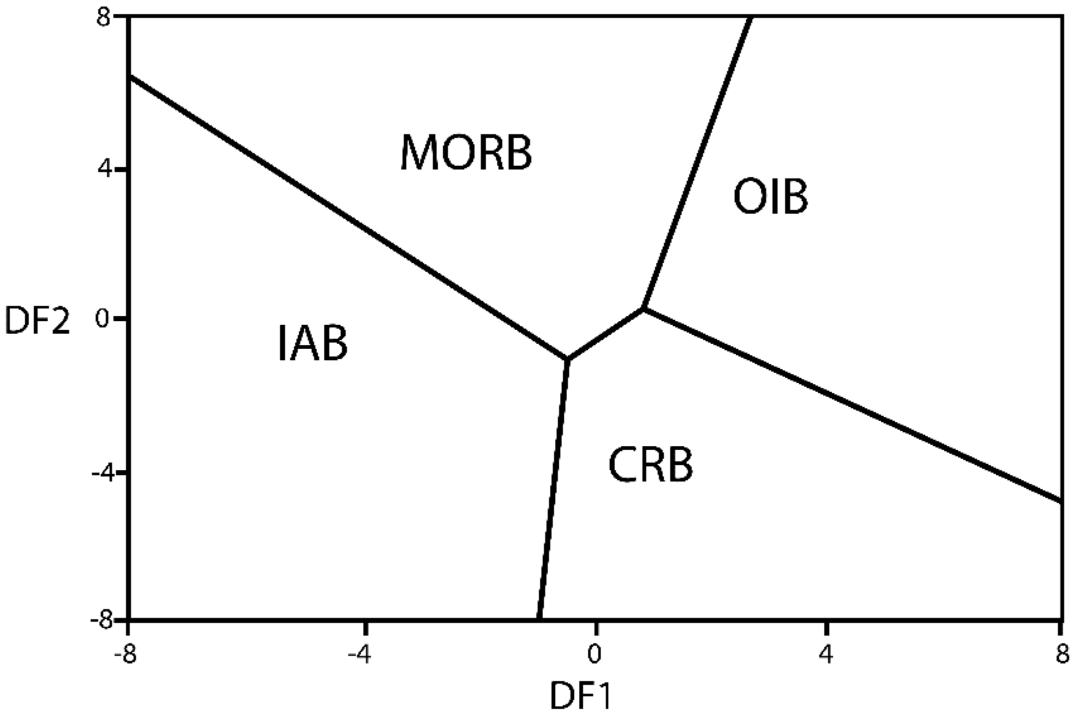

Figure 1.28. Representative discrimination diagram from Agrawal et al. (2004)

Table 1.4. Discrimination functions used in diagrams of Agrawal et al. (2004)

Discrimination Functions	
DF1	$+0.258SiO_2+2.395TiO_2+0.106Al_2O_3+1.019Fe_2O_3-6.778MnO+0.405MgO+0.119CaO+0.071Na_2O-0.198K_2O+0.0613P_2O_5-24.064$
DF2	$+0.730SiO_2+1.119TiO_2+0.156Al_2O_3+1.332Fe_2O_3+4.376MnO+0.493MgO+0.936CaO+0.882Na_2O-0.291K_2O-1.572P_2O_5-59.472$

Verma et al. (2006) published five new discriminant function diagrams (Figure 1.29) based on extensive database representatives of basic and ultrabasic rocks using discrimination functions (Table 1.5). Tectonic settings discriminated are island arc, continental rift, ocean-island, and mid-oceanic ridge. 2732 samples were selected and major element data was used for discriminant analysis. The diagrams were obtained after log-transformation. They also obtained a high success ratio between 82% to 97%.

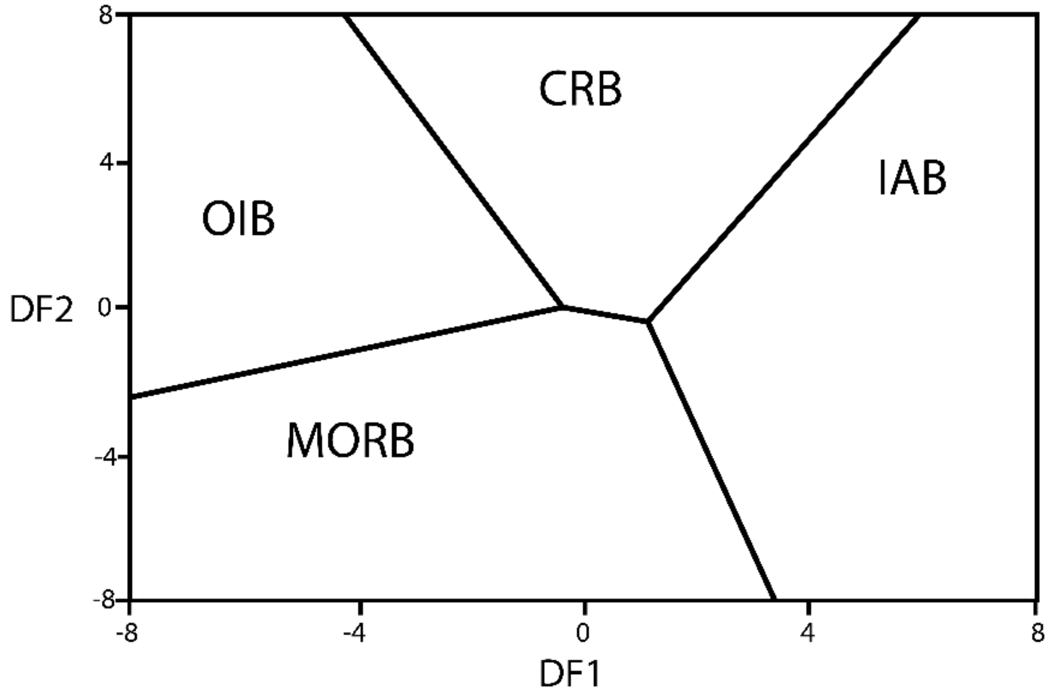

Figure 1.29. Representative discrimination diagram from Verma et al. (2006)

Table 1.5. Discrimination functions used in diagrams of Verma et al. (2006)

Discrimination Functions	
DF1	$-4.6761\,ln(TiO_2/SiO_2)+2.5330\,ln(Al_2O_3/SiO_2)-0.3884\,ln(Fe_2O_3/SiO_2)+3.9688\,ln(FeO/SiO_2)+0.8980\,ln(MnO/SiO_2)-0.5832\,ln(MgO/SiO_2)-0.2896\,ln(CaO/SiO_2)-0.2704\,ln(Na_2O/SiO_2)+1.0810\,ln(K_2O/SiO_2)+0.1845\,ln(P_2O_5/SiO_2)+1.5445$
DF2	$+0.6751\,ln(TiO_2/SiO_2)+4.5895\,ln(Al_2O_3/SiO_2)-2.0897\,ln(Fe_2O_3/SiO_2)+0.8514\,ln(FeO/SiO_2)+0.4334\,ln(MnO/SiO_2)-1.4832\,ln(MgO/SiO_2)-2.3627\,ln(CaO/SiO_2)-1.6558\,ln(Na_2O/SiO_2)+0.6757\,ln(K_2O/SiO_2)+0.4130\,ln(P_2O_5/SiO_2)+13.1639$

Upon the problems in major and trace element based discrimination diagrams, Agrawal et al. (2008) published new discrimination function based diagrams focusing on five trace elements (La, Sm, Yb, Nb, Th) and four log-transformed ratios (La/Th, Sm/Th, Yb/Th, Nb/Th). The tectonic settings discriminated are island arc, continental rift, ocean island, and mid-ocean ridges. A total of 1645 samples were selected for linear discriminant analysis. Agrawal presented a multidimensional discrimination diagram (Figure 1.30) based on discriminant functions of DF1 and DF2 (Table 1.6) in which continental rifts and ocean islands are plotted in a single region when all four tectonic settings are to be discriminated at the same time. They also presented four diagrams discriminating three settings out of four each time: IAB, OI, and CRB; MOR, IAB, CRB; MOR, IAB, OI and OI, CRB, MOR.

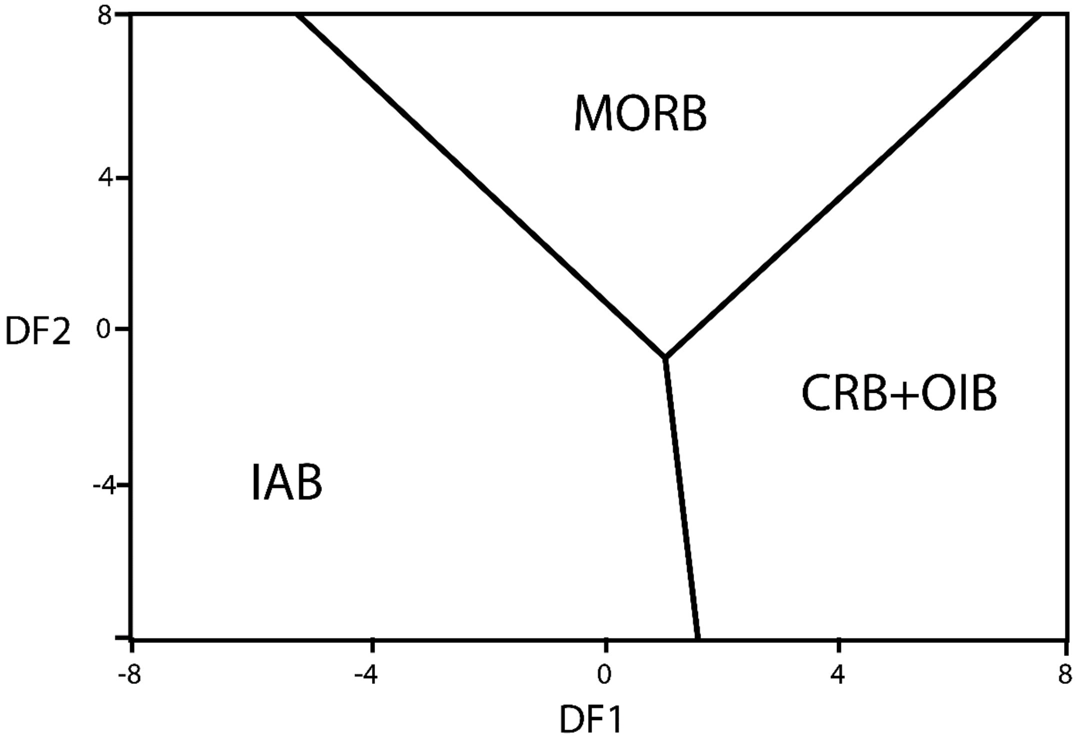

Figure 1.30. Representative discrimination diagram from Agrawal et al. (2008)

Table 1.6. Discrimination functions used in diagrams of Verma et al. (2006)

Discrimination Functions	
DF1	$0.3518\,ln(La/Th)+0.6013\,ln(Sm/Th)-1.3450\,ln(Yb/Th)+2.1056\,ln(Nb/Th)-5.4763$
DF2	$-0.305\,ln(La/Th)-1.1801\,ln(Sm/Th)+1.6189\,ln(Yb/Th)+1.226\,ln(Nb/Th)-0.9944$

Verma and Agrawal (2011) published new tectonic discrimination diagrams for basic and ultrabasic volcanic rocks (Figure 1.31). They applied log-transformation to five HFSE: TiO_2, Nb, V, Y, and Zr. The database was compiled from previous studies of Verma et al. (2006), Agrawal et al. (2004, 2008), and Verma (2010). 1877 analyses were used for discriminant analysis. The tectonic settings discriminated are island arcs, continental rifts, ocean-islands, and mid-ocean ridges. Five HFSE elements and their log-transformed ratios (Nb/TiO_2, V/TiO_2, Y/TiO_2, and Zr/TiO_2) were used in discriminant functions obtaining success ratios between 80% and 94%. Verma and Agrawal (2011) also published one diagram in which continental rifts and ocean islands are plotted on the same region and four diagrams their triple combinations of four tectonic settings were discriminated separately.

1.2.6. Discrimination using Machine Learning Methods

Vermeesch (2006a) used the decision tree learning method of machine learning and built two decision trees in order to discriminate between three different tectonic settings for basaltic rocks; mid-ocean ridges, ocean islands, and island arcs. He used 756 samples from global geochemical datasets of PetDB and GEOROC with their major and trace element and isotope ratio measurements in order to build decision trees. The first tree uses all samples with all elements and isotope ratios (Figure 1.32). The second one only uses altered samples and immobile elements, thus expected to be resistant against weathering and/or metamorphism (Figure 1.33). He stated that the success ratio for the application of the decision tree reaches up to 89% for the first tree and 84% for the second tree.

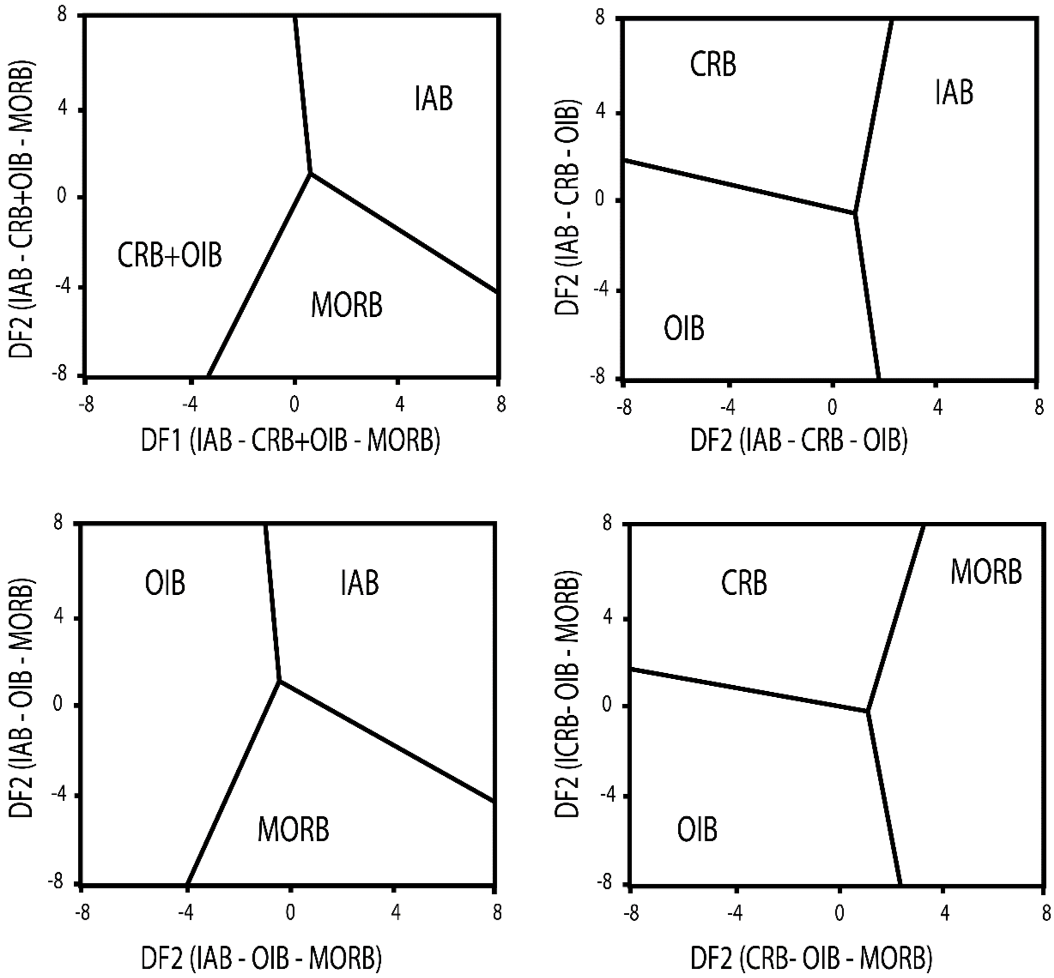

Figure 1.31. Representative discrimination diagrams from Verma and Agrawal et al. (2011)

Agrawal and Verma (2007), on the other hand, stated several problems for Vermeesch (2006a): The dataset included major deficiencies, classification results are irreproducible, reported success ratios are inaccurate, the criteria of classification is not objective, comparison of classification tree with LDA is inadequate and inviolable rules of multivariate nature of geochemical compositions have been violated.

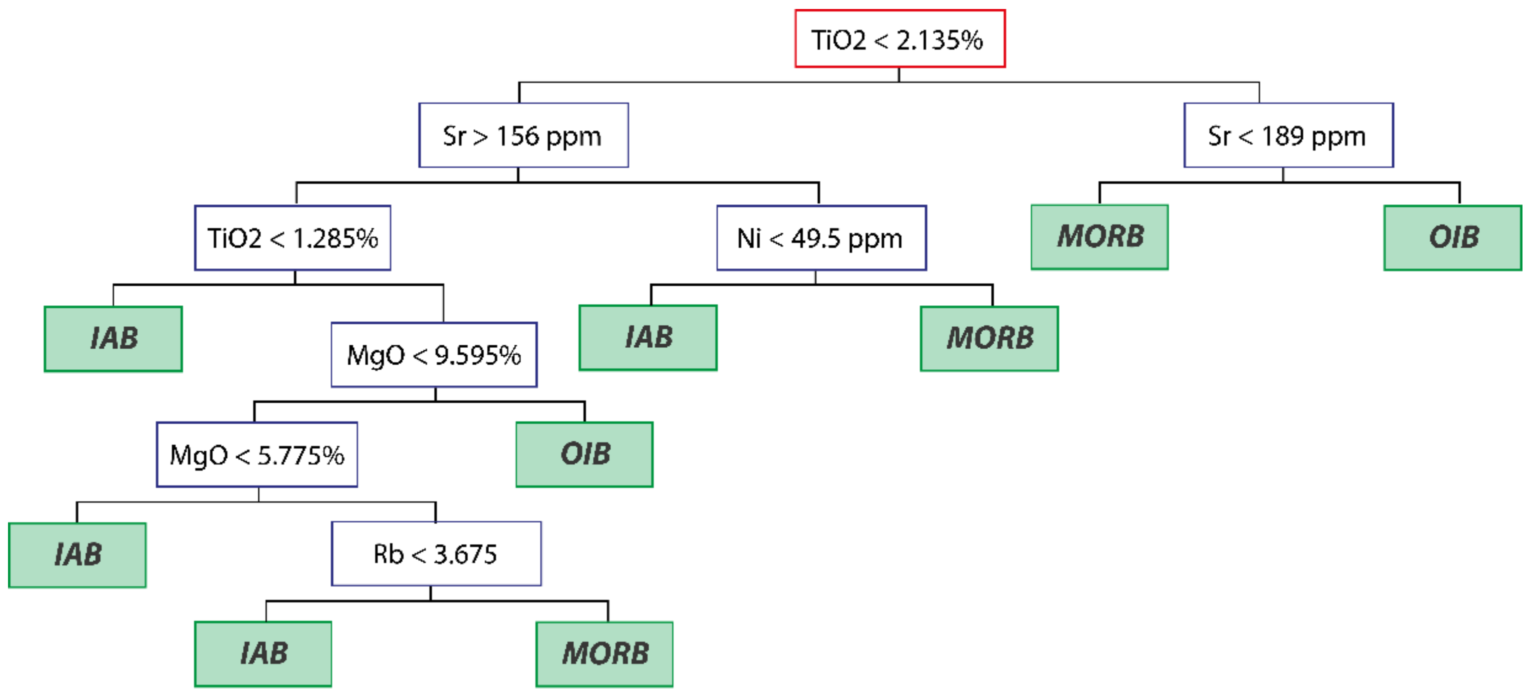

Figure 1.32. Decision tree from Vermeesch (2006a) using all elements

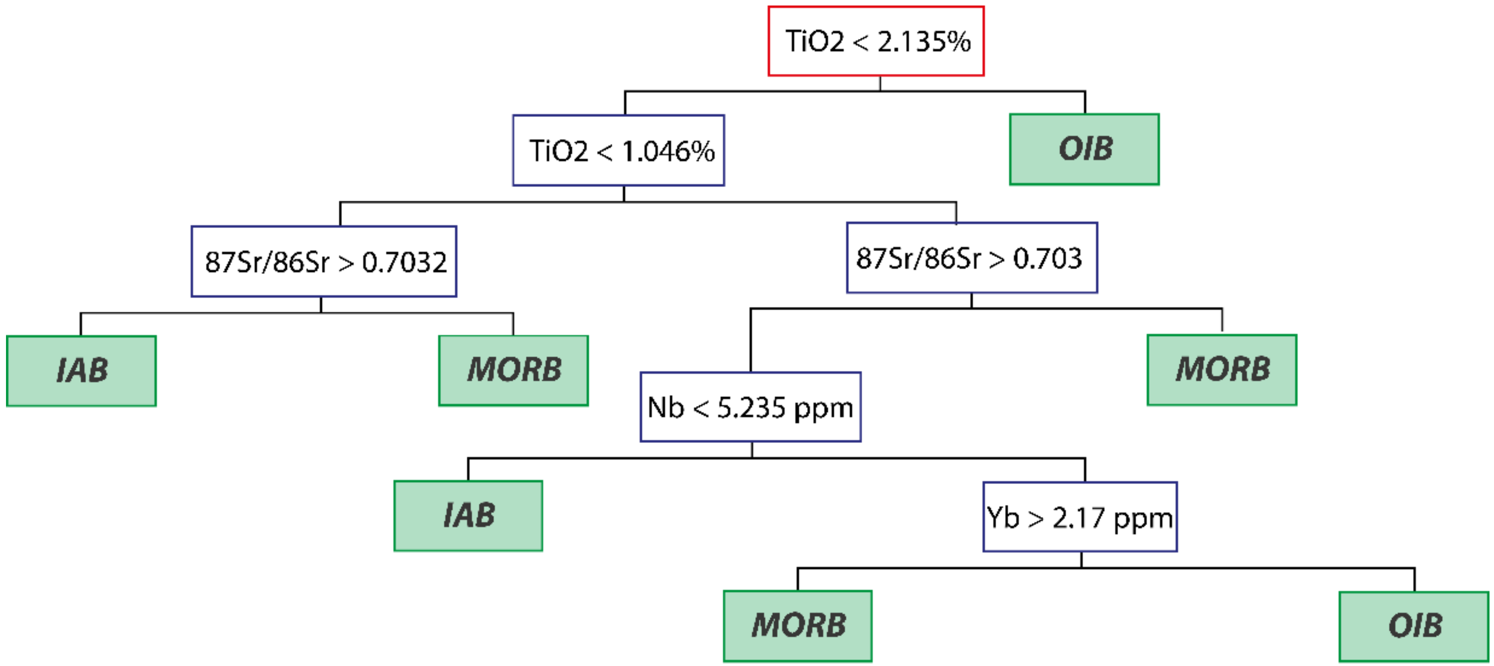

Figure 1.33. Decision tree from Vermeesch (2006a) using only relatively immobile elements

Ueki (2017) applied three different machine learning techniques (support vector machine, sparse multinomial regression, and random forest) in order to discriminate magmas from eight different tectonic settings using representative basalt compositions from global geochemical datasets (PetDB and GEOROC). Data published before 1990 were eliminated in order to prevent analytical uncertainties, and outliers were excluded. The samples from problematic localities such as Azores, the Galapagos, Iceland, and Chile, etc) were eliminated. A total of 2074 samples were used for discrimination. The tectonic settings to be discriminated are back-arc basins, continental arcs, continental floods, island arcs, intra-oceanic arcs, mid-oceanic ridges, oceanic islands, and oceanic plateaus. For discrimination, 20 elements including major elements (SiO_2, TiO_2, Al_2O_3, Fe_2O_3, CaO, MgO, Na_2O, K_2O), along with selected trace element (Sr, Ba, Rb, Zr, Nb, La, Ce, Nd, Hf, Sm, Gd, Y, Yb, Lu, Ta, Th) and 5 isotopic ratios ($^{206}Pb/^{204}Pb$, $^{207}Pb/^{204}Pb$, $^{208}Pb/^{204}Pb$, $^{87}Sr/^{86}Sr$ and $^{143}Nd/^{144}Nd$) were used. Ueki used geochemical compositional data normalized using a one-parameter Box-Cox transform before the application of machine learning algorithms. The performance of discriminations obtained by machine learning techniques was evaluated by 10-fold cross-validation. Ueki showed that modern techniques of machine learning can be a better option for tectono-magmatic discrimination of igneous rocks having high success ratios for support vector machine, sparse multinomial regression, and random forest.

These modern techniques of machine learning along with the traditional methods are still being tested by other researchers (Verma, 2017; Gomez and Verma, 2016; Verma and Oliveira, 2015; Verma et al., 2015; Li, 2015, Pandarinath, 2014; Pandarinath and Verma, 2013, Verma et al., 2012; Verma, 2010; Sheth, 2008) and compared with traditional discrimination methods (bivariate and ternary diagrams)..

CHAPTER 2

DATABASE AND METHODOLOGY

2.1. Data Gathering and Import

The complete database is compiled for 5,114 samples of mainly basic and to a lesser extent ultrabasic igneous rocks from known locations of uncontroversial tectonic settings from all over the world directly from published literature. The database includes the articles generally published after 1995 (with some exceptions). The aim is to include the chemical analyses with high precision and accuracy so that the ratios would reflect the true fractionation between the elements. This is actually very critical, since any false fractionation effect, which may have raised from analytical errors, have the potential of misclassification of the data. Therefore, the database is constructed on high-quality data that best reflects the true geochemical nature of the investigated basic lithology.

The geology, lithology, mineralogy, and geochemistry of samples along with source rock characteristics of each location are referred from the original articles. Global geochemical databases such as GEOROC-Mainz or PetDB are avoided in the construction of the database as they have significant errors that may result in false interpretations (Gomez and Verma, 2016).

2.2. Data Cleaning

The database initially included all available samples from related articles. However, a variety of samples are eliminated in three-stages based on certain criteria.

Initially, the problematic samples are eliminated from the database. Some of the problematic samples include non-igneous lithologies. These are characterized by sedimentary or metamorphic samples, which are analyzed to get petrogenetic inferences, such as slab-derived contributions, nature of the source, crustal contamination. Some other problematic samples, however, are characterized by apparent numerical inconsistencies with the rest of the samples in the dataset, which result in unrealistic element ratios. This problem can be related to analytical errors or can be simply attributed to typos made during the preparation of the manuscript. If all samples from a certain data source are problematic, then the data source is completely removed from the database or transferred to another database.

On the second stage, the data cleaning is solely based on the rock type of samples. The rock type is evaluated by chemical classification using the plot of LeMaitre (1987). Since this study intends to discriminate the basic rocks, the igneous varieties included in the database are basalts, trachybasalts, picrobasalts, foidites, tephrites/basanites. Apart from continental arcs, there is a vast number of basaltic rocks sampled from the other tectonic settings. Continental arcs, however, include a somewhat limited amount of mafic compositions. The reason is mainly that continental arcs have a thick continental lithospheric cap, which increases the change of mafic magmas to interact with the continental crust whose composition significantly differs from that of oceanic crust (e.g. Davidson et al.,1989; Bryant et al.,2006; Stern 2010). Thus, the increasing interaction between continental crust and greater residence times of the magmas within the crustal magma chambers results in the extensive fractionation of mafic magmas, which in turn produces a significant amount of highly evolved varieties (i.e. intermediate and silicic members) (e.g. Wilson 1989). Therefore, for continental arcs only, basaltic andesites and basaltic trachyandesites are also included in the database in order to increase the number of samples for this tectonic setting, which allowed to make a better comparison by homogenizing the sample distribution. All other rock types (i.e. intermediate and acidic varieties) are eliminated from the database at this stage.

On the final stage, all samples with missing values for critical elements are eliminated from the database. The elements, determined as "critical element" are Th, La, Nb, Y, Yb, Zr, Hf, Sm, Nd, and TiO_2, which are selected due to their petrogenetic significance in different tectonic settings (which will be explained in the following paragraphs).

2.3. Classes (Tectonic Settings)

Classes (target features) in the database are characterized by seven tectonic settings, namely continental arc, continental within-plate (including continental rifts and continental flood basalts), mid-ocean ridge, oceanic arc, oceanic back-arc basin, oceanic island, and oceanic plateau. The classification is intended to include nearly all the tectonic settings. The continental back-arcs, however, is excluded due to the limited number of samples available in the literature, which considerably inhibits evaluating their petrogenetic features for discrimination. The continental back-arcs, therefore, are ignored here for the construction of discrimination methods.

Another issue related to the classes is about oceanic back-arcs. Oceanic back-arcs genetically stay in between the mid-ocean ridges and arcs. They begin their life by rifting of the arcs, which can be triggered by the slab roll-back (e.g. Martinez and Taylor, 2002; 2006). This processes result in extension and rifting of the arc, as well as the upwelling of the asthenosphere. This stage is accompanied by diffuse magmatism (e.g. Todd et al.,2010). The rifting and thinning of the arc crust eventually reach a point where the oceanic crust is generated and spreading starts. Thus, the life of an oceanic back-arc can be simply divided into two stages as rifting and spreading. It is important to note that since the rifting back-arcs are immature (i.e not evolved to spreading stage), they display arc-like geochemical characteristics. The spreading back-arcs, on the other hand, are mature, and they show geochemical features between what is called "BABB-type" and MORB-type. In this study, only spreading back-arcs are taken into account into the evaluation, since they represent the true geochemical nature of oceanic back-arc systems. Brief information about the tectonic settings included in the classification is as follows:

- Continental arcs represent divergent plate boundaries, where the oceanic lithosphere is subducted beneath the continental lithosphere. The generation of primary magmas primarily occurs via flux-induced melting and may be sourced from asthenospheric and/or continental lithospheric mantle. The presence of continental crust may add some chemical complexities to the mantle-derived magmas en route the surface.

- Continental within-plate settings are away from the plate boundaries, and the magmatism here does not involve any recent subduction contribution. The magmatism can be induced by mantle plumes, which results in continental flood magmatism or occurs via rifting (can be associated with/without plumes), resulting in continental rift magmatism.

- Mid-oceanic ridges represent divergent plate boundaries where the two lithospheric are moving apart from each other. A great amount of oceanic lithosphere is created at mid-ocean ridges. The magmatism is generated by adiabatic decompression melting, which mainly leads to large degrees of melting. While most of the magmatism occurs at the axis, some appear to be concentrated off-axis in the form of seamounts.

- Oceanic arcs are similar to continental arcs in that they also represent the convergent plate boundaries, and subduction is involved. However, in oceanic arcs, the subduction occurs beneath another oceanic lithosphere, so the system is entirely oceanic (i.e. the continental lithosphere is not involved). The melting is similarly occurring through mainly the flux-melting. Oceanic arcs are relatively simple systems compared to the continental arcs since they do not include continental crust in their petrogenesis.

- Oceanic back-arcs are extensional systems created behind the arcs. They are somewhat between mid-ocean ridges and oceanic arcs. Mature back-arcs are characterized by spreading, creating oceanic lithosphere like mid-ocean ridges. However, because subduction is involved, unlike mid-ocean ridges, they may have a subduction component similar to oceanic arcs. Melting takes place via flux-induced melting and/or decompression melting.

- Oceanic plateaus are among oceanic within-plate settings (Richards et al., 1989). They include a large volume of basaltic products, covering vast areas on the ocean floor. The magmatism is believed to be created by decompression melting of large plume-heads, which results in the production of very large volumes of mafic magma in a short period. They are somewhat similar to continental flood magmatism in this respect.

- Oceanic islands are also oceanic within-plate settings, like the oceanic plateaus (Davies, 1990). Oceanic islands are generally characterized by chains of volcanoes, whose origins are generally thought to be linked to mantle plumes. Although oceanic islands are mainly made up of voluminous mafic products, the size is not comparable to those of oceanic plateaus.

Brief information (tectonic settings, number of compiled references, number of locations, number of samples) is given in Table 2.1.

Table 2.1. Brief Information on Tectonic Settings

Tectonic setting	**Number of references**	**Number of locations**	**Number of samples**
Continental Arcs	15	6	322
Continental Within-Plates	28	15	678
Mid-Oceanic Ridges	17	8	2,213
Oceanic Arcs	26	15	604
Oceanic Back-Arcs	11	9	208
Oceanic Islands	15	11	715
Oceanic Plateaus	13	5	374
TOTAL	**125**	**69**	**5,114**

Several locations selected for database are Andes, Aeolian and Aegean Sea for continental arcs, Africa, Brazil and Paraguay for continental within-plates, East

Pacific Rise, Mid-Atlantic Ridge, Indian and Atlantic Ridges for mid-oceanic ridges, Greater and Lesser Antilles, Mariana and Vanuatu for oceanic arcs, Manus Basin, Lau Basin and Izu Bonin for oceanic back-arcs, Hawaii, Iceland and Young Rurutu for oceanic islands and Kerguelen, Ontong Java and Manihiki for oceanic plateaus.

2.4. Feature Selection

The database initially included all available information in related articles such as major elements (SiO_2, TiO_2, Na_2O, K_2O, FeO / Fe_2O_3, MgO, MnO, CaO, Al_2O_3, P_2O_5), minor and trace elements (Th, La, Nb, Y, Yb, Zr, Hf, Sm, Nd, Ce, Dy, Pr, Eu, Gd, Tb, Ho, Er, Tm, Lu, Pb, Rb, Sr, Ba, Cs, Ta, U, Sc, V, Cr, Ni, Cu, Co, Sb, Zn) and isotope ratios ($^{87}Sr/^{86}Sr$, $^{143}Nd/^{144}Nd$, $^{206}Pb/^{204}Pb$, $^{207}Pb/^{204}Pb$, $^{208}Pb/^{204}Pb$).

Although there are many elements available to consider, it is not so straightforward to apply all of them when the effects of alteration considered. Alteration of the igneous rock can occur during weathering or metamorphism. The igneous rocks generated at mid-ocean ridges, for example, start experiencing hydrothermal metamorphism immediately after their production at the ridge axis (e.g. Bach and Früh-Green, 2010). During this process, which may involve temperatures up to ~400°C, can modify the oceanic crustal lithologies up to amphibolite facies (e.g. Seyfried et al.,1991; Bach and Früh-Green, 2010). With the ongoing spreading, the effect of hydrothermal metamorphism diminishes, as the lithologies are displaced away from the ridge axis. Following this, the alteration continues, but under very low-temperature conditions this time (low-T alteration/weathering). The altered oceanic crust can be further modified during subduction (e.g. Pearce and Peate, 1995; Spandler et al.,2004). The crustal lithologies undergo dehydration with increasing temperature, and they can be metamorphosed, for example, under blueschist to eclogite facies following a cold subduction.

Whether it is of continental or oceanic origin, old igneous rocks are likely to be altered. In addition, as mentioned above, some lithologies may go through multiple stages of alteration as the fate of subducted oceanic crustal rocks. The critical thing here is that the introduction of fluid phase may mobilize some elements, causing their loss or gain in the host lithology. The mobilization is known to primarily effect the low-ionic potential elements, such as Rb, Ba, K, Si etc. In contrast, the elements with intermediate ionic potential, like HFSE and REE (Rare Earth Element) are mainly known to be fluid-immobile (e.g. Pearce 1975; Staudigel et al.,1996; Bach and Früh-Green, 2010). Although the stability of the latter group of elements (HFSE and REE) are mostly valid under weathering and low-grade metamorphic conditions (greenschist facies), their relative immobility have also been reported for higher-grade metamorphic conditions (i.e. amphibolite, blueschist, and eclogite facies; Spandler et al.,2004; John et al.,2010; Sayit et al.,2016). Mobilization may cause significant fractionation of the mobile elements (among themselves and/or relative to immobile ones). Their use (either as absolute abundances or ratios) should be carefully handled or avoided when making petrogenetic inferences. Therefore, for altered rocks, the use of fluid-immobile elements would be a better choice to infer pristine geochemical features inherited from the protolith/original rock.

Considering the potential effects of mobilization on the altered rocks as explained above, only the fluid-immobile elements are considered in this study. It must be noted that most major and minor elements are known to be mobile in fluids. The most resistant ones appear to be Ti, Al, P, and Cr. However, apart from Ti, the others can also be mobilized to some extent under hydrothermal metamorphism (Pearce 1975). Thus, of these, only Ti is included in this study as an element that can reflect the pristine geochemical features under a broad spectrum of alteration conditions.

Isotope ratios are among the least used discriminators when taking into account the tectonomagmatic discrimination methods published thus far. The only study in this regard is that of Vermeesh (2006A), who involved $^{87}Sr/^{86}Sr$ for the decision-tree-based tectonomagmatic discrimination. Sr isotopic ratio, however, can be strongly affected through interaction with seawater (e.g. Bach et al.,2003), which makes it a highly unreliable discriminator. On the other hand, Nd and Pb isotopic ratios remain unaffected upon interaction with seawater, thus they can act as better proxies for the tectonomagmatic discrimination. However, in spite of this petrogenetic superiority, the higher analytical costs of isotopic systems make them less available for most datasets. Also, age-correction poses another problem. Since isotopic ratios can significantly differ from the measured ones, this issue requires the precise age for every sample included for the petrogenetic considerations. However, providing age data for every sample on the ancient rocks is a highly difficult job, especially regarding the ones from the mélanges. Thus, although the isotopic ratios may serve some invaluable information, their low applicability makes them less deserved features for fingerprinting of the igneous rocks.

Another issue to be noted that absolute values of relatively immobile elements are only used for calculation of ratios but not used in the construction of discrimination methods. This is one of the critical points in this study since the Orange software is not able to calculate the elemental ratios from the absolute abundances, which might be suitable for the construction of decision trees. Thus, the consideration of elemental ratios, which is believed to be of a petrogenetic significance, is devised and introduced manually, not by the software. One of the advantages of using ratios over absolute abundances is to minimize the effect of fractional crystallization (FC). Another strong constraint comes from the fact that since the partitioning of fluid-immobile trace elements is highly dependent on the residual mineralogy, they are powerful features in reflecting petrogenetic characteristics, including the nature of mantle source region, degree of partial melting, and contribution of subduction components (e.g. Pearce 1983; McKenzie and O’Nions 1991; Weaver 1991; Shaw 2006).

Using element ratios instead of absolute abundances also increases the discrimination ability of constructed decision trees as an element ratio would be much more discriminating feature when compared to absolute abundance of each element used in calculation of ratio (e.g. Th/Nb compared to Th and Nb) (Figure 2.1).

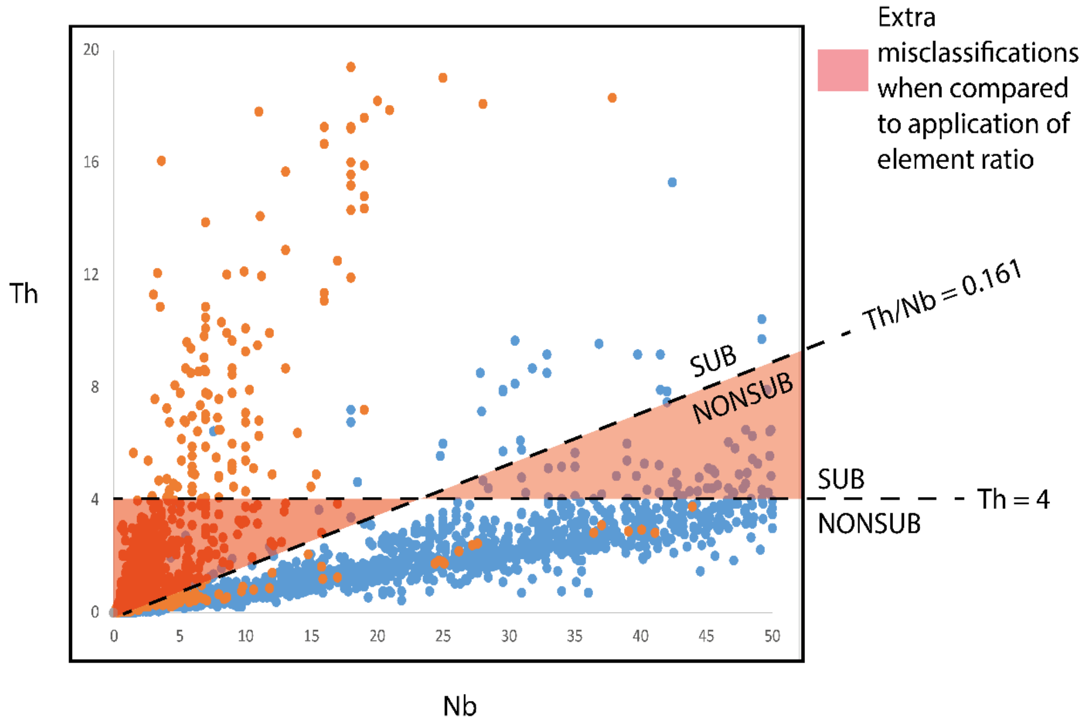

Figure 2.1. The difference between the discrimination potential of element ratios and their absolute abundance

One of the problems when dealing with the datasets is the missing data, which make their use undesirable since this situation would cause in a significant bias and inconsistentiences in the tectonomagmatic discrimination. Thus, although they are relatively immobile, the large amounts of missing data regarding the REE, Ce, Dy, Pr, Eu, Gd, Tb, Ho, Er, Tm, and Lu are ignored as they result in the loss of huge amounts of data. Selected relatively immobile elements are Th, La, Nb, Y, Yb, Zr, Hf, Sm, Nd and TiO_2. Selected relatively immobile elements are highly correlated with elements ignored due to the large amount of missing data, therefore, their elimination has no negative effect on the performance of constructed decision trees (Figure 2.2).

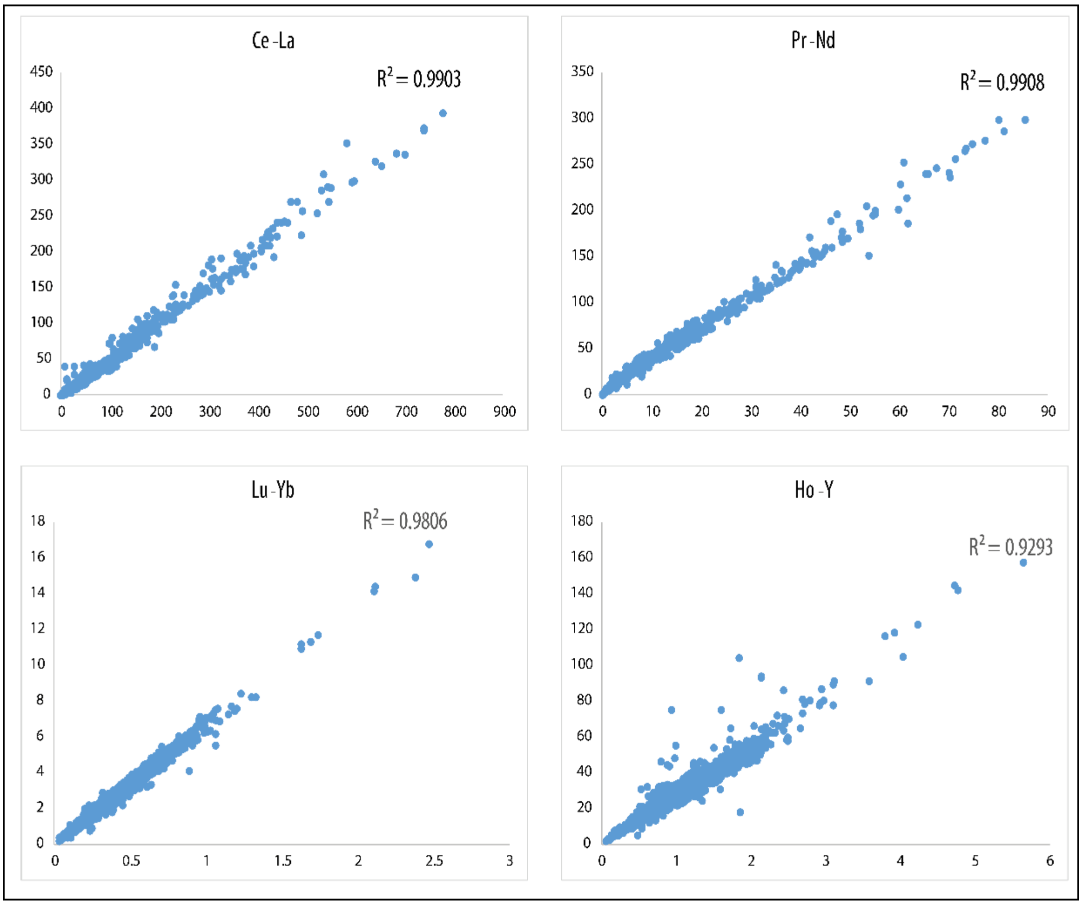

Figure 2.2. Representative example to strong correlation between selected relatively immobile elements and elements eliminated due to high amount of missing data

Applied ratios of immobile elements are Th/Nb, La/Nb, Th/La, Zr/Hf, Zr/Nb, La/Y, La/Yb, Nb/Y, Nb/Yb, Sm/Y, Sm/Yb, Nd/Zr, La/Sm, Sm/Hf, Y/Yb, Zr/Sm, Zr/Y, Zr/Yb, Th/Y, Th/Yb, Sm/Nd, Sm/Nb, Zr/TiO_2, Nd/TiO_2, Nb/TiO_2, TiO_2/Y and TiO_2/Yb. An additional feature as Nb/Nb* is also added with a formula of

$$\frac{Nb}{Nb^*} = \frac{\frac{Nb}{0.658}}{\sqrt{\frac{Th}{0.0795} \cdot \frac{La}{0.648}}}$$

2.5. Splitting Database

The database is first divided into two datasets: Training-test dataset and external dataset. Then, training-test dataset is randomly divided by Orange software as training dataset and test dataset in proportions of 80% and 20%, with respectively. Training dataset is the dataset used in the construction of discrimination methods. The test dataset is the dataset similar to training dataset and used for the initial test for the performance of discrimination methods. The external dataset is the dataset different than the training and test datasets and used for the test for external applicability of discrimination methods to different tectonic settings and locations all over the world.

2.6. Methodology (Decision Tree Learning)

2.6.1. Non-Mathematical Explanation of Decision Tree Learning

Data science is the discipline of processing and analyzing data for the purpose of extracting valuable knowledge. The term “data science” was first used in the 1960s but became popular recently with developments in technology. Various domains such as commerce, medicine, and research are applying data-driven discovery and prediction in order to gain some new insights, such as Google, which tracks user clicks in order to improve its search engine results and ads.

Data science is the science of exploring data in order to discover useful patterns and obtain valuable insights. The use of decision trees is one of the promising and popular approaches of data science. Decision trees are simple but also successful techniques for predicting and explaining the relationship between various features (such as element concentration or ratio of element concentration) of an item (such as a rock) and its target value (such as its tectonic setting).

Decision trees are multi-purpose applications especially for classification problems as they are self-explanatory and easy to follow, flexible in handling a variety of input data, adaptable in processing datasets with errors and missing data, and useful for large datasets. They are successful predictors for a relatively small computational effort.

When a decision tree is used for a task of classification instead of regression, it is generally defined as "classification tree". Classification trees are used to classify an object or an instant (such as a rock) into a predefined set of classes (such as tectonic settings) based on their attribute values (geochemical features such as element concentrations or ratios of element concentrations). Decision trees have a typical structure which is like a tree, starting with a root node and ending with leaf nodes (Figure 2.3).

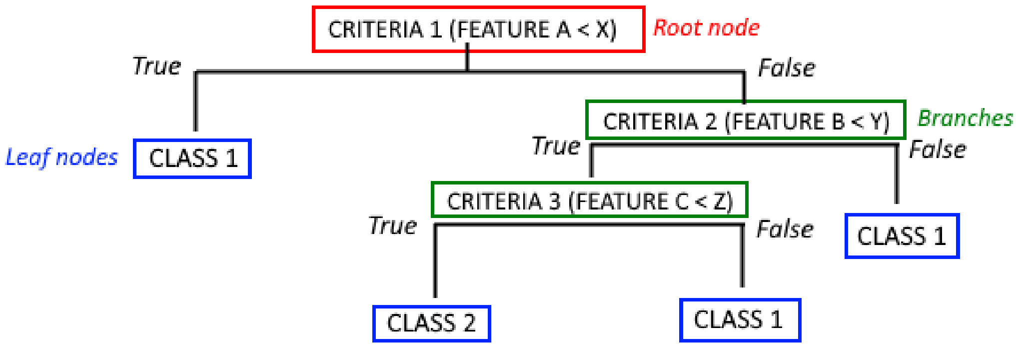

Figure 2.3. Structure of a decision tree

Decision trees are very popular techniques due to their simplicity and transparency. A decision tree can be defined as a classifier as a recursive partition of the instance space or as a predictor, h: $X \rightarrow Y$, that predicts a label associated with an instance x following a route from a root node to a leaf node. Y can be defined as classes, for this case, is tectonic settings, such as mid-oceanic ridge, continental arc, continental within-plate, oceanic arc, oceanic back-arc, oceanic island, oceanic plateau. X can be defined as features, for this case, as ratios of certain relatively immobile elements. Decision trees are widely applied to prediction problems.

The decision tree is made of nodes. The amount of nodes depends on the factors such as complexity of tree, size of tree. A node without any incoming edge is known as root node. Classification starts with root node. Nodes with one incoming edge and at least two outgoing edges are called as either internal node or test node. All other nodes are called either leave or terminal node or decision node.

Depending on the level of depth, each internal node splits internal space into at least two sub-spaces based on the result of a discrete function. At the end of the classification by a decision tree, each leaf is assigned to one class representing the most appropriate target value.

Instances are classified by navigating from the root of the tree until a leaf node based on the tests along the path, including root node, each internal node and finally a leaf node. Decision tree induction is closely related to rule induction. Each path from the root of a decision tree to one of the leaves can be transformed into a rule simply by combination of all conditions along the way.

Generally, decision trees that are not complex are preferred in order to prevent overfitting. Tree complexity has a significant effect on accuracy. Complexity of a tree can be measured by these metrics: total number of nodes, total number of leaves, tree depth and number of attributes used.

Decision tree learning requires three main components: task T, experience E, and performance P. In this case, T is classifying rocks based on their tectonic settings, E is the tectonic settings of rock samples in training set, and P is the percentage of samples correctly classified.

The data used to train the model is called the training set. The training set is presented in the form of a table, in which each row represents rocks, and each column represents the feature of those rocks such as element concentrations or ratios of element concentrations. One column, on the other hand, corresponds to the target attribute, which is the tectonic setting of rock.

The concept of overfitting is essential for the success of decision trees. If a decision tree classifier perfectly fits training data but fails to classify external datasets successfully, it is called "overfitting" (Figure 2.4). That means that the decision tree did not learn but summarized the data. In the decision trees, overfitting is generally observed as a result of too many nodes relative to the amount of training data.

Another concept is underfitting, on which decision tree fails both for the training data and external dataset. In bigger trees, the classifier tends to overfit; yet in smaller trees, there is a tendency of classifier towards underfitting (Figure 2.4).

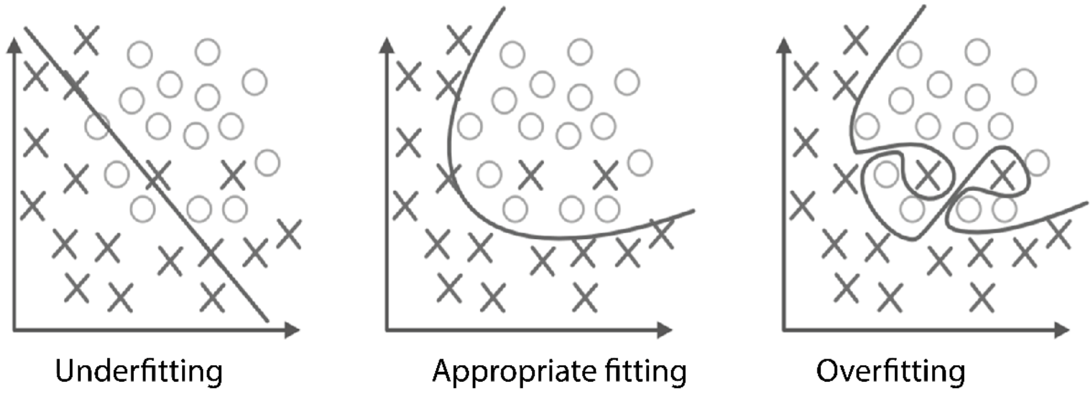

Figure 2.4. Underfitting and overfitting examples

However, the classification of all instances successfully is not possible of selected feature space. Therefore, we have to restrict decision tree to a small portion of possible solutions and to find the optimum size for decision tree (Figure 2.5). The optimum size for decision tree avoids both underfitting and overfitting.

Decision trees are one of the effective techniques for classification. They assure computational feasibility and allow the representation of multi-dimensional decision space as a two-dimensional tree graph. Building a tree may seem to be complicated. On the other hand, using a classification tree is extremely simple.

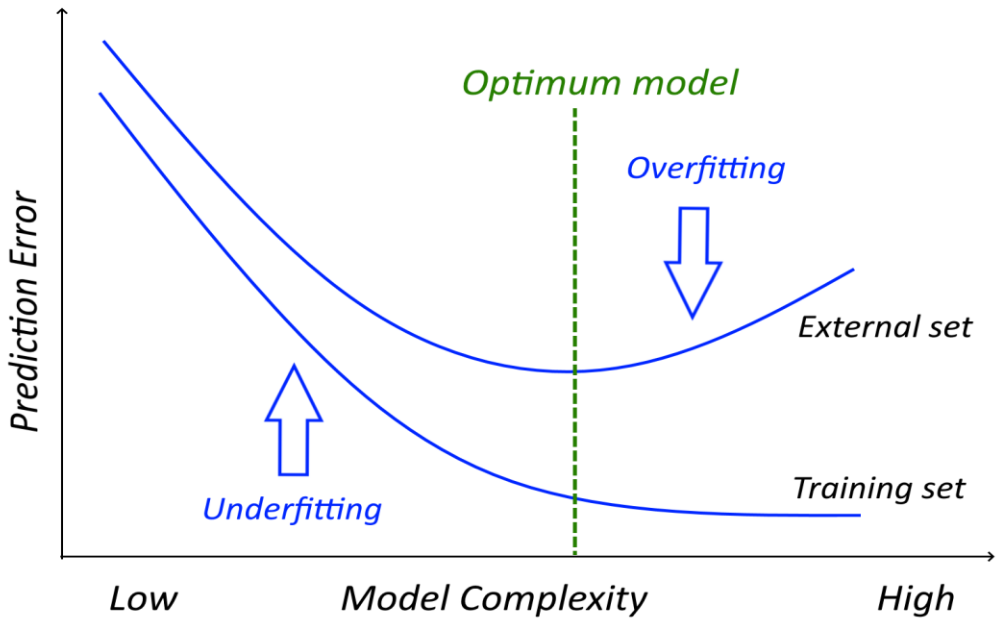

Figure 2.5. Representation of optimum model based on prediction errors on training and external datasets

2.6.2. Mathematical Explanation of Decision Tree Learning

Only brief information is given for the mathematical explanation of decision tree learning. For detailed information, Breiman (2017) shall be referred.

In a typical decision tree, a training set is introduced, and the goal is to form a classification model to predict previously unseen samples, which are known as test set or external set.

A training set is denoted as $S = B(A \cup y)$ where A denotes the set of input attributes containing n attributes: $A = \{a_1, \ldots, a_i, \ldots, a_n\}$ and y represents the class variable or the target attribute. Attributes can be either nominal or numeric.

For a training set S with input attributes set A = {a1, a2, . . ., an} and a nominal target attribute y from an unknown fixed distribution D over the labeled instance space, the goal is to induce an optimal classifier with minimum generalization error.

The generalization error is defined as the misclassification rate over the distribution D, which can be expressed by the equation

$$\varepsilon(DT(S), D) = \sum_{(x,y)\in U} D(x, y). L(y, DT(S)(x))$$

where L (y, DT(S), D) is the zero one loss function defined with equations

$$L(y, DT(S)(x) = \begin{cases} 0 \; if \; y = DT(S)(x) \\ 1 \; if \; y \neq DT(S)(x) \end{cases}$$

The main goal is to induce the best classifier or a set of classifiers that most accurately classify the members of instance space.

An induction algorithm or simply inducer (also known as learner) is an entity that obtains a training set and forms a model that generalizes the relationship between the input attributes and the target attribute and to produce a classifier.

The notation DT represents a decision tree inducer, and DT(S) represents a classification tree that is induced by performing DT on a training set S. Using DT(S), it is possible to predict the target value of a tuple x_q. This prediction is denoted as DT(S)(x_q).

Suppose we have N data points with J dimensions, which can be expressed as $X^n=\{x_1^n,\ldots., x_j^n,\ldots., x_J^n\}$ ($1 \leq n \leq N$). All data points belong to one of K classes Y^N = c_1 | … | c_k | … | c_K and classification of these data points based on the classes is expected by using J features. For this case, N represents the number of basic igneous rock samples, J represents ratios of selected relatively immobile elements, K represents tectonic settings as classes.

The basic idea behind classification trees is to approximate the parameter space by a piece size constant function, in other words, to partition $\underline{X}$ into M disjoint regions $\{R_1,\ldots..,R_m,\ldots..,R_M\}$ (Figure 2.6).

A partition is defined by two quantities at any stage of the recursive process: the split variables j ($1 \leq j \leq J$) and the split point s ($-\infty < s < \infty$). The purpose is to find the partition, where the node impurity $Q_m(T)$ is minimum.

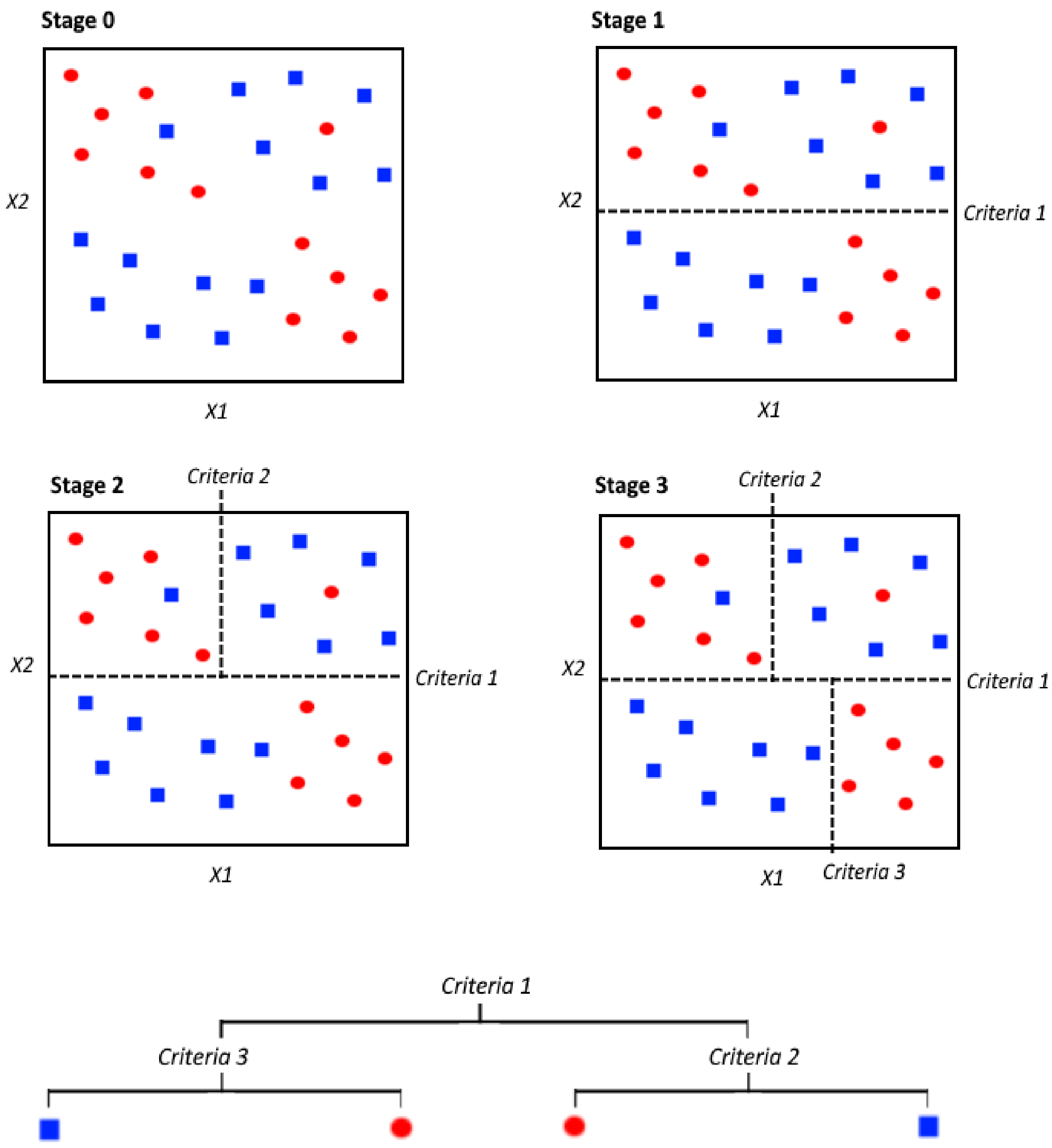

Figure 2.6. Representation of a decision tree in a two-dimensional graph

Let p_{mk} be the proportion of class k observations in node m, then

$$Q_m(T) = \sum_{k=1}^{K} p_{mk}\,(1 - p_{mk})$$

This particular form of Q_m (T) is called the "Gini index of diversity". The recursive partitioning process continues until all the end-nodes are "pure" i.e. all belong to the same class. The maximum sized tree thus obtained perfectly describes the training data. In other words, it has zero bias. However, for the purpose of prediction, this tree is not optimal, because it overfits the training data, causing high variance.

The tree with optimal predictive power is smaller than the largest possible tree and can be found by "cost-complexity" pruning. Define the "cost-complexity criterion" of a tree T as

$$cp_{\propto}(T) = \sum_{m=1}^{|T|} N_m Q_m(T) + \propto |T|$$

with |T| the number of terminal nodes in T, N_m the number of observations in the mth terminal node, Q_m(T) the "node impurity" defined by equation and α a tuning parameter. For a given α ≥ 0, it is possible to find the subtree $T_\alpha \subset T_0$ that minimizes cp_α(T) over all possible subtrees of the largest possible tree T_0

$$T_{\propto} = \underset{T \subset T_0}{argmin}\, cp_{\propto}(T)$$

Repeating this procedure for a range of values 0 ≤ α ≤ ∞ produces a finite nested sequence of trees $\{T_0, T_{\alpha 1}, ..., T_{\alpha max}\}$. Except for T_0, these trees no longer have only pure end-nodes. Impure end-nodes are assigned the class that dominates them. Prediction errors versus the number of nodes are plotted for each of the nested subtrees.

Trees with fewer nodes tend to have a larger bias. The smallest tree with misclassification error not exceeding minimum misclassification error plus one standard error is selected as the final decision tree.

2.6.3. Evaluation of Decision Trees

Several indicators are evaluated in order to determine and evaluate the quality of the decision tree. Evaluation of the decision tree performance is a fundamental aspect of data science and machine learning. The inducer receives a training set as input data and constructs a decision tree. Both the decision trees and inducer can be evaluated as an evaluation criterion.

2.6.3.1. Generalization Error and Classification Accuracy

Let DT(S) be a decision tree for a training set S. The generalization error of DT(S) is its probability to misclassify an instance selected from instance space.

The classification accuracy of a decision tree is one minus the generalization error, and is the primary evaluation criteria for decision trees.

The training error is defined as the percentage of correctly classified samples in the training set. The training error can also be used instead of the classification accuracy, but it can result in bias especially with an inducer with a risk of overfitting.

2.6.3.2. Alternatives for Accuracy Measurement

Precision is an alternative to measure the performance of decision tree. Precision measures the number of positive samples also classified as positive by decision tree.

$$\text{Precision} = (\text{True positive}) / (\text{True positive} + \text{False positive})$$

Another parameter is sensitivity (which is also known as recall), which is the ratio of true positives to the total number of positives.

$$\text{Sensitivity} = \text{True positive} / \text{Positive}$$

Generally, there is a tradeoff between precision and sensitivity. An increase in one parameter results in a decrease in the other one (Figure 2.7). The problem, in this case, is known as multi-criteria decision making, which can easily be solved by weighted sum model. Using this technique, two criteria are combined into a single criterion by using appropriate weighting. The basic principle is the additive utility assumption. The F-measure can be calculated with the formula: F = 2.P.R /(P+R), which can also be explained graphically as the difference between classification (false positive + true positive) with actual (true positive + false negative) (Figure 2.8).

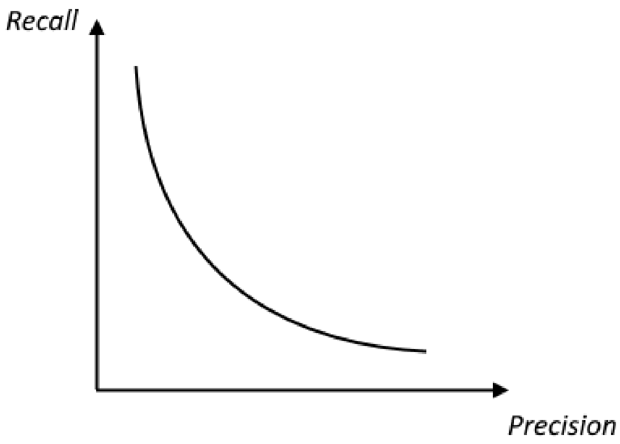

Figure 2.7. Graph of recall versus precision

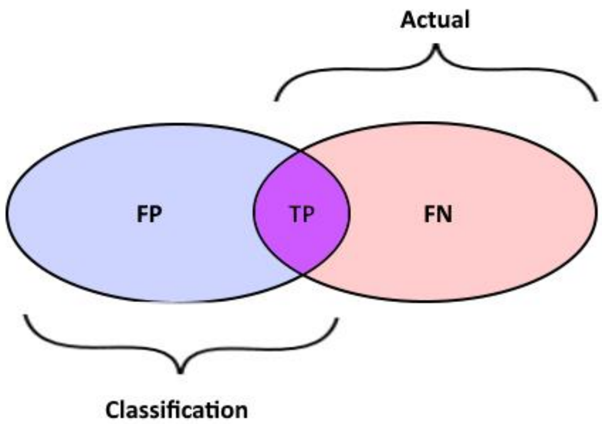

Figure 2.8. Representation of false positive (FP), true positive (TP) and false negative (FN)

The F-measure can have a value between 0 and 1. It obtains its highest value when two sets (classification and actual) are identical and the lowest value when they are completely different.

2.6.3.3. Confusion Matrix

The confusion matrix gives information about the number of correctly and incorrectly classified samples for each class (Table 2.2). A positive example, classified correctly is defined as a true positive (TP), misclassified defined as false positive (FP). Likewise, a negative example, classified correctly is defined as a true negative (TN), misclassified defined as false negative (FN).

Table 2.2. Structure of a confusion matrix

	Predictive Negative	*Predictive Positive*
Negative Examples	A	B
Positive Examples	C	D

Based on TP, TN, FP, FN; which are shown as c, d, a, b in the figure, with respectively; several calculations can be made:

- Accuracy is (a+d)/(a+b+c+d)
- Misclassification rate is (b+c)/(a+b+c+d)
- Precision is d/(b+d)
- True positive rate (recall) is d/(c+d)
- False positive rate is b/(a+b)
- True negative rate (specificity) is a/(a+b)
- False negative rate is c/(c+d)

2.6.3.4. ROC Curve

ROC (Receiver Operating Characteristics) curve is another measure, which is the graphical representation for the tradeoff between true positive and false positive rates (Figure 2.9). The ideal point on the ROC curve would be (0,1) where all positive examples are classified correctly, and no negative examples are misclassified.

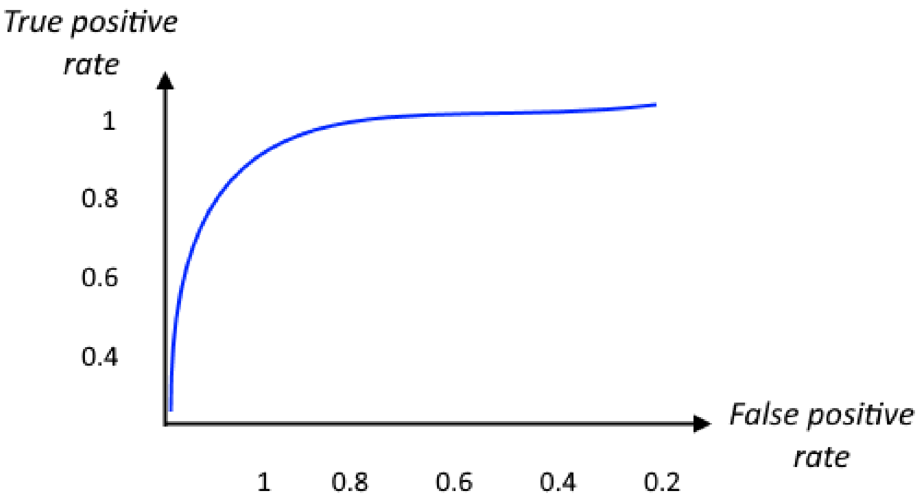

Figure 2.9. Graph of true positive rate versus false positive rate

2.6.3.5. Lift Curve

Lift is another popular method for the evaluation of probabilistic methods. (Figure 2.10). Lift is a measure of the effectiveness of a classification model calculated as the ratio between the results obtained with and without the model. Lift curves are visual aids for evaluating performance of classification models. However, confusion matrix evaluates models on the whole population, whereas lift curves evaluate a part or portion of population.

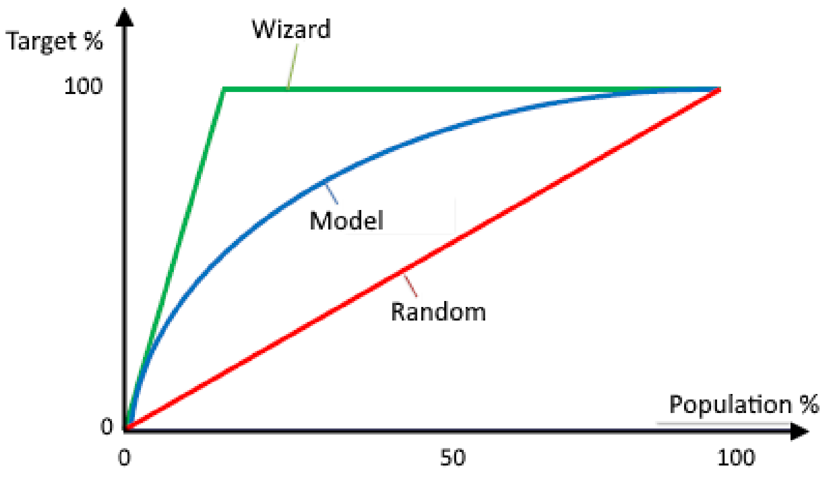

Figure 2.10. Lift curve graph

2.6.3.6. Area Under Curve (AUC)

Area under curve (AUC) is a useful metric for the performance of classifier as it is not affected by the imbalance of training set. Therefore, it is more informative to evaluate AUC instead of misclassification rate. It can be used to compare different models if their ROC curves are intersecting (Figure 2.11). Bigger AUC is an indicator for a better model.

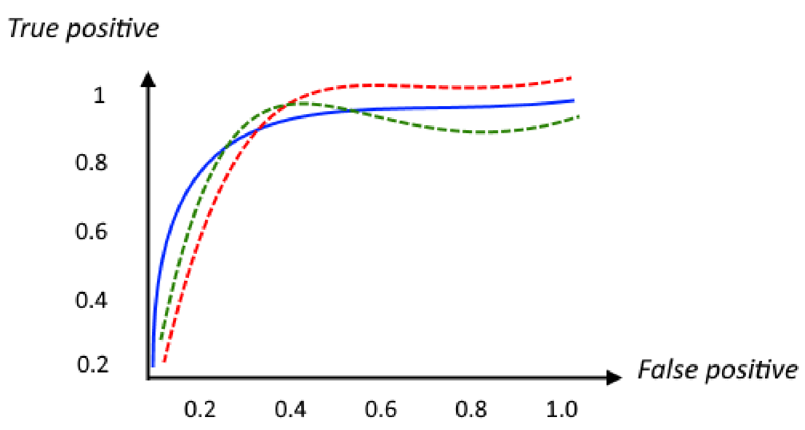

Figure 2.11. Graph of true positive versus false positive

2.6.4. Splitting Decision Trees

Decision tree induces generally split decision trees using univariate discrete splitting functions. In other words, an internal node is split according to the value of a single attribute.

2.6.4.1. Impurity-based criteria

Given a random variable x with k discrete values, distributed according to P = (p1, p2, . . ., pk), an impurity measure is a function φ: [0, 1] k → R that satisfies the following conditions:

• φ (P)≥0.

• φ (P) is minimum if ∃i such that component pi = 1.

• φ (P) is maximum if ∀i, 1 ≤ i ≤ k, pi = 1/k.

• φ (P) is symmetric with respect to components of P.

• φ (P) is smooth (differentiable everywhere) in its range

It should be noted that if the probability vector has a component of 1 (the variable x gets only one value), then the variable is defined as pure. On the other hand, if all components are equal the level of impurity reaches the maximum.

Given a training set S the probability vector of the target attribute y is defined as:

$$P_y(S) = \left(\frac{\left|\sigma_{y=c1} = S\right|}{|S|}, \dots, \frac{\left|\sigma_{y=c|dom(y)|} = S\right|}{|S|}\right)$$

2.6.4.2. Information Gain

Information Gain is an impurity-based criterion that uses the entropy measure (originating from information theory) as the impurity measure.

Information gain is closely related to the maximum likelihood estimation (MLE), which is a popular statistical method used to make inferences about parameters of the underlying probability distribution from a given dataset.

2.6.4.3. Gini Index

The Gini index is an impurity-based criterion that measures the divergences between the probability distributions of the target attributes values.

2.6.4.4. Gain Ratio

The gain ratio normalizes the information gain with this equation:

$$Gain\ Ratio(a_i, S) = \frac{Information\ Gain(a_i, S)}{Entropy(a_i, S)}$$

The information gain is calculated for all attributes. As a consequence of considering only attributes that have performed at least as well as the average information gain, the attribute that has obtained the best ratio gain is selected. Quinlan (1988) has shown that the gain ratio tends to outperform simple information gain criteria, both in accuracy and in terms of classifier complexity. A penalty is assessed for the information gain of a continuous attribute with many potential splits.

2.6.5. Stopping Decision Trees

A decision tree is grown until a stopping criterion is provided. The following conditions are generally accepted and applied as effective stopping criteria:

1. All instances in each leaf of the training set are correctly classified (belonging to the same class)
2. The maximum tree depth is reached.
3. The number of cases in the terminal node is less than the minimum number of cases for parent nodes.
4. If nodes are split, the number of cases in one or more child nodes would be less than the minimum number of cases for child nodes.

5. The best splitting criterion is not greater than a certain threshold.

2.6.6. Pruning Decision Trees

If a constructed decision tree results in overfitting, then the pruning of decision tree is applied, and the common method is cost-complexity pruning.

Cost complexity pruning (also known as weakest link pruning or error complexity pruning) proceeds in two stages (Breiman, 2017). In the first stage, a sequence of trees T0, T1, . . ., Tk is built on the training data where T0 is the original tree before pruning and Tk is the root tree. In the second stage, one of these trees is chosen as the pruned tree, based on its generalization error estimation. The tree Ti+1 is obtained by replacing one or more of the sub-trees in the predecessor tree Ti with suitable leaves. The sub-trees that are pruned are those that obtain the lowest increase in the apparent error rate per pruned leaf:

$$\alpha = \frac{\varepsilon(pruned(T,t),S) - \varepsilon(T,S)}{|leaves(T)| - |leaves(pruned(T,t))|}$$

where ε (T, S) indicates the error rate of the tree T over the sample S and |leaves (T)| denotes the number of leaves in T. Pruned (T, t) denotes the tree obtained by replacing the node t in T with a suitable leaf. In the second phase, the generalization error of each pruned tree is estimated. The best pruned tree is then selected. If the given dataset is large enough, the authors suggest breaking it into a training set and a pruning set. The trees are constructed using the training set and evaluated on the pruning set. On the other hand, if the given dataset is not large enough, they propose using cross-validation methodology, despite the computational complexity implications.

2.6.7. Advantages and Disadvantages of Decision Trees

The main advantages of decision trees can be listed as:

1. They are self-explanatory and easy to follow. A decision tree can be easily understood and followed by non-professional user.
2. They can handle both nominal and numeric input attributes.

3. Their representation is rich.
4. They can handle datasets with errors and missing data.
5. Decision trees are considered to be non-parametric. In other words, they do not include any assumptions about the spatial distribution or about classifier structure.
6. Decision trees are simple as they only require to follow conditions along a single path from the root to the leaf.

On the other hand, the disadvantages of a decision tree can be listed as:

1. They mostly require that the target attribute to have only discrete values.
2. They show low performance when complex interactions are present.
3. They are over-sensitive to irrelevant attributes or to noises making decision trees unstable. A minor change in one split may change everything from that split to the leaf nodes.
4. Missing data and errors can be handled, but extreme effort and attention are required.

2.6.8. Application of Decision Tree Learning to Tectono-Magmatic Discrimination

Tectono-magmatic discrimination methods for mafic igneous rocks are constructed and suggested by using the Decision Tree Method in Orange (a free Data Mining software) based on tectonic settings as classes and ratios of relatively immobile elements as features. The database is divided into three groups: Training dataset, test dataset, and external dataset. The training dataset is used to construct the tectono-magmatic discrimination methods. The test dataset is used to run an initial control for the quality of constructed trees. External datasets are used to check the external applicability of constructed trees in varying conditions (such as geographical location, geological setting, geochemical characteristics, geological age, alteration etc). Multiple decision trees are constructed for the tectono-magmatic discrimination of basic and ultrabasic igneous rocks (Figure 2.12). First, subduction-related settings are discriminated from non-subduction-related settings. Subduction settings are continental arcs, oceanic arcs, and oceanic back-arcs, whereas non-subduction settings are continental within-plates, mid-oceanic ridges, oceanic islands and oceanic plateaus.

Three alternative decision trees are constructed for tectono-magmatic discrimination between subduction settings and non-subduction settings. The first decision tree involves only ratios of relatively immobile elements and has only one branch. The second decision tree is a multi-branched decision tree that involves ratios of relatively immobile elements and also Nb/Nb* ratio. Element ratios using TiO_2 are eliminated for the third decision tree to propose an alternative decision tree.

As the first alternative of tectono-magmatic discrimination between subduction and non-subduction settings, a decision stump is constructed.

Out of 2.642 samples (training and test set), 2.114 samples are used to construct the decision tree, and 528 samples are used to test the decision tree.

Selected features are only element ratios of selected immobile elements (Th, La, Nb, Y, Yb, Zr, Hf, Sm, Nd, TiO_2). Absolute values of immobile elements are only used for calculation of element ratios and then ignored in the construction of decision trees.

Out of selected element ratios (Th/Nb, La/Nb, Th/La, Zr/Hf, Zr/Nb, La/Y, La/Yb, Nb/Y, Nb/Yb, Sm/Y, Sm/Yb, Nd/Zr, La/Sm, Sm/Hf, Y/Yb, Zr/Sm, Zr/Y, Zr/Yb, Th/Y, Th/Yb, Sm/Nb, Sm/Nd, Zr/TiO_2, TiO_2/Y, TiO_2/Yb, Nd/TiO_2, Nb/TiO_2), Th/Nb is the feature with highest information gain (0.528), gain ratio (0.264), and gini index (0.276) (Table 2.3) for the tectono-magmatic discrimination between subduction and non-subduction settings.

As the second alternative of tectono-magmatic discrimination between subduction and non-subduction settings, a multi-branched decision tree is constructed.

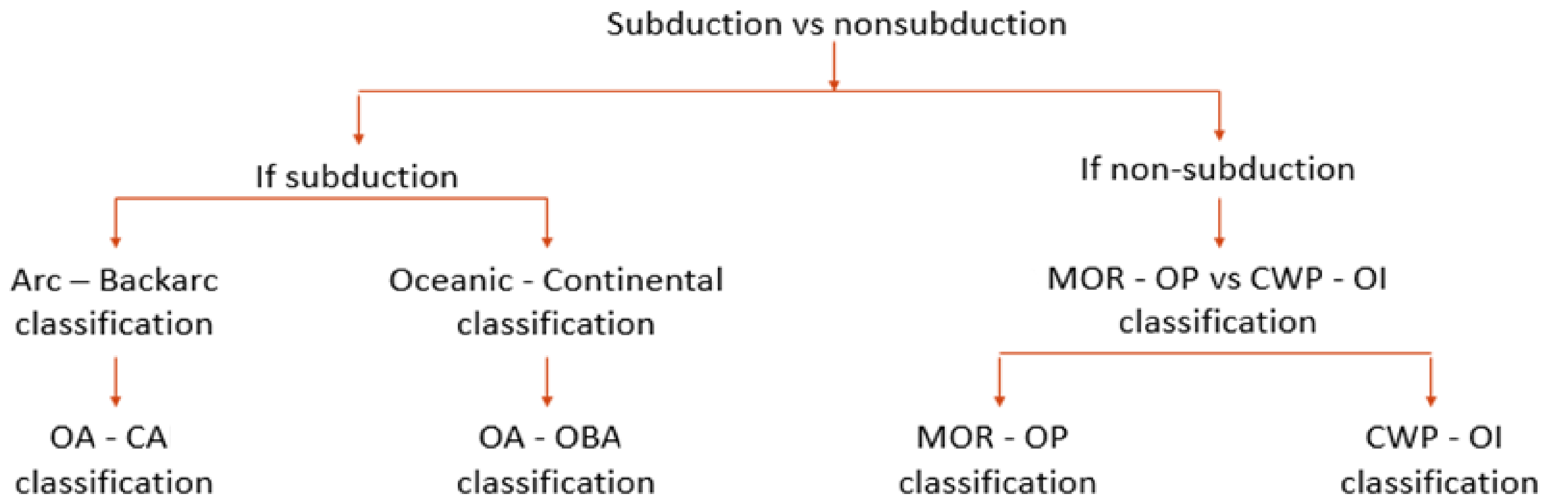

Figure 2.12. Flowchart for the tectono-magmatic discrimination of rocks

Selected features are only element ratios of selected immobile elements (Th, La, Nb, Y, Yb, Zr, Hf, Sm, Nd, TiO_2). Absolute values of immobile elements are only used for calculation of element ratios and then ignored in the construction of decision trees.

Table 2.3. Information gain, gain ratio and gini index of most discriminative features

Feature	Information Gain	Gain Ratio	Gini Index
Th/Nb	0.528	0.264	0.276
La/Nb	0.445	0.222	0.229
Sm/Nb	0.214	0.107	0.098
Zr/Nb	0.173	0.086	0.072
Sm/Hf	0.155	0.078	0.085

Selected ratios of relatively immobile elements are Th/Nb, La/Nb, Th/La, Zr/Hf, Zr/Nb, La/Y, La/Yb, Nb/Y, Nb/Yb, Sm/Y, Sm/Yb, Nd/Zr, La/Sm, Sm/Hf, Y/Yb, Zr/Sm, Zr/Y, Zr/Yb, Th/Y, Th/Yb, Sm/Nb, Sm/Nd, Zr/TiO_2, TiO_2/Y, TiO_2/Yb, Nd/TiO_2, Nb/TiO_2 along with Nb/Nb* ratio.

As the third alternative of tectono-magmatic discrimination between subduction and non-subduction settings, another multi-branched decision tree is constructed.

Selected features are only element ratios of selected immobile elements (Th, La, Nb, Y, Yb, Zr, Hf, Sm, Nd, TiO_2). Absolute values of immobile elements are only used for calculation of element ratios and then ignored in the construction of decision trees.

Selected ratios of relatively immobile elements are Th/Nb, La/Nb, Th/La, Zr/Hf, Zr/Nb, La/Y, La/Yb, Nb/Y, Nb/Yb, Sm/Y, Sm/Yb, Nd/Zr, La/Sm, Sm/Hf, Y/Yb, Zr/Sm, Zr/Y, Zr/Yb, Th/Y, Th/Yb, Sm/Nb, Sm/Nd along with Nb/Nb* ratio. Ratios of relatively immobile elements including TiO_2 (Zr/TiO_2, TiO_2/Y, TiO_2/Yb, Nd/TiO_2, and Nb/TiO_2) are ignored for the alternative decision tree.

If this classification returns with a result of subduction-related settings, then one of two approaches would be selected.

At the first approach, the arc-related settings are discriminated from the back-arc setting and then arc-related settings are discriminated from each other.

For discrimination of arc and back-arc settings, out of 668 samples (training and test set), 535 samples are used to construct the decision tree, and 133 samples are used to test decision tree. Later, for discrimination of oceanic arc from continental arc settings within arc-related samples, out of 562 samples (training and test set), 450 samples are used to construct decision tree, and 112 samples are used to test decision tree.

At the second approach, oceanic settings are discriminated from continental settings, and then oceanic settings are discriminated from each other.

For the discrimination of oceanic and continental settings, out of 668 samples (training and test set), 535 samples are used to construct the decision tree, and 133 samples are used to test the decision tree. Later, for discrimination of oceanic arc from oceanic back-arc settings within samples of oceanic setting, out of 487 samples (training and test set), 390 samples are used to construct decision tree, and 97 samples are used to test decision tree.

If the classification returns with a result of non-subduction-related settings, then first mid-oceanic ridges and oceanic plateaus are discriminated from continental within-plates and oceanic islands.

If non-subduction-related setting is either mid-oceanic ridge or oceanic plateau, then these are discriminated from each other. If it is either continental within-plate or oceanic island, then these are discriminated from each other.

For the discrimination of non-subduction-related settings into two parts as mid-oceanic ridge and oceanic plateau as first part and continental within-plates and oceanic islands as second part, out of 1.974 samples (training and test set), 1.580 samples are used to construct decision tree, and 394 samples are used to test decision tree. Later, for discrimination of mid-oceanic ridges from oceanic plateaus within the first part, out of 1.120 samples (training and test set), 896 samples are used to construct decision tree, and 224 samples are used to test decision tree. For discrimination of continental within-plates from oceanic islands within the second part, out of 854 samples (training and test set), 684 samples are used to construct decision tree, and 170 samples are used to test decision tree.

CHAPTER 3

RESULTS

3.1. Constructed Decision Trees

Multiple sets of decision trees are constructed for the tectono-magmatic discrimination for basic igneous rocks (1) between subduction (SUB) and non-subduction (NONSUB) settings, (2) between arc and back-arc-related settings, (3) within arc-related settings, (4) between oceanic and continental settings, (5) within oceanic settings, (6) between mid-oceanic ridge (MOR) / oceanic plateau (OP) and oceanic island (OI) / continental within-plate (CWP), (7) between MOR and OP, (8) between OI and CWP. Two multi-branched decision trees are constructed for each sets.

For the first decision tree, all element ratios are included as features; yet, for the second one, TiO_2-related ratios are not included in order to construct an alternative decision tree.

3.1.1. Discrimination Between Subduction and Non-Subduction Settings

The first set of decision trees is constructed for the tectono-magmatic discrimination between SUB and NONSUB settings. SUB settings are continental arcs (CA), oceanic arcs (OA) and oceanic back-arc basins (OBAB) whereas NONSUB settings are MOR, OP, OI and CWP.

In addition to the decision trees, a decision stump (Figure 3.1) is also constructed in order to examine if it may result underfitting even when an effective discriminating feature (e.g. Th/Nb) is applied. Nb/Nb* ratio is not included in the construction of decision stump.

The first decision tree has 4 levels in depth using Nb/Nb* at first level, TiO_2/Yb at the second level, Zr/Nb at third level, and La/Nb at the fourth level (Figure 3.2). Nb/Nb* is an effective discriminating feature due to the diverse behavior of Th and La relative to Nb. The second decision tree has only 2 levels in depth, using Nb/Nb* at first level and Nb/Y at the second level (Figure 3.3). No further levels could be constructed for further discrimination.

Decision rules for constructed decision trees are given in Figure 3.4, Figure 3.5 and Figure 3.6, respectively.

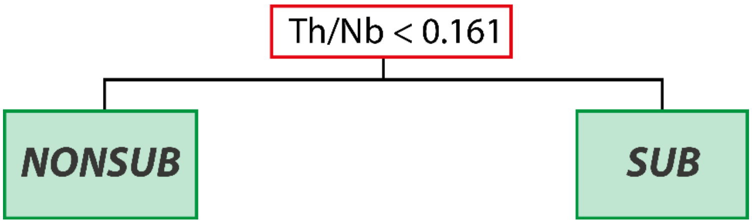

Figure 3.1. Decision stump for discrimination between subduction and non-subduction settings

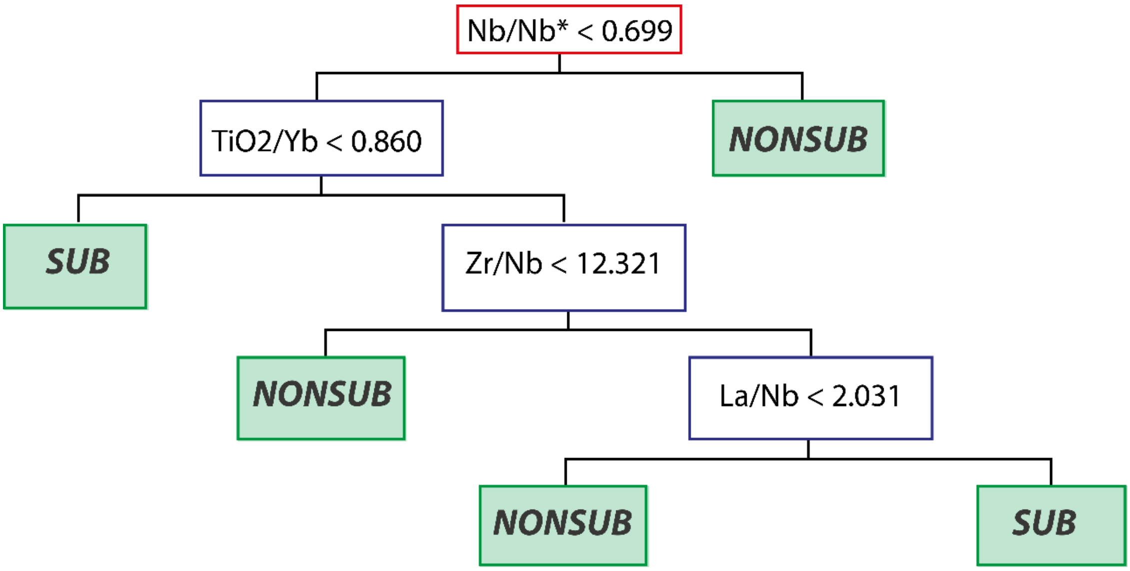

Figure 3.2. The first decision tree to discriminate between subduction and non-subduction settings

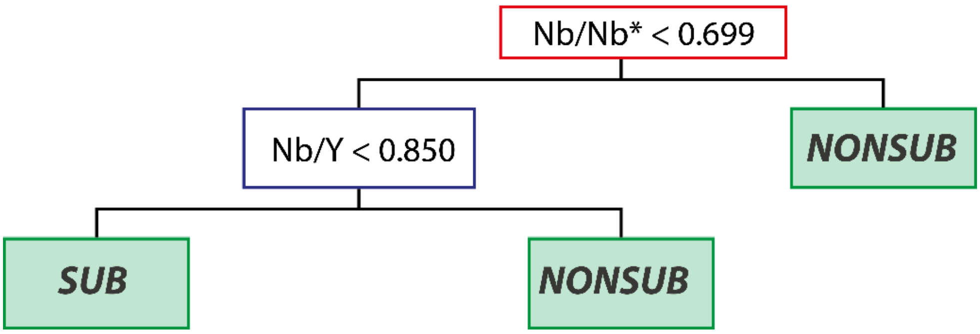

Figure 3.3. The second decision tree to discriminate between subduction and non-subduction settings

```
IF (Th/Nb < 0.161) :
        Classification: Nonsub
ELSE :
        Classification: Sub
```

Figure 3.4. Decision rule for the decision stump

```
IF (Nb/Nb* < 0.699) :
        IF (TiO2/Yb < 0.860) :
                Classification: Sub
        ELSEIF (Zr/Nb < 12.321) :
                Classification: Nonsub
        ELSEIF (La/Nb < 2.031) :
                Classification: Sub
ELSE :
        Classification: Nonsub
```

Figure 3.5. Decision rule for the first decision tree

```
IF (Nb/Nb* < 0.699) :
        IF (Nb/Y < 0.850) :
                Classification: Sub
        ELSE :
                Classification: Nonsub
ELSE :
        Classification: Nonsub
```

Figure 3.6. Decision rule for the second decision tree

3.1.2. Discrimination Within Subduction Settings

The second set of decision trees is constructed for the tectono-magmatic discrimination within subduction-related settings. Subduction-related settings are OA, CA and OBAB (Table 3.1).

If the sample is either classified or already known as "SUB", a further discrimination within subduction-related settings is required. Two alternative paths are provided at this stage: discrimination between (1) arc and back-arc-related settings, (2) oceanic and continental settings.

Table 3.1 Subduction settings

<table>
<tr><th>Subduction Settings</th><th>Arc vs Back-Arc</th><th>Oceanic vs Continental</th></tr>
<tr><td>Oceanic Back-Arcs</td><td>Back-Arc</td><td rowspan="2">Oceanic</td></tr>
<tr><td>Oceanic Arcs</td><td rowspan="2">Arc</td></tr>
<tr><td>Continental Arcs</td><td>Continental</td></tr>
</table>

3.1.2.1. The First Path for Discrimination Within Subduction Settings

The first path involves two-stage discrimination within subduction settings: (1) between arc and back-arc-related settings, (2) within arc-related settings.

3.1.2.1.1. Discrimination Between Arc and Back-Arc-Related Settings

Two decision trees are constructed for the tectono-magmatic discrimination between arc and back-arc-related settings. Both decision trees have 5 levels of depth. The first decision tree (Figure 3.7) use Nb/Nb* at first level, Nd/Zr at the second level, TiO_2/Y, and Nd/TiO_2 at the third level, Y/Yb at fourth level and Zr/Hf at fifth level. The second decision tree (Figure 3.8), on the other hand, use Nb/Nb* at first level, Nd/Zr at second level, Zr/Hf and Zr/Nb at third level, Zr/Y and Y/Yb at fourth level and Nd/Zr and Zr/Hf at fifth level.

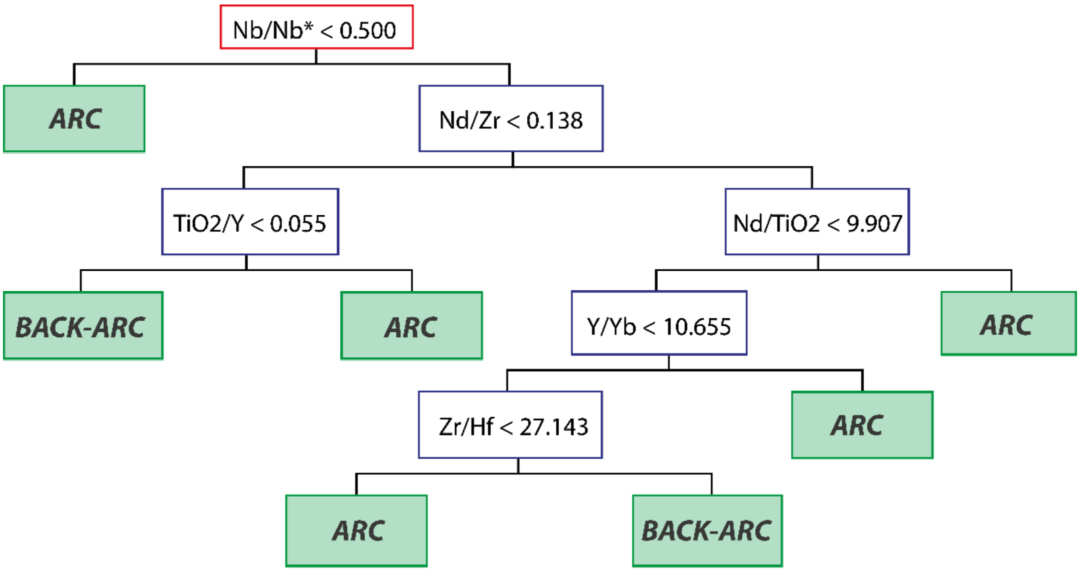

Figure 3.7. The first decision tree to discriminate between arc and back-arc-related settings

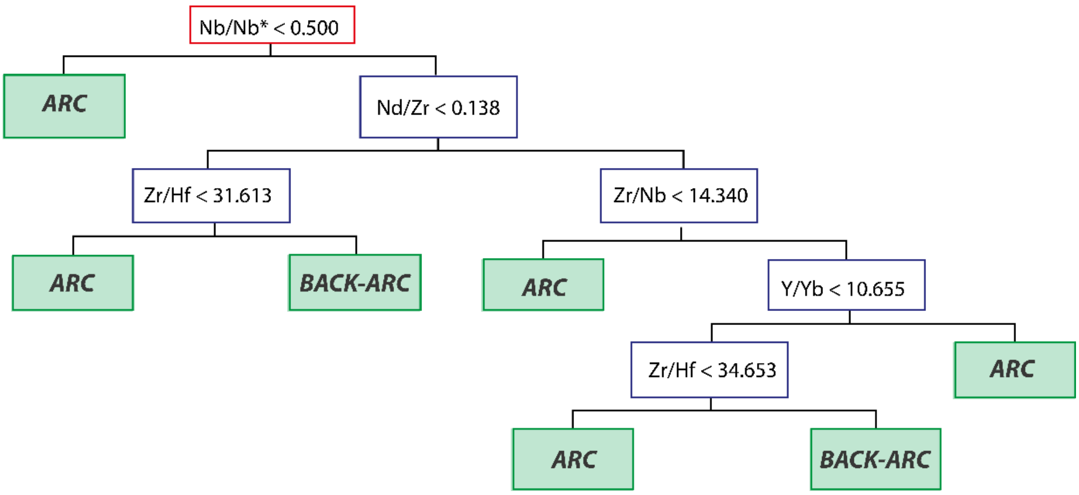

Figure 3.8. The second decision tree to discriminate between arc and back-arc-related settings

Decision rules for constructed decision trees are given in Figure 3.9 and Figure 3.10, respectively.

```
IF (Nb/Nb* < 0.500) :
        Classification: Arc
ELSEIF (Nd/Zr < 0.138) :
        IF (TiO2/Y < 0.055) :
                Classification: Back-Arc
        ELSE :
                Classification: Arc
ELSEIF (Nd/TiO2 < 9.907) :
        IF (Y/Yb < 10.655) :
                IF (Zr/Hf < 27.143) :
                        Classification: Arc
                ELSE :
                        Classification: Back-Arc
        ELSE :
                Classification: Arc
ELSE:
        Classification: Arc
```

Figure 3.9. Decision rule for the first decision tree

```
IF (Nb/Nb* < 0.500) :
        Classification: Arc
ELSEIF (Nd/Zr < 0.138) :
        IF (Zr/Hf < 31.613) :
                Classification: Arc
        ELSE :
                Classification: Back-Arc
ELSEIF (Zr/Hf < 14.340) :
        Classification: Arc
ELSEIF (Y/Yb < 10.655) :
        IF (Y/Yb < 34.653) :
                Classification: Arc
        ELSE :
                Classification: Back-Arc
ELSE:
        Classification: ARC
```

Figure 3.10. Decision rule for the second decision tree

3.1.2.1.2. Discrimination Within Arc-Related Settings

Two decision trees are constructed for the tectono-magmatic discrimination within arc-related settings (oceanic arcs and continental arcs from each other). Both decision trees have 7 levels of depth. The first decision tree (Figure 3.11) use Zr/TiO_2 at first level, Th/Nb and La/Nb at second level, Nd/TiO_2 and Zr/Yb at third level, Zr/TiO_2, La/Yb and Y/Yb at fourth level, Y/Yb, Sm/Hf and Zr/Hf at fifth level, Nb/Nb*, Zr/Sm and La/Nb at sixth level and Nb/Y, Th/Y, Sm/Hf and Zr/Hf at seventh level. The second decision tree (Figure 3.12) use Zr/Sm at first level, La/Nb and Sm/Y at second level, Nb/Nb* and Y/Yb at third level, Th/La, Sm/Hf and Zr/Y at fourth level, La/Y, Sm/Nd, Nb/Nb*, Sm/Hf and La/Nb at fifth level, Sm/Hf, Zr/Nb, La/Y, Th/La and Nb/Y at sixth level and Sm/Y, Nb/Nb* and Zr/Hf at seventh level. Decision rules for constructed decision trees are given in Figure 3.13 and Figure 3.14, respectively.

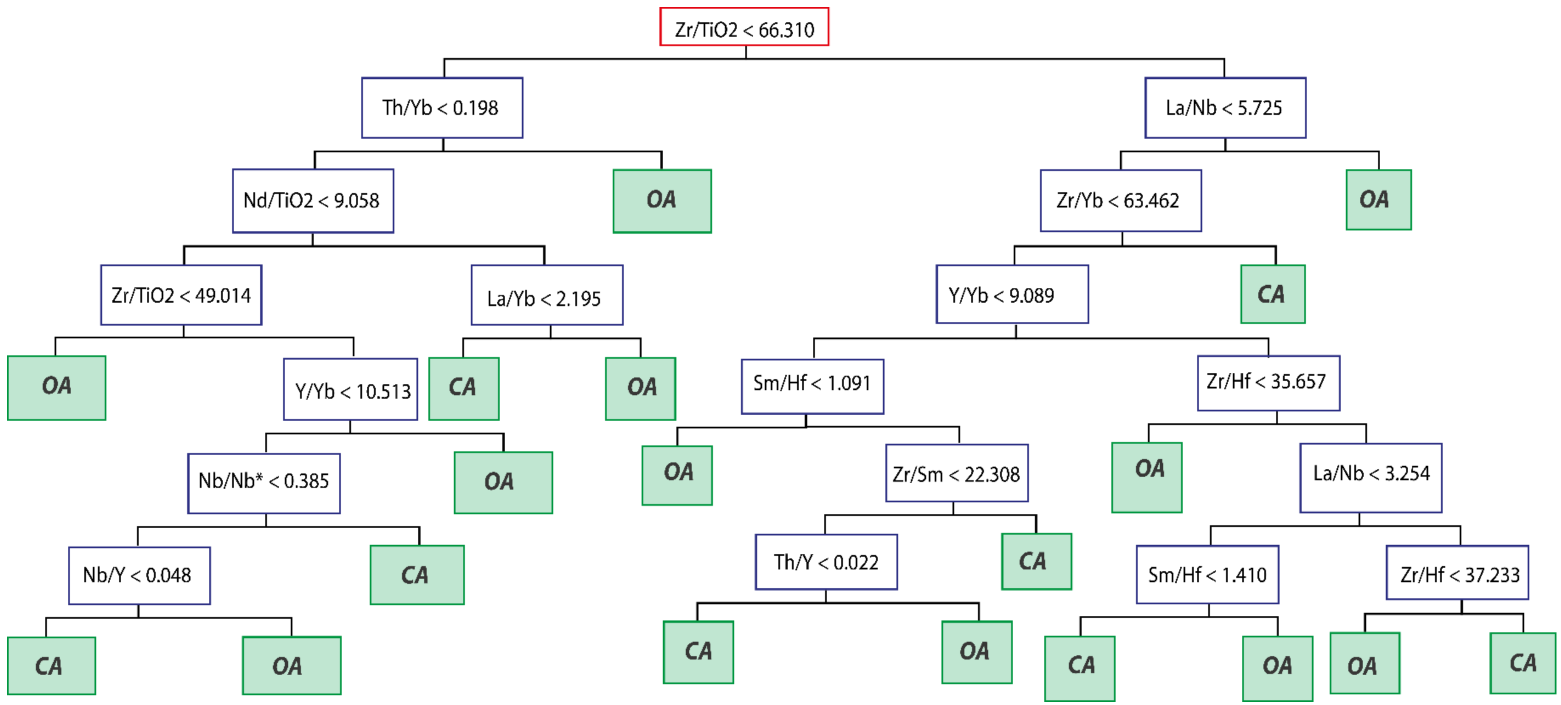

Figure 3.11. The first decision tree to discriminate within arc-related settings

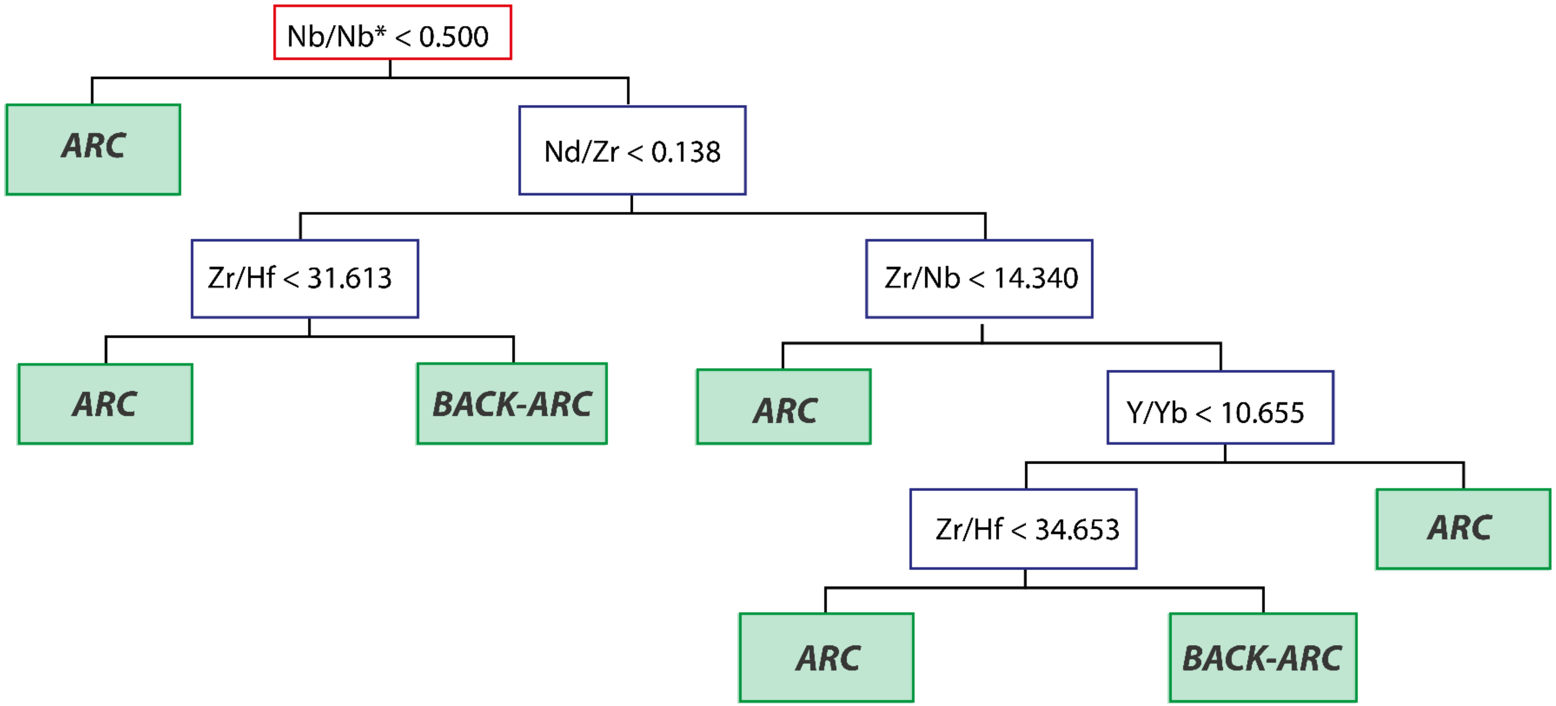

Figure 3.12. The second decision tree to discriminate within arc-related settings

```
IF (Zr/TiO2 < 66.310) :
    IF (Th/Yb < 0.198) :
        IF (Nd/TiO2 < 9.058) :
            IF ( Zr/TiO2 < 49.014) :
                Classification : OA
            ELSEIF (Y/Yb < 10.513) :
                IF (Nb/Nb* < 0.385) :
                    IF (Nb/Y < 0.048) :
                        Classification: CA
                    ELSE :
                        Classification: OA
                ELSE :
                    Classification: CA
            ELSE :
                Classification: OA
        ELSEIF (La/Yb < 2.195) :
            Classification : CA
        ELSE :
            Classification: OA
    ELSE:
        Classification: OA
ELSEIF (La/Nb < 5.725) :
    IF (Zr/Yb < 63.462) :
        IF (Y/Yb < 9.089) :
            IF (Sm/Hf < 1.091) :
                Classification: OA
            ELSEIF (Zr/Sm < 22.308) :
                IF (Th/Y < 0.022) :
                    Classification: CA
                ELSE :
                    Classification: OA
            ELSE:
                Classification: CA
        ELSEIF (Zr/Hf < 35.657) :
            Classification: OA
        ELSEIF (La/Nb < 3.254) :
            IF (Sm/Hf < 1.410) :
                Classification: CA
            ELSE :
                Classification : OA
        ELSEIF ( Zr/Hf < 37.233) :
            Classification: OA
        ELSE:
            Classification: CA
    ELSE :
        Classification : CA
ELSE:
    Classification: OA
```

Figure 3.13. Decision rule for the first decision tree

```
IF (Zr/Sm < 22.480) :
    IF (La/Nb < 4.930):
        IF (Nb/Nb* < 0.403) :
            IF (Th/La < 0.083) :
                IF (La/Y <  0.291) :
                    Classification: CA
                ELSE :
                    Classification: CA
            ELSEIF (Sm/Nd < 0.247) :
                IF (Sm/Hf < 1.731) :
                    Classification: OA
                ELSE :
                    Classification: CA
            ELSEIF (Zr/Nb < 39.773) :
                Classification: OA
            ELSEIF (Sm/Y < 0.121) :
                Classification: OA
            ELSE :
                Classification: CA
        ELSE :
            Classification: CA
    ELSE :
        Classification: OA
ELSEIF (Sm/Y < 0.129) :
    IF (Y/Yb < 10.248) :
        IF (Sm/Hf < 1.091) :
            Classification: OA
        ELSEIF (Nb/Nb* < 0.385) :
            IF (La/Y < 0.268) :
                IF (Nb/Nb* < 0.373) :
                    Classification: OA
                ELSE :
                    Classification: CA
            ELSE :
                Classification: CA
        ELSE :
            Classification: CA
    ELSEIF (Sm/Hf < 1.533) :
        Classification: OA
    ELSEIF (Sm/Hf < 1.581) :
        Classification: CA
    ELSE:
        Classification: OA
ELSEIF (Y/Yb < 9.967) :
    Classification: CA
ELSEIF (Zr/Y < 5.280) :
    IF (La/Nb < 2.932) :
        IF (Th/La < 0.128) :
            Classification: CA
        ELSE :
            Classification: OA
    ELSEIF (Nb/Y < 0.065) :
        Classification: OA
    ELSEIF (Zr/Hf < 38.023) :
        Classification: OA
    ELSE :
        Classification: CA
ELSE:
    Classification: CA
```

Figure 3.14. Decision rule for the second decision tree

3.1.2.2. The Second Path for Discrimination Within Subduction Settings

The second path involves two-stage discrimination within subduction settings: (1) between oceanic and continental settings, (2) within oceanic settings.

3.1.2.2.1. Discrimination Between Oceanic and Continental Settings

Two decision trees are constructed for the tectono-magmatic discrimination between oceanic and continental settings. Both decision trees have 7 levels of depth. The first decision tree (Figure 3.15) use Sm/Yb at first level, Nd/Zr at second level, Th/Nb and Y/Yb at third level, Zr/TiO_2, La/Nb, Nb/Nb* and La/Sm at fourth level, La/Nb, Nd/Zr and Nb/Yb at fifth level, TiO_2/Y, Nb/Nb* and Th/Nb at sixth level and Zr/Hf and Th/La at seventh level. The second decision tree (Figure 3.16) use Sm/Yb at first level, Nd/Zr at second level, Th/Nb and Y/Yb at third level, Th/La, La/Nb, Nb/Nb* and La/Sm at fourth level, Sm/Hf, Nd/Zr and Nb/Yb at fifth level, La/Nb, Nb/Nb* and Th/Nb at sixth level and Nb/Y, Zr/Hf and Th/La at seventh level. Decision rules for constructed decision trees are given in Figure 3.17 and Figure 3.18, respectively.

3.1.2.2.2. Discrimination Within Oceanic Settings

Two decision trees are constructed for the tectono-magmatic discrimination within oceanic settings (oceanic arcs and oceanic back-arc basins from each other). Both decision trees have 6 levels of depth. The first decision tree (Figure 3.19) use Th/Nb at first level, Sm/Yb and Zr/Hf at second level, La/Nb and Th/Nb at third level, Nb/Nb*, Nd/Zr and TiO_2/Yb at fourth level, Nb/Nb* and Zr/Hf at fifth level and Y/Yb and Nb/Yb at sixth level. The second decision tree (Figure 3.20) use Th/Nb at first level, Sm/Yb and Zr/Hf at second level, La/Nb and Th/Nb at third level, Nb/Nb*, Nd/Zr and La/Sm at fourth level, Nb/Nb* and Sm/Y at fifth level and Y/Yb at sixth level. Decision rules for constructed decision trees are given in Figure 3.21 and Figure 3.22, respectively.

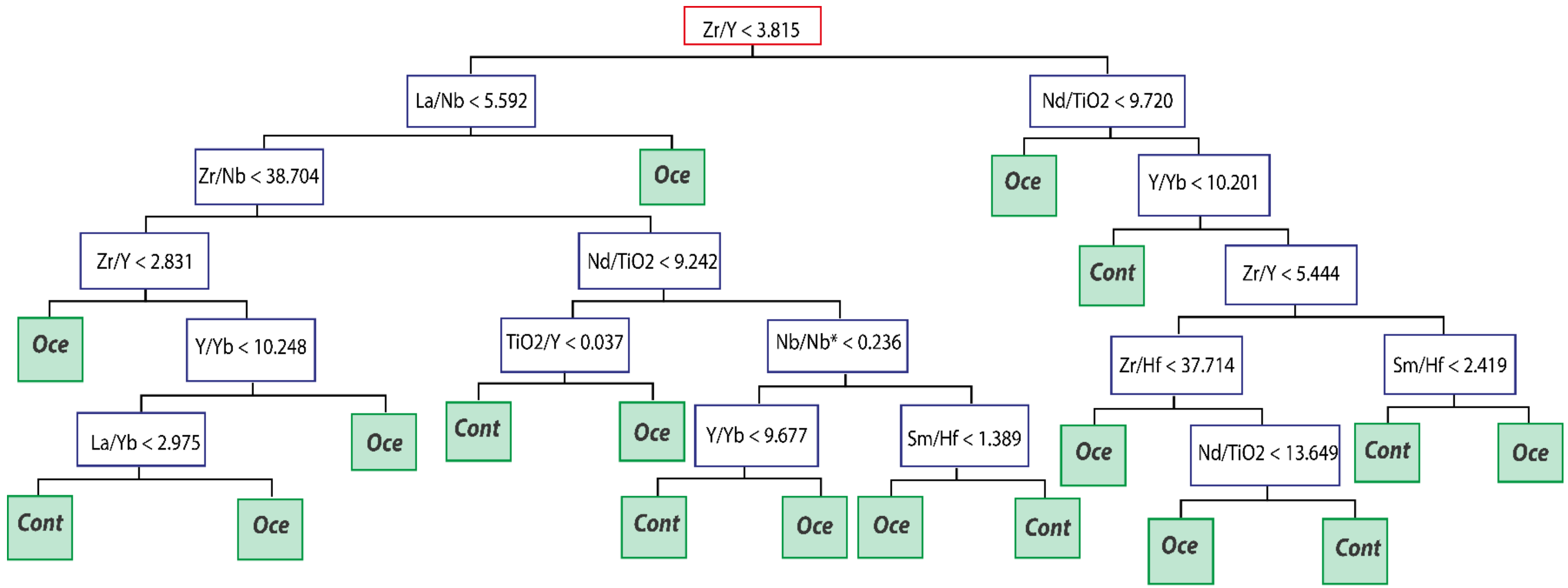

Figure 3.15. The first decision tree to discriminate between oceanic and continental settings

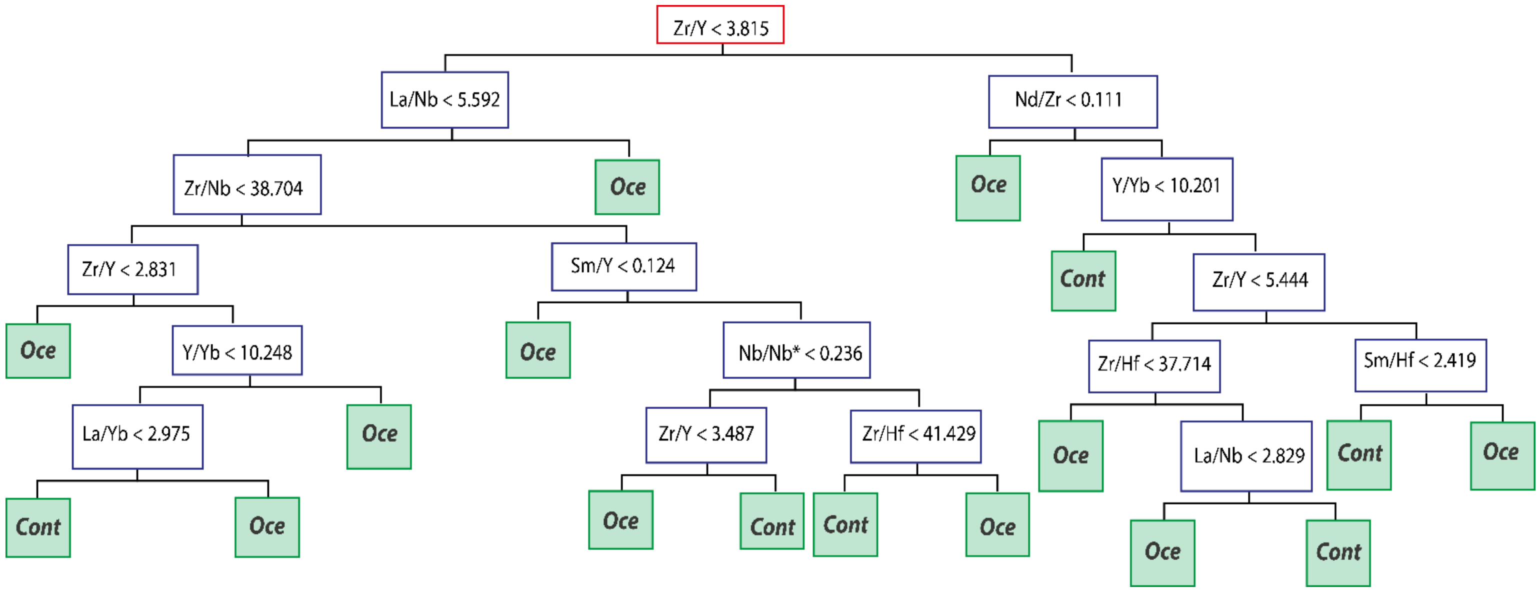

Figure 3.16. The second decision tree to discriminate between oceanic and continental settings

```
IF (Zr/Y < 3.815) :
        IF (La/Nb < 5.592) :
                IF (Zr/Nb < 38.704) :
                        IF (Zr/Y < 2.831) :
                                Classification: Oceanic
                        ELSEIF (Y/Yb < 10.248) :
                                IF (La/Yb < 2.975) :
                                        Classification: Continental
                                ELSE :
                                        Classification: Oceanic
                        ELSE:
                                Classification: Oceanic
                ELSEIF (Nd/TiO2 < 9.242) :
                        IF ( TiO2/Y < 0.037) :
                                Classification: Continental
                        ELSE :
                                Classification: Oceanic
                ELSEIF (Nb/Nb* < 0.236) :
                        IF (Y/Yb < 9.677) :
                                Classification: Continental
                        ELSE :
                                Classification: Oceanic
                ELSEIF (Sm/Hf < 1.389) :
                        Classification: Oceanic
                ELSE :
                        Classification: Continental
ELSEIF (Nd/TiO2 < 9.720) :
        Classification: Oceanic
ELSEIF (Y/Yb < 10.201) :
        Classification: Continental
ELSEIF ( Zr/Y < 5.444) :
        IF (Zr/Hf < 37.714) :
                Classification: Oceanic
        ELSEIF (Nd/TiO2 < 13.649) :
                Classification: Oceanic
        ELSE :
                Classification: Continental
ELSEIF (Sm/Hf < 2.419) :
        Classification: Continental
ELSE:
        Classification: Oceanic
```

Figure 3.17. Decision rule for the first decision tree

```
IF (Zr/Y < 3.815) :
        IF (La/Nb < 5.592) :
                IF (Zr/Nb < 38.704) :
                        IF (Zr/Y < 2.831) :
                                Classification: Oceanic
                        ELSEIF (Y/Yb < 10.248) :
                                IF (La/Yb < 2.975) :
                                        Classification: Continental
                                ELSE :
                                        Classification: Oceanic
                        ELSE:
                                Classification: Oceanic
                ELSEIF (Sm/Y < 0.124) :
                        Classification: Oceanic
                ELSEIF (Nb/Nb* < 0.236) :
                        IF (Zr/Y < 3.487) :
                                Classification: Oceanic
                        ELSE :
                                Classification: Continental
                ELSEIF (Zr/Hf < 41.429) :
                        Classification: Continental
                ELSE :
                        Classification: Oceanic
ELSEIF (Nd/Zr < 0.111) :
        Classification: Oceanic
ELSEIF (Y/Yb < 10.201) :
        Classification: Continental
ELSEIF ( Zr/Y < 5.444) :
        IF (Zr/Hf < 37.714) :
                Classification: Oceanic
        ELSEIF (La/Nb<2.829) :
                Classification: Oceanic
        ELSE :
                Classification: Continental
ELSEIF (Sm/Hf < 2.419) :
        Classification: Continental
ELSE:
        Classification: Oceanic
```

Figure 3.18. Decision rule for the second decision tree

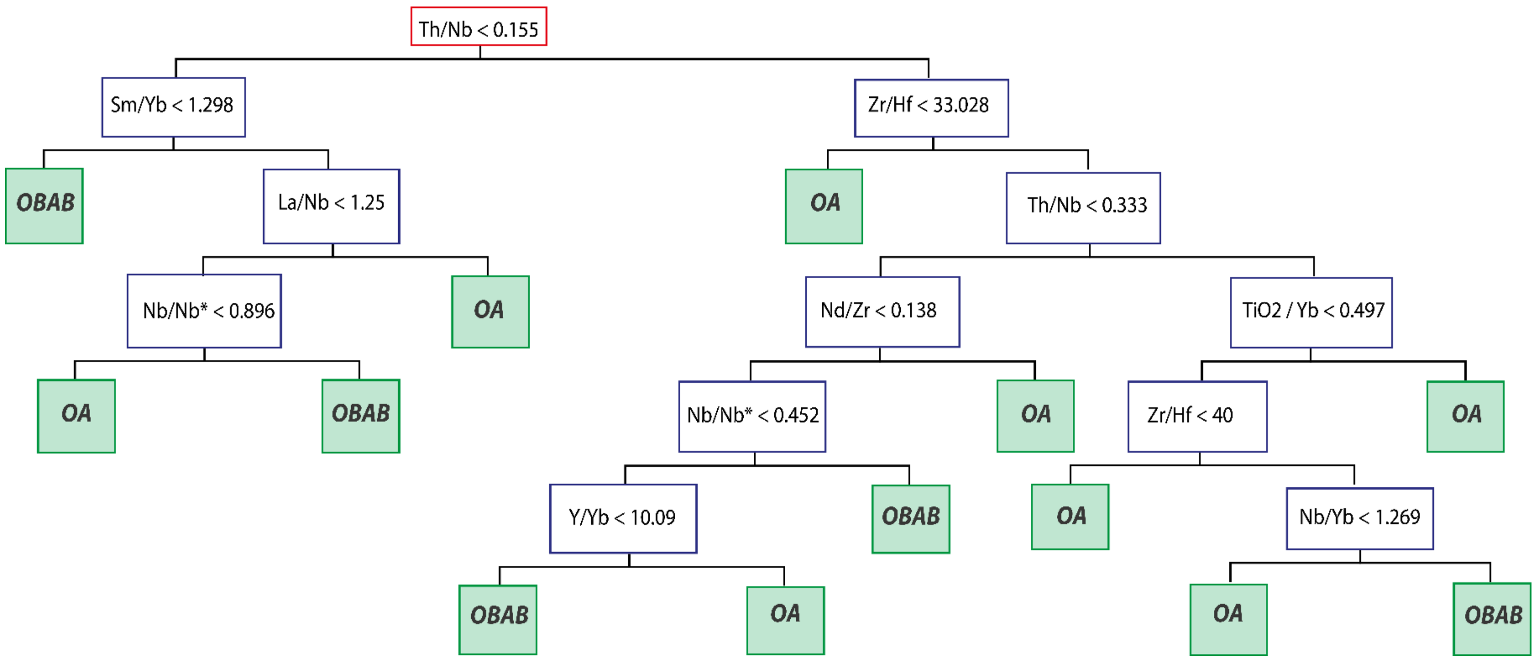

Figure 3.19. The first decision tree to discriminate within oceanic settings

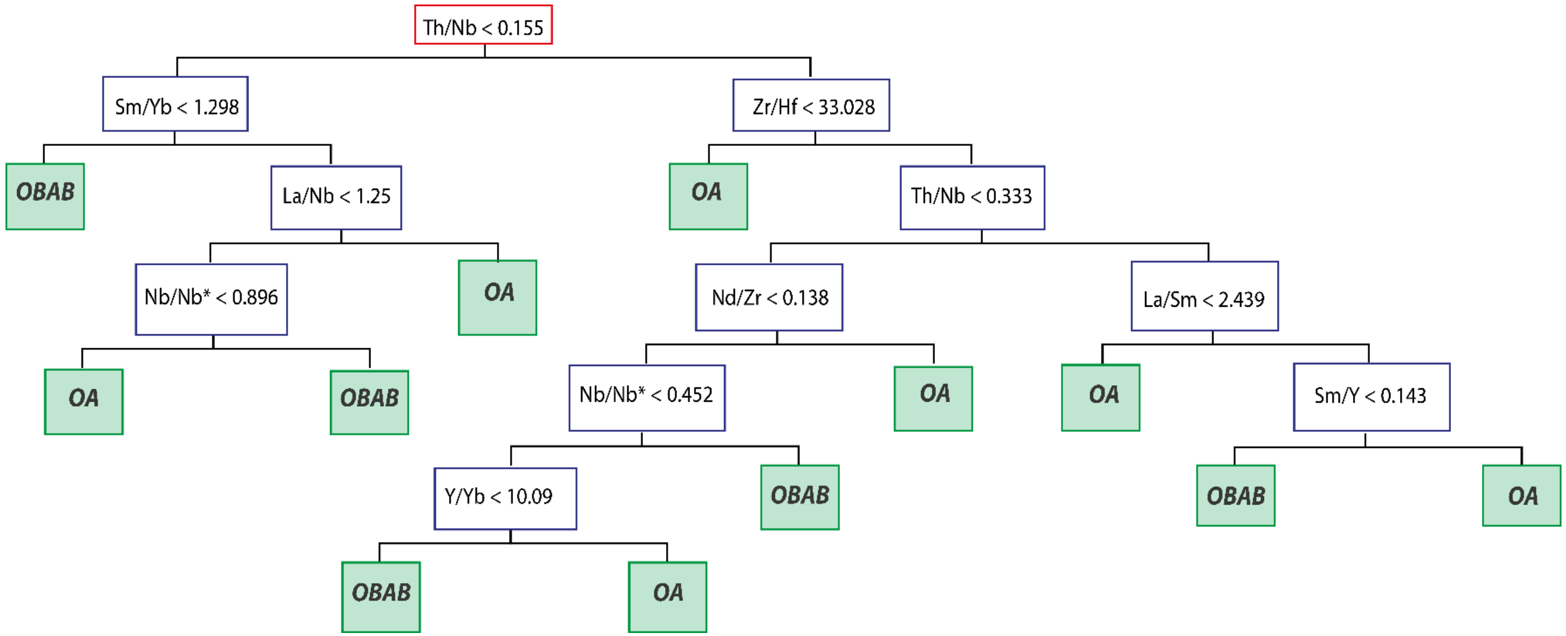

Figure 3.20. The second decision tree to discriminate within oceanic settings

```
IF (Th/Nb < 0.155) :
        IF (Sm/Yb < 1.298) :
                Classification: OBAB
        ELSEIF (La/Nb < 1.25) :
                IF (Nb/Nb* < 0.896) :
                        Classification: OA
                ELSE :
                        Classification: OBAB
        ELSE :
                Classification: OA
ELSEIF (Zr/Hf < 33.028) :
        Classification: OA
ELSEIF (Th/Nb < 0.333) :
        IF (Nd/Zr < 0.138) :
                IF (Nb/Nb* < 0.452) :
                        IF (Y/Yb < 10.09) :
                                Classification: OBAB
                        ELSE :
                                Classification: OA
                ELSE :
                        Classification: OBAB
        ELSE:
                Classification: OA
ELSEIF (TiO2/Yb < 0.497) :
        IF (Zr/Hf < 40) :
                Classification: OA
        ELSEIF (Nb/Yb < 1.269) :
                Classification: OA
        ELSE :
                Classification: OBAB
ELSE :
        Classification: OA
```

Figure 3.21. Decision rule for the first decision tree

```
IF (Th/Nb < 0.155) :
        IF (Sm/Yb < 1.298) :
                Classification: OBAB
        ELSEIF (La/Nb < 1.25) :
                IF (Nb/Nb* < 0.896) :
                        Classification: OA
                ELSE :
                        Classification: OBAB
        ELSE :
                Classification: OA
ELSEIF (Zr/Hf < 33.028) :
        Classification: OA
ELSEIF (Th/Nb < 0.333) :
        IF (Nd/Zr < 0.138) :
                IF (Nb/Nb* < 0.452) :
                        IF (Y/Yb < 10.09) :
                                Classification: OBAB
                        ELSE :
                                Classification: OA
                ELSE :
                        Classification: OBAB
        ELSE:
                Classification: OA
ELSEIF (La/Sm < 2.439) :
        Classification: OA
ELSEIF (Sm/Y < 0.143) :
        Classification: OBAB
ELSE :
        Classification: OA
```

Figure 3.22. Decision rule for the second decision tree

3.1.3. Discrimination Within Non-Subduction Settings

The third set of decision trees is constructed for the tectono-magmatic discrimination within non-subduction settings. Subduction settings are MOR, OP, OI and CWP. At first stage, MOR and OP (Group 1) are discriminated from OI and CWP (Group 2). If the sample is classified as Group 1, a further discrimination is required between MOR and OP. If the sample is classified as Group 2, a discrimination is applied between OI and CWP.

3.1.3.1. Discrimination Between Group 1 (Mid-Oceanic Ridge and Oceanic Plateau) and Group 2 (Oceanic Island and Continental Within-plate) Settings

The first step of discrimination within non-subduction settings is discrimination of samples into two sub-groups: group 1 consisting samples of mid-oceanic ridges and oceanic plateaus and group 2 consisting samples of oceanic islands and continental within-plates.

Two decision trees are constructed for the tectono-magmatic discrimination within non-subduction settings (MOR and OP as Group 1, OI and CWP as Group 2). Both decision trees have 7 levels of depth. The first decision tree uses Sm/Yb at first level, Nd/Zr at second level, Th/Nb and Y/Yb at third level, Zr/TiO_2, La/Nb, Nb/Nb* and La/Sm at fourth level, La/Nb, Nd/Zr and Nb/Yb at fifth level, TiO_2/Y, Nb/Nb* and Th/Nb at sixth level and Zr/Hf and Th/La at seventh level (Figure 3.23).

The second decision tree uses Sm/Yb at first level, Nd/Zr at second level, Th/Nb and Y/Yb at third level, Th/La, La/Nb, Nb/Nb* and La/Sm at fourth level, Sm/Hf, Nd/Zr and Nb/Yb at fifth level, La/Nb, Nb/Nb* and Th/Nb at sixth level and Nb/Y, Zr/Hf and Th/La at seventh level (Figure 3.24).

Decision rules for constructed decision trees are given in Figure 3.25 and Figure 3.26, respectively.

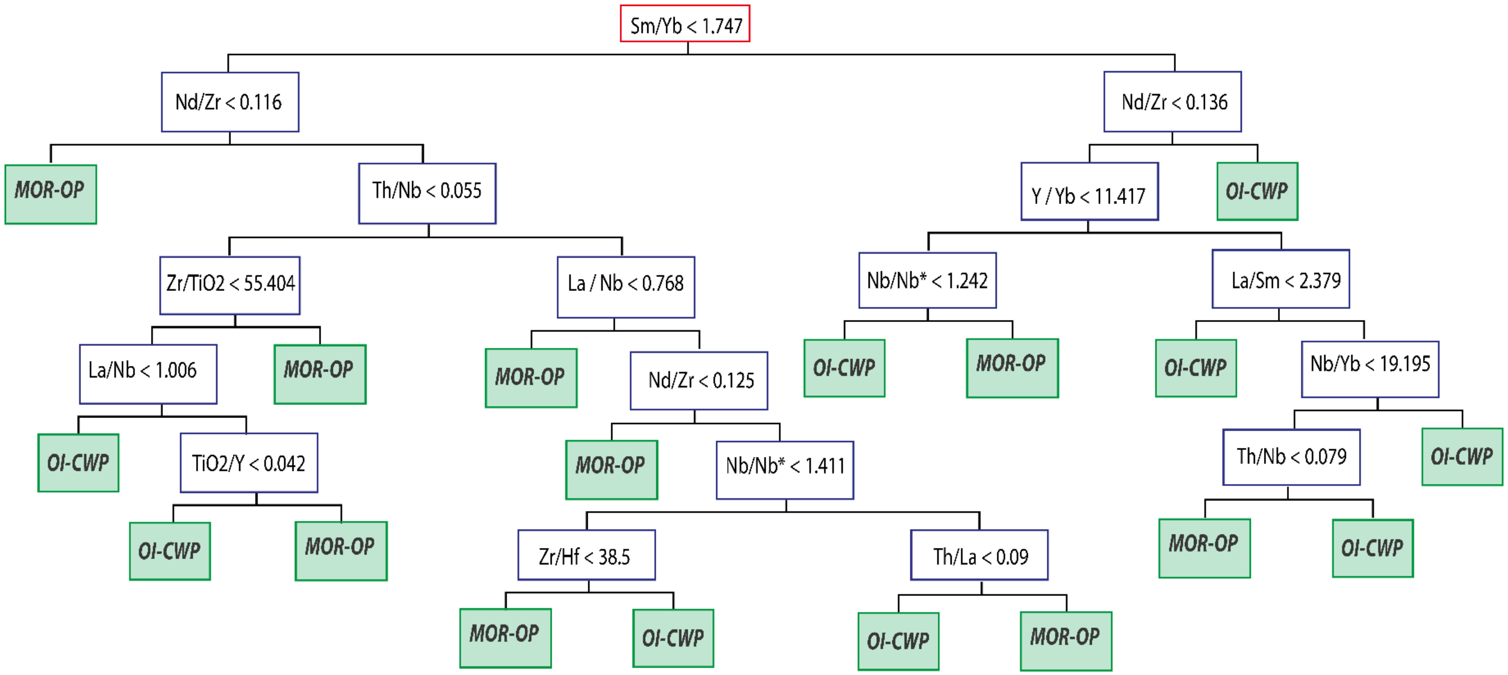

Figure 3.23. The first decision tree to discriminate within non-subduction settings

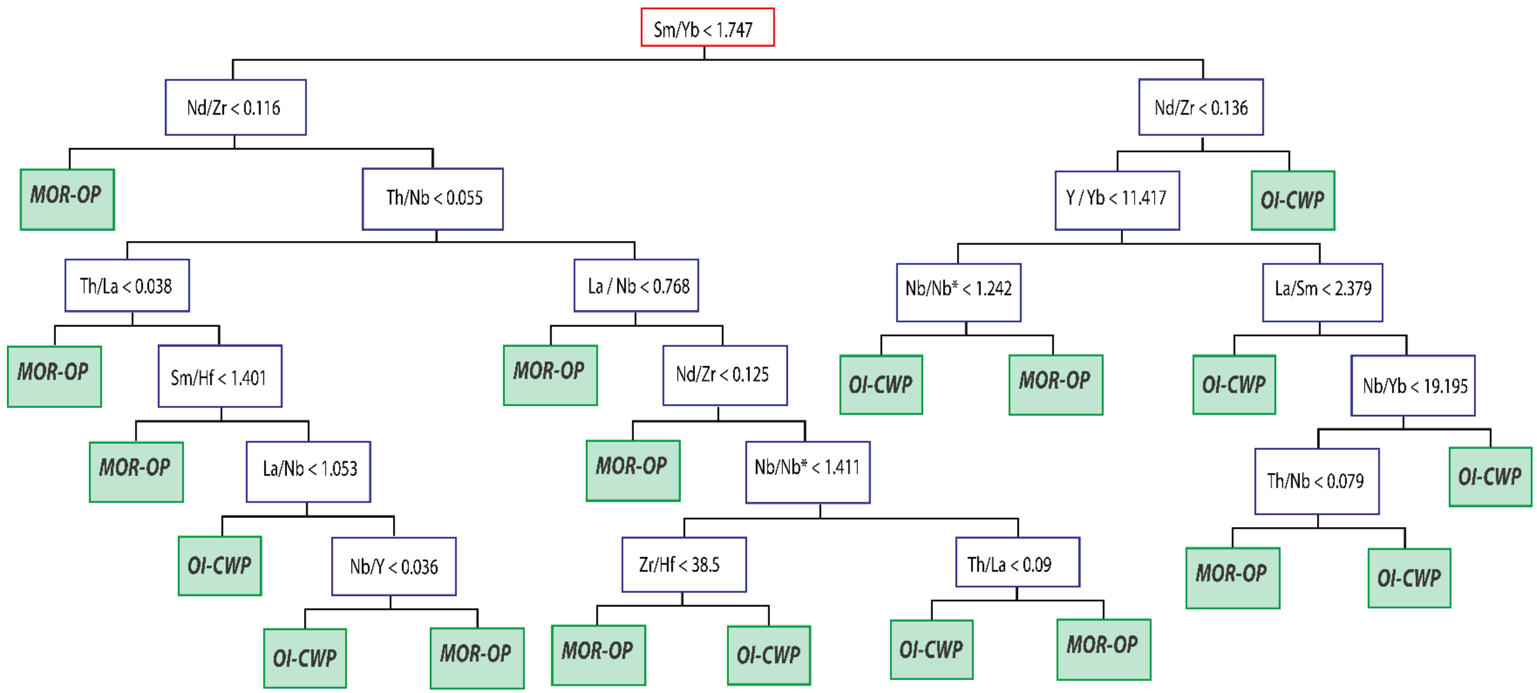

Figure 3.24. The second decision tree to discriminate within non-subduction settings

```
IF (Sm/Yb < 1.747) :
        IF (Nd/Zr < 0.116) :
                Classification: MOR-OP
        ELSEIF (Th/Nb < 0.055) :
                IF (Zr/TiO2 < 55.404) :
                        IF (La/Nb < 1.006) :
                                Classification: OI-CWP
                        ELSEIF (TiO2/Y < 0.042) :
                                Classification: OI-CWP
                        ELSE :
                                Classification: MOR-OP
                ELSE :
                        Classification: MOR-OP
        ELSEIF (La/Nb < 0.768) :
                Classification: MOR-OP
        ELSEIF (Nd/Zr < 0.125) :
                Classification: MOR-OP
        ELSEIF (Nb/Nb* < 1.411) :
                IF (Zr/Hf < 38.5) :
                        Classification: MOR-OP
                ELSE :
                        Classification: OI-CWP
        ELSEIF (Th/La < 0.09) :
                Classification: OI-CWP
        ELSE:
                Classification: MOR-OP
ELSEIF (Nd/Zr < 0.136) :
        IF (Y/Yb < 11.417) :
                IF (Nb/Nb* < 1.242) :
                        Classification: OI-CWP
                ELSE :
                        Classification: MOR-OP
        ELSEIF (La/Sm < 2.379) :
                Classification: OI-CWP
        ELSEIF (Nb/Yb < 19.195) :
                IF (Th/Nb < 0.079) :
                        Classification: MOR-OP
                ELSE :
                        Classification: OI-CWP
        ELSE:
                Classification: OI-CWP
ELSE :
        Classification: OI-CWP
```

Figure 3.25. Decision rule for the first decision tree

```
IF (Sm/Yb < 1.747) :
        IF (Nd/Zr < 0.116) :
                Classification: MOR-OP
        ELSEIF (Th/Nb < 0.055) :
                IF (Th/La < 0.038) :
                        Classification: MOR-OP
                ELSEIF (Sm/Hf < 1.401) :
                        Classification: MOR-OP
                ELSEIF (La/Nb < 1.053) :
                        Classification: OI-CWP
                ELSEIF (Nb/Y < 0.036) :
                        Classification: OI-CWP
                ELSE :
                        Classification: MOR-OP
        ELSEIF (La/Nb < 0.768) :
                Classification: MOR-OP
        ELSEIF (Nd/Zr < 0.125) :
                Classification: MOR-OP
        ELSEIF (Nb/Nb* < 1.411) :
                IF (Zr/Hf < 38.5) :
                        Classification: MOR-OP
                ELSE :
                        Classification: OI-CWP
        ELSEIF (Th/La < 0.09) :
                Classification: OI-CWP
        ELSE:
                Classification: MOR-OP
ELSEIF (Nd/Zr < 0.136) :
        IF (Y/Yb < 11.417) :
                IF (Nb/Nb* < 1.242) :
                        Classification: OI-CWP
                ELSE :
                        Classification: MOR-OP
        ELSEIF (La/Sm < 2.379) :
                Classification: OI-CWP
        ELSEIF (Nb/Yb < 19.195) :
                IF (Th/Nb < 0.079) :
                        Classification: MOR-OP
                ELSE :
                        Classification: OI-CWP
        ELSE:
                Classification: OI-CWP
ELSE :
        Classification: OI-CWP
```

Figure 3.26. Decision rule for the second decision tree

3.1.3.2. Discrimination Between Mid-Oceanic Ridges and Oceanic Plateaus

Two decision trees are constructed for the tectono-magmatic discrimination between MOR and OP. The first decision tree has 6 and the second one has 7 levels of depth. The first decision tree uses Th/Y at first level, Zr/Hf at second level, Nb/ TiO_2 at third level, Th/Y and Zr/Y at fourth level, Zr/Y, Zr/Nb, and Th/La at fifth level, Th/La and Nb/Nb* at sixth level (Figure 3.27).

The second decision tree uses Th/Y at first level, Zr/Hf at second level, Zr/Nb at third level, Sm/Yb and Zr/Hf at fourth level, Zr/Nb, La/Nb, Y/Yb and Zr/Hf at fifth level, Th/La, La/Y and Zr/Nb at sixth level and Sm/Y at seventh level (Figure 3.28).

Decision rules for constructed decision trees are given in Figure 3.29 and Figure 3.30, respectively.

3.1.3.3. Discrimination Between Oceanic Islands and Continental Within-plates

Two decision trees are constructed for the tectono-magmatic discrimination between OI and CWP. Both decision trees have 8 levels of depth. The first decision tree uses Nb/Y at first level, Zr/Yb at second and third levels, Sm/Nb and Zr/Y at fourth level, Th/Nb and TiO_2/Y at fifth level, Th/Nb, Nb/ TiO_2, Y/Yb and Zr/Hf at sixth level, Sm/Nd, Th/La, Sm/Yb, Nb/Y and Th/La at seventh level and La/Y, Zr/Nb, Zr/Yb, Sm/Nb and La/Sm at eighth level (Figure 3.31).

The second decision tree uses Nb/Y at first level, Zr/Yb at second and third levels, Sm/Nb and Zr/Y at fourth level, Th/Nb and Sm/Nb at fifth level, Th/Nb, Sm/Nb, Zr/Y and Zr/Hf at sixth level, Sm/Nd, Y/Yb, Zr/Yb and Nb/Yb at seventh level and La/Y, Zr/Nb and Sm/Nd at eighth level (Figure 3.32).

Decision rules for constructed decision trees are given in Figure 3.33 and Figure 3.34, respectively.

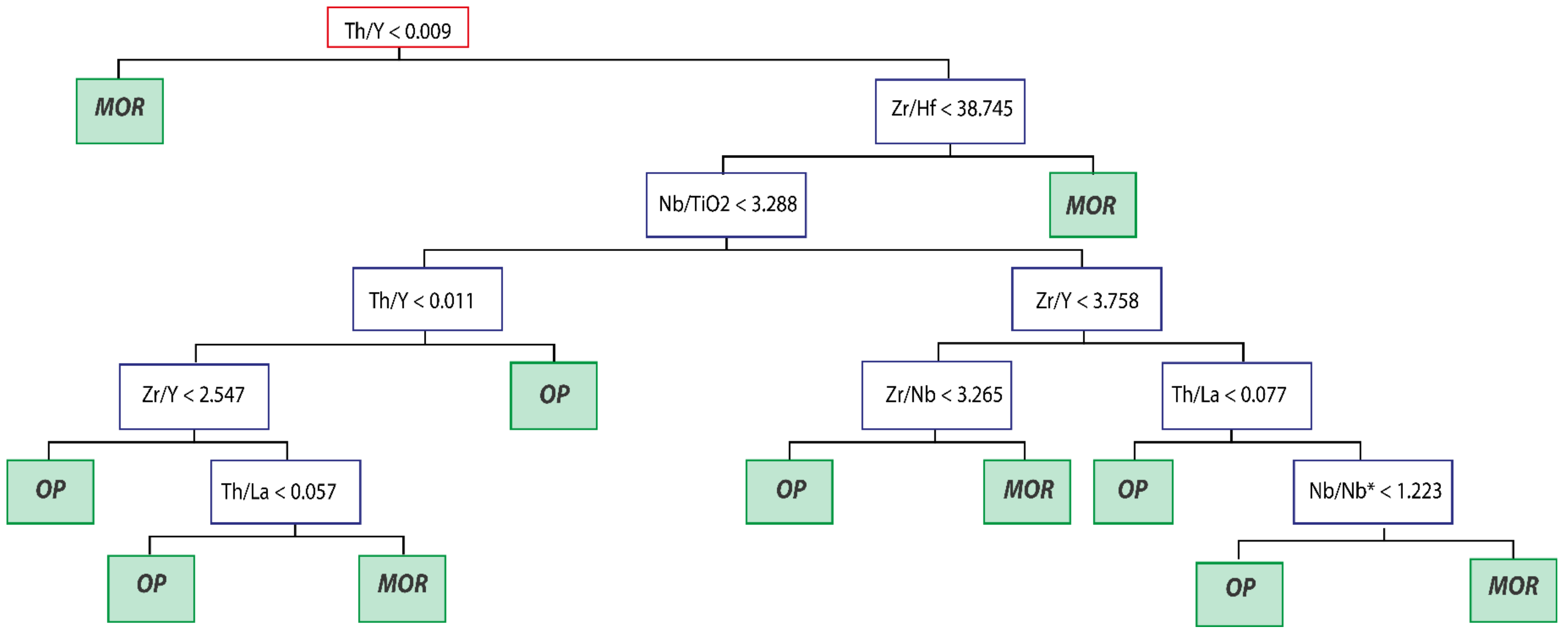

Figure 3.27. The first decision tree to discriminate between Mid-Oceanic Ridges and Oceanic Plateaus

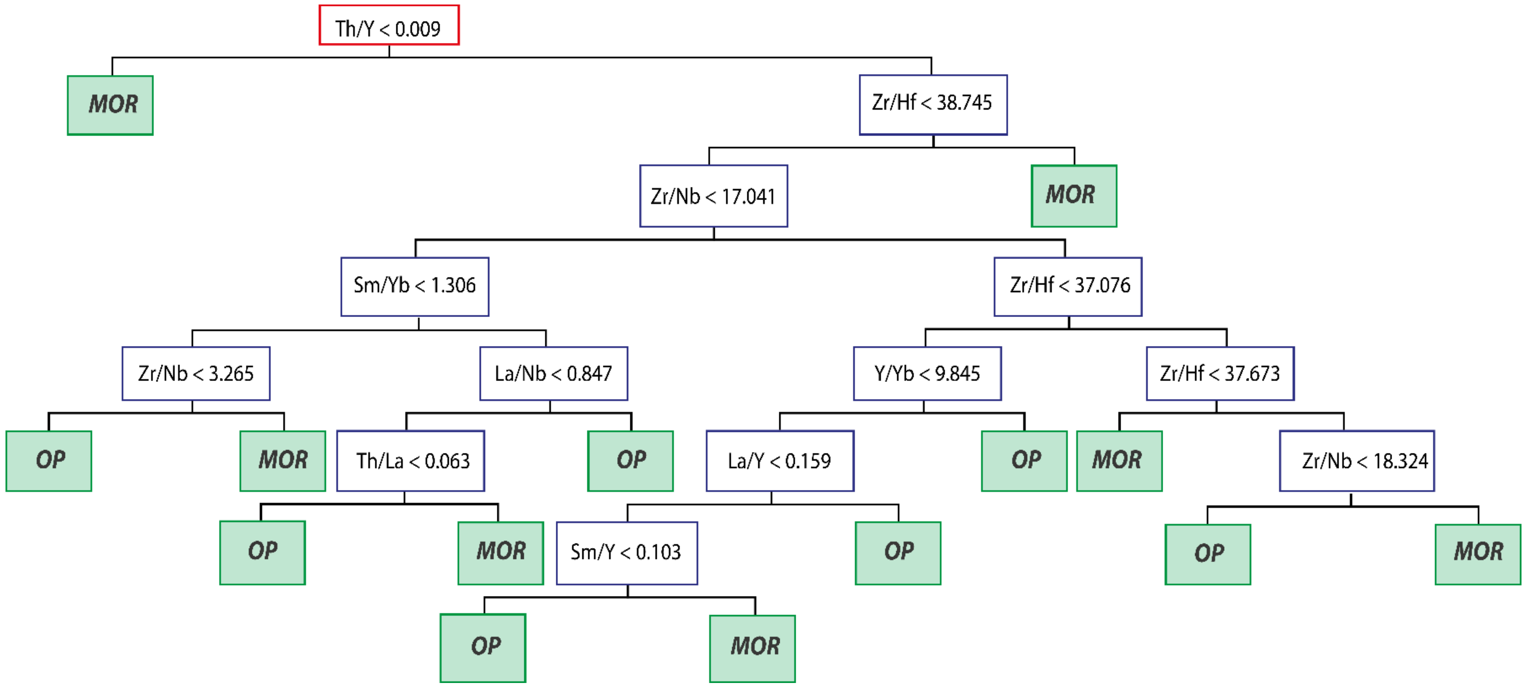

Figure 3.28. The second decision tree to discriminate between Mid-Oceanic Ridges and Oceanic Plateaus

```
IF (Th/Y < 0.009) :
        Classification: MOR
ELSEIF (Zr/Hf < 38.745) :
        IF (Nb/TiO2 < 3.288) :
                IF (Th/Y < 0.011) :
                        IF (Zr/Y < 2.547) :
                                Classification: OP
                        ELSEIF (Th/La < 0.057) :
                                Classification: OP
                        ELSE :
                                Classification: OP
                ELSE :
                        Classification: OP
        ELSEIF (Zr/Y < 3.758) :
                IF (Zr/Nb < 3.265) :
                        Classification: OP
                ELSE:
                        Classification: MOR
        ELSEIF (Th/La < 0.077) :
                Classification: OP
        ELSEIF (Nb/Nb* < 1.223) :
                Classification: OP
        ELSE :
                Classification: MOR
ELSE :
        Classification: MOR
```

Figure 3.29. Decision rule for the first decision tree

```
IF (Th/Y < 0.009) :
        Classification: MOR
ELSEIF (Zr/Hf < 38.745) :
        IF (Zr/Nb < 17.041) :
                IF (Sm/Yb < 1.306) :
                        IF (Zr/Nb < 3.265) :
                                Classification: OP
                        ELSE :
                                Classification: MOR
                ELSEIF (La/Nb < 0.847) :
                        IF (Th/La < 0.063) :
                                Classification: OP
                        ELSE :
                                Classification: MOR
                ELSE :
                        Classification: OP
        ELSEIF (Zr/Hf < 37.076) :
                IF (Y/Yb < 9.845) :
                        IF (La/Y < 0.159) :
                                IF (Sm/Y < 0.103) :
                                        Classification: OP
                                ELSE :
                                        Classification: MOR
                ELSE :
                        Classification: OP
        ELSEIF (Zr/Hf < 37.673):
                Classification: MOR
        ELSEIF (Zr/Nb < 18.324) :
                Classification: OP
        ELSE :
                Classification: MOR
ELSE :
        Classification: MOR
```

Figure 3.30. Decision rule for the second decision tree

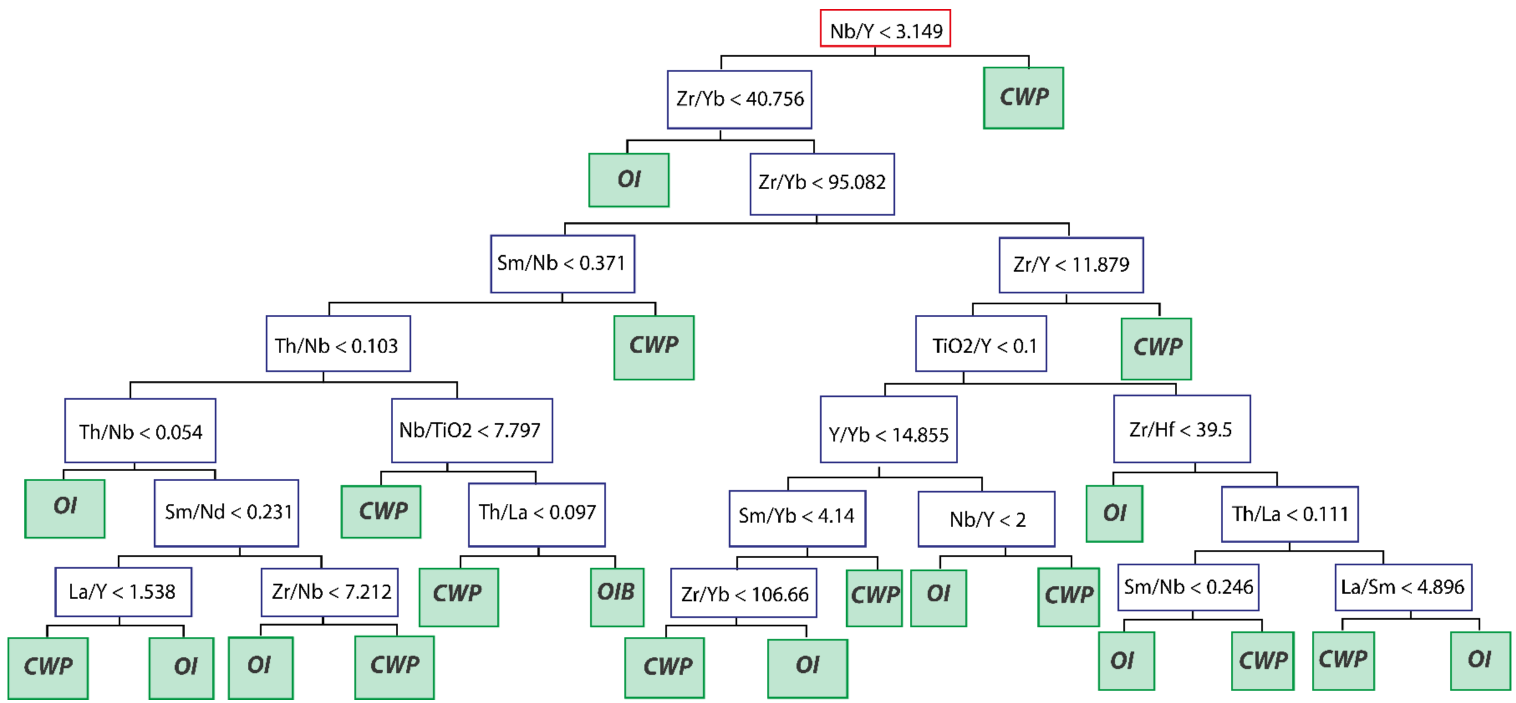

Figure 3.31. The first decision tree to discriminate between Ocean Islands and Continental Within-Plates

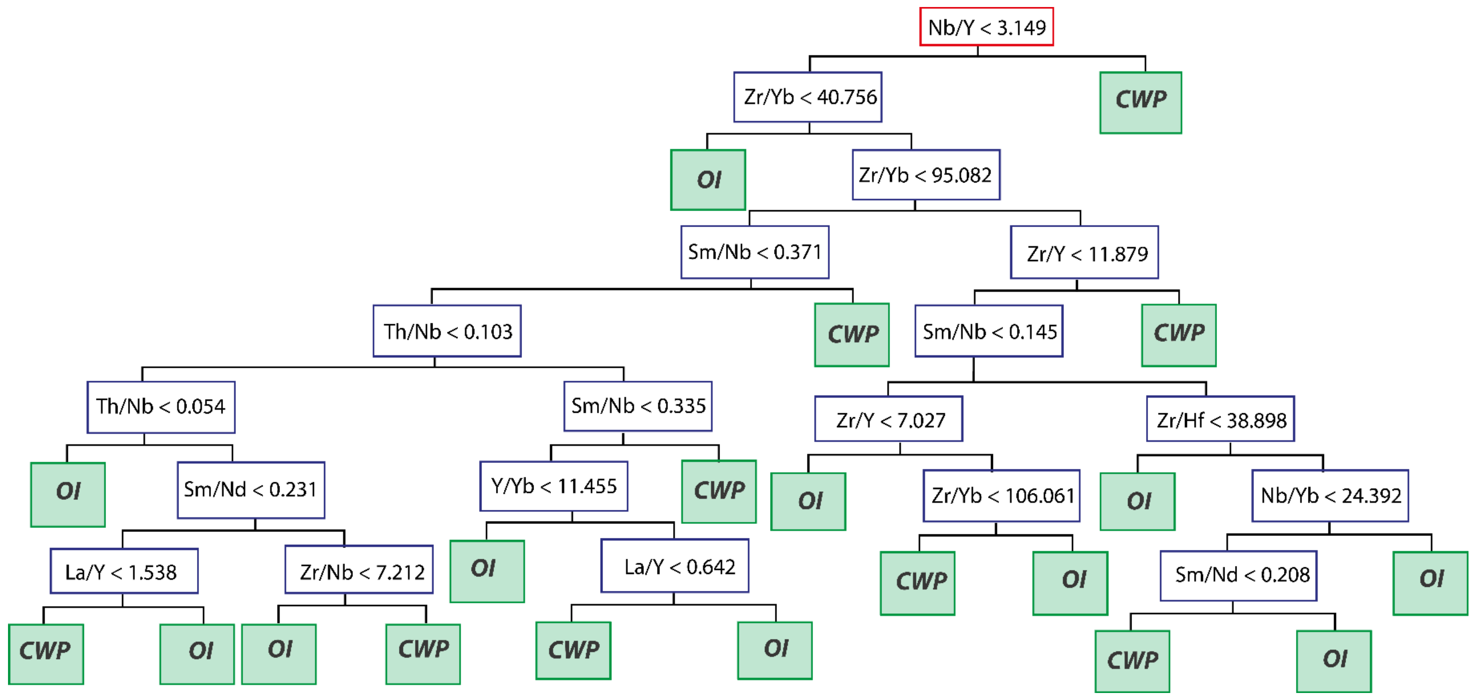

Figure 3.32. The second decision tree to discriminate between Ocean Islands and Continental Within-Plates

```
IF (Nb/Y < 3.149) :
    IF (Zr/Yb < 40.756) :
        Classification: OI
    ELSEIF (Zr/Yb < 95.082) :
        IF (Sm/Nb < 0.371) :
            IF (Th/Nb < 0.103) :
                IF (Th/Nb < 0.054) :
                    Classification: OI
                ELSEIF (Sm/Nd < 0.231) :
                    IF (La/Y < 1.538) :
                        Classification: CWP
                    ELSE :
                        Classification: OI
                ELSEIF (Zr/Nb < 7.212) :
                    Classification: OI
                ELSE :
                    Classification: CWP
            ELSEIF (Nb/TiO2) :
                Classification: CWP
            ELSEIF (Th/La < 0.097) :
                Classification: CWP
            ELSE :
                Classification: OI
        ELSE :
            Classification: CWP
    ELSEIF (Zr/Y < 11.879) :
        IF (TiO2/Y < 0.1) :
            IF (Y/Yb < 14.855) :
                IF (Sm/Yb < 4.14) :
                    IF (Zr/Yb < 106.66) :
                        Classification: CWP
                    ELSE :
                        Classification: OI
                ELSE :
                    Classification: CWP
            ELSEIF (Nb/Y < 2) :
                Classification: OI
            ELSE:
                Classification: CWP
        ELSEIF (Zr/Hf < 39.5) :
            Classification: OI
        ELSEIF (Th/La <  0.111) :
            IF (Sm/Nb < 0.246) :
                Classification: OI
            ELSE :
                Classification: CWP
        ELSEIF (La/Sm < 4.896) :
            Classification: CWP
        ELSE:
            Classification: OI
    ELSE :
        Classification: CWP
ELSE :
    Classification: CWP
```

Figure 3.33. Decision rule for the first decision tree

```
IF (Nb/Y < 3.149) :
        IF (Zr/Yb < 40.756) :
                Classification: OI
        ELSEIF (Zr/Yb < 95.082) :
                IF (Sm/Nb < 0.371) :
                        IF (Th/Nb < 0.103) :
                                IF (Th/Nb < 0.054) :
                                        Classification: OI
                                ELSEIF (Sm/Nd < 0.231) :
                                        IF (La/Y < 1.538) :
                                                Classification: CWP
                                        ELSE :
                                                Classification: OI
                                ELSEIF (Zr/Nb < 7.212) :
                                        Classification: OI
                                ELSE :
                                        Classification: CWP
                        ELSEIF (Sm/Nb < 0.335) :
                                IF (Y/Yb <11.455) :
                                        Classification: OI
                                ELSEIF (La/Y < 0.642) :
                                        Classification: CWP
                                ELSE :
                                        Classification: OI
                        ELSE :
                                Classification: CWP
                ELSE:
                        Classification: CWP
        ELSEIF (Zr/Y < 11.879) :
                IF (Sm/Nb < 0.145) :
                        IF (Zr/Y < 7.027) :
                                Classification: OI
                        ELSEIF (Zr/Yb < 106.601) :
                                Classification: CWP
                        ELSE :
                                Classification: OI
                ELSEIF (Zr/Hf < 38.898) :
                        Classification: OI
                ELSEIF (Nb/Yb < 24.392) :
                        IF (Sm/Nd < 0.208) :
                                Classification: CWP
                        ELSE :
                                Classification: OI
                ELSE:
                        Classification: OI
        ELSE :
                Classification: CWP
ELSE :
        Classification: CWP
```

Figure 3.34. Decision rule for the second decision tree

3.2. Classification Results (Decision Trees)

3.2.1. Discrimination Between Subduction and Non-Subduction Settings

One decision stump using Th/Nb ratio (Figure 3.35) and two multi-branched decision trees (Figure 3.36 and Figure 3.37) are constructed for the discrimination between subduction and non-subduction settings. Using training set, success ratios for discrimination at each level of depth are determined.

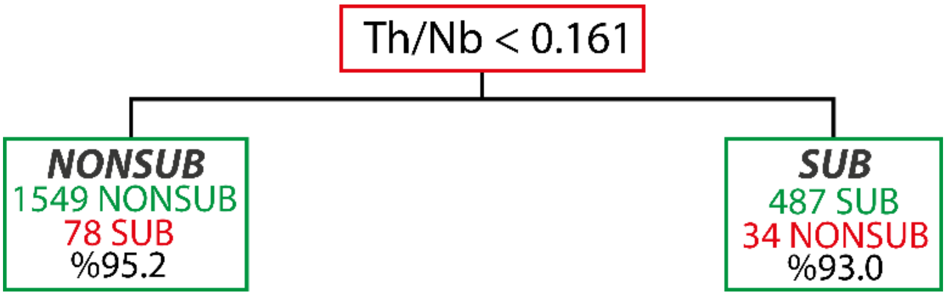

Figure 3.35. Classification results of the decision stump to discriminate between subduction and non-subduction settings

For confusion matrix, showing the tectono-magmatic discrimination results for training+test and external datasets; true positive (TP) represents samples of subduction settings classified as subduction, true negative (TN) represents samples of non-subduction settings classified as non-subduction, false positive (FP) represents samples of non-subduction settings classified as subduction and false negative (FN) represents samples of subduction settings classified as non-subduction.

When confusion matrix for training and test datasets are evaluated, the overall success ratio for tectono-magmatic discrimination between subduction and non-subduction settings is high for all levels of three decision trees (Table 3.2).

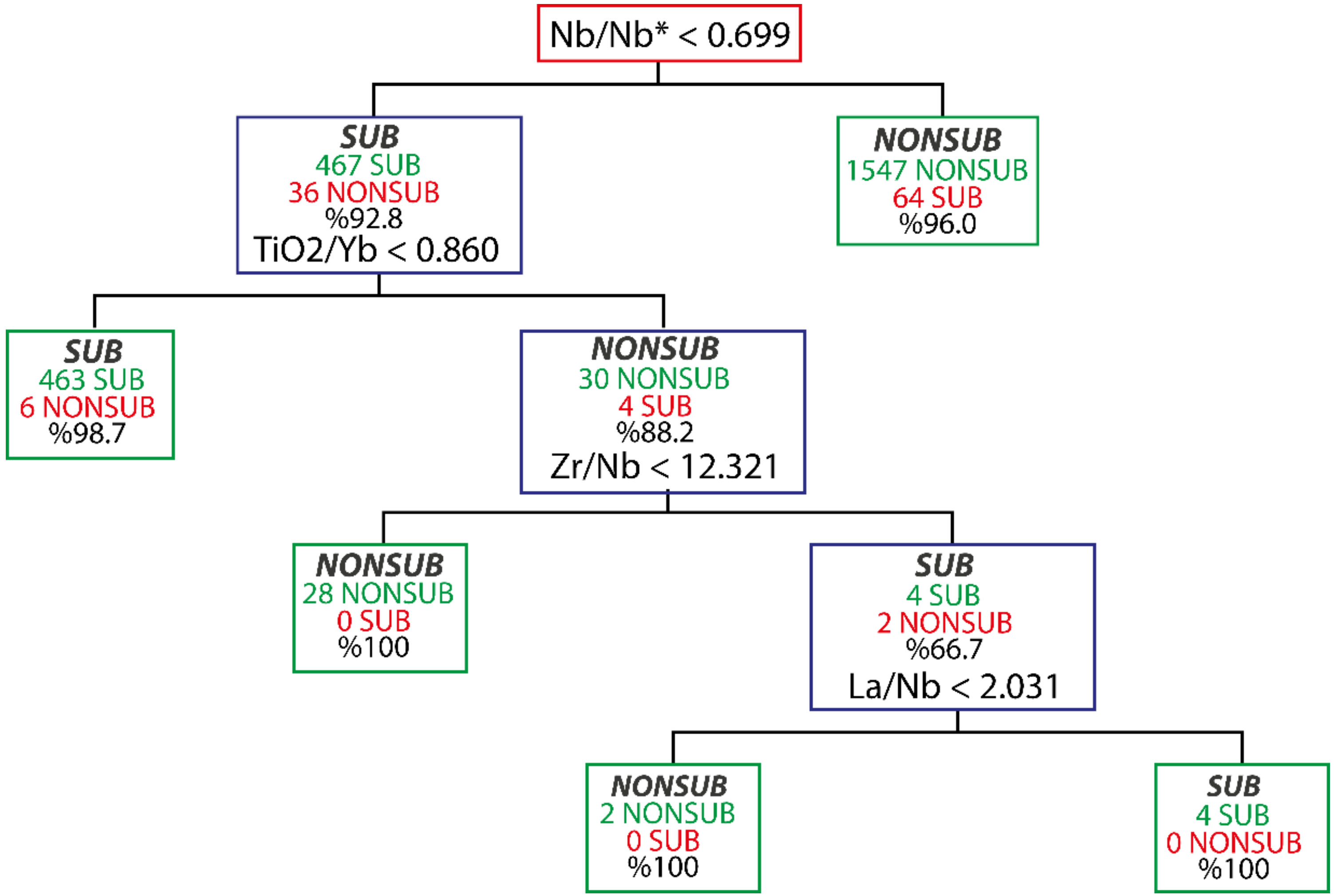

Figure 3.36. Classification results of the first decision tree to discriminate between subduction and non-subduction settings

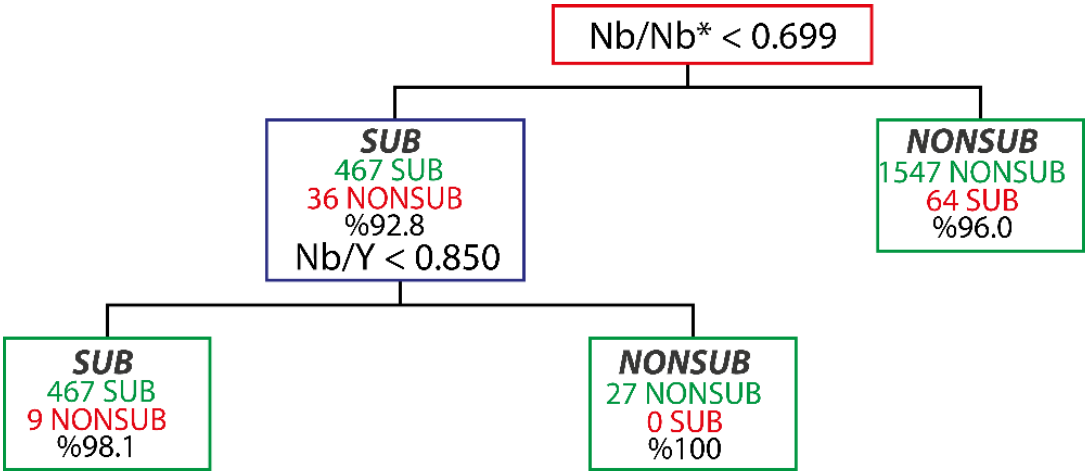

Figure 3.37. Classification results of the second decision tree to discriminate between subduction and non-subduction settings

Table 3.2. Confusion Matrix Summary for Training and Test Datasets for Tectono-Magmatic Discrimination Between Subduction and Non-Subduction Settings

	Tree 1	Tree 2				Tree 3	
	Level 1	Level 1	Level 2	Level 3	Level 4	Level 1	Level 2
TP	577	591	587	591	591	591	591
TN	1,932	1,928	1,964	1,962	1,964	1,928	1,962
FP	42	46	10	12	19	46	12
FN	91	77	81	77	77	77	77

When confusion matrix for external datasets are evaluated, the overall success ratio for tectono-magmatic discrimination between subduction and non-subduction settings remain high for all levels of three decision trees (Table 3.3).

Decision stump correctly discriminated all articles except 1 article from CA, 4 articles from CWP, 6 articles from OA, 4 articles from OBAB, 1 article from OI and 1 article from OP (Table 3.4). Only 6 articles have major fails at discrimination between subduction and non-subduction related settings for training and test sets.

Table 3.3. Confusion Matrix Summary for External Datasets for Tectono-Magmatic Discrimination Between Subduction and Non-Subduction Settings

	Tree 1	Tree 2				Tree 3	
	Level 1	Level 1	Level 2	Level 3	Level 4	Level 1	Level 2
TP	375	396	395	396	396	396	393
TN	1,937	1,942	1,981	1,977	1,977	1,942	1,979
FP	69	64	25	29	29	64	27
FN	91	70	71	70	70	70	73

Table 3.4. Misclassifications in training and test datasets by decision trump for discrimination between subduction and non-subduction settings

JOURNAL	CLASS	SAMPLES	LEVEL 1 ERRORS	LEVEL 1 ERROR %
Mullen 2017 Cascade Arc	CA	35	6	17.14
Coe 2008 South Africa	CWP	27	23	85.19
Gibson 2000 Picrite	CWP	16	3	18.75
Janney 2002 South Africa	CWP	11	2	18.18
Mirnejad 2006 Leucite Hills	CWP	10	10	100.00
Bedard 1999 Canada	OA	12	2	16.67
Jolly 2007 Greater Antilles Arc	OA	37	5	13.51
Jolly 2008 Greater Antilles Arc A	OA	98	1	1.02
Pearce 2005 Mariana	OA	11	1	9.09
Todd 2012 Fiji Tonga	OA	13	5	38.46
Tollstrup 2010 Izu Bonin	OA	51	2	3.92
Beier 2015 Manus Basin	OBAB	6	5	83.33
Leat 2004 Sandwich	OBAB	5	3	60.00
Pearce 1995 Lau	OBAB	25	24	96.00
Pearce 2005 Mariana	OBAB	53	33	62.26
Jackson 2010 Samoa	OI	135	1	0.74
Neal 2002 Kerguelen	OP	35	3	8.57

Decision stump mainly sustains its success for external datasets (Table 3.5). All CA and OI are classified correctly. Misclassifications for MOR in external dataset are observed. Other than these, the general trend of misclassifications in training and test datasets is also observed in external dataset.

Table 3.5. Misclassifications in external datasets by decision stump for discrimination between subduction and non-subduction settings

JOURNAL	CLASS	SAMPLES	LEVEL 1 ERRORS	LEVEL 1 ERROR %
Davies 2006 Aldan Shield	CWP	7	7	100.00
Frey 1996 Bunbury	CWP	10	2	20.00
Gibson 1993 Rio Grande Rift	CWP	15	7	46.67
Gibson 1995 Brazil Paraguay	CWP	25	11	44.00
Gibson 1995 Southeast Brazil	CWP	32	5	15.63
Gibson 2005 Tristan	CWP	14	12	85.71
Mana 2015 East African Rift	CWP	29	3	10.34
Olierook 2016 Bunbury	CWP	8	6	75.00
Xu 2001 SW China	CWP	25	11	44.00
Kelley 2013 EPR MAR	MOR	562	2	0.36
Pyle 1995 Indian Pacific	MOR	17	1	5.88
Jolly 2008 Greater Antilles Arc B	OA	78	1	1.28
König 2008 Subduction Zones	OA	6	3	50.00
Straub 2010 Izu Bonin	OA	48	2	4.17
Tamura 2011 Mariana	OA	19	2	10.53
Wharton 1994 Viti Levu	OA	6	1	16.67
Woodhead 2001 Mixed	OA	23	1	4.35
Bezos 2009 Lau Basin	OBAB	34	34	100.00
Harrison 2003 East Scotia	OBAB	5	5	100.00
Ikeda 2016 Mariana	OBAB	15	12	80.00
Ishizuka 2009 Izu Bonin	OBAB	30	21	70.00
Mortimer 2007 South Fiji Northland	OBAB	12	9	75.00
Frey 2002 Kerguelen	OP	17	1	5.88
Weis 2002 Kerguelen	OP	29	1	3.45

The first decision tree is more successful at discrimination of subduction and non-subduction-related settings (Table 3.6). The amount of articles with misclassification slightly increase but number of articles with major fails decrease from 6 to 4. Most of misclassifications are solved at advanced levels of decision tree, using multiple criteria.

Table 3.6. Misclassifications in training and test datasets by first decision tree for discrimination between subduction and non-subduction settings

JOURNAL	CLASS	SAMPLES	LEVEL 1 ERRORS	LEVEL 1 ERROR %	LEVEL 2 ERRORS	LEVEL 2 ERROR %	LEVEL 3 ERRORS	LEVEL 3 ERROR %	LEVEL 4 ERRORS	LEVEL 4 ERROR %
Hickey Vargas 2016 Andean	CA	55			1	2				
Mullen 2017 Cascade Arc	CA	35	6	17	7	20	6	17	6	17
Coe 2008 South Africa	CWP	27	22	81						
Gibson 2000 Picrite	CWP	16	2	13			2	13		
Hanghoj 2003 East Greenland	CWP	103	1	1						
Larsen 2003 West Greenland	CWP	23	1	4	1	4	1	4	1	4
Mirnejad 2006 Leucite Hills	CWP	10	10	100						
Arevalo 2010 Mixed	MOR	512	5	1	5	1	5	1	5	1
Kempton 2002 Indian	MOR	63	2	3	2	3	2	3	2	3
Nauret 2006 Central Indian	MOR	34	1	3	1	3	1	3	1	3
Bedard 1999 Canada	OA	12	3	25	3	25	3	25	3	25
Jolly 2007 Greater Antilles	OA	37	4	11	4	11	4	11	4	11
Jolly 2008 Greater Antilles	OA	98	1	1	1	1	1	1	1	1
Todd 2012 Fiji Tonga	OA	13	3	23	5	38	3	23	3	23
Beier 2015 Manus Basin	OBAB	6	5	83	5	83	5	83	5	83
Leat 2004 Sandwich	OBAB	5	3	60	3	60	3	60	3	60
Pearce 1995 Lau	OBAB	25	17	68	17	68	17	68	17	68
Pearce 2005 Mariana	OBAB	53	31	58	31	58	31	58	31	58
Neal 2002 Kerguelen	OP	35	2	6	1	3	1	3	1	3

The first decision tree is also applicable to external datasets successfully, especially to CA, OI and OP (Table 3.7). Other than this, the trend of misclassifications for training and test dataset is similar to that of external dataset.

Table 3.7. Misclassifications in external datasets by first decision tree for discrimination between subduction and nonsubduction settings

JOURNAL	CLASS	SAMPLES	LEVEL 1 ERRORS	LEVEL 1 ERROR %	LEVEL 2 ERRORS	LEVEL 2 ERROR %	LEVEL 3 ERRORS	LEVEL 3 ERROR %	LEVEL 4 ERRORS	LEVEL 4 ERROR %
Davies 2006 Aldan Shield	CWP	7	7	100	4	57	7	100	7	100
Frey 1996 Bunbury	CWP	10	1	10	1	10	1	10	1	10
Gibson 1993 Rio Grande Rift	CWP	15	7	47	3	20	4	27	4	27
Gibson 2005 Tristan	CWP	14	12	86						
Olierook 2016 Bunbury	CWP	8	5	63	5	63	5	63	5	63
Shuying 2015 South China	CWP	12	1	8	1	8	1	8	1	8
Xu 2001 SW China	CWP	25	4	16	2	8	2	8	2	8
Jenner 2012 Mixed	MOR	588	1	0	1	0	1	0	1	0
Kelley 2013 EPR MAR	MOR	562	7	1	7	1	7	1	7	1
Pyle 1995 Indian Pacific	MOR	17	1	6	1	6	1	6	1	6
Jolly 2008 Greater Antilles	OA	78			1	1				
König 2008 Subduction Zone	OA	6	3	50	3	50	3	50	3	50
Straub 2010 Izu Bonin	OA	48	2	4	2	4	2	4	2	4
Woodhead 2001 Mixed	OA	23	1	4	1	4	1	4	1	4
Bezos 2009 Lau Basin	OBAB	34	21	62	21	62	21	62	21	62
Harrison 2003 East Scotia	OBAB	5	5	100	5	100	5	100	5	100
Ikeda 2016 Mariana	OBAB	15	12	80	12	80	12	80	12	80
Ishizuka 2009 Izu Bonin	OBAB	30	18	60	18	60	18	60	18	60
Mortimer 2007 South Fiji	OBAB	12	8	67	8	67	8	67	8	67

The second decision tree is both simpler in structure and more successful at discrimination of subduction and non-subduction-related settings for training and test datasets (Table 3.8). 18 articles have misclassifications, only 4 of which have major failures. The decision tree is especially successful for CA, OI and OP.

Table 3.8. Misclassifications in training and test datasets by second decision tree for discrimination between subduction and non-subduction settings

JOURNAL	CLASS	SAMPLES	LEVEL 1 ERRORS	LEVEL 1 ERROR %	LEVEL 2 ERRORS	LEVEL 2 ERROR %
Mullen 2017 Cascade Arc	CA	35	6	17	6	17
Coe 2008 South Africa	CWP	27	22	81		
Gibson 2000 Picrite	CWP	16	2	13	2	13
Hanghoj 2003 East Greenland	CWP	103	1	1	1	1
Larsen 2003 West Greenland	CWP	23	1	4		
Mirnejad 2006 Leucite Hills	CWP	10	10	100		
Arevalo 2010 Mixed	MOR	512	5	1	5	1
Kempton 2002 Indian	MOR	63	2	3	2	3
Nauret 2006 Central Indian	MOR	34	1	3	1	3
Bedard 1999 Canada	OA	12	3	25	3	25
Jolly 2007 Greater Antilles Arc	OA	37	4	11	4	11
Jolly 2008 Greater Antilles Arc A	OA	98	1	1	1	1
Todd 2012 Fiji Tonga	OA	13	3	23	3	23
Beier 2015 Manus Basin	OBAB	6	5	83	5	83
Leat 2004 Sandwich	OBAB	5	3	60	3	60
Pearce 1995 Lau	OBAB	25	17	68	17	68
Pearce 2005 Mariana	OBAB	53	31	58	31	58
Neal 2002 Kerguelen	OP	35	2	6	1	3

The second decision tree, similar to the decision stump and decision tree, is also successfully applicable to external datasets (Table 3.9). Only 4 articles (2 CWP, 1 OA and 1 OBAB) have major failures. OI and OP are correctly discriminated.

Table 3.9. Misclassifications in external datasets by second decision tree for discrimination between subduction and non-subduction settings

JOURNAL	CLASS	SAMPLES	LEVEL 1 ERRORS	LEVEL 1 ERROR %	LEVEL 2 ERRORS	LEVEL 2 ERROR %
Bryant 2006 Andes	CA	3			1	33
De Astis 2000 Aeolian	CA	23			1	4
Santo 2004 Aeolian	CA	31			1	3
Davies 2006 Aldan Shield	CWP	7	7	100	7	100
Frey 1996 Bunbury	CWP	10	1	10	1	10
Gibson 1993 Rio Grande Rift	CWP	15	7	47	1	7
Gibson 1995 Brazil Paraguay	CWP	25	12	48		
Gibson 1995 Southeast Brazil	CWP	32	5	16		
Gibson 2005 Tristan	CWP	14	12	86		
Mana 2015 East African Rift	CWP	29	1	3		
Olierook 2016 Bunbury	CWP	8	5	63	5	63
Shuying 2015 South China	CWP	12	1	8	1	8
Xu 2001 SW China	CWP	25	4	16	3	12
Jenner 2012 Mixed	MOR	588	1	0	1	0
Kelley 2013 EPR MAR	MOR	562	7	1	7	1
Pyle 1995 Indian Pacific	MOR	17	1	6	1	6
König 2008 Subduction Zones	OA	6	3	50	3	50
Straub 2010 Izu Bonin	OA	48	2	4	2	4
Woodhead 2001 Mixed	OA	23	1	4	1	4
Bezos 2009 Lau Basin	OBAB	34	21	62	21	62
Harrison 2003 East Scotia	OBAB	5	5	100	5	100
Ikeda 2016 Mariana	OBAB	15	12	80	12	80
Ishizuka 2009 Izu Bonin	OBAB	30	18	60	18	60

The trends of misclassifications for training – test datasets and external datasets are similar to each other.

3.2.2. Discrimination Within Subduction Settings

3.2.2.1. The First Path for Discrimination Within Subduction Settings

The first path involves two-stage discrimination within subduction settings: (1) between arc and back-arc-related settings, (2) within arc-related settings.

3.2.2.1.1. Discrimination Between Arc and Back-arc-related Settings

Two multi-branched decision trees (Figure 3.38 and Figure 3.39) are constructed for the discrimination between arc and back-arc-related settings. Using training set, success ratios for discrimination at each level of depth are determined.

For confusion matrix, showing the tectono-magmatic discrimination results for training+test and external datasets; true positive (TP) represents samples of back-arc-related settings classified as back-arc, true negative (TN) represents samples of arc-related settings classified as arc, false positive (FP) represents samples of arc-related settings classified as back-arc and false negative (FN) represents samples of back-arc-related settings classified as arc.

When confusion matrix for training and test datasets are evaluated, the overall success ratio for tectono-magmatic discrimination between arc and back-arc-related settings are higher for the last two levels of two decision trees (Table 3.10).

When confusion matrix for external datasets are evaluated, the overall success ratio for tectono-magmatic discrimination between arc and back-arc-related settings decreases in varying degrees for the second trees (Table 3.11).

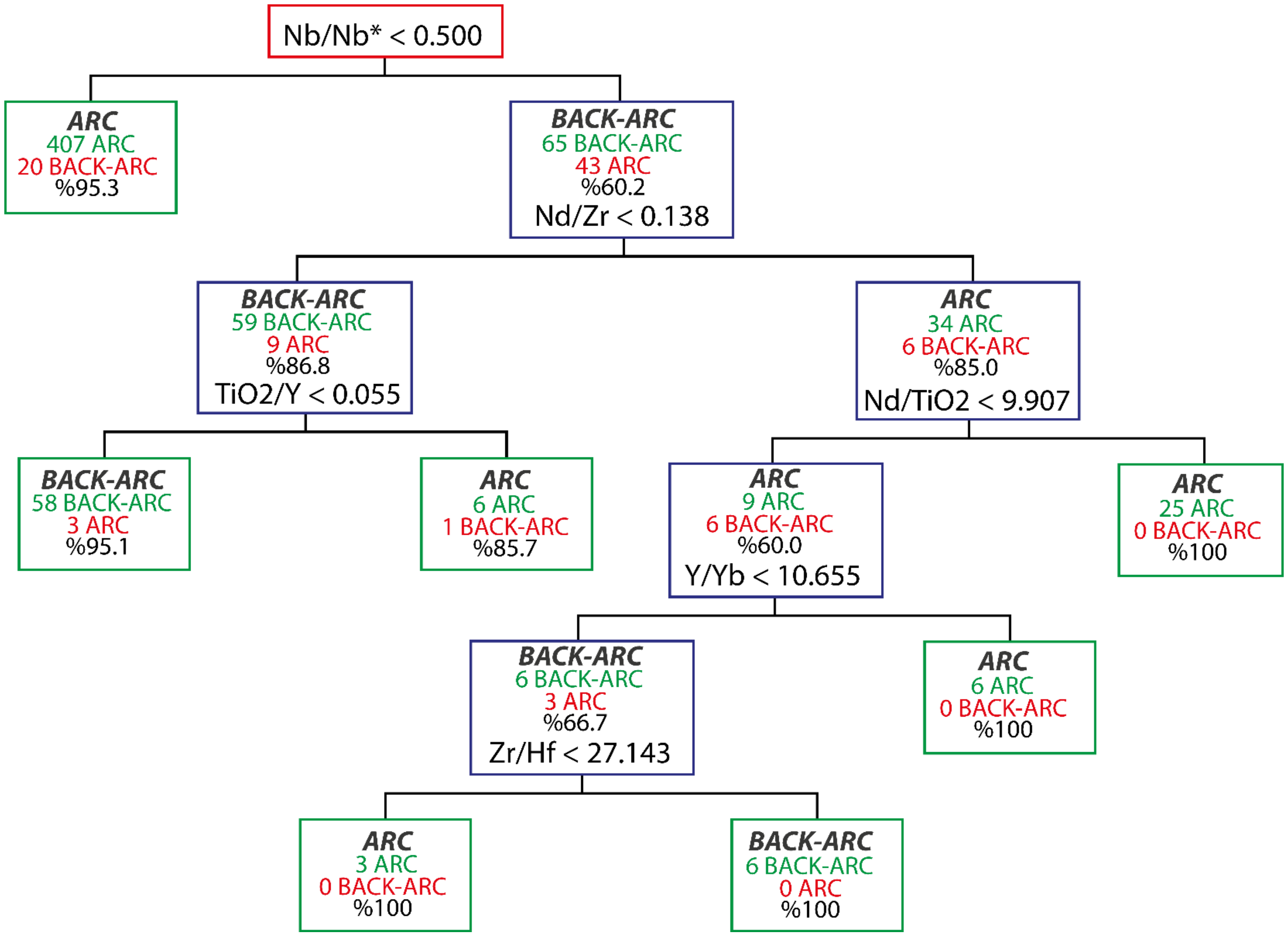

Figure 3.38. Classification results of the first decision tree to discriminate between arc and back-arc-related settings

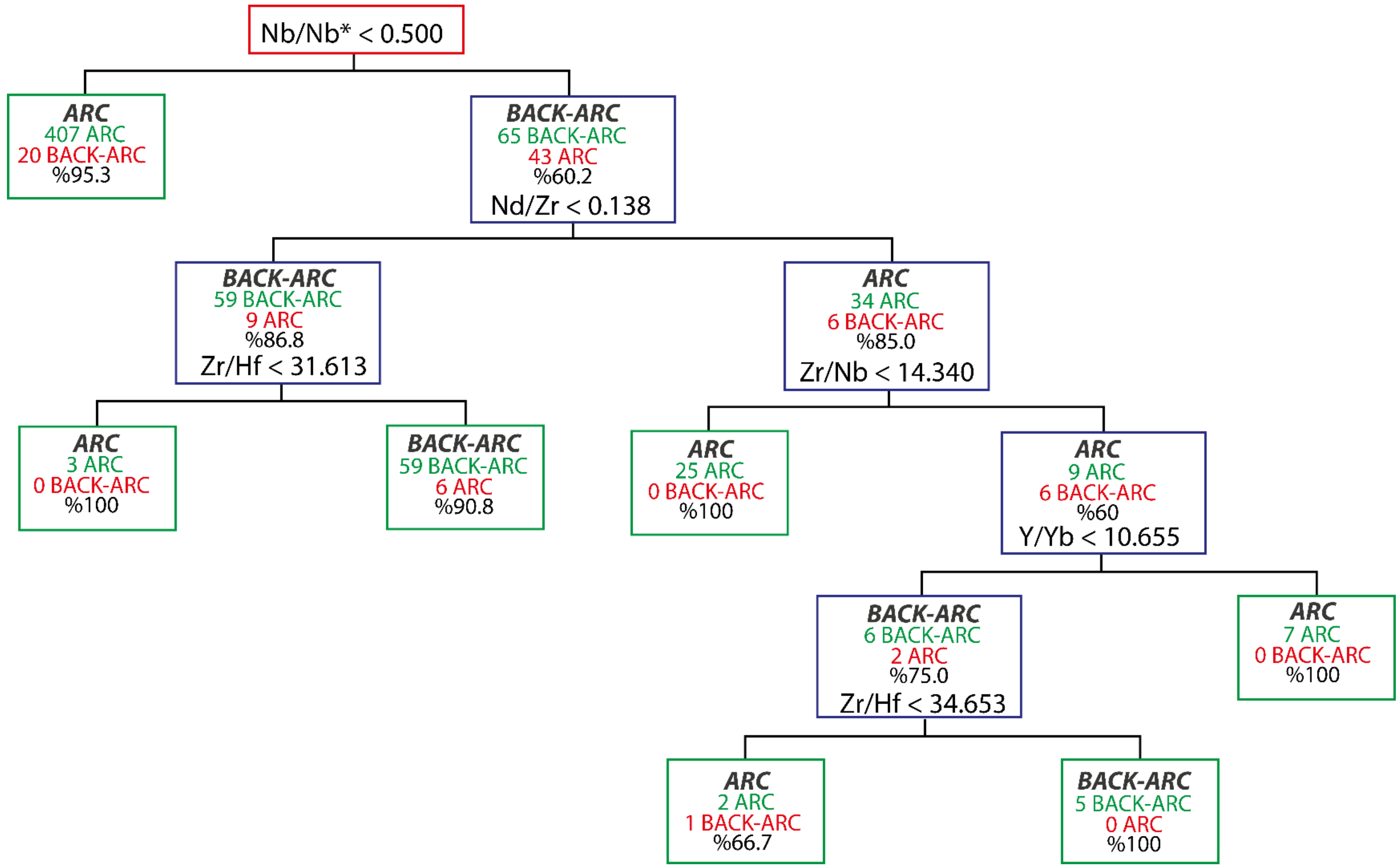

Figure 3.39. Classification results of the second decision tree to discriminate between arc and back-arc-related settings

Table 3.10. Confusion Matrix Summary for Training and Test Datasets for Tectono-Magmatic Discrimination Between Arc and Back-arc-related Settings

Tree	1				2			
Level	2	3	4	5	2	3	4	5
TP	86	84	92	92	86	82	89	88
TN	550	557	553	556	550	554	554	556
FP	12	5	9	6	12	8	8	6
FN	20	22	14	14	20	24	17	18

Table 3.11. Confusion Matrix Summary for External Datasets for Tectono-Magmatic Discrimination Between Arc and Back-arc-related Settings

Tree	1				2			
Level	2	3	4	5	2	3	4	5
TP	68	62	62	62	68	68	58	58
TN	348	348	347	347	348	354	350	351
FP	16	16	17	17	16	10	14	13
FN	34	40	40	40	34	34	44	44

The first decision tree correctly discriminated articles of subduction settings as arc-related and back-arc-related settings except of 8 articles for training and test datasets (Table 3.12). For this 8 articles, no major failures in discrimination is observed. Misclassifications in the first levels are solved through the deeper levels in decision tree.

The first decision tree is relatively more successful at OA and CA with respect to OBAB for the discrimination of arc- and back-arc-related settings in training and test datasets. Only 1 articles from OA has misclassification with a misclassification ratio less than 10%.

Table 3.12. Misclassifications by first decision tree for discrimination between arc and back-arc settings

JOURNAL	CLASS	SAMPLES	LEVEL 2 ERRORS	LEVEL 2 ERROR %	LEVEL 3 ERRORS	LEVEL 3 ERROR %	LEVEL 4 ERRORS	LEVEL 4 ERROR %	LEVEL 5 ERRORS	LEVEL 5 ERROR %
Mullen 2017 Cascade Arc	CA	35	4	11	3	9	3	9	3	9
Bedard 1999 Canada	OA	12	2	17	1	8	3	25	1	8
Jolly 2007 Greater Antilles	OA	37					1	3		
Jolly 2008 Greater Antilles	OA	98					1	1	1	1
Pearce 2005 Mariana	OA	11	1	9	1	9	1	9	1	9
Beier 2015 Manus Basin	OBAB	6	1	17	1	17	1	17	1	17
Pearce 1995 Lau	OBAB	25	6	24	6	24	2	8	2	8
Pearce 2005 Mariana	OBAB	53	13	25	13	25	11	21	11	21

The first decision tree sustains its success for discrimination between arc and back-arc-related settings for external datasets (Table 3.13). External articles from CA can be correctly classified, whereas misclassifications are observed for OA and OBAB. 3 articles (1 from OA and 2 from OBAB) completely fail at discrimination. Other than these 3 articles, 3 more articles also have major failure. However, decrease in the classification ratio in these articles does not affect the overall success ratio as their sample amounts are rather limited to less than 10 samples per article. The general trend of misclassifications in external dataset is similar to that of training and test datasets.

Table 3.13. Misclassifications by first decision tree for discrimination between arc and back-arc settings

JOURNAL	CLASS	SAMPLES	LEVEL 2 ERRORS	LEVEL 2 ERROR %	LEVEL 3 ERRORS	LEVEL 3 ERROR %	LEVEL 4 ERRORS	LEVEL 4 ERROR %	LEVEL 5 ERRORS	LEVEL 5 ERROR %
König 2008 Subduction	OA	6	6	100	6	100	6	100	6	100
König 2010 Subduction	OA	4	2	50	2	50	2	50	2	50
Pearce 1999 W. Pacific	OA	5	1	20	1	20	1	20	1	20
Straub 2010 Izu Bonin	OA	48	2	4	2	4	2	4	2	4
Tamura 2011 Mariana	OA	19	4	21	4	21	5	26	5	26
Woodhead 2001 Mixed	OA	23	1	4	1	4	1	4	1	4
Harrison 2003 East Scotia	OBAB	5	5	100	5	100	5	100	5	100
Ikeda 2016 Mariana	OBAB	15	3	20	3	20	3	20	3	20
Ishizuka 2009 Izu Bonin	OBAB	30	15	50	20	67	20	67	20	67
Mortimer 2007 South Fiji	OBAB	12	5	42	6	50	6	50	6	50
Sinton 2003 Manus	OBAB	6	6	100	6	100	6	100	6	100

The second decision tree is also successful at discrimination between arc and back-arc-related settings (Table 3.14). 8 articles have misclassifications with only 1 major failure. The misclassifications in the first levels are later solved with increasing levels of depth. Only 1 article from CA has misclassification. These two decision trees give similar results for training and test dataset when considered.

Table 3.14. Misclassifications by second decision tree for discrimination between arc and back-arc settings

JOURNAL	CLASS	SAMPLES	LEVEL 2 ERRORS	LEVEL 2 ERROR %	LEVEL 3 ERRORS	LEVEL 3 ERROR %	LEVEL 4 ERRORS	LEVEL 4 ERROR %	LEVEL 5 ERRORS	LEVEL 5 ERROR %
Mullen 2017 Cascade Arc	CA	35	4	11	4	11	5	14	4	11
Bedard 1999 Canada	OA	12	2	17			1	8		
Pearce 2005 Mariana	OA	11	1	9	1	9	1	9	1	9
Peate 1997 Vanuatu	OA	37	1	3	1	3				
Todd 2012 Fiji Tonga	OA	13	4	31	2	15	1	8	1	8
Beier 2015 Manus Basin	OBAB	6	1	17	5	83	5	83	5	83
Pearce 1995 Lau	OBAB	25	6	24	6	24	2	8	2	8
Pearce 2005 Mariana	OBAB	53	13	25	13	25	11	21	11	21

The second decision tree sustains its success for external dataset (Table 3.15). Similar to the first decision tree, all articles from CA in external dataset are correctly discriminated and the general trend for misclassification through the articles and tectonic settings for external dataset is similar to that for training and test dataset.

Two articles of OBAB completely fails at discrimination, however, the amount of samples per articles is limited so their effect on overall ratio of success remain limited.

Table 3.15. Misclassifications by second decision tree for discrimination between arc and back-arc settings

JOURNAL	CLASS	SAMPLES	LEVEL 2 ERRORS	LEVEL 2 ERROR %	LEVEL 3 ERRORS	LEVEL 3 ERROR %	LEVEL 4 ERRORS	LEVEL 4 ERROR %	LEVEL 5 ERRORS	LEVEL 5 ERROR %
Jolly 2008 Greater Antilles B	OA	78					1	1		
König 2008 Subduction	OA	6	6	100	1	17	1	17	1	17
König 2010 Subduction	OA	4	2	50	1	25	1	25	1	25
Pearce 1999 Western Pacific	OA	5	1	20	1	20	1	20	1	20
Straub 2010 Izu Bonin	OA	48	2	4	2	4	2	4	2	4
Tamura 2011 Mariana	OA	19	4	21	4	21	6	32	6	32
Wharton 1994 Viti Levu	OA	6					1	17	1	17
Woodhead 2001 Mixed	OA	23	1	4	1	4	1	4	1	4
Harrison 2003 East Scotia	OBAB	5	5	100	5	100	5	100	5	100
Ikeda 2016 Mariana	OBAB	15	3	20	3	20	4	27	4	27
Ishizuka 2009 Izu Bonin	OBAB	30	15	50	15	50	22	73	22	73
Mortimer 2007 South Fiji	OBAB	12	5	42	5	42	7	58	7	58
Sinton 2003 Manus	OBAB	6	6	100	6	100	6	100	6	100

3.2.2.1.2. Discrimination Within Arc-related Settings

Two multi-branched decision trees (Figure 3.40 and Figure 3.41) are constructed for the discrimination within arc and related settings. Using training set, success ratios for discrimination at each level of depth are determined.

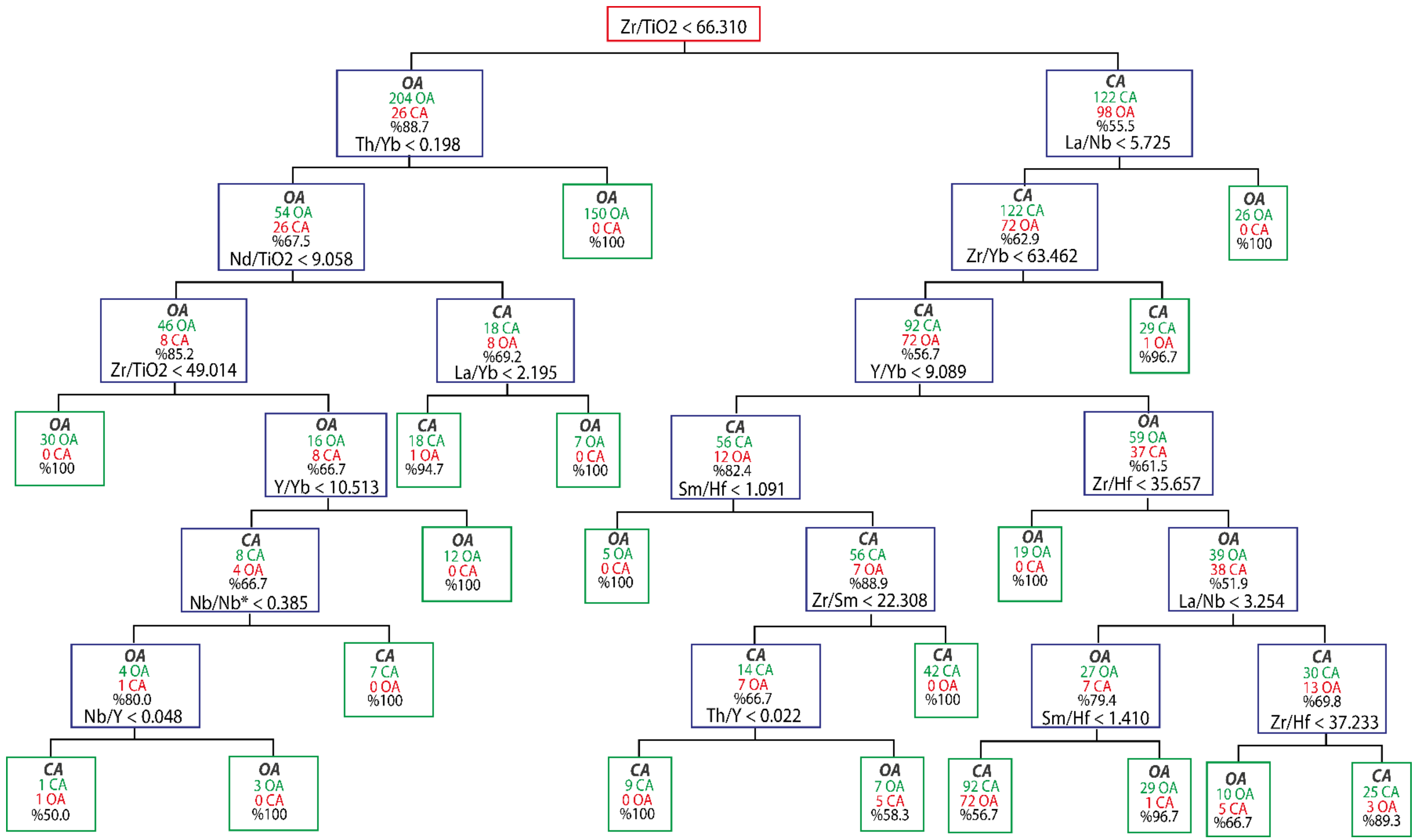

Figure 3.40. Classification results of the first decision tree to discriminate within arc-related settings

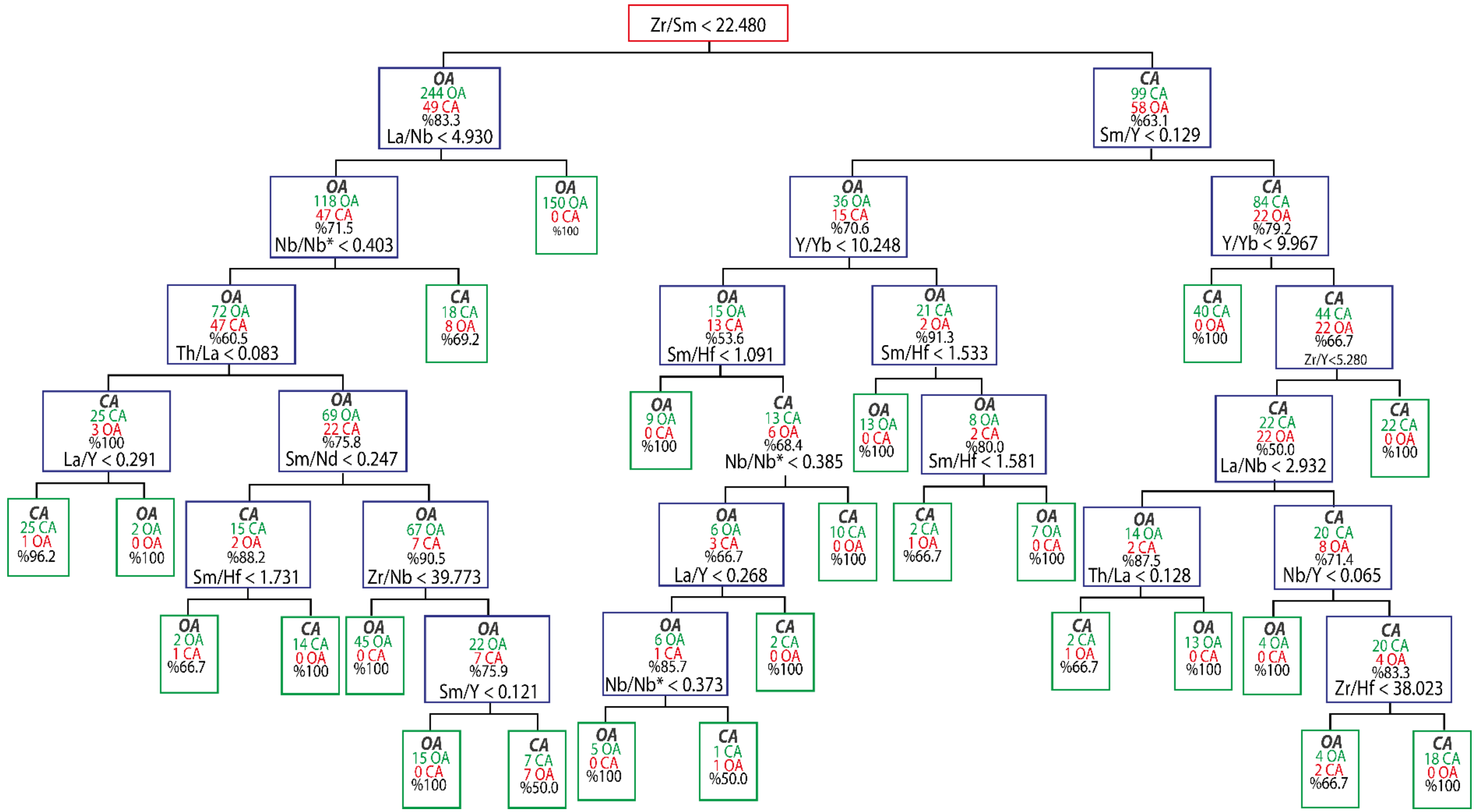

Figure 3.41. Classification results of the second decision tree to discriminate within arc-related settings

For confusion matrix, showing the tectono-magmatic discrimination results for training+test and external datasets; true positive (TP) represents samples of oceanic arcs classified as oceanic arc, true negative (TN) represents samples of continental arcs classified as continental arc, false positive (FP) represents samples of continental arcs classified as oceanic arc and false negative (FN) represents samples oceanic arcs classified as continental arc.

When confusion matrix for training and test datasets are evaluated, the overall success ratio for tectono-magmatic discrimination between oceanic arc and continental arc settings have an increasing trend with increasing levels in depth for both decision trees (Table 3.16).

When their applicability to external datasets are evaluated, both decision trees with their all levels shall be accepted to be applicable for tectono-magmatic discrimination between oceanic arc and continental arc settings with a decrease in their success ratios (Table 3.17).

Table 3.16. Confusion Matrix Summary for Training and Test Datasets for Tectono-Magmatic Discrimination Between Oceanic Arc and Continental Arc Settings

Tree	1						2					
Level	2	3	4	5	6	7	2	3	4	5	6	7
TP	308	298	368	367	362	370	360	360	352	367	372	368
TN	147	168	120	128	162	160	105	105	149	160	166	171
FP	34	13	61	53	19	21	76	76	32	21	15	10
FN	73	83	13	14	19	11	21	21	29	14	9	13

The first decision tree is successful at the discrimination between OA and CA (Table 3.18). The amount of articles with misclassifications are higher when compared to that in previous discriminations. However, amount of misclassifications per articles are small so that only 1 article has major failure at discrimination.

Table 3.17. Confusion Matrix Summary for External Dataset for Tectono-Magmatic Discrimination Between Oceanic Arc and Continental Arc Settings

Tree	1						2					
Level	2	3	4	5	6	7	2	3	4	5	6	7
TP	106	99	175	176	164	157	176	176	139	163	169	178
TN	136	136	83	68	75	72	54	54	73	95	108	107
FP	5	5	58	73	66	69	87	87	68	46	33	34
FN	117	124	48	47	59	66	47	47	84	60	54	45

The first decision tree is also applicable to external datasets yet, the amount of misclassifications per articles slightly increase with more major failures. (Table 3.19). The second decision tree is similar to the first decision tree for discrimination of training and test dataset (Table 3.20) and for external dataset (Table 3.21). The trends of misclassification are similar between first and second decision tree and between training-test dataset and external dataset. There is no unexpected abrupt change in success ratio for a specific tectonic setting or an article.

3.2.2.2. The Second Path for Discrimination Within Subduction Settings

3.2.2.2.1. Discrimination Between Oceanic and Continental Settings

Two multi-branched decision trees (Figure 3.42 and Figure 3.43) are constructed for the discrimination between oceanic and continental settings. Using training set, success ratios for discrimination at each level of depth are determined. For confusion matrix, showing the tectono-magmatic discrimination results for training+test and external datasets; true positive (TP) represents samples of oceanic settings classified as oceanic, true negative (TN) represents samples of continental settings classified as continental, false positive (FP) represents samples of continental settings classified as oceanic and false negative (FN) represents samples of oceanic settings classified as continental.

Table 3.18. Misclassifications by first decision tree for discrimination between oceanic arc and continental-arc settings

JOURNAL	CLASS	SAMPLES	LEVEL 2 ERRORS	LEVEL 2 ERROR %	LEVEL 3 ERRORS	LEVEL 3 ERROR %	LEVEL 4 ERRORS	LEVEL 4 ERROR %	LEVEL 5 ERRORS	LEVEL 5 ERROR %	LEVEL 6 ERRORS	LEVEL 6 ERROR %	LEVEL 7 ERRORS	LEVEL 7 ERROR %
Gertisser 2000 Aeolian	CA	5					1	20	1	20			4	80
Hickey Vargas 2016 Andean	CA	55	1	2	1	2	8	15	8	15	3	5	5	9
Hickey Vargas 2016 Chile	CA	34	1	3	1	3	26	76	26	76	1	3	4	12
Metrich 2001 Aeolian	CA	10					2	20	2	20	2	20	2	20
Mullen 2017 Cascade Arc	CA	35	9	26	9	26	18	51	11	31	11	31	3	9
Portnyagin 2015 Kamchatka	CA	3					3	100	3	100				
Simon 2014 Kamchatka	CA	39	23	59	2	5	3	8	2	5	2	5	3	8
Bedard 1999 Canada	OA	12	5	42	5	42	5	42						
Hickey Vargas 2013 Daito	OA	8	4	50	4	50					2	25	1	13
Jolly 2007 Greater Antilles	OA	37	14	38	14	38	3	8	3	8	4	11	1	3
Jolly 2008 Greater Antilles	OA	98	15	15	20	20	8	8	7	7	8	8	1	1
Pearce 1995 South Sandwich	OA	14							1	7			1	7
Pearce 2005 Mariana	OA	11	2	18	2	18								
Peate 1997 Vanuatu	OA	37	8	22	10	27	1	3	5	14	4	11	2	5
Rojas Agramonte 2017 Lesser Antilles	OA	15	9	60	9	60	3	20	3	20	4	27	4	27
Singer 2007 Auletian	OA	48	18	38	18	38					8	17	4	8
Todd 2012 Fiji Tonga	OA	13	2	15	2	15			2	15	1	8	3	23
Tollstrup 2010 Izu Bonin	OA	51	4	8	7	14	1	2	1	2	3	6	2	4
Yogodzinski 2015 Western Auletian	OA	19	7	37	7	37								

Table 3.19. Misclassifications by first decision tree for discrimination between oceanic arc and continental-arc settings

JOURNAL	CLASS	SAMPLES	LEVEL 2 ERRORS	LEVEL 2 ERROR %	LEVEL 3 ERRORS	LEVEL 3 ERROR %	LEVEL 4 ERRORS	LEVEL 4 ERROR %	LEVEL 5 ERRORS	LEVEL 5 ERROR %	LEVEL 6 ERRORS	LEVEL 6 ERROR %	LEVEL 7 ERRORS	LEVEL 7 ERROR %
Bailey 2009 Santorini	CA	45	1	2	1	2	12	27	27	60	26	58	18	40
Bryant 2006 Andes	CA	3					1	33	1	33	1	33	1	33
Calanchi 2002 Aeolian	CA	8	2	25	2	25	8	100	8	100	8	100	8	100
De Astis 1997 Aeolian	CA	18					2	11	2	11	1	6	3	17
De Astis 2000 Aeolian	CA	23	1	4	1	4	8	35	8	35	4	17	6	26
Ianelli 2017 North Patagonian	CA	9	1	11	1	11	4	44	4	44	4	44	3	33
Santo 2004 Aeolian	CA	31					20	65	20	65	19	61	28	90
Zelenski 2018 Kamchatka	CA	4					3	75	3	75	3	75	2	50
Finney 2008 Okmok	OA	3												
Jolly 2008 Greater Antilles Arc	OA	78	43	55	50	64	13	17	14	18	23	29	13	17
König 2008 Subduction Zones	OA	6							1	17	1	17	1	17
König 2010 Subduction Zones	OA	4							1	25	1	25	1	25
Leslie 2009 Fiji Arc	OA	11	6	55	6	55					2	18		
Pearce 1999 Western Pacific	OA	5	4	80	4	80	3	60	1	20	1	20	2	40
Stellin 2002 Shishaldin	OA	4	1	25	1	25								
Straub 2010 Izu Bonin	OA	48	33	69	33	69	27	56	24	50	22	46	28	58
Tamura 2011 Mariana	OA	19	9	47	9	47					3	16	3	16
Wharton 1994 Viti Levu	OA	6	1	17	1	17	1	17						
Woodhead 2001 Mixed	OA	23	5	22	5	22	2	9	4	17	3	13	3	13

Table 3.20. Misclassifications by second decision tree for discrimination between oceanic arc and continental-arc settings

JOURNAL	CLASS	SAMPLES	LEVEL 2 ERRORS	LEVEL 2 ERROR %	LEVEL 3 ERRORS	LEVEL 3 ERROR %	LEVEL 4 ERRORS	LEVEL 4 ERROR %	LEVEL 5 ERRORS	LEVEL 5 ERROR %	LEVEL 6 ERRORS	LEVEL 6 ERROR %	LEVEL 7 ERRORS	LEVEL 7 ERROR %
Gertisser 2000 Aeolian	CA	5	5	100	5	100	5	100	2	40	2	40	2	40
Hickey Vargas 2016 Andean	CA	55	3	5	3	5	2	4	3	5	3	5	3	5
Hickey Vargas 2016 Chile	CA	34	5	15	5	15	5	15			1	3	3	9
Metrich 2001 Aeolian	CA	10	10	100	10	100	10	100						
Mullen 2017 Cascade Arc	CA	35	19	54	19	54	4	11	10	29	3	9	2	6
Simon 2014 Kamchatka	CA	39	34	87	34	87	6	15	6	15	6	15		
Bedard 1999 Canada	OA	12					1	8	1	8	1	8	1	8
Hickey Vargas 2013 Daito	OA	8	3	38	3	38	3	38	3	38			2	25
Hochstaedter 2001 Izu Bonin	OA	2					1	50						
Jolly 2007 Greater Antilles	OA	37	5	14	5	14	6	16	3	8	3	8	3	8
Jolly 2008 Greater Antilles	OA	98	2	2	2	2	6	6	3	3	3	3	3	3
Pearce 1995 South Sandwich	OA	14					4	29						
Pearce 2005 Mariana	OA	11											1	9
Peate 1997 Vanuatu	OA	37	5	14	5	14	5	14	2	5	2	5		
Rojas Agramonte 2017 Lesser Antilles	OA	15	3	20	3	20	3	20	1	7	1	7	1	7
Singer 2007 Auletian	OA	48	10	21	10	21	12	25	5	10	4	8	3	6
Todd 2012 Fiji Tonga	OA	13	1	8	1	8	3	23	3	23	2	15	3	23
Tollstrup 2010 Izu Bonin	OA	51					1	2	1	2	1	2	2	4
Yogodzinski 2015 W Auletian	OA	19											2	11

Table 3.21. Misclassifications by second decision tree for discrimination between oceanic arc and continental-arc settings

JOURNAL	CLASS	SAMPLES	LEVEL 2 ERRORS	LEVEL 2 ERROR %	LEVEL 3 ERRORS	LEVEL 3 ERROR %	LEVEL 4 ERRORS	LEVEL 4 ERROR %	LEVEL 5 ERRORS	LEVEL 5 ERROR %	LEVEL 6 ERRORS	LEVEL 6 ERROR %	LEVEL 7 ERRORS	LEVEL 7 ERROR %
Bailey 2009 Santorini	CA	45	27	60	27	60	8	18	28	62	10	22	10	22
Bryant 2006 Andes	CA	3	1	33	1	33	1	33						
Calanchi 2002 Aeolian	CA	8	8	100	8	100	8	100	1	13	2	25	2	25
De Astis 1997 Aeolian	CA	18	10	56	10	56	10	56	3	17	3	17	3	17
De Astis 2000 Aeolian	CA	23	14	61	14	61	14	61	4	17	5	22	5	22
Ianelli 2017 N Patagonian	CA	9							2	22	2	22	2	22
Santo 2004 Aeolian	CA	31	27	87	27	87	27	87	8	26	11	35	12	39
Jolly 2008 Antilles Arc B	OA	78	18	23	18	23	22	28	27	35	18	23	10	13
König 2008 Subduction	OA	6					2	33	2	33	2	33	2	33
König 2010 Subduction	OA	4					3	75	3	75	3	75	3	75
Leslie 2009 Fiji Arc	OA	11					1	9	1	9	1	9	1	9
Pearce 1999 W Pacific	OA	5					1	20	1	20	1	20	1	20
Straub 2010 Izu Bonin	OA	48	9	19	9	19	30	63	12	25	14	29	14	29
Tamura 2011 Mariana	OA	19	4	21	4	21	4	21	4	21	4	21	3	16
Wharton 1994 Viti Levu	OA	6					1	17	1	17	1	17	1	17
Woodhead 2001 Mixed	OA	23					4	17	1	4	2	9	3	13

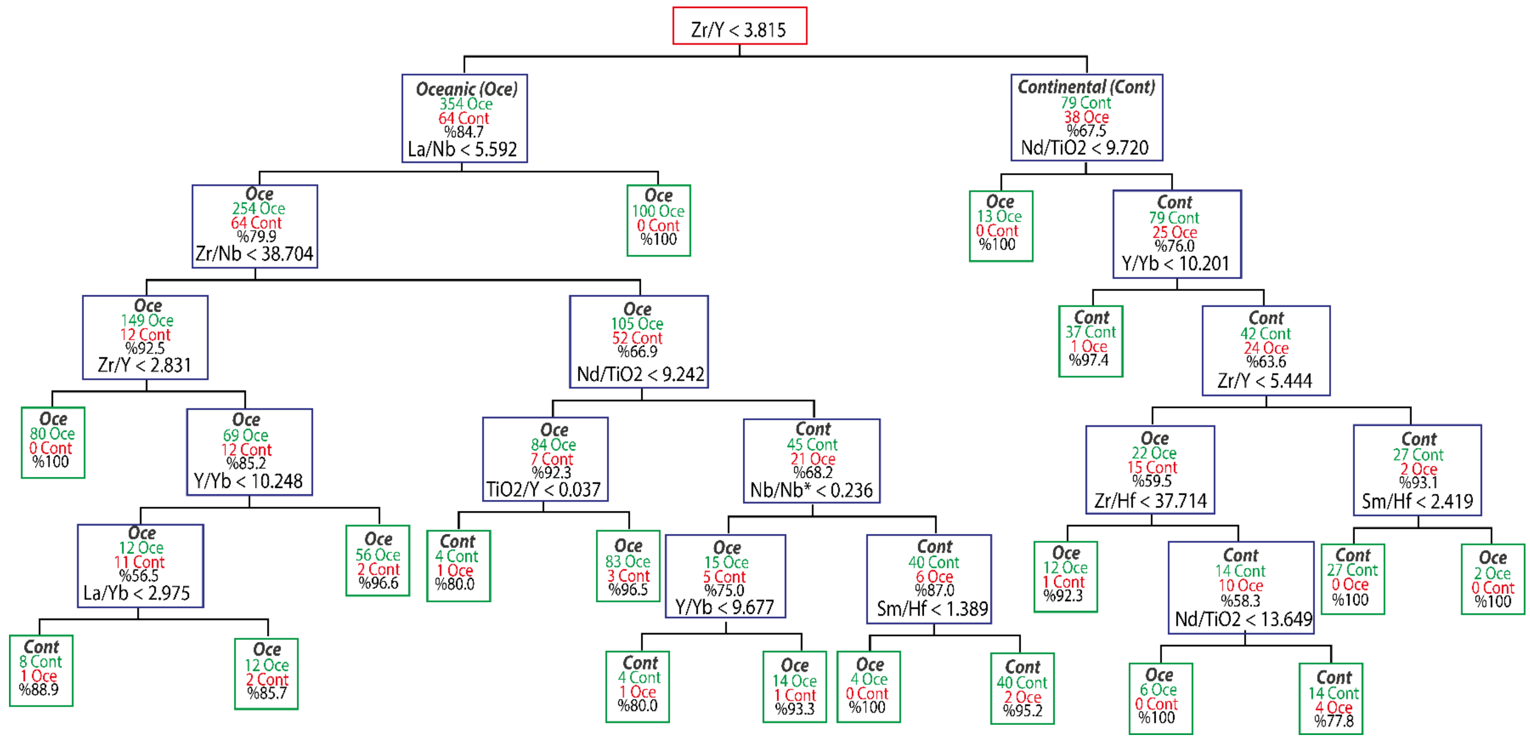

Figure 3.42. Classification results of the first decision tree to discriminate between oceanic and continental settings

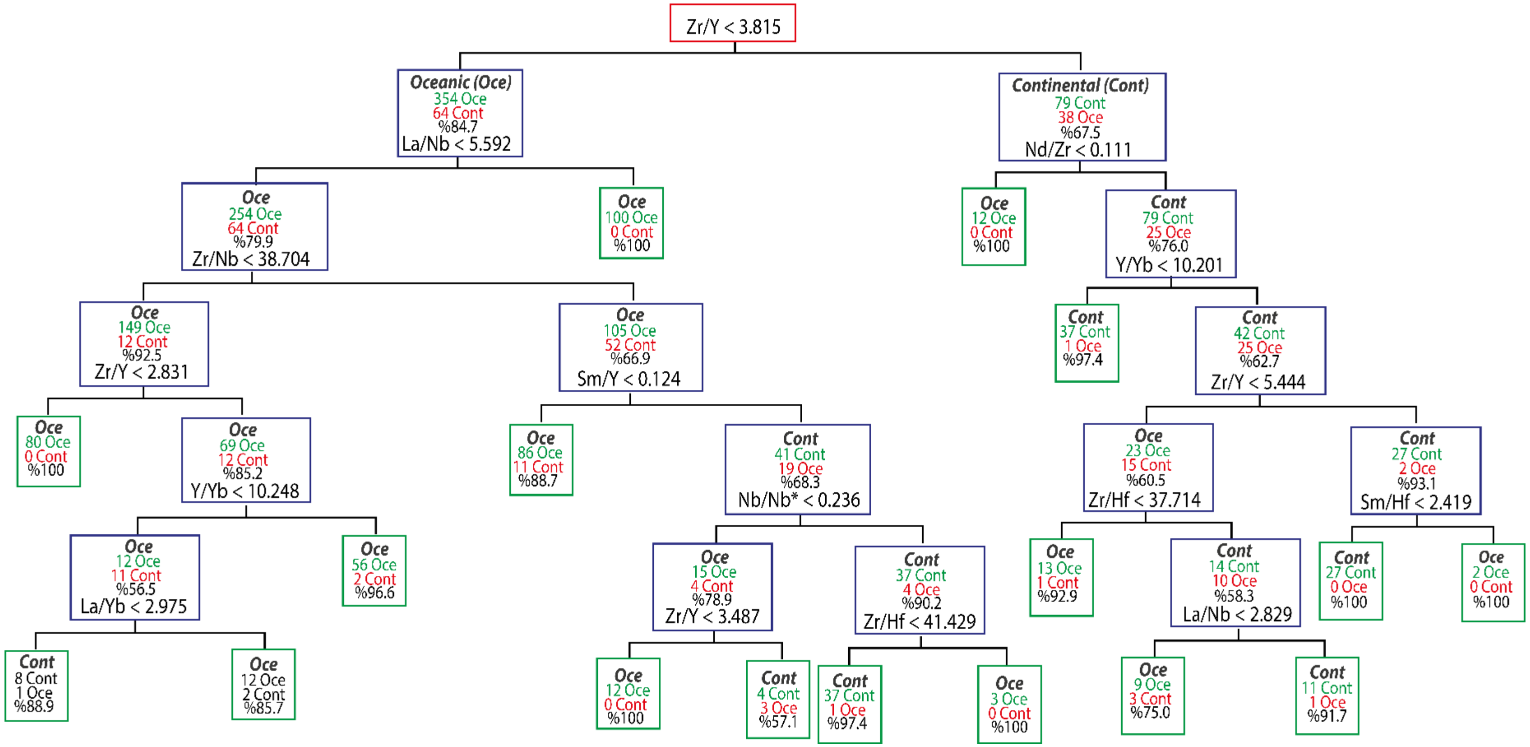

Figure 3.43. Classification results of the second decision tree to discriminate between oceanic and continental settings

When confusion matrix for training and test datasets are evaluated, the overall success ratio for tectono-magmatic discrimination between oceanic and continental settings have an increasing trend with increasing levels in depth for both decision trees (**Error! Not a valid bookmark self-reference.**). When their applicability to external datasets is evaluated, the first decision tree seems to fail as a result of overfitting for both tectonic settings, oceanic and continental, whereas the second decision tree seems to fail as a result of overfitting only for discrimination of continental settings (Table 3.23).

Table 3.22. Confusion Matrix Summary for Training and Test Datasets for Tectono-Magmatic Discrimination Between Oceanic and Continental Settings

Tree	1					2				
Level	2	3	4	5	6	2	3	4	5	6
TP	452	452	455	459	467	451	451	454	460	467
TN	101	101	133	151	163	100	100	131	145	151
FP	80	80	48	30	18	81	81	50	36	30
FN	35	35	32	28	20	36	36	33	27	20

Table 3.23. Confusion Matrix Summary for External Dataset for Tectono-Magmatic Discrimination Between Oceanic and Continental Related Settings

Tree	1					2				
Level	2	3	4	5	6	2	3	4	5	6
TP	274	274	271	268	264	284	284	294	292	302
TN	113	113	84	97	100	100	100	72	84	75
FP	28	28	57	44	41	41	41	69	57	66
FN	51	51	54	57	61	41	41	29	33	23

Two decision trees have similar results on discrimination of samples from articles of subduction-related settings for both training and external datasets. First decision tree is successful for the discrimination of training dataset (Table 3.24) with only 1 major failure and sustains its success for external dataset (Table 3.25).

Table 3.24. Misclassifications by first decision tree for discrimination between oceanic and continental settings

JOURNAL	CLASS	SAMPLES	LEVEL 2 ERRORS	LEVEL 2 ERROR %	LEVEL 3 ERRORS	LEVEL 3 ERROR %	LEVEL 4 ERRORS	LEVEL 4 ERROR %	LEVEL 5 ERRORS	LEVEL 5 ERROR %	LEVEL 6 ERRORS	LEVEL 6 ERROR %
Gertisser 2000 Aeolian	CA	5	5	100	5	100	5	100	5	100	5	100
Hickey Vargas 2016 Andean	CA	55	6	11	6	11	2	4	6	11	2	4
Hickey Vargas 2016 Chile	CA	34	14	41	14	41	14	41	3	9	3	9
Metrich 2001 Aeolian	CA	10					2	20				
Mullen 2017 Cascade Arc	CA	35	19	54	19	54	18	51	11	31	5	14
Portnyagin 2015 Kamchatka	CA	3					2	67				
Simon 2014 Kamchatka	CA	39	36	92	36	92	5	13	5	13	3	8
Bedard 1999 Canada	OA	12									2	17
Hickey Vargas 2013 Daito	OA	8	2	25	2	25	4	50	2	25	2	25
Jolly 2007 Greater Antilles Arc	OA	37	6	16	6	16	3	8	3	8	3	8
Jolly 2008 Greater Antilles Arc A	OA	98	2	2	2	2	7	7	4	4	3	3
Pearce 2005 Mariana	OA	11					2	18				
Peate 1997 Vanuatu	OA	37	7	19	7	19	2	5	3	8	2	5
Rojas Agramonte 2017 Lesser Antilles	OA	15	5	33	5	33	3	20	3	20	2	13
Singer 2007 Auletian	OA	48	9	19	9	19	4	8	7	15	2	4
Tollstrup 2010 Izu Bonin	OA	51					2	4	1	2	2	4
Yogodzinski 2015 W Auletian	OA	19	2	11	2	11	3	16				
Pearce 1995 Lau	OBAB	25					1	4	1	4		
Pearce 2005 Mariana	OBAB	53	1	2	1	2	1	2	3	6	1	2

The trend of misclassifications through the articles of training (Table 3.26) and external (Table 3.27) datasets are similar in the second decision tree.

Table 3.25. Misclassifications by first decision tree for discrimination between oceanic and continental settings

JOURNAL	CLASS	SAMPLES	LEVEL 2 ERRORS	LEVEL 2 ERROR	LEVEL 3 ERRORS	LEVEL 3 ERROR	LEVEL 4 ERRORS	LEVEL 4 ERROR	LEVEL 5 ERRORS	LEVEL 5 ERROR	LEVEL 6 ERRORS	LEVEL 6 ERROR
Bailey 2009 Santorini	CA	45	14	31	14	31	18	40	14	31	11	24
Bryant 2006 Andes	CA	3							1	33	1	33
Calanchi 2002 Aeolian	CA	8	5	63	5	63	8	100	8	100	8	100
De Astis 1997 Aeolian	CA	18	1	6	1	6	4	22	5	28	5	28
De Astis 2000 Aeolian	CA	23	1	4	1	4	5	22	6	26	6	26
Ianelli 2017 N Patagonian Andes	CA	9					2	22	1	11	1	11
Santo 2004 Aeolian	CA	31	7	23	7	23	20	65	9	29	9	29
Jolly 2008 Greater Antilles Arc B	OA	78	11	14	11	14	19	24	9	12	13	17
König 2008 Subduction Zones	OA	6							1	17	1	17
König 2010 Subduction Zones	OA	4							1	25	1	25
Leslie 2009 Fiji Arc	OA	11	3	27	3	27			1	9	1	9
Pearce 1999 Western Pacific	OA	5	3	60	3	60	3	60	3	60	4	80
Straub 2010 Izu Bonin	OA	48	11	23	11	23	27	56	18	38	25	52
Wharton 1994 Viti Levu	OA	6	1	17	1	17	2	33	1	17	2	33
Woodhead 2001 Mixed	OA	23	1	4	1	4	3	13	1	4	2	9
Bezos 2009 Lau Basin	OBAB	34							2	6	2	6
Harrison 2003 East Scotia	OBAB	5	4	80	4	80			4	80		
Ikeda 2016 Mariana	OBAB	15	1	7	1	7			1	7	1	7
Ishizuka 2009 Izu Bonin	OBAB	30	11	37	11	37	6	20	14	47	10	33
Mortimer 2007 South Fiji	OBAB	12	5	42	5	42	2	17	4	33	2	17
Sinton 2003 Manus	OBAB	6							1	17	1	17

Table 3.26. Misclassifications by second decision tree for discrimination between oceanic and continental settings

JOURNAL	CLASS	SAMPLES	LEVEL 2 ERRORS	LEVEL 2 ERROR %	LEVEL 3 ERRORS	LEVEL 3 ERROR %	LEVEL 4 ERRORS	LEVEL 4 ERROR %	LEVEL 5 ERRORS	LEVEL 5 ERROR %	LEVEL 6 ERRORS	LEVEL 6 ERROR %
Gertisser 2000 Aeolian	CA	5	5	100	5	100	5	100	5	100	5	100
Hickey Vargas 2016 Andean	CA	55	6	11	6	11	2	4	6	11	1	2
Hickey Vargas 2016 Chile	CA	34	14	41	14	41	13	38	2	6	3	9
Metrich 2001 Aeolian	CA	10					2	20			2	20
Mullen 2017 Cascade Arc	CA	35	20	57	20	57	23	66	20	57	18	51
Portnyagin 2015 Kamchatka	CA	3					2	67				
Simon 2014 Kamchatka	CA	39	36	92	36	92	3	8	3	8	1	3
Bedard 1999 Canada	OA	12									2	17
Hickey Vargas 2013 Daito	OA	8	3	38	3	38	4	50	2	25	1	13
Jolly 2007 Greater Antilles Arc	OA	37	6	16	6	16	3	8	3	8	2	5
Jolly 2008 Greater Antilles Arc A	OA	98	2	2	2	2	6	6	1	1	2	2
Pearce 2005 Mariana	OA	11					1	9				
Peate 1997 Vanuatu	OA	37	7	19	7	19	3	8	3	8	2	5
Rojas 2017 Lesser Antilles	OA	15	5	33	5	33	3	20	3	20	2	13
Singer 2007 Auletian	OA	48	9	19	9	19	4	8	8	17	5	10
Todd 2012 Fiji Tonga	OA	13					1	8	1	8		
Tollstrup 2010 Izu Bonin	OA	51					5	10	4	8	1	2
Yogodzinski 2015 West Auletian	OA	19	2	11	2	11	3	16			2	11
Pearce 2005 Mariana	OBAB	53	1	2	1	2			1	2		

Table 3.27. Misclassifications by second decision tree for discrimination between oceanic and continental settings

JOURNAL	CLASS	SAMPLES	LEVEL 2 ERRORS	LEVEL 2 ERROR %	LEVEL 3 ERRORS	LEVEL 3 ERROR %	LEVEL 4 ERRORS	LEVEL 4 ERROR %	LEVEL 5 ERRORS	LEVEL 5 ERROR %	LEVEL 6 ERRORS	LEVEL 6 ERROR %
Bailey 2009 Santorini	CA	45	25	56	25	56	28	62	25	56	24	53
Bryant 2006 Andes	CA	3							1	33	1	33
Calanchi 2002 Aeolian	CA	8	5	63	5	63	8	100	8	100	8	100
De Astis 1997 Aeolian	CA	18	1	6	1	6	4	22	5	28	5	28
De Astis 2000 Aeolian	CA	23	1	4	1	4	5	22	6	26	7	30
Ianelli 2017 Patagonian Andes	CA	9	1	11	1	11	3	33	2	22	2	22
Santo 2004 Aeolian	CA	31	7	23	7	23	20	65	9	29	18	58
Zelenski 2018 Kamchatka	CA	4	1	25	1	25	1	25	1	25	1	25
Finney 2008 Okmok	OA	3										
Jolly 2008 Greater Antilles Arc B	OA	78	11	14	11	14	20	26	10	13	12	15
Leslie 2009 Fiji Arc	OA	11	3	27	3	27			1	9	1	9
Pearce 1999 Western Pacific	OA	5									1	20
Straub 2010 Izu Bonin	OA	48	3	6	3	6	5	10	4	8	5	10
Wharton 1994 Viti Levu	OA	6	1	17	1	17	2	33	1	17	1	17
Woodhead 2001 Mixed	OA	23	1	4	1	4	3	13				
Harrison 2003 East Scotia	OBAB	5	5	100	5	100			5	100		
Ikeda 2016 Mariana	OBAB	15									1	7
Ishizuka 2009 Izu Bonin	OBAB	30	12	40	12	40	5	17	12	40	6	20
Mortimer 2007 South Fiji	OBAB	12	5	42	5	42	2	17	4	33	2	17

3.2.2.2.2. Discrimination Within Oceanic Settings

Two multi-branched decision trees (Figure 3.44 and Figure 3.45) are constructed for the discrimination within oceanic settings. Using training set, success ratios for discrimination at each level of depth are determined.

For confusion matrix, showing the tectono-magmatic discrimination results for training+test and external datasets; true positive (TP) represents samples of oceanic back-arcs classified as oceanic back-arcs, true negative (TN) represents samples of oceanic arcs classified as oceanic arcs, false positive (FP) represents samples of oceanic arcs classified as oceanic back-arcs and false negative (FN) represents samples of oceanic back-arcs classified as oceanic arcs. When confusion matrix for training and test datasets are evaluated (Table 3.28), the overall success ratio for tectono-magmatic discrimination between oceanic arc and oceanic back-arc settings have an increasing trend with increasing levels in depth for classification of oceanic back-arcs but decreasing trend for classification of oceanic arcs at both decision trees. When their applicability to external datasets are evaluated, both decision trees with their all levels shall be accepted to be applicable for tectono-magmatic discrimination between oceanic arc and oceanic back-arc settings without a significant decrease in their success ratios (Table 3.29).

The first decision tree successfully discriminates OA and OBAB from each other for both training (Table 3.30) and external (Table 3.31) dataset with only 6 articles for training and 10 articles for external dataset with misclassifications. Each dataset has only 1 article with major failure. Misclassifications through articles have similar trends. The second decision tree is also very similar to the first one for both training (Table 3.32) and external (Table 3.33) datasets.

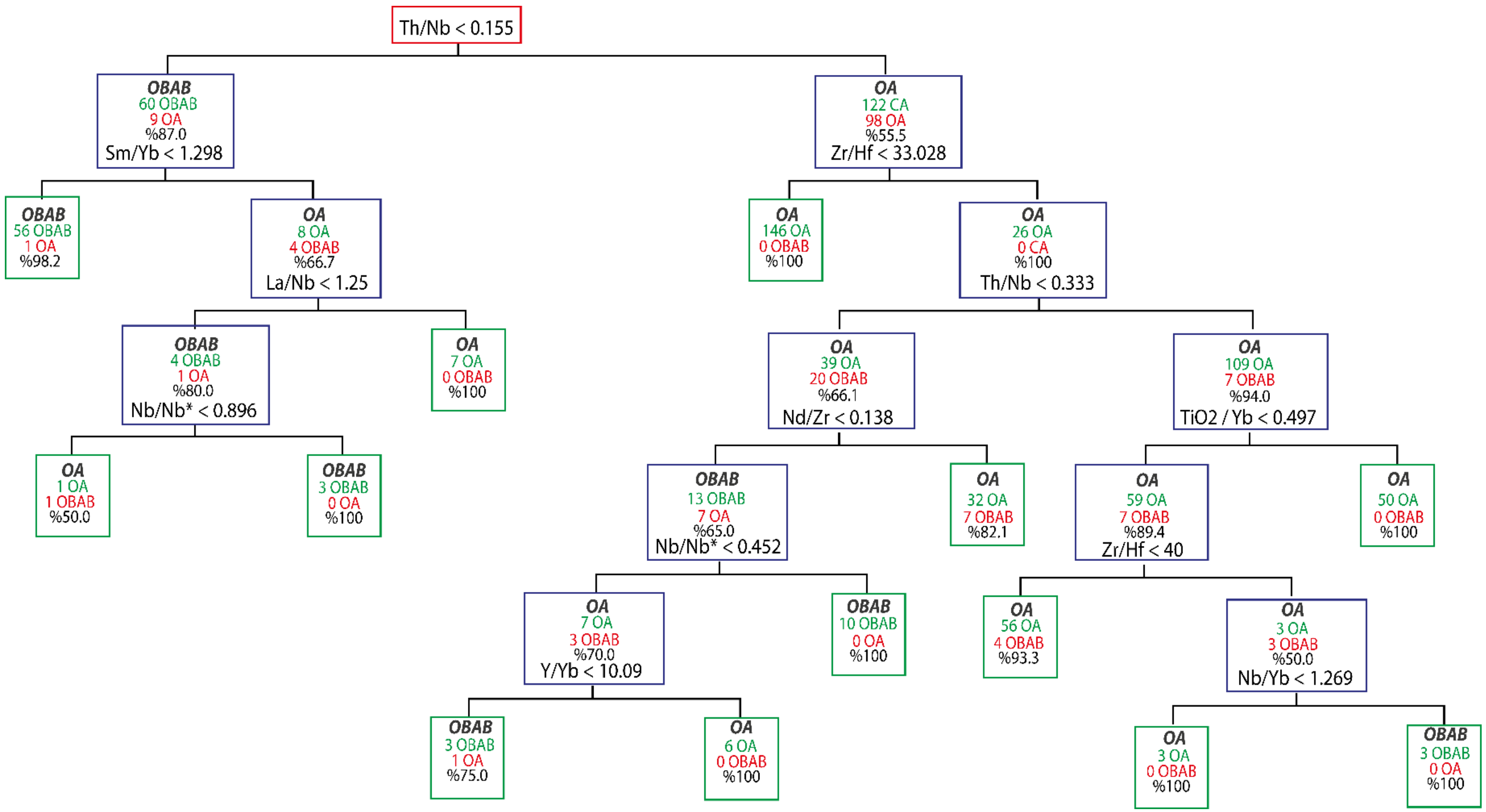

Figure 3.44. Classification results of the first decision tree to discriminate within oceanic settings

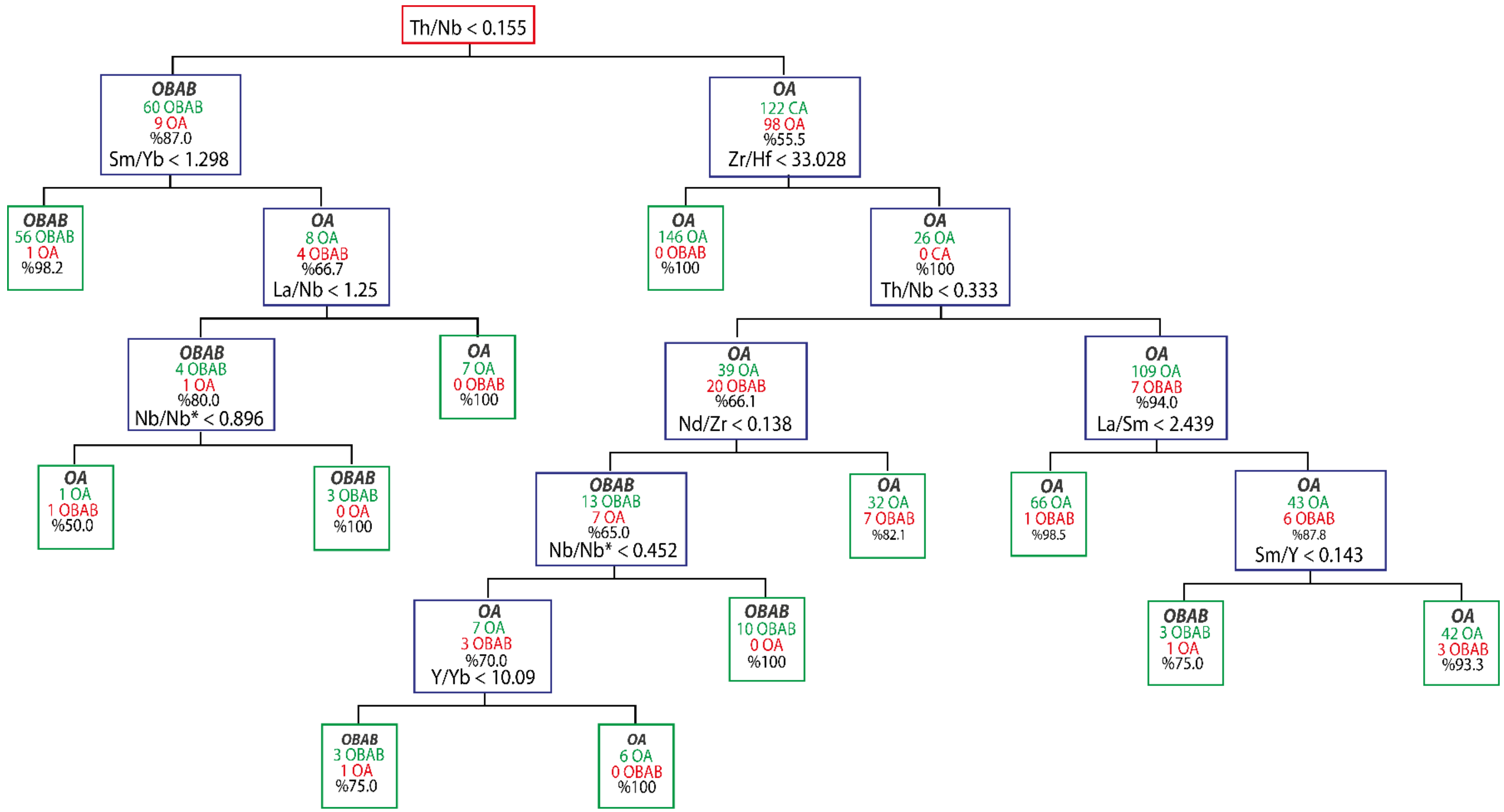

Figure 3.45. Classification results of the second decision tree to discriminate within oceanic settings

Table 3.28. Confusion Matrix Summary for Training and Test Datasets for Tectono-Magmatic Discrimination Between Oceanic Arc and Oceanic Back-Arc Settings

Tree	1					2				
Level	2	3	4	5	6	2	3	4	5	6
TP	77	83	97	94	98	77	83	97	98	99
TN	378	377	366	376	374	378	377	366	371	369
FP	3	4	15	5	7	3	4	15	10	12
FN	29	23	9	12	8	29	23	9	8	7

Table 3.29. Confusion Matrix Summary for External Dataset for Tectono-Magmatic Discrimination Between Oceanic Arc and Oceanic Back-Arc Settings

Tree	1					2				
Level	2	3	4	5	6	2	3	4	5	6
TP	54	77	80	80	81	54	77	80	81	81
TN	219	219	211	213	208	219	219	211	197	195
FP	4	4	12	10	15	4	4	12	26	28
FN	48	25	22	22	21	48	25	12	21	21

Table 3.30. Misclassifications by first decision tree for discrimination between oceanic arc and oceanic back-arc settings

JOURNAL	CLASS	SAMPLES	LEVEL 2 ERRORS	LEVEL 2 ERROR %	LEVEL 3 ERRORS	LEVEL 3 ERROR %	LEVEL 4 ERRORS	LEVEL 4 ERROR %	LEVEL 5 ERRORS	LEVEL 5 ERROR %	LEVEL 6 ERRORS	LEVEL 6 ERROR %
Bedard 1999 Canada	OA	12	2	17	2	17	2	17	2	17	2	17
Hochstaedter 2001 Izu Bonin	OA	2					1	50			1	50
Peate 1997 Vanuatu	OA	37					1	3	1	3	1	3
Todd 2012 Fiji Tonga	OA	13	1	8	1	8	7	54	2	15	3	23
Beier 2015 Manus	OBAB	6	1	17	1	17	1	17	1	17	1	17
Pearce 2005 Mariana	OBAB	53	21	40	20	38	12	23	14	26	11	21

Table 3.31. Misclassifications by first decision tree for discrimination between oceanic arc and oceanic back-arc settings

JOURNAL	CLASS	SAMPLES	LEVEL 2 ERRORS	LEVEL 2 ERROR %	LEVEL 3 ERRORS	LEVEL 3 ERROR %	LEVEL 4 ERRORS	LEVEL 4 ERROR %	LEVEL 5 ERRORS	LEVEL 5 ERROR %	LEVEL 6 ERRORS	LEVEL 6 ERROR %
König 2008 Subduction	OA	6	1	17	1	17	1	17	1	17	1	17
Pearce 1999 W. Pacific	OA	5					1	20	1	20	2	40
Straub 2010 Izu Bonin	OA	48	2	4	2	4	3	6	2	4	5	10
Tamura 2011 Mariana	OA	19					4	21	4	21	4	21
Wharton 1994 Viti Levu	OA	6					2	33	1	17	2	33
Woodhead 2001 Mixed	OA	23	1	4	1	4	1	4	1	4	1	4
Ikeda 2016 Mariana	OBAB	15	5	33	5	33	5	33	5	33	5	33
Ishizuka 2009 Izu Bonin	OBAB	30	24	80	9	30	7	23	7	23	6	20
Mortimer 2007 South Fiji	OBAB	12	8	67	5	42	4	33	4	33	4	33
Sinton 2003 Manus	OBAB	6	6	100	6	100	6	100	6	100	6	100

Table 3.32. Misclassifications by second decision tree for discrimination between oceanic arc and oceanic back-arc settings

JOURNAL	CLASS	SAMPLES	LEVEL 2 ERRORS	LEVEL 2 ERROR %	LEVEL 3 ERRORS	LEVEL 3 ERROR %	LEVEL 4 ERRORS	LEVEL 4 ERROR %	LEVEL 5 ERRORS	LEVEL 5 ERROR %	LEVEL 6 ERRORS	LEVEL 6 ERROR %
Bedard 1999 Canada	OA	12	2	17	2	17	2	17	3	25	3	25
Hochstaedter 2001 Izu Bonin	OA	2					1	50			1	50
Jolly 2007 Greater Antilles Arc	OA	37					1	3	3	8	3	8
Jolly 2008 Greater Antilles Arc A	OA	98			1	1	1	1	1	1	1	1
Peate 1997 Vanuatu	OA	37					1	3	1	3	1	3
Todd 2012 Fiji Tonga	OA	13	1	8	1	8	7	54	2	15	3	23
Beier 2015 Manus Basin	OBAB	6	1	17	1	17	1	17	1	17	1	17
Pearce 2005 Mariana	OBAB	53	21	40	20	38	12	23	11	21	9	17

Table 3.33. Misclassifications by second decision tree for discrimination between oceanic arc and oceanic back-arc settings

JOURNAL	CLASS	SAMPLES	LEVEL 2 ERRORS	LEVEL 2 ERROR %	LEVEL 3 ERRORS	LEVEL 3 ERROR %	LEVEL 4 ERRORS	LEVEL 4 ERROR %	LEVEL 5 ERRORS	LEVEL 5 ERROR %	LEVEL 6 ERRORS	LEVEL 6 ERROR %
König 2008 Subduction	OA	6	1	17	1	17	1	17	1	17	1	17
Pearce 1999 Western Pacific	OA	5					1	20	2	40	2	40
Straub 2010 Izu Bonin	OA	48	2	4	2	4	3	6	5	10	6	13
Tamura 2011 Mariana	OA	19					4	21	12	63	12	63
Wharton 1994 Viti Levu	OA	6					2	33	1	17	2	33
Woodhead 2001 Mixed	OA	23	1	4	1	4	1	4	1	4	1	4
Ikeda 2016 Mariana	OBAB	15	5	33	5	33	5	33	5	33	5	33
Ishizuka 2009 Izu Bonin	OBAB	30	24	80	9	30	7	23	6	20	6	20
Mortimer 2007 South Fiji	OBAB	12	8	67	5	42	4	33	4	33	4	33
Sinton 2003 Manus	OBAB	6	6	100	6	100	6	100	6	100	6	100

3.2.3. Discrimination Within Non-Subduction Settings

3.2.3.1. Discrimination Between Group 1 (Mid-Oceanic Ridge and Oceanic Plateau) and Group 2 (Oceanic Island and Continental Within-plate) Settings

Two multi-branched decision trees (Figure 3.46 and Figure 3.47) are constructed for the discrimination between group 1 (mid-oceanic ridge and oceanic plateau) and group 2 (oceanic island and continental within-plate) of non-subduction settings. Using training set, success ratios for discrimination at each level of depth are determined.

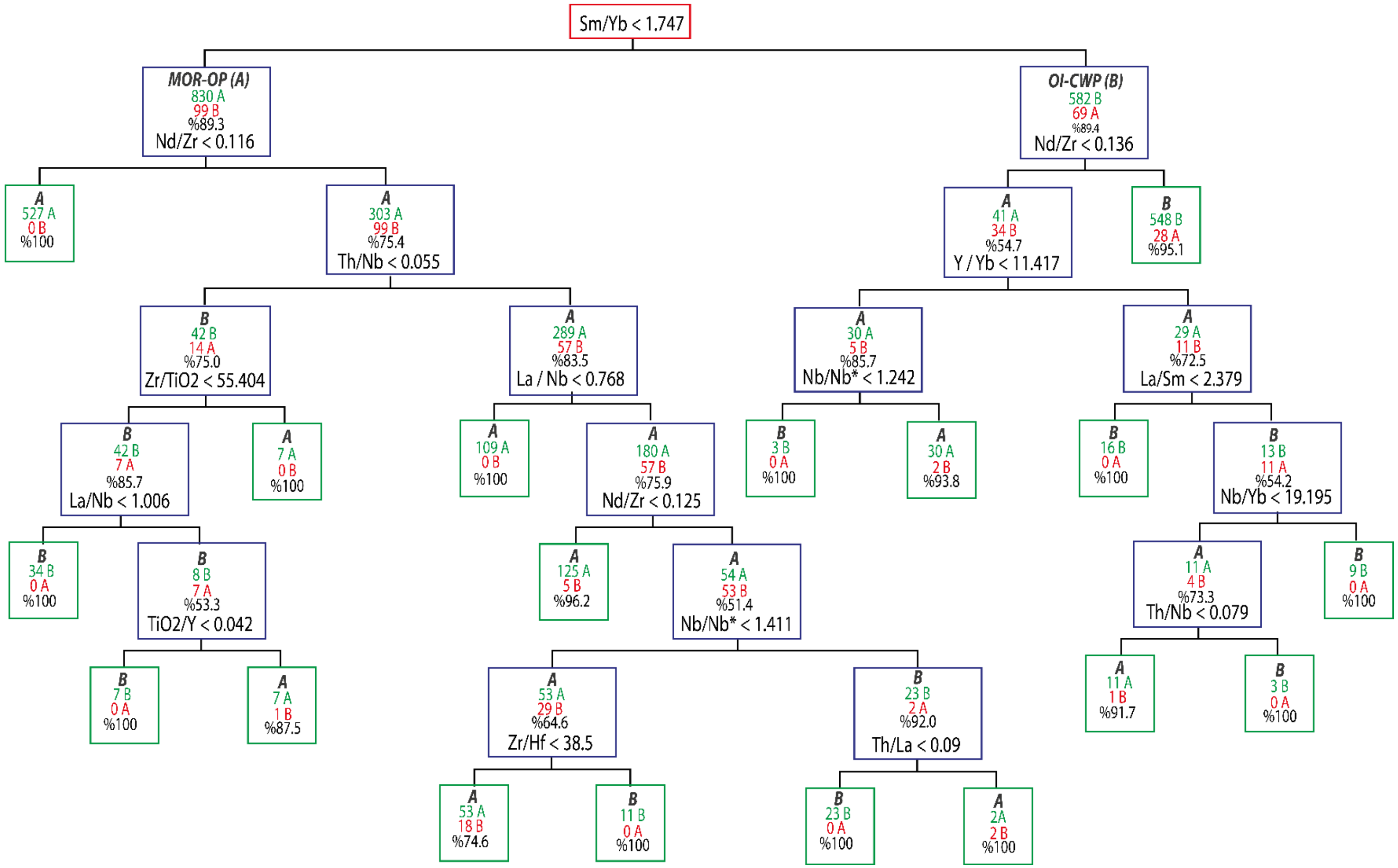

Figure 3.46. Classification results of the first decision tree to discriminate between mid-oceanic ridge + oceanic plateau and oceanic island + continental-within plates

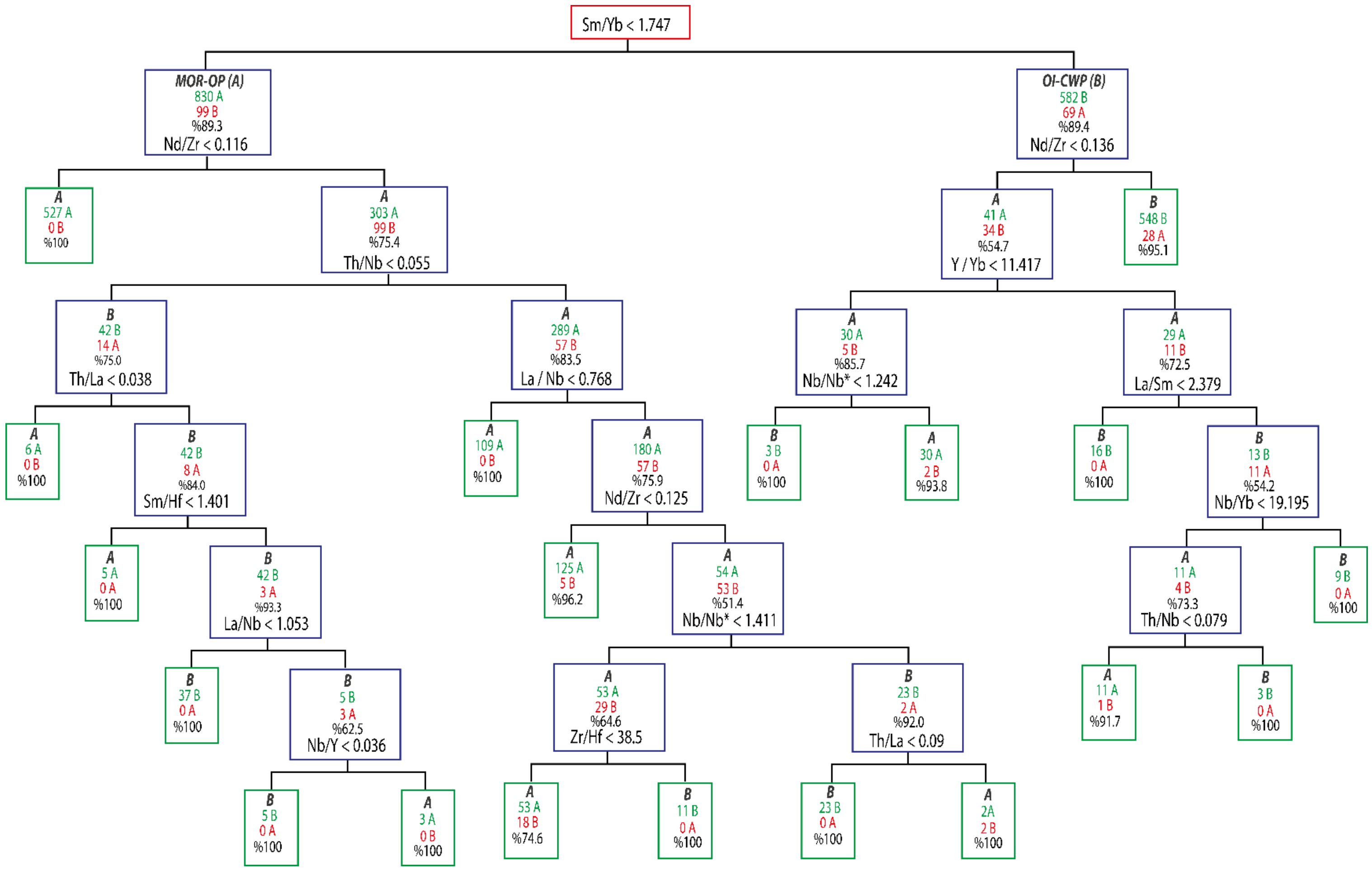

Figure 3.47. Classification results of the second decision tree to discriminate between mid-oceanic ridge + oceanic plateau and oceanic island + continental-within plates

For confusion matrix, showing the tectono-magmatic discrimination results for training+test and external datasets; true positive (TP) represents samples of group 2 classified as group 2, true negative (TN) represents samples of group 1 classified as group 1, false positive (FP) represents samples of group 1 classified as group 2 and false negative (FN) represents samples of group 2 classified as group 1.

When confusion matrix for training and test datasets are evaluated, the overall success ratio for tectono-magmatic discrimination between group 1 (mid-oceanic ridges and oceanic plateaus) and group 2 (oceanic islands and continental within-plates) settings are increasing with the increasing depth of the first decision tree (Table 3.34). For the second decision tree, on the other hand, it is increasing for group 2 but nearly stable for group 1 with slight fluctuations at third and fourth levels.

Table 3.34. Confusion Matrix Summary for Training and Test Datasets for Tectono-Magmatic Discrimination Between Group 1 and Group 2 of Non-Subduction Settings

ree	1						2					
Level	2	3	4	5	6	7	2	3	4	5	6	7
TP	680	765	769	763	763	812	680	765	769	763	763	814
TN	1,082	1,048	1,057	1,071	1,071	1,078	1,082	1,048	1,056	1,077	1,077	1,077
FP	38	72	63	49	49	42	38	72	64	43	43	43
FN	174	89	85	91	91	42	174	89	85	91	91	40

When confusion matrix for external datasets are evaluated, the overall success ratio for tectono-magmatic discrimination between group 1 (mid-oceanic ridge and oceanic plateaus) and group 2 (oceanic islands and continental within-plates) related settings decreases in varying but not significant degrees for the second trees (Table 3.35). Both decision trees obtain very similar success for discrimination of group 2 with increasing level of depth but a reverse pattern for discrimination of group 1 is observed so that the success ratio for the discrimination of group 1 decreases with increasing level of depth for both decision trees, which can imply the potential of overfitting for group 1.

Table 3.35. Confusion Matrix Summary for External Dataset for Tectono-Magmatic Discrimination Between Group 1 and Group 2 of Non-Subduction Settings

Tree	1						2					
Level	2	3	4	5	6	7	2	3	4	5	6	7
TP	406	473	479	461	461	489	406	473	479	461	461	489
TN	1,432	1,258	1,298	1,318	1,318	1,350	1,432	1,258	1,320	1,372	1,372	1356
FP	35	209	169	149	149	117	35	209	147	95	95	111
FN	133	66	60	78	78	50	133	66	60	78	78	50

Both decision trees successfully discriminate group 1 (MOR and OP) and group 2 (OI and CWP) from each other for both training and external datasets. There are no major failures for the discrimination of training set by the first decision tree (Table 3.36). 4 articles from CWP, 4 articles from MOR, 5 articles from OI and 3 articles OP have misclassifications. The first decision tree is successfully applicable to external datasets (Table 3.37) with only 2 articles completely misclassified. Trend of misclassification through the articles are similar to each other for both training and external datasets.

Second decision tree is quite similar to the first decision tree based on the distribution of misclassifications through the training (Table 3.38) and external (Table 3.39) datasets. Both decision tree is successful for discrimination of training set and applicable to external datasets without having any abrupt change in success ratios.

Second decision tree has also no major failures in training dataset but a few articles with major and complete failures, which does not effect the overall ratio of success for this decision tree as the amount of samples in these articles are limited.

Table 3.36. Misclassifications by first decision tree for discrimination between group 1 and group 2 of non-subduction settings

JOURNAL	CLASS	SAMPLES	Level 2	Level2 %	Level 3	Level3 %	Level 4	Level 4 %	Level 5	Level 5%	Level 6	Level 6%	Level 7	Level 7%
Hanghoj 2003 E Greenland	CWP	103	15	15	9	9	8	8	9	9	9	9	4	4
Larsen 2003 W Greenland	CWP	23	6	26	5	22	5	22	5	22	5	22	5	22
Peate 2003 E Greenland	CWP	41	13	32					1	2	1	2	1	2
Rooney 2012 Afar Plume	CWP	33	1	3	1	3	1	3	1	3	1	3	1	3
Arevalo 2010 Mixed	MOR	512	11	2	27	5	23	4	19	4	19	4	12	2
Gale 2011 MAR	MOR	70	12	17	14	20	14	20	12	17	12	17	12	17
Kempton 2002 Indian	MOR	63			1	2	1	2	1	2	1	2		
Yi 2000 Atlantic	MOR	15	4	27	8	53	8	53	4	27	4	27	4	27
Dixon 2008 Hawaii	OI	52	7	13	6	12	6	12	6	12	6	12	2	4
Jackson 2010 Samoa	OI	135	6	4					1	1	1	1	1	1
Kokfelt 2006 Iceland	OI	80	53	66	33	41	33	41	33	41	33	41	15	19
Salters 2010 Walvis	OI	37	19	51	17	46	17	46	19	51	19	51	6	16
Stracke 2003 Iceland	OI	43	43	100	15	35	15	35	15	35	15	35	7	16
Neal 2002 Kerguelen	OP	35	11	31	12	34	12	34	11	31	11	31	13	37
Sano 2012 Shatsky	OP	99			4	4	1	1	1	1	1	1		
Tim 2011 Manihiki	OP	13			1	8	1	8	1	8	1	8	1	8

Table 3.37. Misclassifications by first decision tree for discrimination between group 1 and group 2 of non-subduction settings

JOURNAL	CLASS	SAMPLES	Level 2	Level2 %	Level 3	Level3 %	Level 4	Level 4 %	Level 5	Level 5%	Level 6	Level 6%	Level 7	Level 7%
Davies 2006 Aldan Shield	CWP	7	1	14					1	14	1	14		
Endress 2011 Egypt	CWP	14	12	86	6	43			6	43	6	43		
Frey 1996 Bunbury	CWP	10	10	100	10	100	10	100	10	100	10	100	10	100
Furman 2006 Afar Plume	CWP	37	2	5	1	3	1	3	2	5	2	5	2	5
Gibson 1995 SE Brazil	CWP	32	1	3	1	3	1	3	1	3	1	3	1	3
Mana 2015 EAR	CWP	29	2	7	1	3	1	3	1	3	1	3	1	3
Olierook 2016 Bunbury	CWP	8	7	88	6	75	6	75	6	75	6	75	6	75
Shuying 2015 South China	CWP	12	4	33	3	25	3	25	4	33	4	33	3	25
Xu 2001 SW China	CWP	25	1	4	1	4	1	4	1	4	1	4	1	4
Jenner 2012 Mixed	MOR	588	7	1	23	4	19	3	19	3	19	3	25	4
Kelley 2013 EPR MAR	MOR	562	21	4	80	14	63	11	45	8	45	8	50	9
Zhang 2014 South Pacific	MOR	118			72	61	48	41	48	41	48	41		
Gibson 2005 Tristan	OI	32	24	75	19	59	19	59	22	69	22	69	13	41
Kitagawa 2008 Iceland	OI	107	35	33	17	16	17	16	22	21	22	21	12	11
Peate 2010 Iceland	OI	18	2	11	1	6	1	6	2	11	2	11	1	6
Borisova 2002 Kerguelen	OP	7	3	43	7	100	7	100	7	100	7	100	7	100
Frey 2002 Kerguelen	OP	17	1	6	1	6	2	12	2	12	2	12	8	47
Shafer 2004 Ontong Java	OP	10			1	10	1	10	1	10	1	10		
Tejada 2002 Ontong Java	OP	63			1	2	1	2	1	2	1	2	1	2
Trela 2015 Kerguelen	OP	19			15	79	15	79	13	68	13	68	13	68
Weis 2002 Kerguelen	OP	29					5	17	5	17	5	17	5	17

Table 3.38. Misclassifications by second decision tree for discrimination between group 1 and group 2 of non-subduction settings

JOURNAL	CLASS	SAMPLES	Level 2	Level2 %	Level 3	Level3 %	Level 4	Level 4%	Level 5	Level 5%	Level 6	Level 6%	Level 7	Level 7%
Hanghoj 2003 East Greenland	CWP	103	15	15	9	9	8	8	9	9	9	9	4	4
Larsen 2003 West Greenland	CWP	23	6	26	5	22	5	22	5	22	5	22	5	22
Peate 2003 East Greenland	CWP	41	13	32					1	2	1	2	1	2
Rooney 2012 Afar Plume	CWP	33	1	3	1	3	1	3	1	3	1	3	1	3
Arevalo 2010 Mixed	MOR	512	11	2	27	5	21	4	15	3	15	3	13	3
Brandl 2012 EPR	MOR	10			2	20	2	20						
Gale 2011 MAR	MOR	70	12	17	14	20	14	20	12	17	12	17	12	17
Yi 2000 Atlantic	MOR	15	4	27	8	53	8	53	4	27	4	27	4	27
Dixon 2008 Hawaii	OI	52	7	13	6	12	6	12	6	12	6	12	2	4
Jackson 2010 Samoa	OI	135	6	4					1	1	1	1	1	1
Kokfelt 2006 Iceland	OI	80	53	66	33	41	33	41	33	41	33	41	15	19
Salters 2010 Walvis	OI	37	19	51	17	46	17	46	19	51	19	51	6	16
Stracke 2003 Iceland	OI	43	43	100	15	35	15	35	15	35	15	35	5	12
Neal 2002 Kerguelen	OP	35	11	31	12	34	12	34	11	31	11	31	13	37
Sano 2012 Shatsky	OP	99			4	4	4	4	1	1	1	1		
Tim 2011 Manihiki	OP	13			1	8							1	8

Table 3.39. Misclassifications by second decision tree for discrimination between group 1 and group 2 of non-subduction settings

JOURNAL	CLASS	SAMPLES	Level 2	Level2 %	Level 3	Level3 %	Level 4	Level 4%	Level 5	Level 5%	Level 6	Level 6%	Level 7	Level 7%
Davies 2006 Aldan Shield	CWP	7	1	14					1	14	1	14		
Endress 2011 Egypt	CWP	14	12	86	6	43			6	43	6	43		
Frey 1996 Bunbury	CWP	10	10	100	10	100	10	100	10	100	10	100	10	100
Furman 2006 Afar Plume	CWP	37	2	5	1	3	1	3	2	5	2	5	2	5
Gibson 1995 SE Brazil	CWP	32	1	3	1	3	1	3	1	3	1	3	1	3
Mana 2015 EAR	CWP	29	2	7	1	3	1	3	1	3	1	3	1	3
Olierook 2016 Bunbury	CWP	8	7	88	6	75	6	75	6	75	6	75	6	75
Shuying 2015 South China	CWP	12	4	33	3	25	3	25	4	33	4	33	3	25
Xu 2001 SW China	CWP	25	1	4	1	4	1	4	1	4	1	4	1	4
Jenner 2012 Mixed	MOR	588	7	1	23	4	22	4	22	4	22	4	28	5
Kelley 2013 EPR MAR	MOR	562	21	4	80	14	79	14	36	6	36	6	41	7
Pyle 1995 Indian Pacific	MOR	17			1	6	1	6	1	6	1	6	1	6
Gibson 2005 Tristan	OI	32	24	75	19	59	19	59	22	69	22	69	13	41
Kitagawa 2008 Iceland	OI	107	35	33	17	16	17	16	22	21	22	21	12	11
Peate 2010 Iceland	OI	18	2	11	1	6	1	6	2	11	2	11	1	6
Borisova 2002 Kerguelen	OP	7	3	43	7	100	7	100	7	100	7	100	7	100
Frey 2002 Kerguelen	OP	17	1	6	1	6	2	12	2	12	2	12	8	47
Shafer 2004 Ontong Java	OP	10			1	10	1	10	1	10	1	10		
Trela 2015 Kerguelen	OP	19			15	79	15	79	13	68	13	68	13	68
Weis 2002 Kerguelen	OP	29					5	17	5	17	5	17	5	17

3.2.3.2. Discrimination Between Mid-Oceanic Ridges and Oceanic Plateaus

Two multi-branched decision trees (Figure 3.48 and Figure 3.49) are constructed for the discrimination between mid-oceanic ridge and oceanic plateau. Using training set, success ratios for discrimination at each level of depth are determined.

For confusion matrix, showing the tectono-magmatic discrimination results for training+test and external datasets; true positive (TP) represents samples of oceanic plateaus classified as oceanic plateaus, true negative (TN) represents samples of mid-oceanic ridges classified as mid-oceanic ridges, false positive (FP) represents samples of mid-oceanic ridges classified as oceanic plateaus and false negative (FN) represents samples of oceanic plateaus classified as mid-oceanic ridges.

When confusion matrix for training and test datasets are evaluated, the overall success ratio for tectono-magmatic discrimination between mid-oceanic ridges and oceanic plateaus are continuously increasing with the increasing level of depth in both decision trees with a few exceptions (Table 3.40).

When confusion matrix for external datasets are evaluated, the overall success ratio for tectono-magmatic discrimination between mid-oceanic ridges and oceanic plateaus decreases in varying degrees for the second trees (Table 3.41).

The first decision tree is quite successful at the discrimination of MOR and OP for training dataset, especially for samples of articles from MOR (Table 3.42). Only 1 article from MOR has misclassification and this is solved at sixth level.

The same success is also observed in external dataset with a similar trend for the distribution of misclassification through the articles of MOR and OP (Table 3.43).

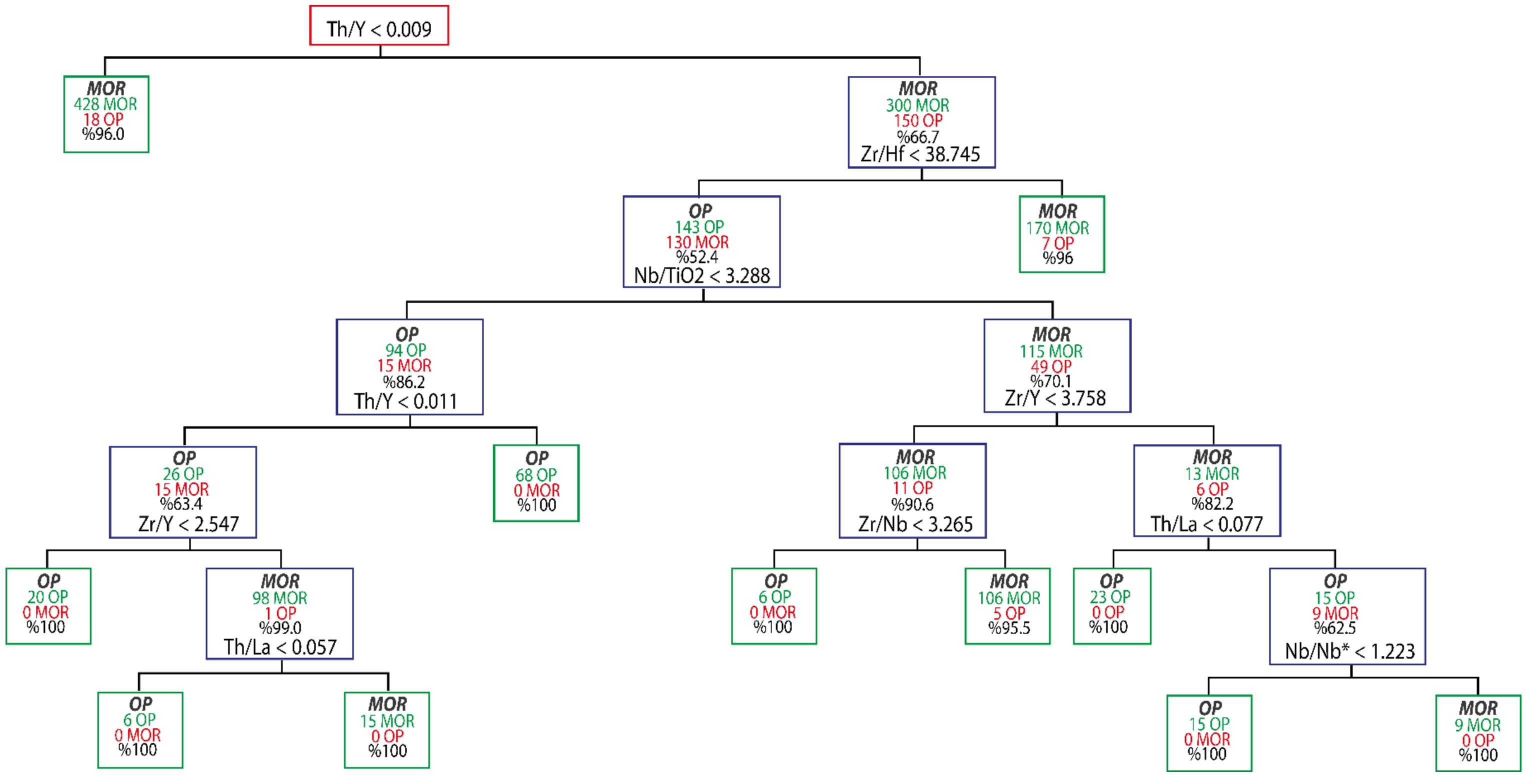

Figure 3.48. Classification results of the first decision tree to discriminate between mid-oceanic ridge and oceanic plateaus

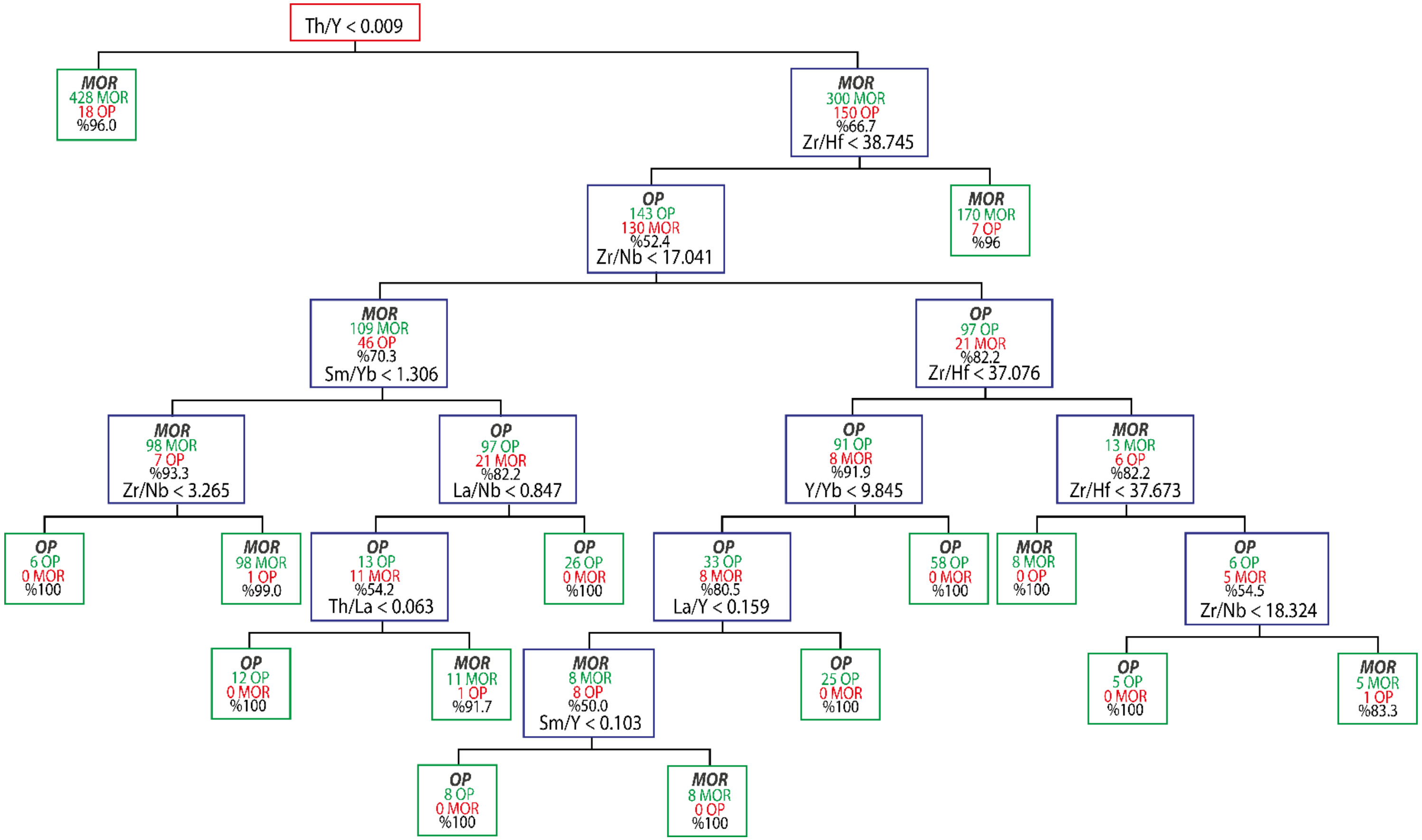

Figure 3.49. Classification results of the second decision tree to discriminate between mid-oceanic ridge and oceanic plateaus

Table 3.40. Confusion Matrix Summary for Training and Test Datasets for Tectono-Magmatic Discrimination Between Mid-Oceanic Ridge and Oceanic Plateau Settings

Tree	1						2					
Level	2	3	4	5	6	7	2	3	4	5	6	7
TP	176	118	162	159	167	167	176	121	161	175	175	171
TN	744	891	879	895	907	907	744	883	882	877	877	906
FP	165	18	30	14	2	2	165	26	27	32	32	3
FN	35	93	49	52	44	44	35	90	50	36	36	40

Table 3.41. Confusion Matrix Summary for External Dataset for Tectono-Magmatic Discrimination Between Mid-Oceanic Ridge and Oceanic Plateaus

Tree	1					2					
Level	2	3	4	5	6	2	3	4	5	6	7
TP	113	52	66	64	53	113	50	61	66	66	38
TN	966	1,236	1,206	1,252	1,277	966	1,210	1,217	1,188	1,188	1,270
FP	388	68	98	52	27	388	94	87	116	116	34
FN	50	111	97	99	110	50	113	102	97	97	125

The second decision tree is also quite similar to the first decision tree on the basis of the success ratios and the distributions of misclassifications through the articles and the tectonic settings.

It is quite successful at the discrimination of MOR and OP at training dataset (Table 3.44) and also applicable to external dataset (Table 3.45).

For both decision trees, MOR is much more successfully discriminated with respect to OP and the trend of misclassifications through the articles in training set and external dataset is similar to each other without any abrupt change in success ratio for any specific articles or tectonic settings.

Table 3.42. Misclassifications by first decision tree for discrimination between mid-oceanic ridge and oceanic plateaus

JOURNAL	CLASS	SAMPLES	Level 2	Level 2%	Level 3	Level3%	Level 4	Level4%	Level 5	Level 5%	Level 6	Level 6%
Arevalo 2010 Mixed	MOR	51	85	17	15	3	27	5	14	3	2	0
Fitton 2004 Ontong Java	OP	64	6	9	10	16	10	16	10	16	10	16
Neal 2002 Kerguelen	OP	35	6	17	35	10	8	23	8	23	8	23
Sano 2012 Shatsky	OP	99	21	21	39	39	22	22	32	32	24	24
Tim 2011 Manihiki	OP	13	2	15	9	69	9	69	2	15	2	15

Table 3.43. Misclassifications by first decision tree for discrimination between mid-oceanic ridge and oceanic plateaus

JOURNAL	CLASS	SAMPLES	Level 2	Level 2%	Level 3	Level3%	Level 4	Level4%	Level 5	Level 5%	Level 6	Level 6%
Jenner 2012 Mixed	MO	58	16	28	46	8	53	9	23	4	18	3
Kelley 2013 EPR MAR	MO	56	16	29	20	4	38	7	24	4	8	1
Zhang 2014 South Pacific	MO	11	7	6	2	2	7	6	5	4	1	1
Borisova 2002 Kerguelen	OP	7	7	10	7	10	7	10	7	10	7	10
Frey 2002 Kerguelen	OP	17	9	53	10	59	10	59	10	59	10	59
Hastie 2016 Curacao	OP	4			2	50	2	50	2	50	2	50
Shafer 2004 Ontong Java	OP	10	5	50	6	60	6	60	7	70	6	60
Tejada 2002 Ontong Java	OP	63	1	2	45	71	43	68	43	68	43	68
Trela 2015 Kerguelen	OP	19	6	32	19	10	7	37	7	37	19	10
Weis 2002 Kerguelen	OP	29	13	45	13	45	13	45	13	45	13	45
White 2004 Ontong Java	OP	6	1	17	1	17	1	17	2	33	2	33

Table 3.44. Misclassifications by second decision tree for discrimination between mid-oceanic ridge and oceanic plateaus

JOURNAL	CLASS	SAMPLES	Level 2	Level 2%	Level 3	Level3%	Level 4	Level4%	Level 5	Level 5%	Level 6	Level 6%	Level 7	Level 7%
Arevalo 2010 Mixed	MOR	51	85	17	22	4	26	5	29	6	29	6	3	1
Gale 2011 MAR	MOR	70	33	47			1	1	1	1	1	1		
Nauret 2006 Central Indian	MOR	34	5	15	2	6			1	3	1	3		
Niu 1997 2002 EPR	MOR	77	1	1	1	1			1	1	1	1		
Fitton 2004 Ontong Java	OP	64	6	9	8	13	12	19	7	11	7	11	7	11
Neal 2002 Kerguelen	OP	35	6	17	35	10	6	17	6	17	6	17	6	17
Sano 2012 Shatsky	OP	99	21	21	38	38	22	22	21	21	21	21	24	24
Tim 2011 Manihiki	OP	13	2	15	9	69	10	77	2	15	2	15	3	23

Table 3.45. Misclassifications by second decision tree for discrimination between mid-oceanic ridge and oceanic plateaus

JOURNAL	CLASS	SAMPLES	Level 2	Level 2%	Level 3	Level3%	Level 4	Level4%	Level 5	Level 5%	Level 6	Level 5%	Level 7	Level 7%
Jenner 2012 Mixed	MOR	588	166	28	48	8	33	6	45	8	45	8	6	1
Kelley 2013 EPR MAR	MOR	562	163	29	43	8	46	8	62	11	62	11	27	5
Pyle 1995 Indian Pacific	MOR	17	2	12	1	6	1	6	2	12	2	12		
Zhang 2014 South Pacific	MOR	118	7	6	2	2	7	6	7	6	7	6	1	1
Borisova 2002 Kerguelen	OP	7	7	100	7	100	7	100	7	100	7	100	7	100
Frey 2002 Kerguelen	OP	17	9	53	16	94	15	88	14	82	14	82	14	82
Hastie 2016 Curacao	OP	4			4	100	4	100	4	100	4	100	4	100
Shafer 2004 Ontong Java	OP	10	5	50	6	60	6	60	6	60	6	60	8	80
Tejada 2002 Ontong Java	OP	63	1	2	34	54	31	49	31	49	31	49	33	52
Trela 2015 Kerguelen	OP	19	6	32	19	100	7	37	7	37	7	37	19	100
Weis 2002 Kerguelen	OP	29	13	45	13	45	18	62	14	48	14	48	26	90
White 2004 Ontong Java	OP	6	1	17	6	100	6	100	6	100	6	100	6	100

3.2.3.3. Discrimination Between Oceanic Islands and Continental Within-plates

Two multi-branched decision trees (Figure 3.50 and Figure 3.51) are constructed for the discrimination between oceanic island and continental within-plates. Using training set, success ratios for discrimination at each level of depth are determined.

For confusion matrix, showing the tectono-magmatic discrimination results for training+test and external datasets; true positive (TP) represents samples of ocean islands classified as ocean islands, true negative (TN) represents samples of continental within-plates classified as continental within-plates, false positive (FP) represents samples of continental within-plates classified as ocean islands and false negative (FN) represents samples of ocean islands classified as continental within-plates.

When confusion matrix for training and test datasets (Table 3.46) and external datasets (Table 3.47) are evaluated, the overall success ratio for tectono-magmatic discrimination between oceanic islands and continental within-plates are continuously increasing with increasing level of depth in both decision trees. The success ratios for the discrimination of both oceanic islands and continental within-plates reach their maximum at the highest level of depth in both decision trees.

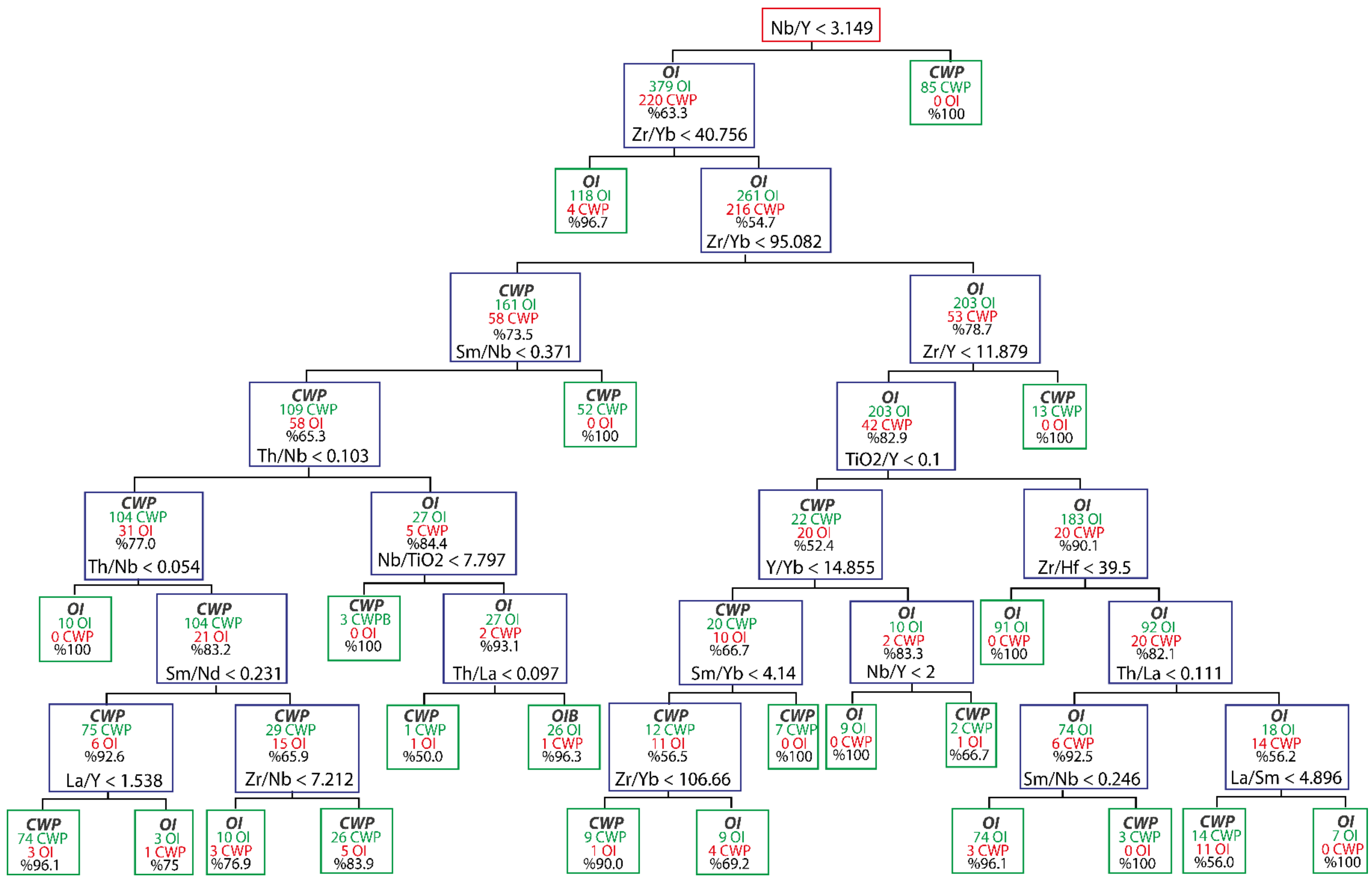

Figure 3.50. Classification results of the first decision tree to discriminate between oceanic island and continental-within plates

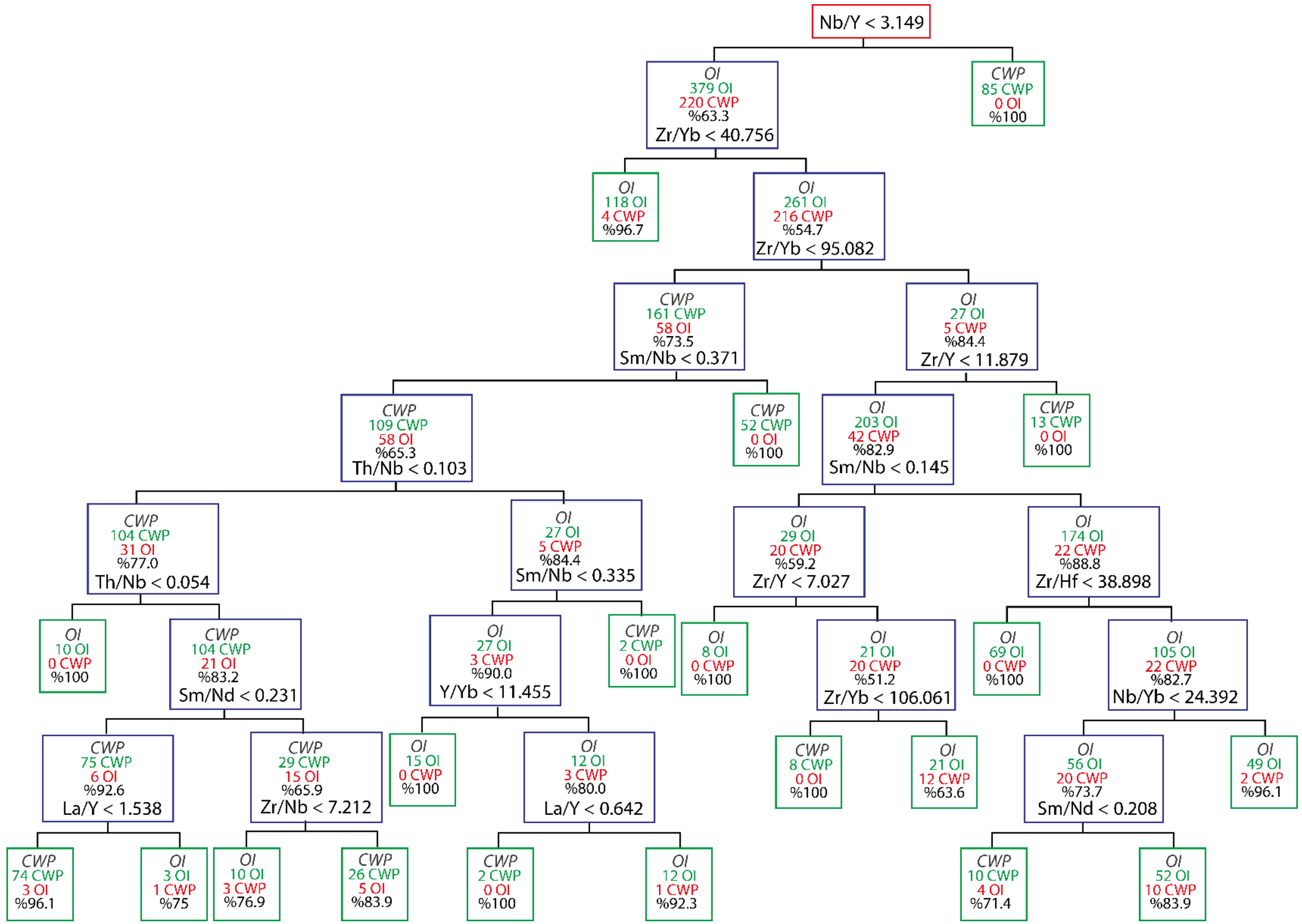

Figure 3.51. Classification results of the second decision tree to discriminate between oceanic island and continental-within plates

Table 3.46. Confusion Matrix Summary for Training and Test Datasets for Tectono-Magmatic Discrimination Between Ocean Islands and Continental Within-plates

Tree	1						2					
Level	3	4	5	6	7	8	3	4	5	6	7	8
TP	397	394	399	399	419	431	397	394	425	425	425	445
TN	298	315	334	334	337	345	298	315	309	309	309	327
FP	78	61	42	42	39	31	78	61	67	67	67	49
FN	81	84	79	79	59	47	81	84	53	53	53	33

Table 3.47. Confusion Matrix Summary for External Dataset for Tectono-Magmatic Discrimination Between Oceanic Islands and Continental Within-plates

Tree	1						2					
Level	3	4	5	6	7	8	3	4	5	6	7	8
TP	51	48	54	54	61	63	51	48	58	58	58	64
TN	231	251	247	247	242	237	231	251	225	225	225	226
FP	71	51	55	55	60	65	71	51	77	77	77	76
FN	186	189	183	183	176	174	186	189	179	189	179	173

Both decision trees are quite successful for the discrimination between ocean islands and continental within-plates for training sets. The first decision tree has no major failures through the articles of both tectonic settings for training dataset (Table 3.48). The success ratio for discrimination of ocean islands and continental within-plates are close to each other. However, the success ratio of decision tree for the discrimination of ocean islands at external datasets falls drastically (Table 3.49). This is not an indication of an overfitting. This is the complex nature of misclassified samples from ocean islands and continental within-plates that makes nearly impossible for decision tree to correctly discriminate them from each other. The same trend of misclassifications are also observed for the second decision tree at discrimination of samples from both training (Table 3.50) and external (Table 3.51) datasets.

Table 3.48. Misclassifications by first decision tree for discrimination between oceanic islands and continental within-plates

JOURNAL	CLASS	SAMPLES	Level 3	Level 3%	Level 4	Level4%	Level 5	Level5%	Level 6	Level6%	Level 7	Level7%	Level 8	Level8%
Aviado 2015 West Antarctic	CWP	19	12	63	12	63	5	26	5	26	5	26	6	32
Furman 2006 Turkana Kenya	CWP	42	7	17	7	17	1	2	1	2	1	2	2	5
Gibson 2000 Picrite	CWP	16	2	13	2	13	3	19	3	19	2	13		
Hanghoj 2003 East Greenland	CWP	103	11	11	11	11	11	11	11	11	8	8	8	8
Johnson 2005 Siberia	CWP	18	15	83	15	83	9	50	9	50	10	56	2	11
Larsen 2003 West Greenland	CWP	23	6	26	6	26	5	22	5	22	5	22	6	26
Peate 2003 East Greenland	CWP	41	24	59	8	20	8	20	8	20	8	20	4	10
Rooney 2012 Afar Plume	CWP	33											3	9
Dixon 2008 Hawaii	OI	52	5	10	5	10	5	10	5	10	4	8	2	4
Geldmacher 2000 Madeira	OI	49	7	14	8	16	14	29	14	29	14	29	6	12
Gurenko 2006 Canary	OI	44					2	5	2	5			1	2
Jackson 2010 Samoa	OI	135	9	7	11	8	12	9	12	9	12	9	16	12
Kokfelt 2006 Iceland	OI	80	32	40	32	40	31	39	31	39	22	28	14	18
Millet 2009 Azores	OI	21	1	5	1	5	3	14	3	14	3	14	2	10
Woodhead 1996 Mangaia	OI	17					11	65	11	65	4	24	6	35

Table 3.49. Misclassifications by first decision tree for discrimination between oceanic islands and continental within-plates

JOURNAL	CLASS	SAMPLES	Level 3	Level 3%	Level 4	Level4%	Level 5	Level5%	Level 6	Level6%	Level 7	Level7%	Level 8	Level8%
Davies 2006 Aldan Shield	CWP	7	3	43	2	29					1	14	1	14
Endress 2011 Egypt	CWP	14	1	7			12	86	12	86	10	71	10	71
Frey 1996 Bunbury	CWP	10	3	30	3	30	3	30	3	30	3	30	3	30
Furman 2004 East African Rift	CWP	29									1	3	4	14
Furman 2006 Afar Plume	CWP	37	2	5	2	5	2	5	2	5	5	14	7	19
Gibson 1993 Rio Grande Rift	CWP	15	9	60	9	60	1	7	1	7	1	7	1	7
Gibson 1995 Brazil Paraguay	CWP	25	11	44	4	16	3	12	3	12	4	16	4	16
Gibson 1997 Trindade	CWP	3					2	67	2	67	2	67	2	67
Gibson 2005 Tristan	CWP	14	13	93	2	14	1	7	1	7	1	7	1	7
Mana 2015 East African Rift	CWP	29	10	34	10	34	8	28	8	28	9	31	7	24
Olierook 2016 Bunbury	CWP	8	5	63	5	63	5	63	5	63	5	63	5	63
Shuying 2015 South China	CWP	12	4	33	4	33	2	17	2	17	2	17	5	42
Xu 2001 SW China	CWP	25	10	40	10	40	16	64	16	64	16	64	15	60
Gibson 2005 Tristan	OI	32	22	69	22	69	16	50	16	50	13	41	11	34
Hanyu 2011 Young Rurutu	OI	21	6	29	9	43	9	43	9	43	9	43	9	43
Kitagawa 2008 Iceland	OI	10	97	91	97	91	95	89	95	89	94	88	94	88
Lassiter 2003 Raivavae	OI	14	6	43	6	43	8	57	8	57	7	50	9	64
Morgan 2009 Hawaii	OI	45	45	100	45	10	45	100	45	10	45	100	45	10
Peate 2010 Iceland	OI	18	18	100	18	10	18	100	18	10	16	89	14	78
Davies 2006 Aldan Shield	CWP	7	3	43	2	29					1	14	1	
Endress 2011 Egypt	CWP	14	1	7			12	86	12	86	10	71	10	

Table 3.50. Misclassifications by second decision tree for discrimination between oceanic islands and continental within-plates

JOURNAL	CLASS	SAMPLES	Level 3	Level 3%	Level 4	Level4%	Level 5	Level5%	Level 6	Level6%	Level 7	Level7%	Level 8	Level8%
Aviado 2015 West Antarctic	CWP	19	12	63	12	63	5	26	5	26	5	26	6	32
Furman 2006 Turkana Kenya	CWP	42	7	17	7	17	1	2	1	2	1	2	2	5
Gibson 2000 Picrite	CWP	16	2	13	2	13	3	19	3	19	2	13		
Hanghoj 2003 East Greenland	CWP	10	11	11	11	11	11	11	11	11	8	8	8	8
Janney 2002 South Africa	CWP	11	1	9										
Johnson 2005 Siberia	CWP	18	15	83	15	83	9	50	9	50	10	56	2	11
Larsen 2003 West Greenland	CWP	23	6	26	6	26	5	22	5	22	5	22	6	26
Mirnejad 2006 Leucite Hills	CWP	10												
Peate 2003 East Greenland	CWP	41	24	59	8	20	8	20	8	20	8	20	4	10
Rooney 2012 Afar Plume	CWP	33											3	9
Tappe 2011 Greenland	CWP	33												
Dixon 2008 Hawaii	OI	52	5	10	5	10	5	10	5	10	4	8	2	4
Geldmacher 2000 Madeira	OI	49	7	14	8	16	14	29	14	29	14	29	6	12
Gurenko 2006 Canary	OI	44					2	5	2	5			1	2
Jackson 2010 Samoa	OI	13	9	7	11	8	12	9	12	9	12	9	16	12
Kokfelt 2006 Iceland	OI	80	32	40	32	40	31	39	31	39	22	28	14	18
Millet 2009 Azores	OI	21	1	5	1	5	3	14	3	14	3	14	2	10
Salters 2010 Walvis	OI	37	26	70	26	70								
Stracke 2003 Iceland	OI	43	1	2	1	2	1	2	1	2				
Woodhead 1996 Mangaia	OI	17					11	65	11	65	4	24	6	35

Table 3.51. Misclassifications by second decision tree for discrimination between oceanic islands and continental within-plates

JOURNAL	CLASS	SAMPLES	Level 3	Level 3%	Level 4	Level4%	Level 5	Level5%	Level 6	Level6%	Level 7	Level7%	Level 8	Level8%
Carlson 1996 Southern Brazil	CWP	14												
Davies 2006 Aldan Shield	CWP	7	3	43	2	29	2	29	2	29	2	29	2	29
Endress 2011 Egypt	CWP	14	1	7			12	86	12	86	12	86	10	71
Frey 1996 Bunbury	CWP	10	3	30	3	30	3	30	3	30	3	30	3	30
Furman 2004 East African Rift	CWP	29											4	14
Furman 2006 Afar Plume	CWP	37	2	5	2	5	3	8	3	8	3	8	5	14
Gibson 1993 Rio Grande Rift	CWP	15	9	60	9	60	10	67	10	67	10	67	9	60
Gibson 1995 Brazil Paraguay	CWP	25	11	44	4	16	4	16	4	16	4	16	4	16
Gibson 1995 Southeast Brazil	CWP	32												
Gibson 1997 Trindade	CWP	3					2	67	2	67	2	67	2	67
Gibson 2005 Tristan	CWP	14	13	93	2	14	2	14	2	14	2	14	2	14
Leroex 2003 Kimberlite Africa	CWP	28												
Mana 2015 East African Rift	CWP	29	10	34	10	34	11	38	11	38	11	38	9	31
Olierook 2016 Bunbury	CWP	8	5	63	5	63	5	63	5	63	5	63	5	63
Shuying 2015 South China	CWP	12	4	33	4	33	4	33	4	33	4	33	5	42
Xu 2001 SW China	CWP	25	10	40	10	40	19	76	19	76	19	76	16	64
Gibson 2005 Tristan	OI	32	22	69	22	69	14	44	14	44	14	44	13	41
Hanyu 2011 Young Rurutu	OI	21	6	29	9	43	9	43	9	43	9	43	9	43
Kitagawa 2008 Iceland	OI	10	97	91	97	91	95	89	95	89	95	89	96	90
Lassiter 2003 Raivavae	OI	14	6	43	6	43	6	43	6	43	6	43	4	29
Morgan 2009 Hawaii	OI	45	45	100	45	10	45	100	45	10	45	100	45	10
Peate 2010 Iceland	OI	18	18	100	18	10	18	100	18	10	18	100	14	78

CHAPTER 4

DISCUSSION

4.1. Discussion of Decision Trees

4.1.1. Discussion Based on Information Gain

Information gain is an important parameter for the selection of features in the construction of decisin trees (Table 4.1). Element ratios with greater information gain values are better discriminators and are preferred in decision trees.

Th/Nb and Nb/Nb* are useful discriminating features for discrimination between subduction and non-subduction settings. Th and Nb behave as incompatible elements during peridotitic upper mantle melting (e.g. Sun and McDonough, 1989). The mineral phases in the mantle peridotite (olivine, clinopyroxene, orthopyroxene, spinel, garnet) at these conditions are characterized by very low $D_{melt/liquid}$; thus they have only a minimal effect on the fractionation of Th/Nb. Their behavior, however, may change significantly in subduction systems owing to dehydration and melting of the slab and its mineralogy. During these processes, Th remains highly incompatible; it is partitioned into the sediment melt and transferred into the mantle wedge (e.g. Elliott et al., 1997). In contrast, Nb is retained in the slab, which is mainly linked to the presence of Ti-bearing accessory phases, such as rutile (e.g. Ayers and Watson, 1993). Thus, the transfer of Nb to the overlying mantle wedge is negligible. While the mantle wedge remains pristine in terms of Nb (no addition), it becomes Th-rich with the flux of this element via sediment melt. Therefore, during the subduction process, Th and Nb are significantly fractioned, which causes the generation of magmas with high Th/Nb signatures. It must also be noted that La (a LREE) displays somewhat a similar behavior to Th since it is mobilized by slab-derived sediment melt. However, since Th is relatively more incompatible than La, Th/Nb serves a more sensitive indicator of the subduction component. The use of Nb/Nb* is due to the diverse behavior of Th and La relative Nb, as explained before. Since the subduction-related magmas are generally Th and La rich over Nb, they display negative anomalies. In this respect, Nb/Nb* ratio is useful to see the magnitude of this relative depletion. In addition, because of the integration of both Th and La at the same time, Nb/Nb* may act as a better subduction indicator than Th/Nb.

Table 4.1. Information gain values of selected features for tectono-magmatic discriminations

Feature	Sub Nonsub	Arc Backarc	OA CA	Oceanic Continental	OA OBAB	MOR+OP OI+CWP	MOR OP	OI CWP
La/Nb	0.445	0.166	0.149	0.128	0.208	0.108	0.112	
La/Sm					0.086	0.378		0.052
La/Y			0.016			0.478	0.033	0.056
La/Yb			0.019	0.016		0.482		
Nb/Nb*	0.550	0.203	0.079	0.093	0.262	0.010	0.030	
Nb/TiO_2							0.086	0.075
Nb/Y	0.147		0.029			0.424		0.078
Nb/Yb					0.019	0.460		0.077
Nd/TiO_2		0.132	0.025	0.059				
Nd/Zr		0.175		0.062	0.240	0.520		
Sm/Hf	0.155		0.085	0.044		0.150		
Sm/Nb	0.214							0.051
Sm/Nd			0.023					0.094
Sm/Y		0.147	0.039	0.042	0.165		0.118	0.148
Sm/Yb					0.150	0.477	0.105	0.097
Th/La			0.004			0.169	0.103	0.021
Th/Nb	0.528	0.196			0.253	0.087		0.042
Th/Y			0.019				0.162	
Th/Yb			0.015				0.141	
TiO_2/Y		0.037		0.016		0.416		0.065
TiO_2/Yb	0.115				0.035	0.480		
Y/Yb		0.019	0.046	0.036	0.020	0.396	0.006	0.048
Zr/Hf		0.083	0.091	0.038	0.151	0.062	0.085	0.033
Zr/Nb	0.173	0.039	0.003	0.005			0.151	
Zr/Sm			0.168		0.207			
Zr/TiO_2			0.166	0.141		0.055		
Zr/Y		0.016	0.166	0.141			0.050	0.165
Zr/Yb			0.089	0.075				0.192

In contrast to Th/Nb and Nb/Nb*, which are used to assess the presence of the subduction component, the role of Nb/Y and TiO_2/Yb ratios are different. Nb, Ti, Y, and Yb behave similarly during dehydration and melting of the slab; they are all strongly conservative and retained in the slab (e.g. Pearce and Peate, 1995). Their partitioning during the melting of mantle peridotite, however, is different. Nb is highly incompatible, while Ti, Y, and Yb are all less incompatible than Nb (e.g. Sun and McDonough, 1989). Thus, Nb/Y and TiO_2/Yb can be fractionated under low degrees of melting. In addition to melting, these ratios can also be controlled based on the nature of the mantle source (depleted vs. enriched). For example, N-MORBs, which are thought to be derived from depleted mantle sources (under moderate to high degrees of melting), are characterized by low Nb/Y and TiO_2/Yb ratios (e.g. Sun and McDonough, 1989; Niu and Batiza, 1997; Hoernle et al., 2011). In contrast, enriched magmas, such as E-MORBs and most OIBs, are characterized by high Nb/Y and TiO_2/Yb ratios, owing to the involvement of enriched sources and low-degree of partial melting (e.g. Sun and McDonough, 1989; Chauvel et al., 1992; Workman et al., 2004).

Furthermore, since melt extraction depletes the source more in Nb, the mantle source domains that have previously experienced a melt extraction(s) is characterized by even lower Nb/Y and TiO_2/Yb ratios than those of N-MORBs (e.g. Pearce and Parkinson, 1993). This phenomenon is observed in some MORs and oceanic arcs, which seems to have tapped pre-depleted mantle sources (e.g. Pearce et al., 1995; Niu and Batiza, 1997). Additionally, the presence of residual garnet can make a substantial effect on Y and Yb, since these elements are strongly partitioned into garnet (e.g. McKenzie and O'Nions, 1991). Therefore, melt generation involving garnet-bearing mantle sources can result in magmas with high Nb/Y and TiO_2/Yb ratios.

Although having relatively high information gain, gain ratio and gini index values, Sm/Nb and Sm/Hf ratios are not preferred by any of the three decision trees at all.

For discrimination between arc and back-arc-related settings, the element ratios used in these trees have relatively high information gain. However, features with high information gain values (e.g. Th/Nb, La/Nb, and Sm/Y) are not preferred within two decision trees constructed for discrimination of arc and back-arc-related settings.

In the classification of subduction-related settings, the Nd/Zr ratio appears as a new ratio, not found in the previous discrimination. This element ratio contains trace elements Nd and Zr, which display somewhat similar incompatibilities (e.g. Sun and McDonough, 1989). Thus, except for the small degrees of partial melting, these elements are expected not to fractionate significantly. However, a material like sediment, which can be added to the mantle source of subduction zone magmas, may cause a strong fractionation of this ratio. Sediments are known to be some distinct geochemical features. For example, they are generally depleted in Zr (and Hf) relative to Nd (and Sm) (e.g. Plank and Langmuir 1998). Thus, the addition of sediments with high Nd/Zr ratios (e.g. via sediment melt) to the mantle source would directly affect the composition of resulting magmas, leading to high Nd/Zr signatures.

For discrimination between OA and CA, the element ratios used in these trees have relatively high information gain. However, Zr/Y having high information gain value is not preferred within two decision trees constructed for discrimination of OA and CA. In the discrimination between the oceanic and continental arcs, Zr/TiO_2 and Zr/Sm appear as the main discriminants. Regarding these pairs, Zr is relatively more incompatible than both Ti and Sm (e.g. Sun and Donough, 1989). Zr and Ti are subduction-immobile, while Sm is slightly subduction-mobile (Pearce and Peate 1995), thus it may cause some enrichment to some extent (though not much) in the mantle wedge. Based on the partitioning behavior, the melts derived from depleted sources under medium to high degrees of melting are characterized by lower Zr/TiO_2 and Zr/Sm ratios (relative to the ones originated from enriched sources and/or by low degrees of melting). Similarly, melt extraction would drive any mantle source domain to lower values in both Zr/TiO_2 and Zr/Sm. Sm/Y operates somewhat similarly to Zr/TiO_2 and Zr/Sm since Sm is more incompatible than Y. With increasing Zr/TiO_2

and Zr/Sm, Sm/Y can also be expected to increase due to source enrichment and/or decreasing degree of melting.

For discrimination between oceanic and continental settings, the element ratios used in these trees have relatively high information gain. However, Zr/TiO_2 having maximum information gain value is not preferred within two decision trees. Zr/Y ratio appears to be at the top discrimination between oceanic and continental subduction-related settings. In this pair, both elements are subduction-immobile, thus unaffected by the slab-derived contributions to the mantle wedge (e.g. Pearce and Stern 2006). The operation of this ratio is somewhat similar to Zr/Sm and Zr/Ti, though the incompatibility difference is more significant between Zr and Y (e.g. Sun and McDonough, 1989). The source depletion would tend to lower Zr/Y ratio. In contrast, decreasing degrees of partial melting would tend to increase this ratio.

Also, due to strong partitioning of Y into garnet, Zr/Y can be significantly fractionated, if garnet remains as a residual mineral in the source; thus partial melting processes involving garnet-bearing sources may have a substantial effect in the fractionation of Zr/Y (particularly under low degrees of partial melting).

For discrimination between OA and OBAB, the element ratios used in these trees have relatively high information gain. However, Zr/Sm having high information gain value is not preferred within two decision trees constructed for discrimination of OA and OBAB. The discrimination between oceanic arcs and back-arcs starts with Th/Nb, which has been used also as a major feature in distinguishing between subduction and non-subduction settings. Since the chemical behaviors of these elements are given before, it is repeated here. However, in the discrimination of oceanic arcs and backarcs, Zr/Hf seems to have involved at the upper levels, whose behavior deserves some discussion. Zr and Hf are both subduction-immobile elements; thus their contributions to the mantle wedge are negligible. Zr is slightly more incompatible than Hf, which makes Zr to be concentrated more in the melt. Therefore, small degrees of partial melting may produce magmas with relatively high Zr/Hf ratios when compared with high degrees of melting. Similarly, source depletion would lower the Zr/Hf ratio of the source due to the extraction of Zr with the melt.

For discrimination between MOR+OP and OI+CWP of non-subduction settings, the element ratios used in these trees have relatively high information gain. However, La/Y, La/Yb and TiO_2/Yb having high information gain value are not preferred within two decision trees constructed for discrimination. In the classification of non-subduction settings, Sm/Yb and Nd/Zr appear as the main discriminators. The behavior of Sm/Yb is very similar to Sm/Y (as explained before). Sm is more incompatible than Yb, though the extent of fractionation is strongly controlled by the aluminous mineral phase in the source. Yb, as one the HREE, is highly compatible with garnet (e.g. Johnson 1998). Spinel, on the other hand, with low Dmelt/solid, cannot retain Yb. Thus, while the melting of a garnet-bearing mantle source may lead to an extensively fractionated Sm/Yb ratio, spinel-bearing sources would leave this ratio relatively unfractionated. Consequently, the depth of melting may have a substantial effect on the Sm/Yb ratio, based on which the aluminous phase would be stable. Nd/Zr, on the other hand, is sensitive to the degree of partial melting regardless of the type of aluminous phase. A low degree of partial melting and/or source enrichment would result in higher Nd/Zr ratios.

For discrimination between MOR and OP, the element ratios used in these trees have relatively high information gain. However, Th/Y having high information gain value is not preferred within two decision trees constructed for discrimination. Th/Yb is preferred instead of Th/Y behaving very similar for this discrimination. Th/Y ratio used at the first level display very similar fractionation behavior to Nb/Y during the melting of peridotite under upper mantle conditions. Th is a highly incompatible element, while Y is compatible, especially if garnet remains as a residual phase (e.g. McKenzie and O’Nions 1991). Thus, Th/Y ratio can be easily fractionated during low degrees of partial melting. The involvement of garnet would amplify this effect further. Also, since Th is highly incompatible, depleted sources are characterized by lower Th/Y ratios compared to enriched sources. Similarly, melt extraction also drives Th/Y ratio to lower levels.

For discrimination between OI and CWP, the element ratios used in these trees have relatively high information gain. However, Sm/Y is not preferred within two decision trees constructed for discrimination. Sm/Yb is preferred instead of Sm/Y behaving very similar for this discrimination. The discrimination between CWP and OI probably constitutes the most difficult classification due to the compositional resemblance of lavas generated in these settings (Figure 4.1 and Figure 4.2), which arise from their derivation from similar mantle sources and under similar degree of partial melting (e.g. Furman et al.,2006; Panter et al.,2006).

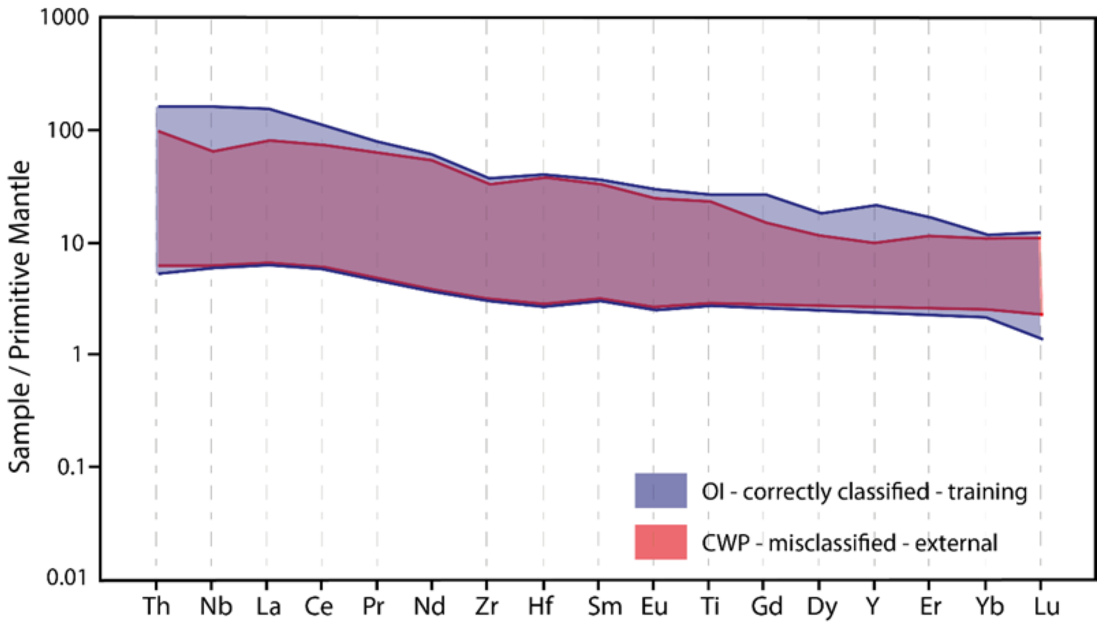

Figure 4.1. Comparison of spider-diagrams between samples from continental within-plates misclassified as oceanic island and samples of oceanic islands correctly classified (normalization coefficients are based on Sun and McDonough, 1995)

Since they include no or minimal subduction component in most cases, subduction-sensitive ratios Th/Nb and Nb/Nb* do not work at the uppermost level. However, some CWP lavas are result of very low degree of melting under great depths. These ones, with potassic/ultrapotassic compositions, are extremely enriched in incompatible elements (e.g. Janney et al.,2002). Thus, a ratio including a highly incompatible element and compatible element that can be retained by garnet (like Nb/Y) can be useful for the first order classification.

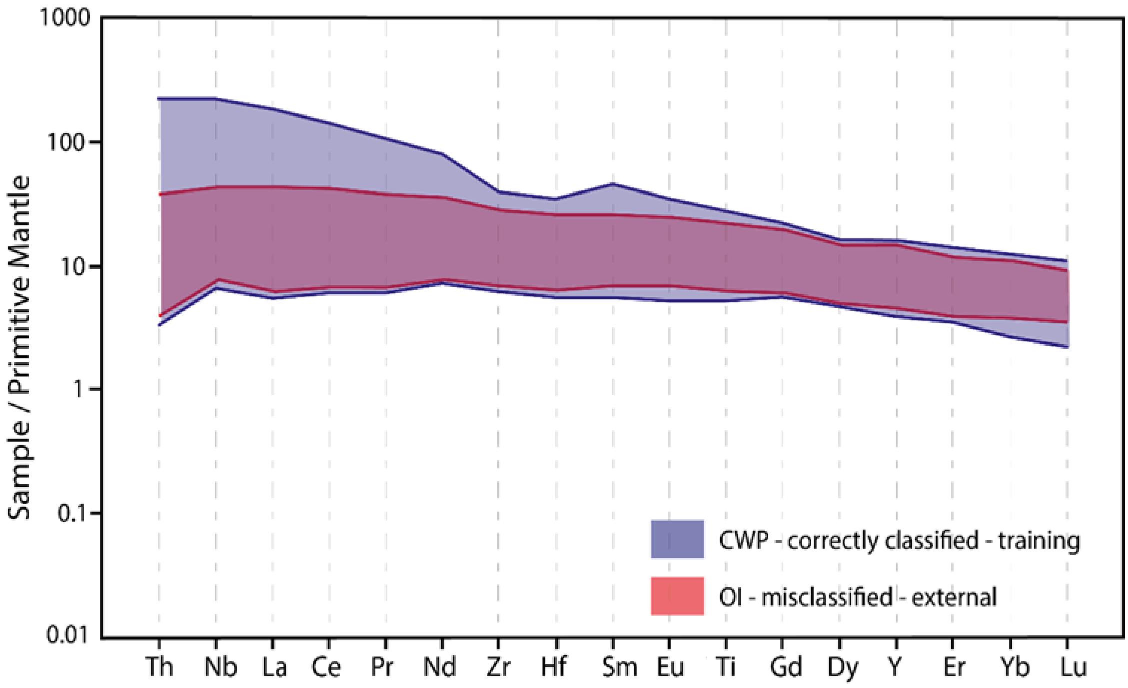

Figure 4.2. Comparison of spider-diagrams between samples oceanic islands misclassified as continental within-plate and samples of continental within-plate correctly classified (normalization coefficients are based on Sun and McDonough, 1995)

From information gain values of element ratios, it can be observed that the complexity of discriminations increases towards the right side of the table as the effectiveness of element ratios to discriminate settings decrease.

4.1.2. Discussion Based on Lift Curves and ROC Curves

When lift curves (Figure 4.3) are evaluated, it can be stated that most of the classifications are constructed based on a model but not random. ROC curve of decision trees (Figure 4.4) also indicates that the decision trees are successful with high AUC values and classification ratios and developed based on a model having AUC values greater than 0.5. Most of the classifications based on decision trees are close to a wizard pattern, especially discrimination of

(1) OA-CA,
(2) Oceanic and continental settings,
(3) OA-OBAB,
(4) MOR+OP and OI+CWP, and
(5) OI-CWP.

Interestingly, decision trees for discrimination of MOR-OP and OI-CWP have problems for the classification of external datasets by correct discrimination of OP, OI and CWP. However, lift curve and ROC curves suggest that these misclassifications are not based on the failure of decision tree models but based on the characteristics of external samples and they can be inseparable due to several geochemical or petrological constraints, which will be discussed and explained using spider-diagrams.

4.1.3. Discussion Based on Statistical Evaluation of Decision Trees

Statistical parameters to consider the quality of decision trees are AUC (Area Under ROC Curve), classification accuracy, f value, precision and recall values. When lift curves and ROC are compared with area under ROC (AUC), classification accuracy, f value, precision and recall values (Table 4.2, 4.3, 4.4, 4.5, 4.6, 4.7, 4.8 and 4.9), nearly all decision trees have high AUC and classification accuracy values, which indicates that they are constructed based on a model, which is successful in discrimination of two settings as classes from each other.

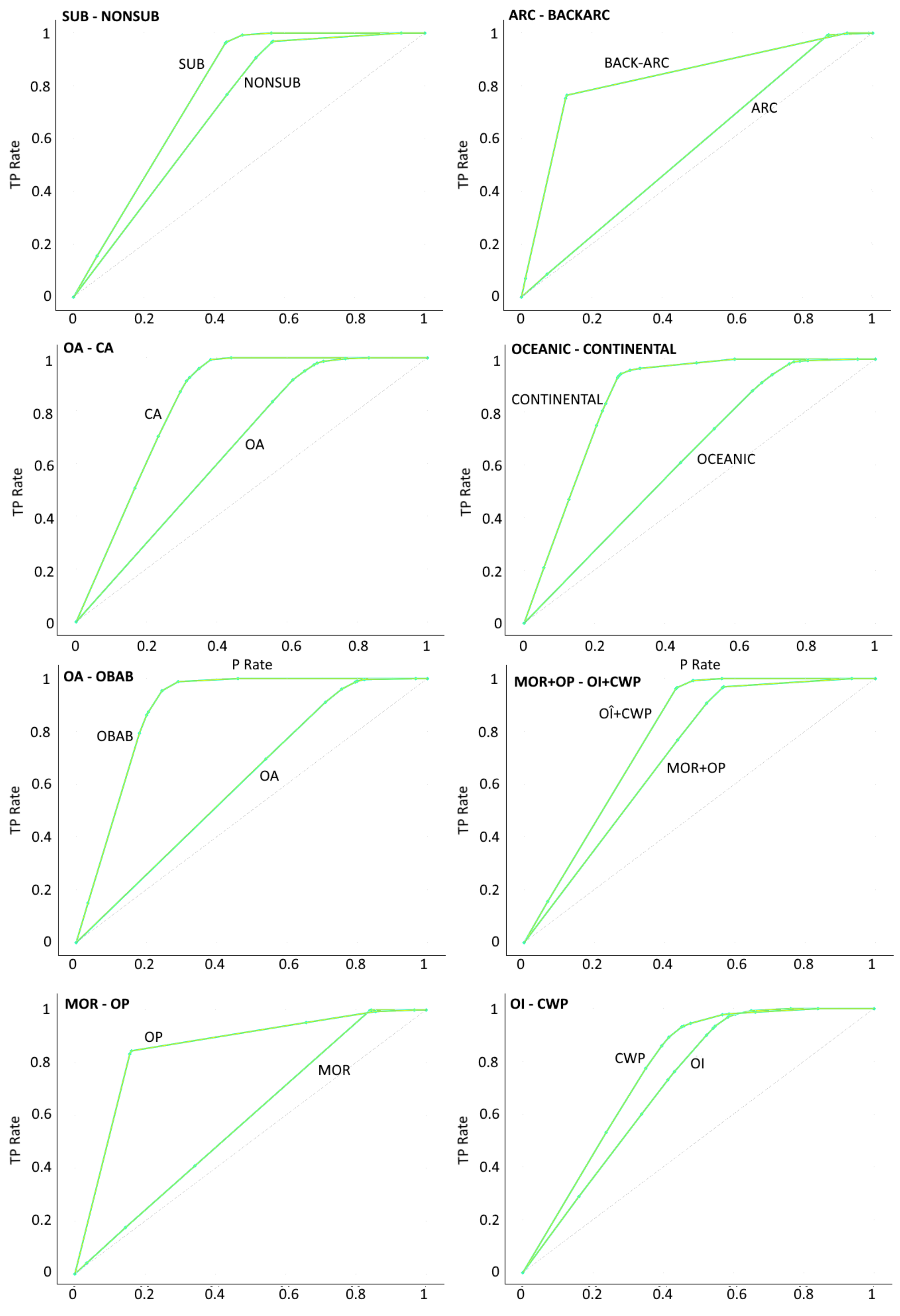

Figure 4.3. Lift curve for tectonic discriminations

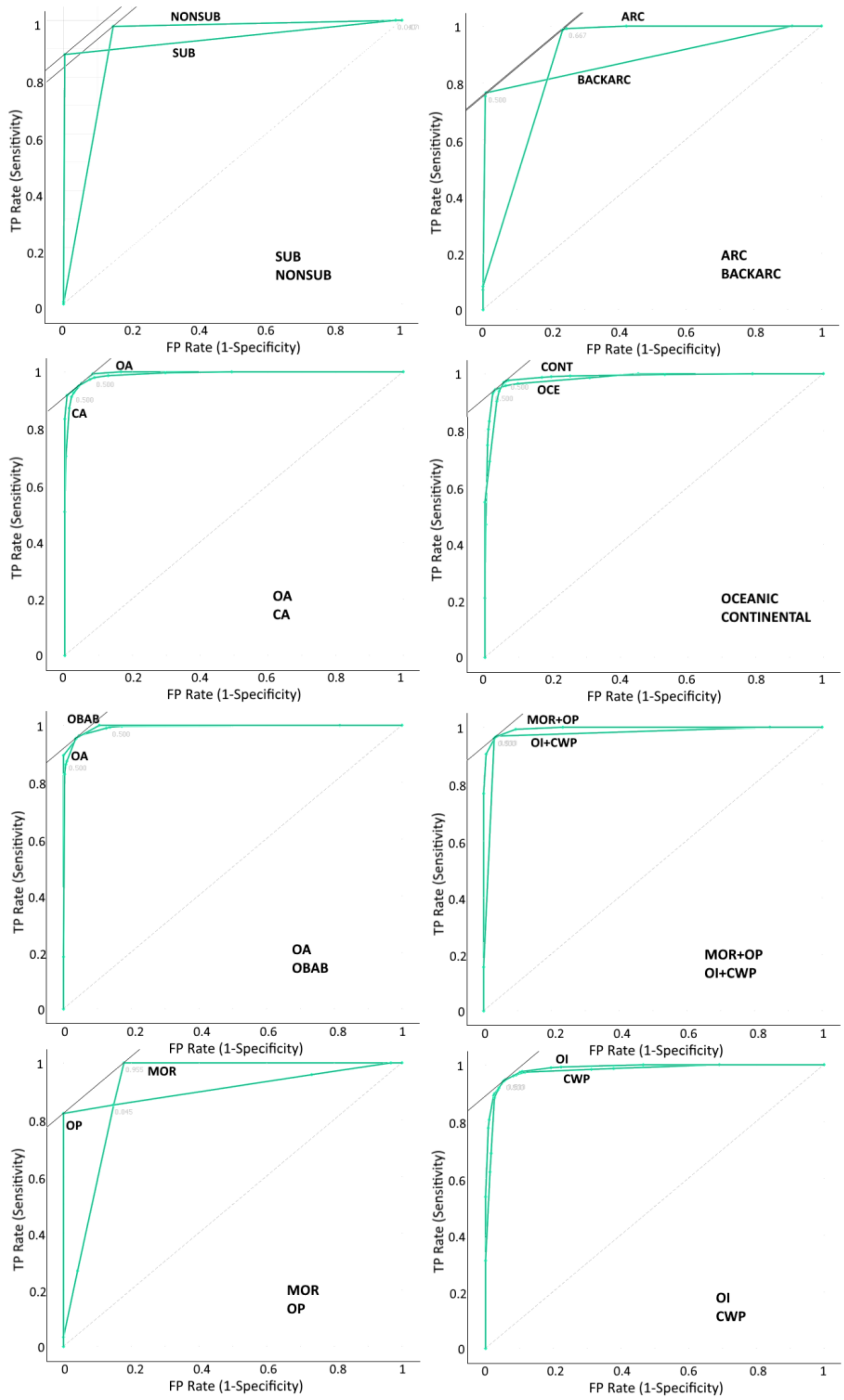

Figure 4.4. ROC for *tectonic* discriminations

Table 4.2. Statistical considerations for discrimination between subduction and non-subduction *settings*

	SUBDUCTION - NONSUBDUCTION						
	Tree 1	Tree 2				Tree 3	
Level	1	1	2	3	4	1	2
AUC	0.912	0.916	0.924	0.925	0.924	0.912	0.925
Cl.Acc.	0.943	0.948	0.960	0.961	0.962	0.943	0.961
F	0.882	0.948	0.959	0.960	0.961	0.882	0.960
Precision	0.915	0.948	0.960	0.961	0.962	0.915	0.962
Recall	0.851	0.948	0.960	0.961	0.962	0.851	0.961

Table 4.3. Statistical considerations for discrimination between arc and back-arc settings

	ARC - BACKARC							
	TREE 1				TREE 2			
Level	2	3	4	5	2	3	4	5
AUC	0.840	0.840	0.835	0.824	0.840	0.847	0.793	0.785
Cl.Acc.	0.906	0.907	0.908	0.908	0.906	0.908	0.905	0.907
F	0.900	0.902	0.904	0.904	0.900	0.903	0.900	0.904
Precision	0.899	0.901	0.903	0.903	0.899	0.902	0.899	0.902
Recall	0.906	0.907	0.908	0.908	0.906	0.908	0.905	0.907

Table 4.4. Statistical considerations for discrimination between oceanic and continental arcs

	Oceanic Arc – Continental Arc											
	TREE 1						TREE 2					
Level	2	3	4	5	6	7	2	3	4	5	6	7
AUC	0.807	0.834	0.849	0.865	0.853	0.833	0.791	0.791	0.860	0.863	0.843	0.818
Cl.Acc.	0.762	0.756	0.778	0.811	0.833	0.822	0.771	0.771	0.798	0.833	0.844	0.827
F	0.767	0.759	0.781	0.815	0.836	0.825	0.755	0.755	0.790	0.833	0.845	0.828
Precision	0.779	0.766	0.786	0.827	0.843	0.832	0.766	0.766	0.793	0.833	0.846	0.829
Recall	0.762	0.756	0.778	0.811	0.833	0.822	0.771	0.771	0.798	0.833	0.844	0.827

Table 4.5. Statistical considerations for discrimination between oceanic and continental settings

	OCEANIC CONTINENTAL									
	TREE 1					TREE 2				
Level	2	3	4	5	6	2	3	4	5	6
AUC	0.735	0.735	0.847	0.878	0.870	0.731	0.731	0.834	0.859	0.845
Cl.Acc.	0.811	0.811	0.813	0.860	0.864	0.807	0.807	0.817	0.856	0.862
F	0.799	0.799	0.818	0.862	0.864	0.795	0.795	0.820	0.854	0.860
Precision	0.801	0.801	0.829	0.865	0.865	0.797	0.797	0.825	0.853	0.860
Recall	0.811	0.811	0.813	0.860	0.864	0.807	0.807	0.817	0.856	0.862

Table 4.6. Statistical considerations for discrimination between Oceanic Arc and Oceanic Back-Arc Basins

	OA - OBAB									
	TREE 1					TREE 2				
Level	2	3	4	5	6	2	3	4	5	6
AUC	0.876	0.889	0.906	0.909	0.898	0.876	0.889	0.912	0.912	0.914
Cl.Acc.	0.905	0.905	0.913	0.921	0.913	0.905	0.905	0.915	0.921	0.918
F	0.898	0.901	0.910	0.917	0.912	0.898	0.901	0.912	0.917	0.915
Precision	0.907	0.903	0.911	0.919	0.911	0.907	0.903	0.913	0.919	0.916
Recall	0.905	0.905	0.913	0.921	0.913	0.905	0.905	0.915	0.921	0.918

Table 4.7. Statistical considerations for discrimination between Group 1 and Group 2 of Non-Subduction Settings

	MOR+OP and OI+CWP									
	TREE 1					TREE 2				
Level	2	3	4	5-6	7	2	3	4	5-6	7
AUC	0.942	0.958	0.966	0.966	0.958	0.942	0.958	0.966	0.965	0.955
Cl.Acc.	0.878	0.893	0.909	0.916	0.938	0.878	0.893	0.909	0.918	0.942
F	0.877	0.893	0.909	0.916	0.938	0.877	0.893	0.908	0.918	0.942
Precision	0.883	0.893	0.911	0.916	0.938	0.883	0.893	0.910	0.919	0.942
Recall	0.878	0.893	0.909	0.916	0.938	0.878	0.893	0.909	0.918	0.942

Table 4.8. Statistical considerations for discrimination between Mid-Ocean Ridge and Oceanic Plateau

	MID-OCEAN RIDGE - OCEANIC PLATEAU										
	TREE 1					TREE 2					
Level	2	3	4	5	6	2	3	4	5	6	7
AUC	0.820	0.845	0.876	0.874	0.849	0.820	0.842	0.867	0.875	0.875	0.842
Cl.Acc.	0.825	0.879	0.925	0.924	0.934	0.825	0.868	0.921	0.922	0.922	0.934
F	0.836	0.868	0.924	0.921	0.931	0.836	0.853	0.919	0.920	0.920	0.932
Precision	0.857	0.872	0.923	0.922	0.933	0.857	0.859	0.918	0.919	0.919	0.932
Recall	0.825	0.879	0.925	0.924	0.934	0.825	0.868	0.921	0.922	0.922	0.934

Table 4.9. Statistical considerations for discrimination between Ocean Island and Continental Within-Plate

	OCEAN ISLAND - CONTINENTAL WITHIN-PLATE								
	TREE 1					TREE 2			
Level	3	4	5-6	7	8	3	4	5-6-7	8
AUC	0.837	0.864	0.897	0.908	0.897	0.837	0.864	0.893	0.886
Cl.Acc.	0.807	0.827	0.851	0.870	0.863	0.807	0.827	0.961	0.855
F	0.807	0.828	0.851	0.870	0.862	0.807	0.828	0.861	0.855
Precision	0.807	0.828	0.851	0.870	0.862	0.807	0.828	0.862	0.855
Recall	0.807	0.827	0.851	0.870	0.863	0.807	0.827	0.861	0.855

4.2. Discussion of Classification Results

4.2.1. Discrimination Between Subduction and Non-Subduction Settings

For training and test datasets, the decision stump correctly classified 1,932 samples of non-subduction out of 1,974 with a success ratio of 97.87% and 577 samples of subduction out of 668 with a success rate of 86.38%. Decision stump using Th/Nb is more effective for the tectono-magmatic discrimination of samples from non-subduction settings compared to those from subduction settings.

The first decision tree is more successful than the decision stump at all levels. The maximum classification ratio for samples of subduction settings is at levels 1, 3 and 4 with a success ratio of 88.47% (591 out of 668) and for samples of non-subduction settings is at level 2 and 4 with a success ratio of 99.49% (1964 out of 1974). The introduction of TiO_2/Yb ratio to the second tree at the second level negatively affects the correct classification of subduction samples with a decrease by 4 and the introduction of Zr/Nb ratio to the second tree at the third level adversely affects the correct classification of non-subduction samples with a decrease by 2.

The second decision tree is also more successful than the decision stump at all levels except its first level for samples of non-subduction. The second decision tree has a simple structure, which makes the application of this tree easier for users. This tree has the same classification ratio of the second tree for the samples of subduction with a success ratio of 88.47% (591 out of 668). However, for non-samples of non-subduction, the second decision tree can only achieve the success ratio of the second tree at its third level with a success ratio of 99.39% (1,962 out of 1,974). For the second decision tree, the introduction of Nb/Y ratio at the second level has no effect on the classification rate of subduction but has a positive impact on samples of non-subduction with an increase by 34.

For external datasets, the decision stump has a correct classification ratio of 96.56% for samples of non-subduction (1,937 out of 2006) and 80.47% for samples of subduction (375 out of 466). Although success ratios decrease about 1% for non-subduction and 6% for subduction, decision stump shall be accepted to be a successful method to discriminate between subduction and non-subduction settings with a single discriminating feature (Th/Nb).

The first decision tree has its maximum classification ratio at levels 1, 3, and 4 for samples of subduction with a success ratio of 84.98% (396 out of 466) and level 2 for samples of non-subduction with success ratio of 98.75% (1,981 out of 2,006). With the introduction of Zr/Nb ratio at the third level of the second tree, the correct classification for samples of non-subduction decreases by 4, and the introduction of La/Nb ratio at the fourth level had no positive or negative effect relative to level 3. The introduction of TiO_2/Yb has a negligible negative impact on correct classification for samples of subduction samples with a decrease by 1. The first decision tree is more applicable to external datasets when compared to decision stump, although success ratios decrease about 1% for non-subduction and 3% for subduction. Both level 2 for its simplicity and level 4 for its maximum success ratio for both training-test and external datasets shall be preferred.

The second decision tree is also more applicable to external datasets when compared to decision stump along with a simple structure with only 2 levels in depth. This tree has its maximum classification ratio at level 1 for samples of subduction with a success ratio of 84.98% (396 out of 466) and level 2 for samples of non-subduction with success ratio of 98.65% (1,979 out of 2,006). The introduction of Nb/Y has a slightly negative effect on the correct classification of subduction with a decrease by 3 but a considerable positive impact on that of non-subduction with an increase by 37. Therefore, the overall success ratio of level 2 of the second decision tree is much better than level 1. The success ratios for application of this decision tree to external datasets decrease by about 1% for non-subduction and 4% for subduction.

The decision trump has only single level of depth using Th/Nb ratio (also known as decision stump) obtained a very high success ratio for all datasets (more than 90% in overall) and became more successful for samples of non-subduction with respect to those of subduction eliminating the risk of underfitting due to its simple structure. The success ratio of this decision tree is distributed homogeneously through the articles from different locations, with a few exceptions for the training and test datasets.

For training and test datasets, 45 articles out of 63 having 2,045 samples are classified correctly with 100% success ratio. 18 articles have misclassifications with varying misclassification ratios. Mid-oceanic ridges are completely classified as "non-subduction setting" with a 100% success ratio. Continental arcs, continental within-plates, oceanic arcs, oceanic islands are quite successful for the discrimination between subduction and non-subduction. Misclassifications for the decision stump are only 6 samples of continental arcs out of 181 samples from 7 articles, 38 samples of continental within-plates out of 376 samples from 12 articles, 16 samples of oceanic arcs out of 381 samples from 14 articles and only 1 samples of oceanic islands out of 478 samples from 9 articles. For continental arcs, Mullen (2017) of Cascade Arcs is the only article, having misclassifications with a misclassification ratio of 17.14% (6 out of 35). For continental within-plates, Mirnejad (2006) of Leucite Hills and Coe (2008) of South Africa are misclassified as "subduction" by decision trump with misclassification rates of 100% and 85.19%, with respectively. Gibson (2000) and Janney (2002), on the other hand, obtained relatively high success ratios with low misclassification rates.

For oceanic arcs, 6 articles have slight misclassification rates ranging from 1% to 38%: Jolly (2008a), Tollstrup (2010), Pearce (2005), Jolly (2007), Bedard (1999) and Todd (2012) with an order of increasing misclassification rate. Oceanic back-arcs generally failed at discrimination between subduction and non-subduction settings. All 5 articles have larger misclassification rates, with 4 of them having a misclassification rate greater than 50%. Pearce (2005) almost completely failed with a misclassification rate of 96% (24 out of 25 samples). Oceanic islands and oceanic plateaus are also quite successful for the discrimination between subduction and non-subduction. Only 1 sample of oceanic island is misclassified out of 478 samples from 9 articles, and only 3 samples of oceanic plateaus are misclassified out of 211 samples from 4 articles.

The decision stump is also successfully applicable to the tectono-magmatic discrimination of external datasets. For external datasets, 38 articles out of 62 having 1,406 samples are classified correctly with 100% success ratio. 24 articles have misclassifications with varying misclassification ratios. Continental arcs and oceanic islands are entirely classified with 100% success ratio. Mid-oceanic ridges and oceanic plateaus are also quite successful for the discrimination between subduction and non-subduction. Only 3 samples of mid-oceanic ridge are misclassified out of 1,304 samples from 5 articles, and only 2 samples are misclassified out of 163 samples from 9 articles. Oceanic back-arcs and continental within-plates generally failed at the discrimination between subduction and non-subduction settings. For oceanic back-arcs, 5 articles out of 6 completely failed for discrimination. For continental within-plates, 9 articles out of 16 have misclassifications with rates ranging between 10% and 100%. Davies (2006) of Aldan Shield, Gibson (2005) of Tristan, and Oliebrook (2016) of Bunbury failed for the discrimination almost completely. In spite of having misclassifications in several articles for oceanic arcs, the only problematic one is König (2008), with samples from various subduction zones with a misclassification rate of 50%.

The first decision tree became more successful compared to the decision stump, and misclassifications have a homogeneous distribution through the articles from different locations for training and test datasets. For training and test datasets, 48 articles out of 63 having 1,674 samples are classified correctly with 100% success ratio. 15 articles have misclassifications with varying misclassification ratios. Oceanic islands are completely classified with 100% success ratio at all levels of this decision tree. Continental arcs, mid-oceanic ridges, oceanic arcs and oceanic plateaus are also quite successful for the discrimination between subduction and non-subduction. Misclassifications for the second tree are only 6 samples of continental arcs out of 181 samples from 7 articles, 8 samples of mid-oceanic ridges out of 909 samples from 12 articles, 11 samples of oceanic arcs out of 381 samples from 14 articles and 1 sample of oceanic plateau out of 211 samples from 4 articles.

The first decision tree is also much more effective for the discrimination of continental within-plates when compared to decision stump with only 1 misclassification out of 376 samples from 12 articles. The problem in tectono-magmatic discrimination of oceanic back-arcs can not be solved at the second tree. All articles from oceanic back-arc have large amounts of misclassifications with ratios more than 50% except one

(24%). When different levels of this decision tree are evaluated, especially the introduction of TiO_2/Yb ratio at level 2 can correctly discriminate most of the continental within-plates, that have been misclassified at level 1. However, interestingly, increasing level of depth for the second decision tree seems to have no positive or negative effect on the misclassifications at the first level. For such articles, there is no apparent difference between level 1 and level 4. Therefore, levels 2, 3 and 4 shall be used for discrimination between subduction and non-subduction without having a significant difference in their success ratios.

The first decision tree is also successfully applicable to the tectono-magmatic discrimination of external datasets. For external datasets, 45 articles out of 62 having 1,055 samples are classified correctly with 100% success ratio. 17 articles have misclassifications with varying misclassification ratios. Continental arcs, oceanic islands, and oceanic plateaus are completely classified with 100% success ratio at all levels of this decision tree. This result indicates that Nb/Nb* ratio is quite effective discriminating feature for these three tectonic settings. Mid-oceanic ridges and oceanic arcs are also quite successful for the discrimination between subduction and non-subduction. Misclassifications for the second tree are only 9 samples of mid-oceanic ridges out of 1,304 samples from 5 articles and 6 samples of oceanic arcs out of 223 samples from 12 articles. The problem in tectono-magmatic discrimination of continental within-plates and oceanic back-arcs can not be solved for the external datasets at the second tree. Only Gibson (2005) of Tristan can be correctly classified with the introduction of TiO_2/Yb ratio at the second level. Other than the introduction of TiO_2/Yb ratio, increasing the level of depth in the second decision tree seems to have no positive or negative effect for the articles misclassified at the first level.

Therefore, for external datasets, levels 2 and 4 of the first decision tree shall be used for discrimination between subduction and non-subduction.

The second decision tree also became more successful compared to the decision stump through articles from different locations in spite of having a simple structure when compared with the first decision tree.

For training and test datasets, 47 articles out of 63 having 1,578 samples are classified correctly with 100% success ratio. 16 articles have misclassifications with varying misclassification ratios. Oceanic islands are completely classified with 100% success ratio at all levels of this decision tree.

Continental arcs, mid-oceanic ridges, oceanic arcs, and oceanic plateaus are quite successful for the discrimination between subduction and non-subduction.

Misclassifications for the second decision tree are only 6 samples of continental arcs out of 181 samples from 7 articles, 8 samples of mid-oceanic ridges out of 909 samples from 12 articles, 11 samples of oceanic arcs out of 381 samples from 14 articles and 1 sample of oceanic plateau out of 211 samples from 4 articles. Continental within-plates cannot be correctly classified at the first level of this decision tree, but with the introduction of Nb/Y ratio at the second level, only 3 samples are misclassified out of 376 samples from 12 articles. Oceanic back-arcs cannot be discriminated with the second decision tree just like the other decision trees, so they are considered as problematic.

The second decision tree is also successfully applicable for tectono-magmatic discrimination of external datasets, just like to previous two decision trees. Among all decision trees constructed for the tectono-magmatic discrimination between subduction and non-subduction, no underfitting or overfitting has been observed.

For external datasets, 45 articles out of 62 having 1,055 samples are classified correctly with 100% success ratio. 17 articles have misclassifications with varying misclassification ratios. Oceanic islands and oceanic plateaus are completely classified correctly with 100% success ratio at all levels of this decision tree. Continental arcs are classified correctly at the first level, but with the addition of Nb/Y ratio at the second level, 3 misclassifications are observed out of 96 samples from 7 articles.

However, Nb/Y ratio is a very effective discriminating feature for continental within-plates as it correctly classifies nearly all samples misclassified in the previous level. Mid-oceanic ridges and oceanic arcs are quite successful for the discrimination between subduction and non-subduction. Misclassifications for the second decision tree are only 9 samples of mid-oceanic ridges out of 1,304 samples from 5 articles and 6 samples of oceanic arcs out of 223 samples from 12 articles. Oceanic back-arcs cannot be discriminated for both training-test and external datasets with the second decision tree just like the other decision trees, so they are considered as problematic.

The success rates obtained from Th/Nb, Nb/Nb*, TiO_2/Yb, and Nb/Y, appear to be consistent with their diverse fractionation in different tectonic settings. The different chemical behavior of Th (and La) and Nb during subduction-related processes make Th/Nb an efficient discriminator.

However, Nb/Nb* when coupled with element ratios TiO_2/Yb and Nb/Y (garnet-sensitive) produces even better results. This is also expected, since Nb/Nb* enables simultaneous use of Th and La, and the TiO_2/Yb and Nb/Y are garnet-sensitive.

The garnet signature (high Ti/Yb and Nb/Y ratios) is not typical in mid-ocean ridges and subduction systems since the melting dominantly takes place in the stability field of spinel (e.g. Pearce and Parkinson, 1993; Niu and Batiza, 1997; Arevalo Jr. and McDonough, 2010). At within-plate settings, however, this feature becomes widespread due to deeper depths of melting that occurs within the stability field of garnet (e.g. McKenzie and O'Nions 1991). Since MORs do not involve subduction component in their petrogenesis, the low Ti/Yb and Nb/Y samples would be expected to include mostly subduction-related ones. As reflected from the success rates, TiO_2/Yb and Nb/Y effectively discriminate subduction-related samples (low Nb/Nb*) having low Ti/Yb and Nb/Y.

Although Th/Nb and Nb/Nb* are very useful discriminants on the subduction-non-subduction classification, there are some instances in which the source-related features cause distinction between these two classes nearly impossible. The kimberlite samples from South Africa (Coe et al.,2008) and the lamproites from the Leucite Hills (Mirnejad and Bell 2006) are two examples that are classified by high misclassification rates based on these two variables. The main reason for such occurrences is the involvement of the SCLM source that has been metasomatized by slab-derived components during a previous/ancient subduction event. Since the SCLM is able to preserve such signatures for an extended period of time (e.g. McKenzie and O'Nions 1983), a recent melting event on the subduction-metasomatized domains on such a mantle source would result in subduction-related geochemical signatures even though there is no active subduction involved (e.g. Gibson et al.,1993). Thus, subduction-related geochemical signatures can also be produced at a CWP setting, which similar to those from subduction settings. The Th-Nb-La systematics of such CWP melts are indistinguishable from those produced at subduction zones, which in turn makes Th/Nb and Nb/Nb* inefficient for the discrimination.

Although some potassic/ultrapotassic kimberlitic magmas carry subduction-related geochemical signatures as discussed above, their highly enriched nature makes them quite different than those originated from the subduction zones. Since the potassic/ultrapotassic magmas form by very small-degree partial melting, their elemental budget is ultra-enriched in terms of highly incompatible elements (e.g. Fraser and Hawkesworth 1992; Araujo et al.,2001; Coe et al.,2008). Therefore, Th, Nb, La abundances of these magmas are too high when compared with those from subduction zones (Figure 4.5). Furthermore, the potassic/ultrapotassic CWP melts are generated at great depths involving garnet as a residual phase. This leads to extensive fractionation between incompatible elements and HREE, which in turn results in extremely high ratios of Nb/Y and Ti/Yb (e.g. LeRoex et al.,2003) (Figure 4.5). Since such extreme values are not common from the subduction zones, the element ratios such as Nb/Y and Ti/Yb can be useful discriminators in the cases that Th/Nb and Nb/Nb* does not work.

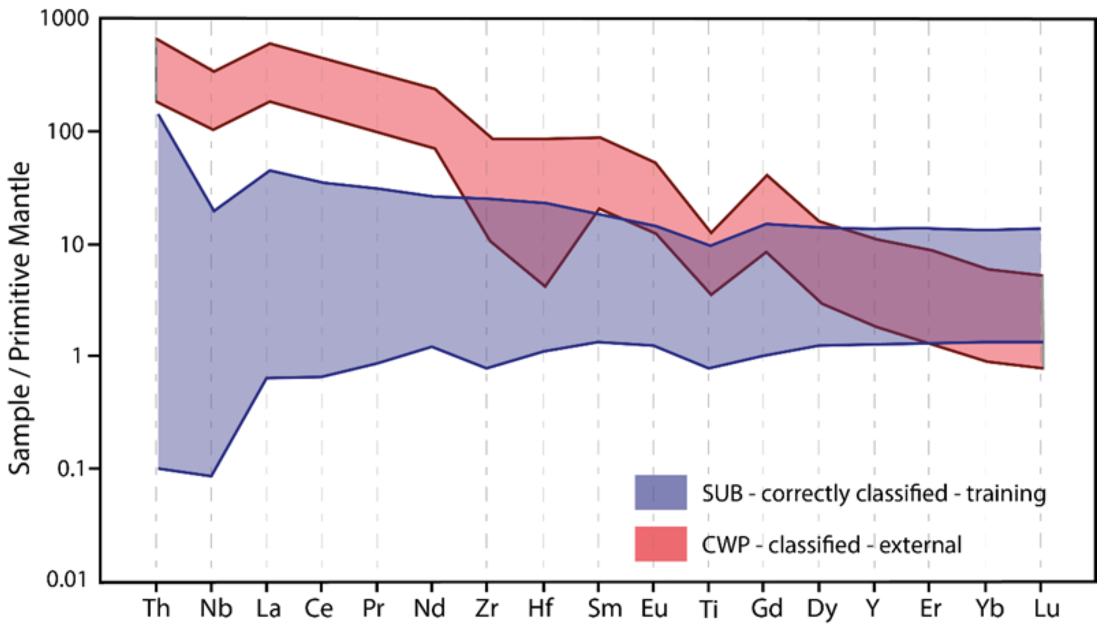

Figure 4.5. Comparison of spider-diagrams between samples continental within-plates and subduction-related settings (normalization coefficients are based on Sun and McDonough, 1995)

It is seen from the above discussion that some lithologies from CWP settings can be recovered in the process of tectonomagmatic classification using some of their petrogenetic features, although they fail at the upper classification levels. Another case in which the classification is difficult comes from BAB settings. As mentioned in Chapter 2, the BABs are like a hybrid between MORs and arcs.

As a natural consequence of this dual nature, the magmas generated at the BABs display a compositional spectrum between these two extremes (e.g. Pearce et al.,1995b; Leat et al.,2004; Pearce et al.,2005). Some BAB magmas show MORB-like subduction-immobile chemistry with the addition of subduction component (relative Th-LREE enrichment), known as "BABB-type" chemistry.

Some, on the other hand, exhibit geochemical characteristics close to the end-members (MORB- and OAB-like). Such BAB magmas are derived from identical mantle sources to either that of MORBs or OABs. The BAB melts produced by decompression melting of MORB-source mantle with no subduction influx would be very akin to melts generated at MORs (Figure 4.6).

Thus, such cases pose a great problem in discrimination of subduction samples (in this case, BAB) from non-subduction ones (MOR). Therefore, the misclassification problem between some BABs and MORs does not appear to arise from the inefficiency of the decision tree classification. Instead, some MOR and BAB melts are indistinguishable in terms of their trace element systematics.

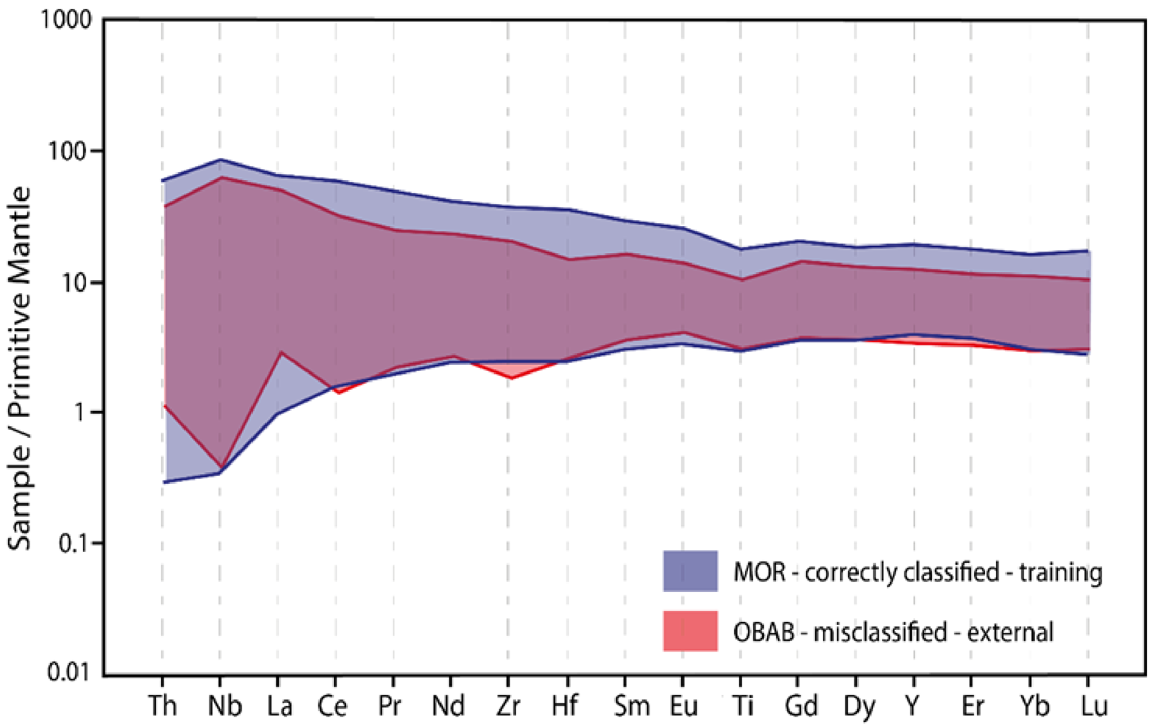

Figure 4.6. Comparison of spider-diagrams between samples from OBAB misclassified as MOR and samples from MOR (normalization coefficients are based on Sun and McDonough, 1995)

4.2.2. Discrimination Within Subduction Settings

4.2.2.1. The First Path for Discrimination Within Subduction Settings

4.2.2.1.1. Discrimination Between Arc and Back-arc-related Settings

For training and test datasets, the first tree correctly classified 556 samples of arcs out of 562 with a success ratio of 98.93% and 92 samples of back-arcs out of 106 with a success ratio of 86.79%. This decision tree is much more successful for the discrimination of arc samples with respect to back-arc samples. However, this may be a result of a limited number of samples in back-arcs as reliable data for back-arcs in literature is also limited. The introduction of Y/Yb at the fourth level increased correctly classified subduction samples by 8 whereas misclassifications in non-subduction samples also increased by 4. These misclassifications are solved by the introduction of Zr/Hf at the fifth level.

A very similar pattern is also observed in the second decision tree. The second decision tree is less successful for the discrimination of back-arc samples with 89 samples out of 106 with a success ratio of 83.96%; however, there are no differences for the discrimination of arc samples.

When the structures of decision trees are evaluated, the first decision tree obtains the highest success ratio at the fifth level for both tectonic settings, whereas the second decision tree at the fourth level for back-arcs and the fifth level for arcs. In the second decision tree, introduction of Zr/Y and Y/Yb at fourth level increased correctly classified subduction samples by 7 but has no positive or negative effect on non-subduction samples and Nd/Zr and Zr/Hf at fifth level increased correctly classified non-subduction samples by 1 whereas misclassifications for subduction samples increased by 1 at this level.

Different than the general trend of their success ratio with an increasing level in depths, both decision trees are more successful in the lower levels at the discrimination of arc and back-arc-related settings for external datasets. Both decision trees have their maximum success ratio at the second level in depth for back-arcs with 68 samples out of 102 (66.67% success ratio).

The first decision tree is the most successful for discrimination of arcs in the second and third levels with 348 samples out of 364 (95.60% success ratio), whereas the second decision tree is the most successful in the third level with 354 samples out of 364 (97.25% success ratio).

For the first decision tree, success for the discrimination of back-arcs decreases with the introduction of TiO_2/Y and Nd/TiO_2 at the third level, and that of arcs decreases with the introduction of Y/Yb at the fourth level. However, these decreases are negligible compared to the decrease in success for the second decision tree at its fourth level with the introduction of Zr/Y and Y/Yb, which results in an additional 10 misclassifications for back-arcs and 4 misclassifications for arcs.

Both decision trees are more successful for the discrimination of arcs with respect to that of back-arcs for both training+test datasets and external datasets.

When the contradiction between the success ratios of both decision trees at the discrimination of training+test datasets and external datasets, it shall be assumed that deeper decision trees may be more successful at the discrimination of training and test set but fail more for the discrimination of external datasets, resulting in overfitting. Therefore, considering the results for training+test sets and external datasets, fourth and fifth levels shall be preferred considering the geochemical and petrological properties of rock samples and comparison with article-based discussion.

The first decision tree obtained a very high success ratio for all datasets (more than 90% overall) and became more successful for samples of arc with respect to those of back-arc-related settings. The success ratio of this decision tree is distributed homogeneously through the articles from different locations, with a few exceptions for the training and test datasets.

For training and test datasets, 18 articles out of 26 having 411 samples are classified correctly with 100% success ratio. 8 articles have misclassifications with varying misclassification ratios. Continental arcs and oceanic arcs quite successful for the discrimination between arc and back-arc-related settings. Misclassifications for the first decision tree are only 3 samples of continental arcs out of 181 from 7 articles and 3 samples of oceanic arcs out of 381 from 14 articles. Similarly, with the discrimination between subduction and non-subduction settings, oceanic back-arcs have misclassification through all articles. Only one article (Leat, 2004 of South Sandwich) can be completely classified.

However, the misclassification rates for this classification are relatively lower than the first set of classifications between subduction and non-subduction. 25 misclassifications through 106 samples of oceanic back-arcs from 5 articles result in a success ratio of 76.42%. The increasing level of depth for the first decision tree seems to have no significant positive or negative effect for the misclassifications at the first level with few exceptions. Todd (2012) of Fiji Tonga and Peate (1997) of Vanuatu are correctly classified at the second level, and Jolly (2007) of Greater Antilles Arcs is only misclassified at the fourth level. For other articles, there is no obvious difference between level 1 and level 5. Therefore, levels 3, 4 and 5 shall be used for discrimination between arc and back-arc-related settings without having a significant difference in their success ratios.

The first decision tree is also successfully applicable for the tectono-magmatic discrimination of external datasets. For external datasets, 15 articles out of 26 having 293 samples are classified correctly with 100% success ratio. 11 articles have misclassifications with varying misclassification ratios. Continental arcs are completely classified with 100% success ratio at all levels of this decision tree. This result indicates that Nb/Nb* ratio is quite effective discriminating feature for these tectonic settings. Oceanic arcs are quite successful for the discrimination between arc and back-arc-related settings. Misclassification for the second tree is 17 samples of oceanic arcs out of 223 from 12 articles. Oceanic back-arcs are still problematic and can be discriminated with relatively lower success ratios in the discrimination between arc and back-arc-related settings. 40 misclassifications out of 102 samples from 6 articles result in a very low success ratio of 60.78%. Harrison (2003) of East Scotia and Sinton (2003) of Mantus are completely misclassified. Only Bezos (2009) of Lau Basin can be correctly classified with 100% success ratio. Ikeda (2003) of Mariana has 3 misclassifications out of 15 samples with a success ratio of 80%. The other two articles have misclassifications 50% and 67%, respectively.

The problem for the correct classification of oceanic back-arcs in the discrimination of arc and back-arc-related settings, as well as between subduction and non-subduction settings can not be solved in training and test datasets and is also observed in external datasets. The second decision tree is successfully applicable for the tectono-magmatic discrimination of training and test datasets, and the results are quite similar to those obtained from the first decision tree but with better success ratios.

For training and test datasets, 19 articles out of 26 having 508 samples are classified correctly with 100% success ratio. 7 articles have misclassifications with varying misclassification ratios. Continental arcs and oceanic arcs quite successful for the discrimination between arc and back-arc-related settings. Misclassifications for the first decision tree are only 4 samples of continental arcs out of 181 from 7 articles and 2 samples of oceanic arcs out of 381 from 14 articles. Similarly, with the first decision tree, oceanic back-arcs have misclassification through all articles. Only one article (Leat, 2004 of South Sandwich) can be completely classified. The misclassification rates for the second decision tree are relatively higher with respect to the first decision tree. 29 misclassifications through 106 samples of oceanic back-arcs from 5 articles result in a success ratio of 72.64%, with a decrease of 3.78%. The increasing level of depth for the second decision tree seems to have no significant positive or negative effect for the misclassifications at the first level with few exceptions. Only Peate

(1997) of Vanuatu are correctly classified at the fourth level, and Jolly (2007) of Greater Antilles Arcs can also be classified at the fourth level. For other articles, there is no obvious difference between level 1 and level 5. Therefore, levels 3, 4 and 5 shall be used for discrimination between arc and back-arc-related settings without having a significant difference in their success ratios.

The second decision tree is also successfully applicable to the tectono-magmatic discrimination of external datasets. For external datasets, 14 articles out of 26 having 287 samples are classified correctly with 100% success ratio. 12 articles have misclassifications with varying misclassification ratios. Continental arcs are completely classified with 100% success ratio at all levels of this decision tree. This result indicates that Nb/Nb* ratio is quite effective discriminating feature for these tectonic settings. Oceanic arcs are quite successful for the discrimination between arc and back-arc-related settings. Misclassification for the second tree is 13 samples of oceanic arcs out of 223 from 12 articles. Oceanic back-arcs are still problematic and can be discriminated with relatively lower success ratios in the discrimination between arc and back-arc-related settings. 44 misclassifications out of 102 samples from 6 articles result in a very low success ratio of 56.86%. Harrison (2003) of East Scotia and Sinton (2003) of Manus are completely misclassified. Only Bezos (2009) of Lau Basin can be correctly classified with 100% success ratio. Ikeda (2003) of Mariana has 4 misclassifications out of 15 samples with a success ratio of 73%. The other two articles have misclassifications 58% and 73%, respectively. The problem for the correct classification of oceanic back-arcs in the discrimination of arc and back-arc-related settings, as well as between subduction and non-subduction settings, can not be solved in training and test datasets and is also observed in external datasets.

The discrimination between arcs and oceanic back-arcs appears to be resolved with relatively high classification rates. One of the reasons for this lies behind the spreading factor of the mature oceanic back-arcs (see Chapter 1 for details), which tend to involve more MORB mantle component with less subduction input (leading to higher Nb/Nb*).

The arcs, on the other hand, include a strong subduction component in their petrogenesis (resulting in lower Nb/Nb*). Thus, Nb/Nb* ratio (found lesser in oceanic back-arcs, but more in arcs) works well as an efficient discriminant for arcs and oceanic back-arcs, by filtering about 90% arcs at the first level of the decision tree. Also, Nd/Zr ratio, which can be strongly fractionated based on the contribution from sediment melt, seem to operate efficiently for the lower levels after Nb/Nb* filter.

In this discrimination, one of the major factors for misclassification of some oceanic backarcs arises from their significant subduction component. Although spreading backarcs mainly tap a mantle source somewhat similar to that of MORs, the amount of subduction component may change among the segments based on factors, including arc proximity and direction of mantle flow. Thus, the lavas produced in some segments can possess strong subduction signatures, with high Nb/Nb* ratios. This causes such backarc lavas to resemble those from arcs, which in turn leads their misclassification.

4.2.2.1.2. Discrimination Within Arc-related Settings

For training and test datasets, the first decision tree correctly classified maximum 370 samples of oceanic arcs out of 381 with a success ratio of 97.11% at its seventh level and 168 samples of continental arcs out of 181 with a success ratio of 92.82% at its third level. The introduction of Zr/TiO_2, La/Yb and Y/Yb at fourth level drastically decreases the successful classification rate of the first decision tree for continental arcs by 48 misclassifications and this negative effect could only be solved with the introduction of Zr/Sm and La/Nb at sixth level. However, the introduction of the ratios at the fourth level has a great positive effect at the classification rate of oceanic arcs with 77 additional correct classifications. Therefore, if a simple decision tree is to be preferred for the first decision tree, the third level shall be preferred for rocks of continental origin, and the fourth level shall be preferred for rocks of oceanic origin.

However, if this information is limited or not available, the seventh level of the first decision tree shall be used for both tectonic settings.

The same trend is also observed for the second decision tree. The introduction of Th/La, Sm/Hf, and Zr/Y at the fourth level has a negative effect on the discrimination of oceanic arcs with a decrease by 16 and positive effect on the discrimination of continental arcs with an increase by 44. However, the general trend is an increase in the success ratio for both tectonic settings with an increase of level in depth for the second decision tree. This decision tree correctly classified 372 samples of oceanic arcs out of 381 with a success ratio of 97.64% and 171 samples of continental arcs out of 181 with a success ratio of 94.48%.

The first decision tree correctly classified maximum 176 samples of continental arcs out of 223 with a success ratio of 78.93% at the fifth level and 136 samples of oceanic arcs out of 141 with a success ratio of 96.45% at second and third levels. The introduction of Zr/TiO_2, La/Yb, and Y/Yb at the fourth level drastically decreases the success ratio for the discrimination of continental arcs with a decrease by 53, and this negative effect cannot be solved for the deeper levels of the first decision tree. Therefore, overfitting for the classification of continental arcs can be assumed starting from the fourth level of the decision tree. Interestingly, the introduction of ratios at the fourth level increases the success ratio for the discrimination of oceanic arcs with an increase by 76. However, starting from the fifth level, the success ratio for the discrimination of oceanic arcs also decreases with an increasing level of depth similar to that of continental arcs in the first decision tree. When the classification results of the first decision tree for the external dataset are examined, second and third levels shall be preferred if the origin of rocks are continental, fourth, and fifth levels shall be preferred if the origin of rocks are oceanic. Deeper levels are assumed to result in overfitting, which results in the failure of a decision tree when applied to external datasets.

The second decision tree correctly classified maximum 178 samples of continental arcs out of 223 with a success ratio of 79.82% at the seventh level and 108 samples of oceanic arcs out of 141 with a success ratio of 76.60% at sixth level. The success ratio for the second decision tree increases with an increasing level of depth. Therefore, no overfitting is observed in the second decision tree. The second decision tree is indeed successful for the discrimination of oceanic arcs in the second and third levels, but this success decreases with the introduction of Th/La, Sm/Hf, and Zr/Y at the fourth level with a decrease by 37. This negative effect is solved with the introduction of La/Y, Sm/Nd, Nb/Nb*, Sm/Hf and La/Nb at the fifth level. For the discrimination of oceanic arcs, on the other hand, there is a continuous increase in the success ratio. When the classification results of the second decision tree for the external dataset are examined, the seventh level shall be preferred for discrimination of oceanic arcs and continental arcs.

The first decision tree is much more successful for the discrimination of continental arcs, and the second decision tree is relatively more successful for the discrimination of oceanic arcs.

The first decision tree obtained a very high success ratio for all datasets and became successful for samples of both oceanic arcs and continental arcs. The success ratio of this decision tree is distributed homogeneously through the articles from different locations, with few exceptions for the training and test datasets.

For training and test datasets, only 6 articles out of 21 having 63 samples are classified correctly with 100% success ratio. 15 articles have misclassifications with varying misclassification ratios. No settings are completely classified with 100% success ratio. Misclassifications for the first decision tree are 18 samples of continental arcs out of 181 from 7 articles and 19 samples of oceanic arcs out of 381 from 14 articles.

For continental arcs, misclassifications generally tend to increase at the fourth and fifth levels with the introduction of Zr/TiO_2, La/Yb and Y/Yb at the fourth level, Y/Yb, Sm/Hf and Zr/Hf at fifth level. Portnyogin (2015) of Kamchatka and Simon (2014) of

Kamchatka can be completely classified with a success ratio of 100%. Gertisser (2000) of Aeolian, on the other hand, can be correctly classified at the sixth level with a success ratio of 100% but with the introduction of Sm/Hf and Zr/Hf at seventh level, 4 misclassifications are observed with a misclassification rate of 80%. Other than this article, misclassification rates for the sixth and seventh levels for all articles of continental arcs are low within a range of 8-20%.

For oceanic arcs, misclassifications are highly dominated in first levels with less and homogeneous distribution through higher levels. Bedard (1999) of Canada, Hochstaedter (2001) of Izu Bonin, Pearce (2005) of Mariana, Schuth (2004) of Solomon Islands and Yogodzinski (2015) of Western Auletian can be completely classified with a success ratio of 100%. Hickey and Vargas (2013) of Daito can be correctly classified at fifth level but 2 and 1 misclassifications with a success ratio of 25% and 13%, with respectively in sixth and seventh levels with the introduction of Sm/Hf, Zr/Nb, La/Y, Th/La and Nb/Y at sixth level and Sm/Y, Nb/Nb* and Zr/Hf at seventh level.

Other than this article, misclassification rates for the sixth and seventh levels for all articles of oceanic arcs are low within a range of 3-27%. The first decision tree is successful for the discrimination of oceanic and continental arcs at its sixth and seventh levels; therefore, these levels shall be preferred.

The first decision tree is more successfully for the tectono-magmatic discrimination of external datasets.

For external datasets, 16 articles out of 26 having 306 samples are classified correctly with 100% success ratio. 10 articles have misclassifications with varying misclassification ratios. For external datasets, the success ratio for the classification of continental arcs decreases much more with respect to that of oceanic arcs, especially with the increasing level of depth. Bryant (2006) of Andes, De Astis (1997) of Aeolian, Santo (2004) of Aeolian and Zelenski (2018) of Kamchatka can be completely classified with a success ratio of 100% whereas Bailey (2009) of Santorini, Calanchi (2002) of Aeolian, De Astis (2000) of Aeolian and Ianelli (2017) of North Patagonian Andes can be classified with 1-2 misclassification errors in the second and third levels. However, for deeper levels of the first decision tree, success ratio drastically falls, and an overfitting is clearly observed for the discrimination of continental arcs for the levels above fourth level, with the introduction of Zr/TiO_2, La/Yb and Y/Yb at fourth level, Y/Yb, Sm/Hf and Zr/Hf at fifth level, Nb/Nb*, Zr/Sm and La/Nb at sixth level and Nb/Y, Th/Y, Sm/Hf and Zr/Hf at seventh level, resulting 64 more misclassifications in continental arcs. However, this situation changes in the opposite direction for the classification of oceanic arcs within the discrimination between continental and oceanic arcs. Most of the articles can be classified more accurately with the increasing level of depth with an increase of correctly classified samples by 51. Finney (2008) of Okmok, König (2008, 2010) of various subduction zones, Stellin (2002) of Shishaldin, Tamura (2011) of Mariana, Bezos (2009) of Lau Basin, Harrison (2003) of East Scotia, Ikeda (2016) of Mariana, Ishizuka (2009) of Izu Bonin, Mortimer (2007) of South Fiji and Sinton (2003) of Manus are all articles, correctly classified with a success ratio of 100%. The misclassification for oceanic arcs decreases down to 66 out of 325, with a success ratio of 79.69%. Therefore, the application of the first decision tree to the discrimination between oceanic arcs and continental arcs are complicated and may require a cross-check with the application of another decision tree developed for the discrimination between oceanic and continental settings. If the sample is known or thought to be of oceanic in origin, then the sixth or seventh levels of the first decision tree shall be preferred more conveniently or the second or third levels shall be preferred if it is of continental in origin. The second decision tree is successfully applicable for the tectono-magmatic discrimination of training and test datasets, and the results are quite similar to those obtained from the first decision tree but with better success ratios. For training and test datasets, 7 articles out of 21 having 121 samples are classified correctly with 100% success ratio. 14 articles have misclassifications with varying misclassification ratios. However, misclassification ratios through articles are more homogeneous and smaller with respect to those in the first decision tree, ranging between 7-20% with quite a few exceptions. For continental arcs, Portnyogin (2015) of Kamchatka, Metrich (2001) of Aeolian, and Simon (2014) of Kamchatka can be correctly classified at either sixth or seventh levels.

Total misclassifications for continental arcs for discrimination between continental and oceanic arcs are 10 samples out of 181 from 7 articles. Only Gertisser (2000) of Aeolian has a misclassification rate of 40% with 2 misclassifications. Other articles have less than 10% misclassification rates with 1-3 misclassifications. For oceanic arcs, Hochstaedter (2001) of Izu Bonin, Hickey and Vargas (2013) of Daito, Pearce (1995) of South Sandwich, Pearce (2005) of Mariana, Peate (1997) of Vanuatu, Schuth (2004) of Solomon Islands and Yogodzinski (2015) of Western Auletian are correctly classified with a success ratio of 100% in either sixth or seventh level of the second decision tree. Similarly, to continental arcs, total misclassifications for oceanic arcs are also more homogeneously distributed through articles with fewer misclassification ratios, ranging between 3% and 25% with misclassifications ranging between 1-3 for each article with one exception (10 misclassifications out of 45).

The second decision tree is also successfully applicable for the tectono-magmatic discrimination of external datasets. For external datasets, only 4 articles out of 20 having 14 samples are classified correctly with 100% success ratio. 16 articles have misclassifications with varying misclassification ratios.

For continental arcs, Bryant (2006) of Andes and Zelenski (2018) of Kamchatka are correctly classified with a success ratio of 100%. Only Santo (2004) of Aeolian has a misclassification rate of 39% with 12 misclassifications out of 31 samples. However, other articles of continental arcs have limited misclassifications with ratios ranging between a narrow range of 17-25% with misclassifications ranging between 2-5%.

For oceanic arcs, Finney (2008) of Okmok and Stellin (2002) of Shishaldin can be correctly classified with a success ratio of 100%. Two articles of oceanic arcs, Jolly (2008) of Greater Antilles Arc and Straub (2010) of Izu Bonin have misclassifications greater than 10. Other articles have misclassifications in a range of 1-3 with misclassification ratios of 9-33%. The second decision tree is much more successful at greater depths for the discrimination of both oceanic arcs and continental arcs.

For oceanic arcs, only for the fourth level, the success ratio decreases drastically with the introduction of Th/La, Sm/Hf and Zr/Y by a decrease of 37. However, these misclassifications are solved with the introduction of La/Y, Sm/Nd, Nb/Nb*, Sm/Hf and La/Nb at the fifth level. The success ratio for discrimination of continental arcs continually increases with the increasing levels of decision tree and reaches its maximum at the sixth level with 108 correct classifications and to 107 at the seventh level. When the success ratio of the second decision tree for discrimination of oceanic arcs and continental arcs are evaluated and compared to the first decision tree, second decision tree shall be accepted to be more successful, especially for the highest levels (sixth and seventh) and shall be preferred for discrimination of both oceanic arcs and continental arcs without requiring any cross-check with other discriminations. The sixth and seventh level of the second decision tree is notably much more successful with respect to the first decision tree and to lowest levels of itself with an increase of correct classifications by 53 (as double as from 54 to 107).

The discrimination between the oceanic and continental arcs is not straightforward, like that between arcs and backarcs. In this case, since both classes (oceanic arcs and continental arcs) include a significant amount of subduction component in their petrogenesis, it is not surprising that the ratios Th/Nb and Nb/Nb* do not work at the uppermost level for the discrimination between oceanic and continental arcs. However, the ratios like Zr/TiO_2 and Zr/Sm are able to make a first-order separation, mainly for the oceanic arcs.

Since the oceanic arcs generally involve highly depleted source regions, they tend to have lower ratios of Zr/Ti and Zr/Sm when compared with continental arcs. This filtering appears to work at the upper levels, by constraining a large number of oceanic arcs. Another useful feature seems to be Sm/Y. High Sm/Y coupled with high Zr/Sm ratios are more common in continental arcs than oceanic arcs. Indeed, the Sm/Y achieves to filter oceanic and continental arcs for a reasonable success rate at the upper levels of the decision tree.

4.2.2.2. The Second Path for Discrimination Within Subduction Settings

4.2.2.2.1. Discrimination Between Oceanic and Continental Settings

For training and test datasets, the first decision tree correctly classified a maximum of 467 samples of oceanic setting out of 487 with a success ratio of 95.89% at the sixth level and 163 samples of continental setting out of 181 with a success ratio of 90.06% at sixth level. The success ratio of classification of the first decision tree continuously increasing with increasing level of depth, therefore, without any doubt for training and test datasets, the sixth level of the first decision tree shall be preferred for the discrimination of oceanic and continental settings.

The second decision tree shows the same trend with the first decision tree, with a continuous increase in the success of classification for both oceanic and continental settings. The second decision tree correctly classified a maximum of 467 samples of oceanic setting out of 487 with a success ratio of 95.89% at the sixth level and 151 samples of continental setting out of 181 with a success ratio of 83.43% at sixth level. When classification results for training and test datasets are examined, both decision trees have the same success for discrimination of oceanic settings but the first decision tree is much more successful for the discrimination of continental settings. Therefore, for a general application, the sixth level of the first decision tree shall be preferred. This is an indication for the positive effect of TiO_2-related ratios.

The first decision tree correctly classified 274 samples of oceanic settings out of 325 with a success ratio of 84.31% at second and third levels and 113 samples of continental settings out of 141 with a success ratio of 80.15% at second and third levels. The success ratio of the decision tree at higher levels gradually decreases as an indicator of overfitting. The introduction of Zr/Y and Nd/TiO_2 at fourth level, Y/Yb, TiO2/Y, Nb/Nb*, Zr/Hf and Sm/Hf at fifth level and La/Yb, Y/Yb, Sm/Hf and Nd/TiO_2 at sixth level affects negatively the classification ratio of oceanic settings. Classification of continental settings, on the other hand, is negatively affected only by the introduction of Zr/Y and Nd/TiO_2 at the fourth level. Therefore, the second and third levels of the first decision tree shall be preferred when classification results of external datasets are considered.

The second decision tree correctly classified 302 samples of oceanic settings out of 325 with a success ratio of 92.92% at the sixth level and 100 samples of continental settings out of 141 with a success ratio of 70.92% at second and third levels. As previously mentioned, the second decision tree fails as a result of overfitting for the discrimination of continental settings. When the classification of external datasets is considered, the sixth level of the second decision tree shall be preferred for the discrimination of oceanic settings if the origin of rock is known to be oceanic. For both decision tree, success ratio decreases drastically for discrimination of continental settings, with a decrease by 29 for the first decision tree with the introduction of Zr/Y and Nd/TiO_2 at fourth level and by 28 for the second decision tree Zr/Y and Sm/Y at the fourth level.

The first decision tree obtained a very high success ratio for all datasets and became more successful for samples of oceanic settings with respect to those of continental settings. The success ratio of this decision tree is distributed homogeneously through the articles from different locations for the training and test datasets.

For training and test datasets, 11 articles out of 26 having 124 samples are classified correctly with 100% success ratio. 15 articles have misclassifications with varying misclassification ratios. The first decision tree is quite successful for the classification of oceanic back-arcs for the discrimination between oceanic and continental settings. Only one article, Pearce (2005) of Mariana has 1 misclassification for each and 2 in total out of 70 samples. Other articles of oceanic back-arcs can be correctly classified with 100% success ratio. The first stage of the second path, which first discriminates between oceanic and continental settings, is more successful in discrimination of oceanic back-arcs rather than discriminating between arc and back-arc-related settings.

For continental arcs, Metrich (2001) of Aeolian, Portnyogin (2015) of Kamchatka can be correctly classified in fifth and sixth levels of the first decision tree. The other articles of continental arcs have limited misclassifications with ratios ranging between 4% and 14%. The only exception is Gertisser (2000) of Aeolian, which completely fails in the first decision tree at all levels.

The fifth and sixth levels of the first decision tree are more successful with respect to lower levels. For instance, the misclassifications in Hickey Vargas (2016) of Chile decreases from 14 (41%) to 3 (9%) with the introduction of Y/Yb, TiO_2/Y, Nb/Nb*, Zr/Hf and Sm/Hf at fifth level and La/Yb, Y/Yb, Sm/Hf and Nd/TiO_2 at sixth level. For oceanic arcs, Bedard (1999) of Canada, Hochstaedter (2001) of Izu Bonin, Pearce (2005) of South Sandwich, Pearce (2005) of Mariana, Schuth (2004) of Solomon Islands, Tollstrup (2010) of Izu Bonin and Yogodzinski (2015) of Western Auleatian can be correctly classified with a success ratio of 100% for the fifth and sixth levels of the first decision tree. Total misclassifications for oceanic arcs in the discrimination between oceanic and continental settings are 18 out of 381 from 14 articles with misclassifications ranging between 2 and 3, with ratios ranging between 3% and 13%. When success ratio of the first decision tree for discrimination between oceanic and continental settings, especially higher levels are much more successful, and their success increases with the introduction of Y/Yb, TiO_2/Y, Nb/Nb*, Zr/Hf and Sm/Hf at fifth level and La/Yb, Y/Yb, Sm/Hf and Nd/TiO_2 at sixth level.

The first decision tree is also successfully applicable for the tectono-magmatic discrimination of external datasets. For external datasets, only 5 articles out of 26 having 35 samples are classified correctly with 100% success ratio. 21 articles have misclassifications with varying misclassification ratios. For continental arcs, Zelenski

(2018) of Kamchatka can be correctly classified with a success ratio of 100% at all levels. However, Bryant (2006) of Andes and Ianelli (2017) of North Patagonian, Andes can be correctly classified at lower levels (second and third) in spite of having misclassifications in higher levels, especially with the introduction of Zr/Y and Nd/TiO_2 at fourth level, Y/Yb, TiO_2/Y, Nb/Nb*, Zr/Hf and Sm/Hf at fifth level. For oceanic arcs, Finney (2008) of Okmok, Stellin (2002) of Shishaldin and Tamura (2011) of Mariana can be correctly classified with a success ratio of 100% at all levels of the first decision tree. Total misclassifications for oceanic arcs are 59 out of 223 from 12 articles, and misclassifications are homogeneously distributed to all articles with quite a few exceptions. Only Pearce (1999) of Western Pacific fails in the discrimination with a misclassification ratio of 80%. For König (2008, 2010) from various subduction zones, the first decision tree is successful for lower levels but misclassifications are observed in higher levels with the introduction of Y/Yb, TiO_2/Y, Nb/Nb*, Zr/Hf and Sm/Hf at fifth level and La/Yb, Y/Yb, Sm/Hf and Nd/TiO_2 at sixth level. For oceanic back-arcs, Harrison (2003) of East Scotia can be correctly classified with a success ratio of 100%. Bezos (2009) of Lau Basin, Ikeda (2016) of Mariana and Sinton (2003) of Manus can be classified in the second or third levels of the first decision tree, but misclassifications are observed at higher levels.

The second decision tree is successfully applicable for the tectono-magmatic discrimination of training and test datasets, and the results are quite similar to those obtained from the first decision tree but with relatively lower success ratios. For training and test datasets, 10 articles out of 26 having 148 samples are classified correctly with 100% success ratio. 16 articles have misclassifications with varying misclassification ratios. The second decision tree is quite successful for the discrimination of oceanic back-arcs. For oceanic back-arcs, Beier (2015) of Manus Basin and Leat (2004) of South Sandwich Pearce (1995) of Lau and Pearce (2005) of Mariana can be correctly classified within the discrimination between oceanic and continental settings.

For continental arcs, Gertisser (2000) of Aeolian fails at classification with a misclassification ratio of 100% out of 5 samples. Mullen (2017) of Cascade Arc also has problems with 50% misclassification ratio. Portnyogin (2015) of Kamchatka can be correctly classified with a success ratio of 100%. Other articles have quite a few misclassifications ranging between 1 and 3. For oceanic arcs, Bedard (1999) of Canada, Hochstaedter (2001) of Izu Bonin, Schuth (2004) of Solomon Islands, Pearce (1995) of Lau and Pearce (2005) of Mariana can be correctly classified at fifth and sixth levels. There are quite a few misclassifications in discrimination of oceanic arcs with misclassification ratios ranging between 2% and 13%. With a few exceptions, fifth and sixth levels of the second tree shall be preferred for discrimination between oceanic and continental settings as success ratio increases with increasing level of the decision tree, by 16 samples for oceanic settings and by 51 for continental settings. Starting from the fourth level, the addition of each level has a positive impact on the classification of both oceanic and continental settings.

The second decision tree is also successfully applicable for the tectono-magmatic discrimination of oceanic settings in external datasets; however, the success ratio for discrimination of continental settings gradually decreases with increasing level of depth in the second decision tree.

For external datasets, 9 articles out of 26 having 104 samples are classified correctly with 100% success ratio. 17 articles have misclassifications with varying misclassification ratios. The second decision tree is also successful for the correct classification of oceanic back-arcs in external datasets. Only 9 misclassifications for oceanic back-arcs are observed out of 102 samples from 6 articles. Bezos (2009) of Lau Basin, Harrison (2003) of East Scotia, and Sinton (2003) of Manus can be correctly classified with a success ratio of 100%. Sixth level of this decision tree is especially quite successful with the positive impacts of the addition of higher levels and introduction of Zr/Y and Sm/Y at fourth level, Y/Yb, Nb/Nb*, Zr/Hf and Sm/Hf at fifth level and La/Yb, Zr/Y, Zr/Hf and La/Nb at sixth level. For oceanic arcs, Finney (2008) of Okmok, König (2008 and 2010) of various subduction zones, Stellin (2002) of Shishaldin, Tamura (2011) of Mariana and Woodhead (2001) of different locations can be correctly classified with a success ratio of 100%. Jolly (2008) of Greater Antilles Arc has 15 misclassifications that form the majority of misclassifications in oceanic arcs.

These misclassifications cannot be solved at any stage of the second decision tree, however, they increase at the fourth level with the introduction of Zr/Y and Sm/Y and decrease at the fifth level with the introduction of Y/Yb, Nb/Nb*, Zr/Hf and Sm/Hf. Other articles have few misclassifications with ratios ranging between 9% and 20%. Discrimination of continental arcs in external datasets is problematic as misclassifications increase in nearly all articles. No articles cannot be correctly classified with all of its samples. Calanchi (2002) of Aeolian fails for discrimination with a misclassification ratio of 100%. Other major failures are Bailey (2009) of Santorini and Santo (2004) of Aeolian with misclassification ratio greater than 50%. Other articles have, on the other hand, misclassifications less than 10. The second decision tree is more successful at the discrimination of oceanic settings with respect to continental settings when the application to external datasets is evaluated. Overfitting can be possible for continental settings, especially for continental arcs. However, as the best choice, the fifth level of the second decision tree shall be preferred.

Among two decision trees, the first decision tree is more successful for discrimination of continental settings, and the second decision tree is more successful for discrimination of oceanic settings. In both decision trees, success ratios decrease with increasing levels of depth for continental settings of external datasets. Therefore, considering the classification results of both training-test and external datasets, the fifth and sixth levels of the first decision tree along with the fifth level of the second decision tree shall be preferred, and a cross-check shall be applied.

For the classification of continental and oceanic settings, the strong subduction fingerprint Nb/Nb* is not preferred at the top of the classification. This case is very similar to that between continental and oceanic arcs since the subduction component is very strong within the two classes, namely continental arcs, and oceanic arcs and back-arcs. This time Zr/Y ratio appears to do a good job at the first level of discrimination. In the oceanic arcs and back-arcs, the source region is generally depleted (characterized by N-MORB source mantle or even depleted) than that of continental arcs. The exceptions are few and include some oceanic arcs and back-arcs that has produced enriched lavas. The continental arcs, on the other hand, may involve relatively a more enriched mantle source with the involvement of continental lithospheric mantle, lower-degrees of partial melting and crustal contamination. Thus, continental arcs can be expected to have higher Zr/Y ratios, in general. This feature really seems to be efficient, allocating a large number of oceanic arcs and back-arcs towards the low Zr/Y side.

4.2.2.2.2. Discrimination Within Oceanic Settings

For training and test datasets, the first decision tree correctly classified a maximum of 378 samples of oceanic arcs out of 381 with a success ratio of 99.21% at the second level, and 98 samples of oceanic back-arc basins out of 106 with a success ratio of 92.45% at sixth level.

The second tree correctly classified maximum 378 samples of oceanic arcs out of 381 with a success ratio of 99.21% at the second level and 99 samples of oceanic back-arc basins out of 106 with a success ratio of 93.4% at sixth level.

When the classification results of two decision trees are examined for training and test datasets, when a simple structure is to be preferred, second level of both decision trees is a good discriminator for oceanic arcs but for a general purpose, sixth level of decision trees shall be preferred for discrimination between oceanic arcs and oceanic back-arcs. If the origin of rock is considered to be of a back-arc, then the second levels of both decision trees shall be applied.

Both decision trees much more successfully discriminate oceanic arcs when compared to oceanic back-arcs for training and test datasets.

The first decision tree correctly classified maximum 219 samples of oceanic arcs out of 223 with a success ratio of 98.21% at second and third levels and 81 samples of oceanic back-arc basins out of 102 with a success ratio of 79.41% sixth levels. The second decision tree obtained the same maximum success ratios at the same levels with the first decision trees.

For both decision trees, the classification rate increases with the increasing level of depth for oceanic back-arcs until the fourth level, but deeper levels have no significant positive or negative effect on the success ratio.

The greater levels in the first decision tree show fluctuations. The success ratio for discrimination of oceanic arcs decreases with the introduction of Nb/Nb*, Nd/Zr and TiO_2/Yb at the fourth level and Y/Yb and Nb/Yb at sixth level but increases with the introduction of Nb/Nb* and Zr/Hf at fifth level.

However, the success ratio for the discrimination of oceanic arcs at the greater levels in the second decision tree continuously decreases with the introduction of Nd/Zr and La/Sm at the fourth level, Nb/Nb* and Sm/Y at fifth level and Y/Yb at sixth level. This is an indication of overfitting that much deeper decision trees ignoring TiO2-related ratios would be expected to fail more at external datasets.

When their success ratios for discrimination of external datasets are examined, if the origin of rock is thought to be arc-related then second and third levels of the first decision tree, otherwise, fifth and sixth levels of the first decision tree shall be preferred. For the second decision tree, the fourth level shall be preferred for discrimination between oceanic arcs and oceanic back-arcs.

The first decision tree obtained a very high success ratio, especially for oceanic arcs. The discrimination of oceanic back-arcs is, on the other hand, is a little problematic with a lower success ratio. The success ratio of this decision tree is distributed homogeneously through the articles from different locations, with a few exceptions for the training and test datasets.

For training and test datasets, 12 articles out of 19 having 347 samples are classified correctly with 100% success ratio. 7 articles have misclassifications with varying misclassification ratios. For oceanic arcs, Hickey and Vargas (2013) of Daito, Jolly (2007 and 2008) of Greater Antilles Arc, Pearce (1995) of South Sandwich, Pearce (2005) of Mariana, Rojas and Agramonte (2017) of Lesser Antilles, Schuth (2004) of Solomon Islands, Singer (2007) of Auletian, Tollstrup (2010) of Izu Bonin and Yogodzinski (2015) of Western Auletian can be correctly classified with a success ratio of 100% at sixth level. Hochstaedter (2001) of Izu Bonin and Peate (1997) of Vanuatu can be correctly classified at third or fifth levels, but with the introduction of Nd/Zr and TiO_2/Yb at fourth level and Y/Yb and Nb/Yb at the sixth level, their discrimination ratios decrease with misclassifications. For oceanic back-arcs, 20 misclassifications out of 106 samples from 5 articles are observed in the discrimination between oceanic arcs and oceanic back-arcs. Leat (2004) of Sandwich and Pearce (1995) of Lau can be correctly classified with a success ratio of 100%. When the classification results for the discrimination of oceanic arcs and oceanic back arcs are evaluated for the first decision tree, fifth and sixth levels shall be preferred. The first decision tree is also successfully applicable for the tectono-magmatic discrimination of external datasets.

For external datasets, 8 articles out of 18 having 155 samples are classified correctly with 100% success ratio. 10 articles have misclassifications with varying misclassification ratios. For oceanic back-arcs, Bezos (2009) of Lau Basin and Harrison (2003) of East Scotia can be correctly classified with a success ratio of 100%. Sinton (2003) of Manus, on the other hand, fails completely for this discrimination. The other three articles have misclassifications ranging between 4 and 6 and ratios between 20% and 33%. For oceanic arcs, Finney (2008) of Okmok, Jolly (2008) of

Greater Antilles Arc, König (2010) of various subduction zones, Leslie (2009) of Fiji Arc and Stellin (2002) of Shishaldin can be correctly classified with a success ratio of 100%. Other articles have misclassifications ranging between 1 and 5 with a broader range misclassification ratio as 4-40%. Pearce (1999) of Western Pacific can be correctly classified at the third level but misclassifications are observed in higher levels of depth. The first decision tree is more successful, especially for the discrimination of oceanic back-arcs at higher levels with the introduction of Nd/Zr and TiO_2/Yb at the fourth level, Nb/Nb* and Zr/Hf at fifth level and Y/Yb and Nb/Yb at sixth level. Therefore, when the classification results for discrimination between oceanic arcs and oceanic back-arcs are evaluated, fifth and sixth levels of the first decision tree shall be preferred for the discrimination between oceanic arc and oceanic back-arcs.

The second decision tree is successfully applicable for the tectono-magmatic discrimination of training and test datasets, and the results are quite similar to those obtained from the first decision tree but with better success ratios.

For training and test datasets, 10 articles out of 19 having 212 samples are classified correctly with 100% success ratio. 9 articles have misclassifications with varying misclassification ratios. For oceanic arcs, Hickey and Vargas (2013) of Daito, Pearce (1995) of South Sandwich, Pearce (2005) of Mariana, Rojas and Agramonte (2017) of Lesser Antilles, Schuth (2004) of Solomon Islands, Singer (2007) of Auletian, Tollstrup (2010) of Izu Bonin and Yogodzinski (2015) of Western Auletian can be correctly classified with a success ratio of 100%. Total misclassifications for oceanic arcs in discrimination between oceanic arcs and oceanic back arcs are 12 out of 381 from 14 articles with a range of 1 to 3 for each article.

The second decision tree is quite successful at oceanic arcs. However, Hochstaedter (2001) of Izu Bonin, Jolly (2007 and 2008) of Greater Antilles Arc and Peate (1997) of Vanuatu can be correctly classified at second and third levels; however, misclassifications are observed in higher levels with introduction of Nd/Zr and La/Sm at fourth level, Nb/Nb* and Sm/Y at fifth level and Y/Yb at sixth level. For oceanic back-arcs, Leat (2004) of Sandwich and Pearce (1995) of Lau can be correctly classified with a success ratio of 100% at the sixth level. Other articles have misclassifications decreasing with increasing level of depth and finally have 19 misclassifications out of 106 samples from 5 articles.

The second decision tree is also successfully applicable for the tectono-magmatic discrimination of external datasets.

For external datasets, 7 articles out of 26 having 139 samples are classified correctly with 100% success ratio. 19 articles have misclassifications with varying misclassification ratios. For oceanic arcs, Finney (2008) of Okmok, Jolly (2008) of Greater Antilles Arc, König (2010) of various subduction zones, Leslie (2009) of Fiji Arc and Stellin (2002) of Shishaldin can be correctly classified with a success ratio of 100% at all levels of the second decision tree. Pearce (1999) of Western Pacific, Tamura (2011) of Mariana and Wharton (1994) of Viti Levu can be classified at second and third levels whereas misclassifications are observed with the introduction of Nd/Zr and La/Sm at fourth level, Nb/Nb* and Sm/Y at fifth level and Y/Yb at sixth level. Ikeda (2016) of Mariana, Ishizuka (2009) of Izu Bonin, Mortimer (2007) of South Fiji and Sinton (2003) of Manus can be classified with misclassifications decreasing with increasing levels of depth.

When the classification results of the second decision tree for both training-test and external datasets are evaluated, fourth, fifth, and sixth levels of both decision trees shall be preferred with an acceptable amount of misclassifications, especially in problematic locations with geochemical, petrological complexities.

The Th/Nb ratio, which appears as the major discriminator, is a very sensitive subduction indicator. The classification this time is very similar to that for arcs and oceanic-back-arcs, so the same ideas are valid here. The arcs have a stronger subduction component due to the fluxing of slab-derived fluids/melts into the mantle wedge (e.g. Pearce et al.,2005). This process, however, is weaker in the oceanic back-arcs with the more contribution from MOR-type mantle, but with less subduction input (e.g. Leat et al.,2004). Indeed, this idea, so the sensitivity of Th/Nb based on the slab-derived influx, is proven by the high classification rates with over 90% arcs being allocated towards the higher Th/Nb ratios. Although it is not effective as Th/Nb, Zr/Hf appears to be useful as separating half of the arcs with very high efficiency, based on the depleted character of the arcs with low Zr/Hf ratios.

4.2.3. Discrimination Within Non-Subduction Settings

4.2.3.1. Discrimination Between Group 1 (Mid-Oceanic Ridge and Oceanic Plateau) and Group 2 (Oceanic Island and Continental Within-plate) Settings

For training and test datasets, the first decision tree correctly classified 812 samples of group 2 (oceanic islands and continental within-plates) out of 854 with a success ratio of 95.08% and 1,082 samples of group 1 (mid-oceanic ridge and oceanic plateaus) out of 1,120 with a success ratio of 96.61%. This decision tree is quite successful for discrimination of both group 1 and group 2 for training and test datasets. Discrimination of group 1 is nearly stable to all levels of the first decision tree with small fluctuations. Misclassification of group 1 increase by 34 with the Th/Nb and Y/Yb at the third level, but, decreases stepwise at higher levels with introduction of Zr/ TiO_2, La/Nb, Nb/Nb* and La/Sm at fourth level, La/Nb, Nd/Zr and Nb/Yb at fifth level, TiO_2/Y, Nb/Nb* and Zr/Hf and Th/La at seventh level. Th/Nb at the sixth level has no positive or negative effect on the classification rate of group 1. The first decision tree becomes much more successful for the discrimination of group 2 with an increasing level of depth and reaches its maximum 812 correct classifications at the seventh level with an increase by 49 following the introduction of Zr/Hf and Th/La at the seventh level. This may indicate that these two ratios seem to be a good indicator for the problematic samples of group 2, which can not be correctly classified at lower levels of depth.

The second decision tree has a very similar pattern at its increasing levels of depth when compared to the first decision tree. For training and test datasets, the second decision tree correctly classified 814 samples of group 2 (oceanic islands and continental within-plates) out of 854 with a success ratio of 95.32% and 1,082 samples of group 1 (mid-oceanic ridge and oceanic plateaus) out of 1,120 with a success ratio of 96.61%. The second decision tree is also quite successful for the discrimination of both group 1 and group 2 for this discrimination for training and test datasets. Discrimination of group 1 is nearly stable to all levels of the first decision tree with small fluctuations. Misclassifications of group 1 increase by 34 with the Th/Nb and Y/Yb at third level, but, decreases again stepwise at higher level with introduction of Zr/TiO_2, Th/La, La/Nb, Nb/Nb* and La/Sm at fourth level, Sm/Hf, Nd/Zr and Nb/Yb at fifth level, La/Nb, Nb/Nb* and La/Nb, Nb/Nb* and Th/Nb at sixth level and Nb/Y, Zr/Hf and Th/La at seventh level have no positive or negative effects on the classification rate of group 1. The second decision tree also becomes much more successful for the discrimination of group 2 with increasing level of depth and reaches to its maximum 814 correct classifications at the seventh level with an increase by 51 following the introduction of Nb/Y, Zr/Hf, and Th/La at the seventh level. This may indicate that these two ratios seem to be a good indicator for the problematic samples of group 2, which can not be correctly classified at lower levels of depth.

When the classification rates of two decision trees for training and test datasets are evaluated and compared to each other, and through different levels of depth, the seventh levels of both decision trees shall be preferred with only difference of element ratios. Therefore, the availability of elements in the dataset shall also be a factor to choose the decision tree or a cross-check shall be done in order to compare their results.

For external datasets, the first decision tree correctly classified 489 samples of group 2 out of 539 with a success ratio of 90.72% and 1,432 samples of group 1 out of 1467 with a success ratio of 97.61%. For discrimination of group 2 (oceanic islands and continental within-plates), the success ratio of classification increases with increasing level of depth in the first decision tree and reaches its maximum at the seventh level. The discrimination of group 1 (mid-oceanic ridges and oceanic plateaus), on the other hand, has its maximum success ratio of classification at the second level, but the success ratio drastically decreases at the third level by 174 with the introduction of Th/Nb and Y/Yb. For higher levels, success ratio increases with increasing level of depth of the first decision tree but can not reach to the ratio at the second ratio (82 correct classifications less than that of the second level with a success ratio difference of 3.34%). The introduction of Th/Nb at the sixth level has no positive or negative effect on the classification rates.

When the classification rates of the first decision tree in the discrimination between group 1 and group 2 are evaluated, the seventh level of this decision tree shall be preferred ignoring the success ratio difference for the discrimination of group 1. The decision tree proves itself to be applicable to external datasets without any serious classification problems.

The second decision tree correctly classified 489 samples of group 2 out of 539 with a success ratio of 90.72% and 1,432 samples of group 1 out of 1467 with a success ratio of 97.61%. The maximum success ratios of two decision trees for discrimination of both groups are exactly the same. There are also no differences at all for the classifications of group 2 at each level but slight differences are observed at the classification of group 1. The success ratio of the second decision tree for group 1 at the seventh level is 1,356 with an increase of 6 with respect to the first decision tree. The introduction of Th/La, La/Nb, Nb/Nb* and La/Sm at fourth level, Sm/Hf, Nd/Zr and Nb/Yb at fifth level, La/Nb, Nb/Nb* and Th/Nb at sixth level, on the other hand, is more effective and successful in the discrimination of group 1. This may indicate that ratios of Th with La and Nb may be more effective with respect to that with Nb only for the discrimination of mid-oceanic ridges and oceanic plateaus in this discrimination.

When the classification rates of the second decision tree in the discrimination between group 1 and group 2 are evaluated and compared with the first decision tree, the seventh level of both decision trees shall be preferred ignoring the success ratio difference for the discrimination of group 1. The decision trees are both successfully applicable to external datasets without any serious classification problems.

The first decision tree obtained a very high success ratio for all datasets and became successful for samples of both group 1 and group 2 of non-subduction settings. The success ratio of this decision tree is distributed homogeneously through the articles from different locations, with few exceptions for the training and test datasets.

For training and test datasets, only 23 articles out of 37 having 782 samples are classified correctly with 100% success ratio. 14 articles have misclassifications with varying misclassification ratios. No settings are entirely classified with 100% success ratio. The first decision tree is quite successful for the classification of continental within-plates. Only 4 articles out of 12 have misclassifications: Hanghoj (2003) of East Greenland, Larsen (2003) of West Greenland, Peate (2003) of East Greenland, and Rooney (2012) of Afar Plume have misclassifications of 4, 5, 1 and 1, with respectively. Total misclassifications for continental within-plates are 11 out of 376 samples. Classification ratios also increase with increasing level of depth. For mid-oceanic ridges, only 2 articles have misclassifications out of 12 articles. Arevalo (2010) of varying ridges and Gale (2011) of Mid-Atlantic Ridge have 12 misclassifications for each. The increasing level of depth and introduction of new features have nearly no effect on the classification of Gale (2011) but decrease misclassifications in Arevalo (2010). For oceanic islands, Geldmacher (2000) of Madeira, Gurenko (2006) of Canary, Millet (2009) of Azores and Woodhead (1996) of Mangaia can be correctly classified with a success ratio of 100%. Kokfelt (2006) has 53 misclassifications (53%) at the second level, but with an increasing level of depth, it decreases down to 15 (19%). Jackson (2010) of Samoa has only 1 misclassification whereas Salters (2010) of Walvis and Stracke (2003) of Iceland have 6 and 7 misclassifications, respectively. For oceanic plateaus, only 1 article is problematic, but the others can be correctly classified. Neal (2002) of Kerguelen has 13 misclassifications with a misclassification ratio of 37%. The increasing level of depth has nearly no effect on these misclassifications.

The first decision tree is more successfully for the tectono-magmatic discrimination of external datasets. For external datasets, 18 articles out of 37 having 403 samples are classified correctly with 100% success ratio. 19 articles have misclassifications with varying misclassification ratios. For external datasets, the first decision tree remains to be successful for the classification of continental within-plates. 7 articles have a total of 24 misclassifications out of 302 samples from 16 articles. Frey (1996) of Bunbury and Olierook (2016) of Bunbury fail with a misclassification ratio of 100% and 75%, respectively. Furman (2006) of Afar Plume, Gibson (1995) of Southeastern Brazil, Mana et al. (2015) of East African Rift, Shuying (2015) of South China and Xu (2001) of SW China have misclassifications in a range of 1-3 with misclassification ratios less than 10%.

For mid-oceanic ridges, 2 articles out of 5 have misclassifications. There are large amounts of misclassifications in these articles but with quite a few misclassification ratios due to great amount of samples in the articles. Jenner (2012) of varying ridges and Kelley (2013) of East Pacific Rise and Mid-Atlantic Ridge have 75 misclassifications in total with misclassification ratios of 4% and 9%, respectively. The second level is the most successful for the discrimination of mid-oceanic ridges, but with the introduction of Th/Nb and Y/Yb at the third level, the success ratio falls drastically. This pattern of success ratios with an increasing level of depth is also observed in oceanic plateaus. For oceanic islands, only 3 articles have misclassifications: Gibson (2005) of Tristan, Kitagawa (2008) of Iceland, and Peate (2010) of Iceland have misclassifications of 13, 12, and 1, with respectively. For oceanic plateaus, Borisova (2002) of Kerguelen fails completely in the classification of oceanic plateaus with a misclassification ratio of 100%. Other problematic articles are Frey (2002) of Kerguelen and Trela (2015) of Kerguelen with 8 and 13 misclassifications and 47% and 68% misclassification ratios, respectively.

When classification ratios for the first decision tree through the training and test datasets and external datasets are evaluated, it can be considered to be more successful for continental within-plates and mid-oceanic ridges and applicable to all settings. The second level of the decision tree is more successful at external datasets, but considering their success ratios through all samples, the seventh level of this decision tree shall be preferred.

The second decision tree is successfully applicable for the tectono-magmatic discrimination of training and test datasets, and the results are quite similar to those obtained from the first decision tree but with better success ratios. For training and test datasets, 23 articles out of 37 having 782 samples are classified correctly with 100% success ratio. 14 articles have misclassifications with varying misclassification ratios. The second decision tree is also quite successful in the discriminations of continental within-plates and mid-oceanic ridges. The same articles have nearly the same misclassifications for all tectonic settings in this decision tree. There are no significant changes in both classifications and misclassifications in the second decision tree with respect to the first one. The only difference is that the second decision tree seems to be more successful at intermediate levels such as the fourth and fifth levels in the classification of training and test datasets. The second decision tree is similar in terms of its applicability for the tectono-magmatic discrimination of external datasets when compared to the first decision tree.

For external datasets, the second decision tree correctly classified 449 samples from 18 articles out of 36 articles. Just similar to the classification results for training and test dataset, the same articles also have nearly the same misclassifications for all tectonic settings in this decision tree. There are no significant changes in both classifications and misclassifications in the second decision tree with respect to the first one. When the classification rates for both decision trees in the discrimination of group 1 and group 2 within non-subduction settings are considered, the seventh level of both decision trees shall be preferred for the discrimination.

The classification within the non-subduction settings is complex, since it includes four tectonic settings. More importantly, some lavas from the diverse settings may display similar signatures due to their derivation from mantle sources with somewhat similar characteristics. With all these complexities, however, the first discrimination factor Sm/Yb works very efficiently. Among the two main classes, the MOR-OP pair involves melt generation mainly taking place in the spinel field and/or high degrees of melting that may cause exhaustion of garnet. Consequently, this results in relatively low Sm/Yb ratios. CWP-OI pair, however, involve deeper melting within the stability field of garnet, which causes melts with high Sm/Yb ratios.

4.2.3.2. Discrimination Between Mid-Oceanic Ridges and Oceanic Plateaus

For both decision trees, the maximum classification rate for oceanic plateaus is obtained at the second level. The classification rate for discrimination of mid-oceanic ridges, on the other hand, increases drastically at the third level and shows a smooth pattern with a slight increase with respect to that in third level. However, the maximum classification rate for mid-oceanic ridges is obtained at the highest level of depth for both decision trees.

For training and test datasets, the first decision tree correctly classified 176 samples of oceanic plateaus out of 211 with a success ratio of 83.41% at the second level and 907 samples of mid-oceanic ridges out of 909 with a success ratio of 99.78% at sixth level. The first decision tree is quite successful at the discrimination of mid-oceanic ridges with only 2 misclassifications.

The introduction of Th/La and Nb/Nb* at the sixth level is quite successful discriminating feature for mid-oceanic ridges increasing the correct classifications by 12. However, the most effective level of the first decision tree is the third level, in which Nb/TiO_2 is introduced, increasing correct classifications by 147. The classification rate of oceanic plateaus is at its maximum at the second level but decreases drastically by 58 with the introduction of Nb/TiO_2 at third level. This decrease can be eliminated with the introduction of Th/Y and Zr/Y at fourth level. Starting from the fourth level, classification rate of oceanic plateaus shows fluctuations through its highest level, and the sixth level has only 9 less correct classifications with respect to the second level.

When classification rates of the first decision tree for the discrimination between oceanic plateaus and mid-oceanic ridges for training and test datasets are evaluated, even though the maximum classification rate for oceanic plateaus are obtained at the second level, the sixth level shall be preferred for the discrimination.

The second decision tree correctly classified 176 samples of oceanic plateaus out of 211 with a success ratio of 83.41% at the second level and 906 samples of mid-oceanic ridges out of 909 with a success ratio of 99.67% at sixth and seventh levels. The first decision tree is quite successful at the discrimination of mid-oceanic ridges with only 3 misclassifications. The introduction of Th/La, La/Y, and Zr/Nb at sixth level and Sm/Y at seventh level is quite a successful discriminating feature for mid-oceanic ridges increasing the correct classifications by 9. However, the most effective level of the first decision tree is the third level, which has the introduction of Zr/Nb, increasing correct classifications by 139. The classification rate of oceanic plateaus is at its maximum at the second level but decreases drastically by 55 with the introduction of Nb/Nb at third level. This decrease can be eliminated with the introduction of Sm/Yb and Zr/Hf at fourth level, Zr/Nb, La/Nb, Y/Yb and Zr/Hf at fifth level. Starting from the fifth level, classification rate of oceanic plateaus shows fluctuations through its highest level, and seventh level has only 5 less correct classifications with respect to the second level.

When classification rates of the second decision tree for the discrimination between oceanic plateaus and mid-oceanic ridges for training and test datasets are evaluated, even though the maximum classification rate for oceanic plateaus are obtained at the second level, the seventh level shall be preferred for the discrimination. As a summary, the highest levels of both decision trees shall be preferred separately or together for cross-check.

For external datasets, the first tree correctly classified 113 samples of oceanic plateaus out of 211 with a success ratio of 53.55% and 1,277 samples of mid-oceanic ridges out of 1,304 with a success ratio of 97.93%. The second decision tree is very similar to the first decision tree with only 7 less classification for mid-oceanic ridges. Both decision trees fail for the discrimination of the oceanic plateaus for external datasets with only a 53.55% maximum success ratio at their second levels. The other levels can only reach half of this success ratio. Therefore, for the classification of oceanic plateaus in the discrimination between oceanic plateau and mid-oceanic ridges, geochemical features may not be sufficient for this external dataset with requirement of additional information. For both decision trees, the seventh levels shall be preferred when their applicability to training and test and external datasets are evaluated, just considering any risk of the failure for classification of oceanic plateaus for external datasets.

The first decision tree obtained a very high success ratio for all datasets and became successful for samples of mid-oceanic ridges but have major failures for the discrimination of oceanic plateaus, especially in external datasets. The success ratio of this decision tree is distributed homogeneously through the articles from different locations, with few exceptions for the training and test datasets.

For training and test datasets, 11 articles out of 16 having 397 samples are classified correctly with 100% success ratio, and all of these are the articles of mid-oceanic ridges. 5 articles have misclassifications with varying misclassification ratios. Mid-oceanic ridges are almost perfectly classified with only 2 misclassifications out of 1120 samples.

For oceanic plateaus, the first decision tree is the most successful at classification of Tim (2011) of Manihiki with 2 misclassifications and 85% success ratio. For other three articles, Fitton (2004) of Ontong Java, Neal (2002) of Kerguelen and Sano

(2012) of Shatsky have 10, 8, and 24 misclassifications with ratios of 16%, 23% and 24%, with respectively. These ratios are acceptable for training and test datasets considering the geological, geochemical and petrological complexity of oceanic plateaus and their similarity to mid-oceanic ridges. However, this complexity makes it more difficult for decision trees to be applicable into external datasets and complete failures can be observed.

For this reason, the first decision tree is still applicable and quite successful to mid-oceanic ridges in discrimination between mid-oceanic ridges and oceanic plateaus, but major failures at the discrimination of oceanic plateaus are observed.

For external datasets, only 2 articles out of 14 having 36 samples are classified correctly with 100% success ratio, and all of these are the articles of mid-oceanic ridges. 12 articles have misclassifications with varying misclassification ratios. Mid-oceanic ridges are quite successfully classified with 27 misclassifications out of 1,304 samples. For oceanic plateaus, Borisova (2002) of Kerguelen and Trela (2015) of Kerguelen completely fail with misclassification ratio of 100%. White (2004) of Ontong Java and Weis (2002) of Kerguelen are the most acceptable classifications with misclassification ratios less than 50% but all others have misclassification ratios greater than 50%.

The second decision tree is successfully applicable for the tectono-magmatic discrimination of training and test datasets, and the results are quite similar to those obtained from the first decision tree but with better success ratios.

Just similar to the classification results for training and test dataset, the same articles also have nearly the same misclassifications for all tectonic settings in this decision tree. There are no significant changes in both classifications and misclassifications in the second decision tree with respect to the first one.

The discrimination between MOR and oceanic plateaus appears to be a difficult task. However, regarding the training and test sets Th/Y ratio achieves to distinguish a good portion of MOR samples at the first level. MORBs are known to largely tap the depleted mantle, associated with moderate to high degrees of partial melting (e.g. Zindler and Hart 1986; Klein and Langmuir 1987; Niu et al.,1996). OPs, on the other hand, are believed to involve plume sources with an intrinsic depleted component (e.g. Kerr et al.,1995; Fitton et al.,2003). However, the depletion levels are more extreme in MORs, perhaps owing to the presence of ultra-depleted, D-DMM-type mantle domains (e.g. Niu and Batiza 1997; Workman and Hart 2005). Thus, Th/Y ratios are lower for at least some MORs, which in turn enables their discrimination at the upper levels from OPs. In spite of relatively high classification rates in training and test sets, the misclassifications encountered in the OP samples appear to be the generation of melts with very similar characteristics to some MORs (Figure 4.7), which in turn is linked to the similarity of their mantle sources.

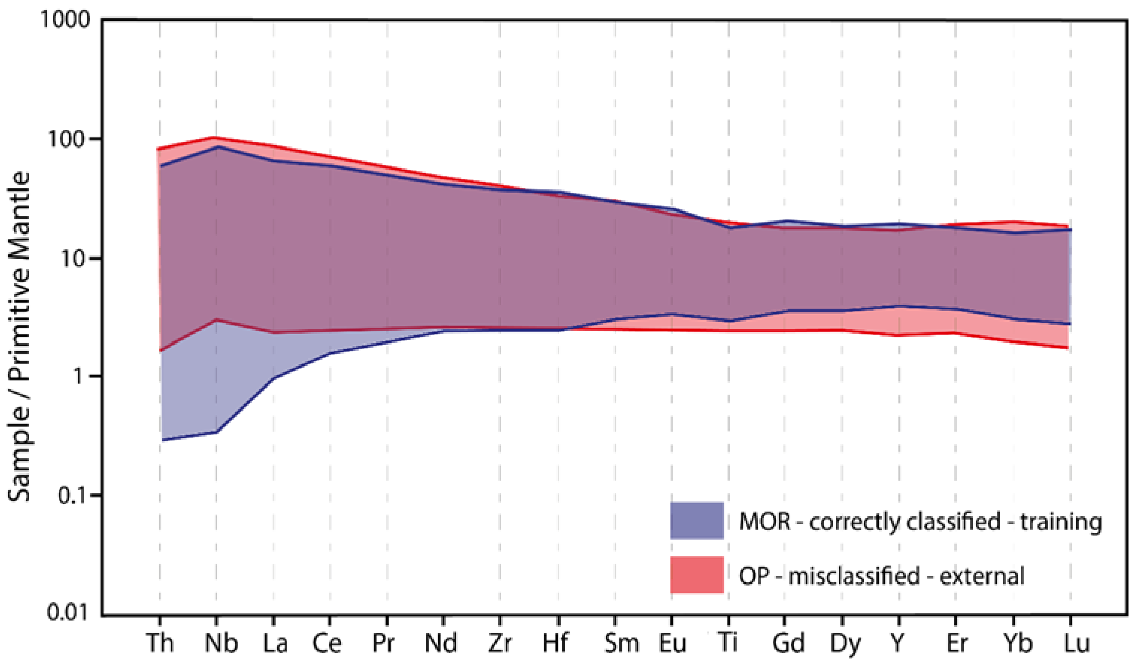

Figure 4.7. Comparison of spider-diagrams between samples from oceanic plateaus misclassified as mid-ocean ridges and samples of mid-ocean ridges correctly classified (normalization coefficients are based on Sun and McDonough, 1995)

4.2.3.3. Discrimination Between Oceanic Islands and Continental Within-plates

For training and test datasets, the first decision tree correctly classified 431 samples of oceanic islands out of 478 with a success ratio of 90.17% at the eighth level and 345 samples of continental within-plates out of 376 with a success ratio of 91.76% at the eighth level. Classification rates of the first decision tree in discrimination of oceanic islands and continental within-plates are increasing for both the oceanic islands and continental within-plates with increasing level of depth and reach to their maximum level at the deepest level. The introduction of each level to the first decision tree has a positive impact for discrimination of either oceanic islands or continental within-plates or even both. Therefore, when the classification rates of first decision tree are evaluated, the eighth level shall be preferred.

The second decision tree correctly classified 445 samples of oceanic islands out of 478 with a success ratio of 93.10% and 327 samples of continental within-plates out of 376 with a success ratio of 86.97%. The first decision tree is more successful for the discrimination of continental within-plates, whereas the second decision tree is more successful for that of oceanic islands.

The classification ratios of the second decision tree are continuously increasing from the third level to its eighth level. However, introduction of Th/Nb and Sm/Nb at fifth level, Th/Nb, Sm/Nb, Zr/Y and Zr/Hf at sixth level, Sm/Nd, Y/Yb, Zr/Yb and Nb/Yb at seventh level has no positive or negative effect for discrimination of either oceanic islands or continental within-plates.

Similar to the first decision tree, when the classification rates of the second decision tree for discrimination of oceanic islands and continental within-plates are evaluated, the eighth level shall be preferred.

For external datasets, the first tree correctly classified 63 samples of oceanic islands out of 237 with a success ratio of 26.25% and 251 samples of continental within-plates out of 302 with a success ratio of 83.11%. The second decision tree is very similar to the first decision tree, with only one more classification for oceanic islands. Both decision trees fail for the discrimination of the oceanic islands for external datasets with only 26.25% maximum success ratio at their eighth levels. The other levels have a similar success ratio to that level. Therefore, for the classification of oceanic plateaus in the discrimination between oceanic islands and continental within-plates, geochemical features may not be sufficient for this external dataset with requirement of additional information. For both decision trees, eighth levels shall be preferred when their applicability to training and test and external datasets are evaluated, just considering any risk of the failure for classification of oceanic plateaus for external datasets.

The first decision tree obtained a very high success ratio for all datasets and became successful for samples of both oceanic islands and continental within-plates in training and test datasets.

The success ratio of this decision tree is distributed homogeneously through the articles from different locations, with a few exceptions for the training and test datasets. For training and test datasets, only 7 articles out of 21 having 177 samples are classified correctly with 100% success ratio. 14 articles have misclassifications with varying misclassification ratios.

For continental within-plates, Aviado (2015) of West Antarctic and Peate (2003) of East Greenland, on the other hand, is correctly classified at the seventh level of the first decision tree. Mirnejad (2006) of Leucite Hills is correctly classified at the second level, but misclassifications are observed at higher levels. For oceanic islands, Gurenko (2006) of Canary has misclassifications with ratio of 63%.

The overall classifications for both oceanic islands and continental within-plates are quite high, and misclassifications are homogeneously distributed through articles for training and datasets other than these articles, misclassifications ranging between 2% and 35%.

For external datasets, only 3 articles out of 22 having 74 samples are classified correctly with 100% success ratio. 19 articles have misclassifications with varying misclassification ratios.

For continental within-plates, Carlson (1996) of South Brazil, Gibson (1995) of Southeast Brazil, and Leroex (2003) of Africa can be classified correctly with classification ratio of 100%. Endress (2011) of Egypt, Xu (2001) of SW China, and Gibson (1997) of Trindade are articles failed at classification of the first decision tree in discrimination between oceanic islands and continental within-plates. The other articles have few misclassifications with relatively small misclassification ratios.

For oceanic islands, on the other hand, classification of oceanic islands failed as all articles have major misclassifications with the misclassification ratios ranging from 34% to a complete failure of 100% for Morgan (2009) of Hawaii.

The second decision tree is similar to those obtained from the first decision tree.

The same articles have nearly the same misclassifications for all tectonic settings in this decision tree. There are no significant changes in both classifications and misclassifications in the second decision tree with respect to the first one. The differences are Gibson (2000) of picrites also has misclassifications at the latest level of this decision tree. Johnson (2005) of Siberia has much higher misclassification ratio of 78%. Woodhead (1996) of Mangaia can be classified correctly with 100% ratio. There are also fewer changes in misclassifications of other articles, but no other major differences are observed between two decision trees for training and test datasets.

The classification results and ratios for the external datasets are also quite similar between two decision trees. Gibson (1995) of Southeast Brazil and Leroex (2003) of Africa can also be correctly classified with second decision trees.

Misclassifications also show slight fluctuations but nearly the same when compared to that of the first decision tree.

The discrimination between CWP and OI probably constitutes the most challenging classification due to compositional resemblance of lavas generated in these settings, which arise from their derivation from similar mantle sources and under similar degree of partial melting. Since they include no or minimal subduction component in most cases, subduction-sensitive ratios Th/Nb and Nb/Nb* do not work at the uppermost level. However, some CWP lavas are result of very low degree of melting under great depths. These ones, with potassic/ultrapotassic compositions, are incredibly enriched in incompatible elements. Thus, a ratio including a highly incompatible element and compatible element that can be retained by garnet (like Nb/Y) can be useful for the first order classification.

4.3. Comparison with Traditional Discrimination Methods

In this section, the decision trees are compared with traditional discrimination methods to understand i) if there is any advantage of using them, and ii) to what extent they are successful over the traditional methods. In fact, when the traditional methods are considered, none of them appear to be able to discriminate all seven tectonic settings. Such result is actually expected since the discrimination of all tectonic settings on a single plot is extremely difficult with the limited number of elements used. Furthermore, considering the published diagrams thus far, even their combination is not able to distinguish all tectonic settings. Thus, in this respect, using the decision trees can be very advantageous in the tectonomagmatic characterization of a sample with no known affinity. Though they can be useful, the applicability of published diagrams seems to be limited compared to the decision trees. For the discrimination between subduction and non-subduction settings, the ternary diagram of Wood (1980) and bivariate diagrams of Pearce (1983) and Saccani (2015) can be applied, whereas for discrimination within subduction settings, Saccani (2015) is useful. However, no traditional discrimination method is available for discrimination within non-subduction settings, which can be compared with the decision trees.

4.3.1. Wood (1980) for Discrimination Between Subduction and Non-Subduction Settings

The ternary diagram of Wood (1980) using Hf/3-Th-Nb/16 can be used in order to discriminate between subduction and non-subduction settings. Samples of both subduction (Figure 4.8) and non-subduction (Figure 4.9) settings are plotted in the diagram separately. Samples of subduction settings are classified with a higher success ratio when compared to those of non-subduction settings. However, the success ratio is about 80% (Figure 4.8). Some of the samples are plotted in unidentified regions whereas others mainly fall into N-MORB with E-MORB, tholeiitic within-plate basalts, and alkaline within-plate basalts with decreasing frequency.

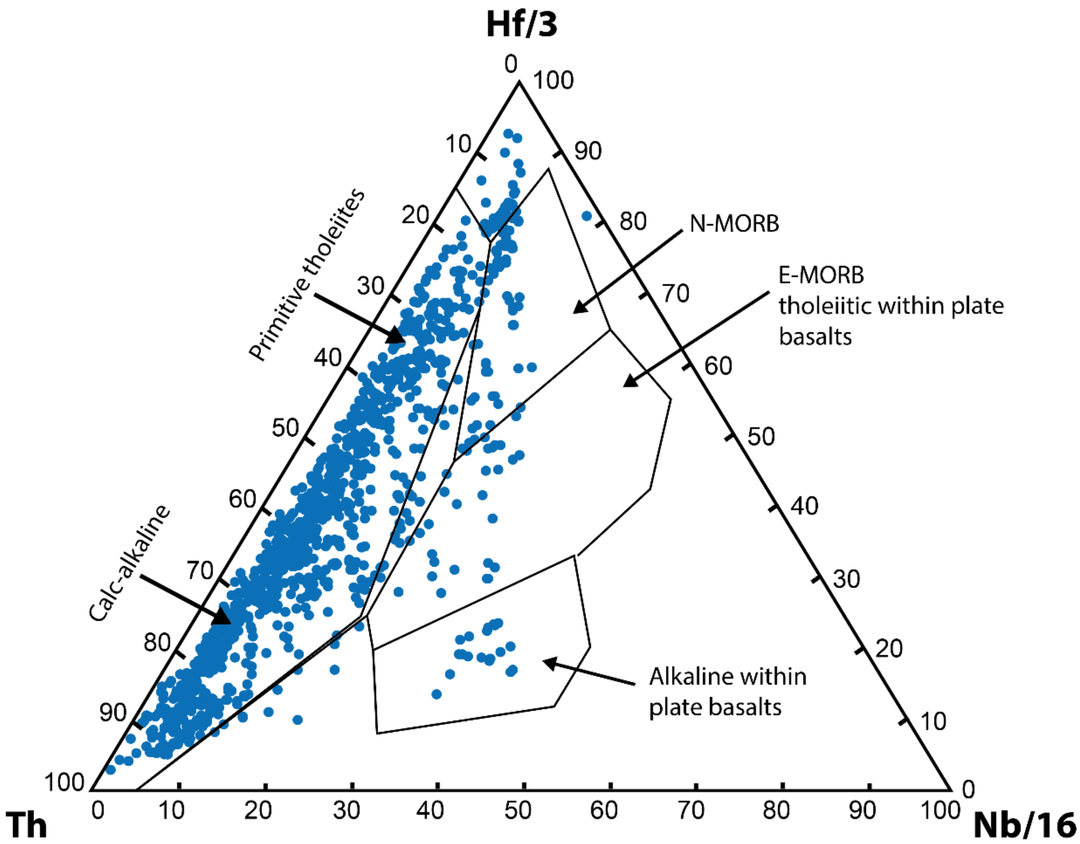

Figure 4.8. Samples of subduction settings plotted on Wood (1980) diagram

Samples of non-subduction settings are, on the other hand, obtained a relatively lower success ratio from the diagram of Wood (1980). Th enrichment in samples resulted in the plot of these samples to calc-alkaline field, and Hf enrichment resulted in the plot of samples to unidentified field (Figure 4.9). There are a large number of samples plotted in the unidentified fields, which decreasing the success ratio of below 70%.

When these diagrams are compared to decision trees, decision trees are much more successful in discrimination of both subduction and non-subduction settings.

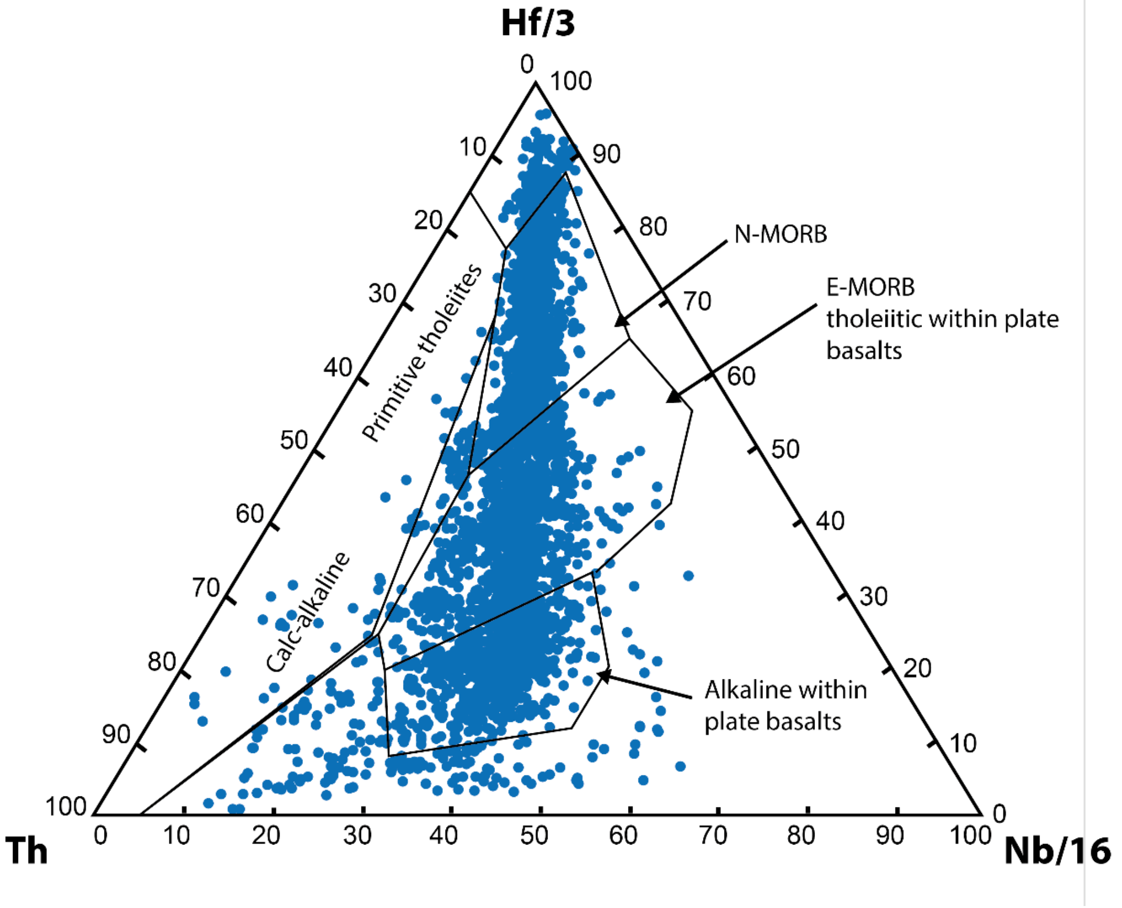

Figure 4.9. Samples of non-subduction settings plotted on Wood (1980) diagram

4.3.2. Pearce and Peate (1995) for Discrimination Between Subduction and Non-Subduction Settings

The bivariate diagram of Pearce and Peate (1995) using Th/Yb and Nb/Yb can be used in order to discriminate between subduction and non-subduction settings. Samples of both subduction (Figure 4.10) and non-subduction (Figure 4.11) settings are plotted in the diagram separately. Samples of non-subduction settings are classified with a higher success ratio when compared to those of subduction samples. A significant amount of samples from subduction settings fall into MORB array or to the field below the MORB array. The success ratio is about 80%. Samples from non-subduction settings generally fall into MORB array. However, there is misclassification of about 80%, due to the samples plotting into subduction field (above the MORB array). When these diagrams are compared to decision trees, decision trees are much more successful in discrimination of both subduction and non-subduction settings.

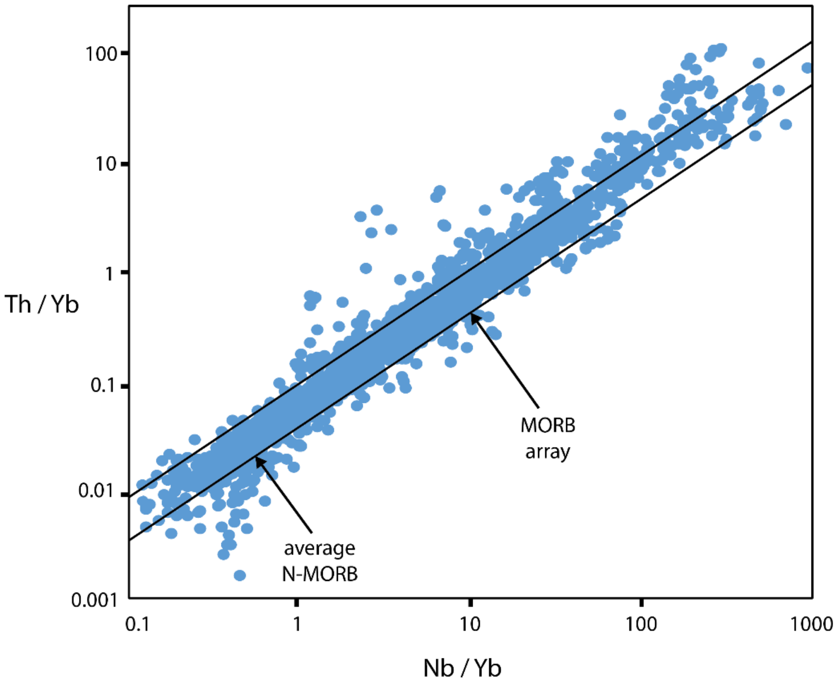

Figure 4.10. Samples of subduction settings plotted on Pearce and Peate (1995) diagram

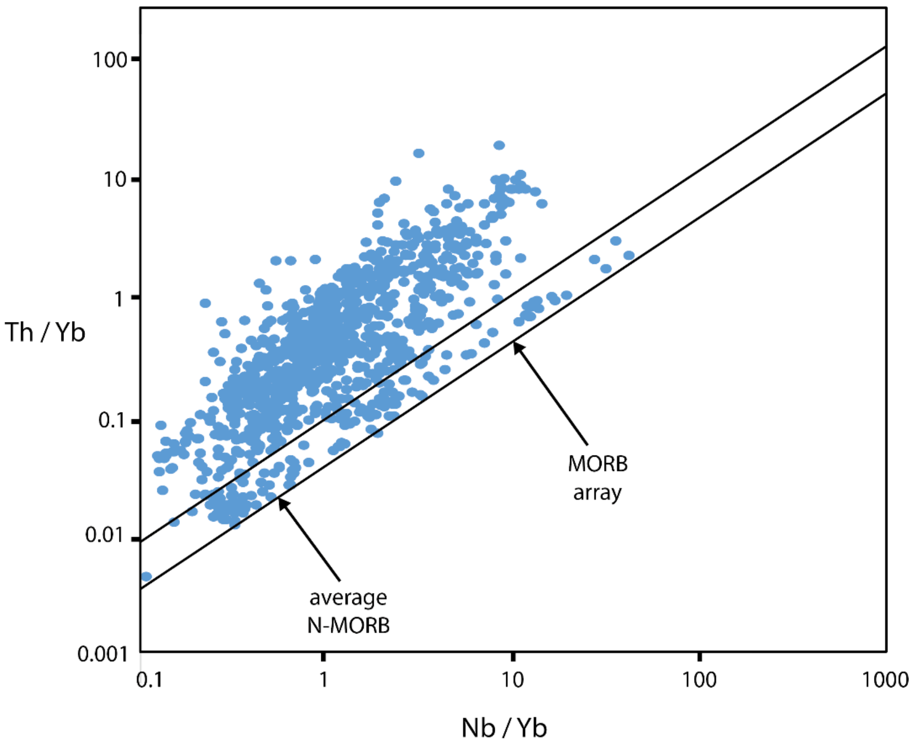

Figure 4.11. Samples of non-subduction settings plotted on Pearce and Peate (1995) diagram

4.3.3. Saccani (2015) for Discrimination Between Subduction and Non-Subduction Settings and Within Subduction Settings

Bivariate diagram of Saccani (2015) using Th_N and Nb_N can be used in order to discriminate between subduction and non-subduction settings. The diagram can also be used in order to discriminate within subduction settings and to discriminate arc settings from back-arc settings. Samples of subduction settings are plotted in the diagram (Figure 4.12). A large amount of samples is plotted in the field defined as divergent plate and within-plate settings. Samples of non-subduction settings are plotted in the diagram (Figure 4.13). Saccani (2015) is relatively more successful in discrimination of non-subduction samples with respect to subduction samples. The samples show a linear trend in overall. However, a large amount of samples is still misclassified as convergent plate setting (nascent forearc).

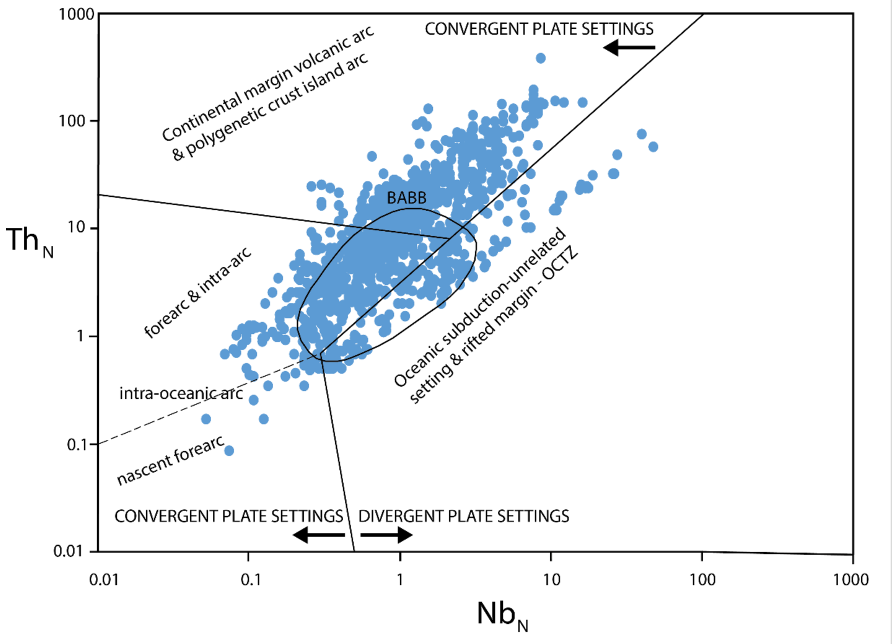

Figure 4.12. Samples of subduction settings plotted on Saccani (2015) diagram

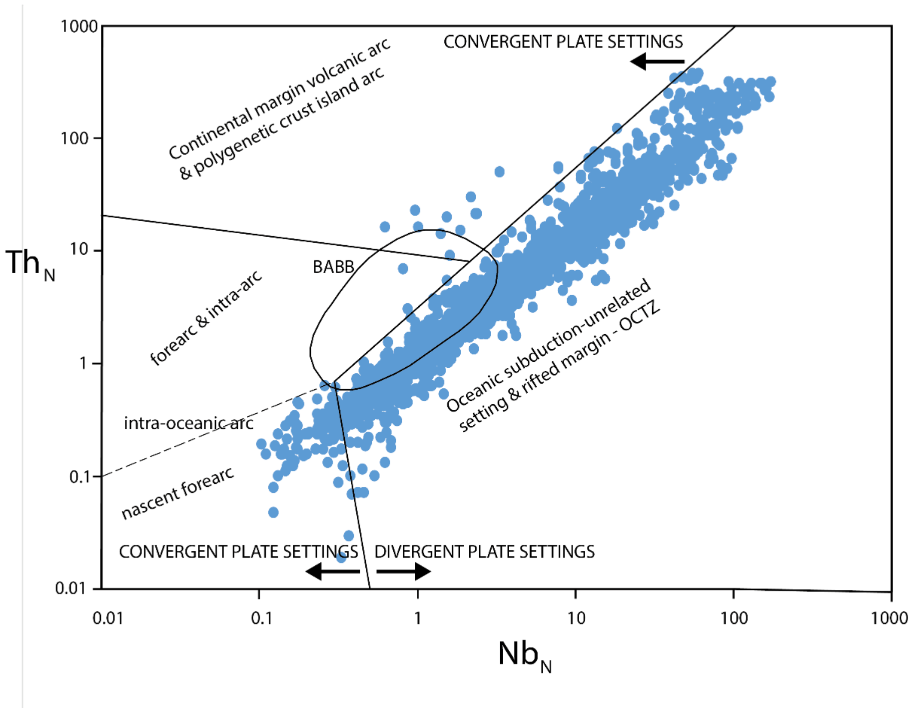

Figure 4.13. Samples of non-subduction settings plotted on Saccani (2015) diagram

Samples of arc settings are plotted in the diagram (Figure 4.14). Saccani (2015) is relatively more successful in discrimination of arc samples with respect to back-arc samples. However, there are samples misclassified as divergent plate and within-plate settings. Many samples are also plotted in the BABB region.

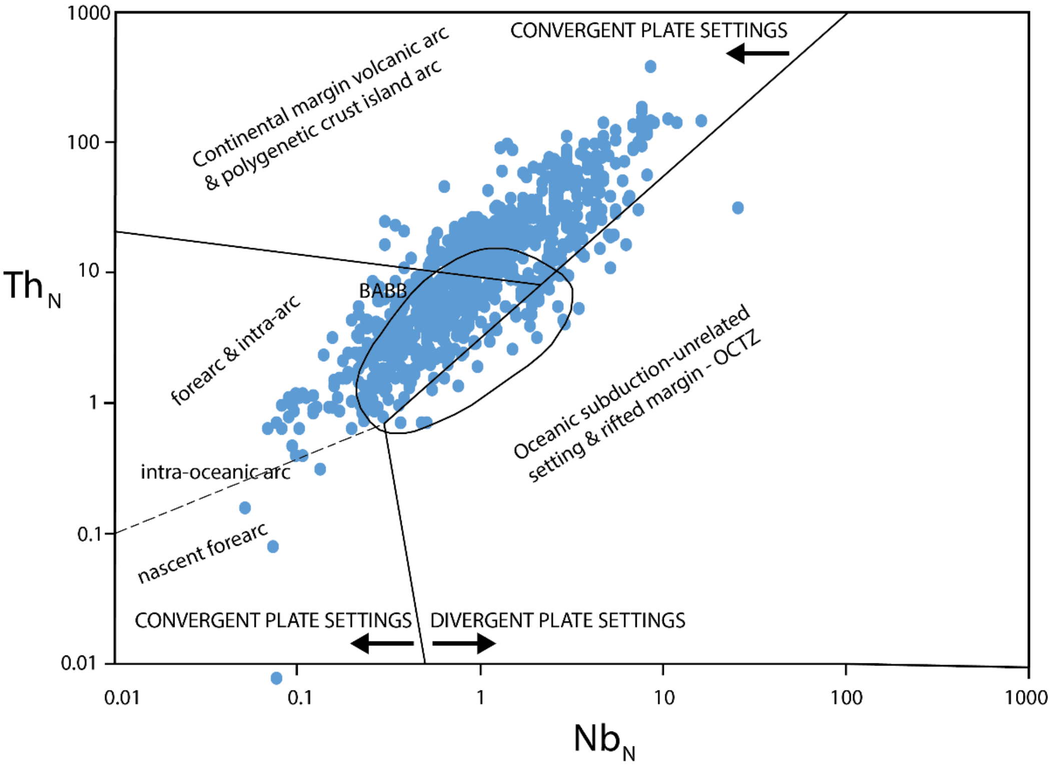

Figure 4.14. Samples of arc settings plotted on Saccani (2015) diagram

Samples of back-arc settings are plotted in the diagram (Figure 4.15). For back-arc settings, the relative ratio of misclassified samples is higher with respect to the discrimination of other settings (subduction, non-subduction, and arc), and Saccani (2015) has the lowest success ratio at the discrimination of back-arc settings. The samples are misclassified either as divergent plate and within-plate settings or arc setting.

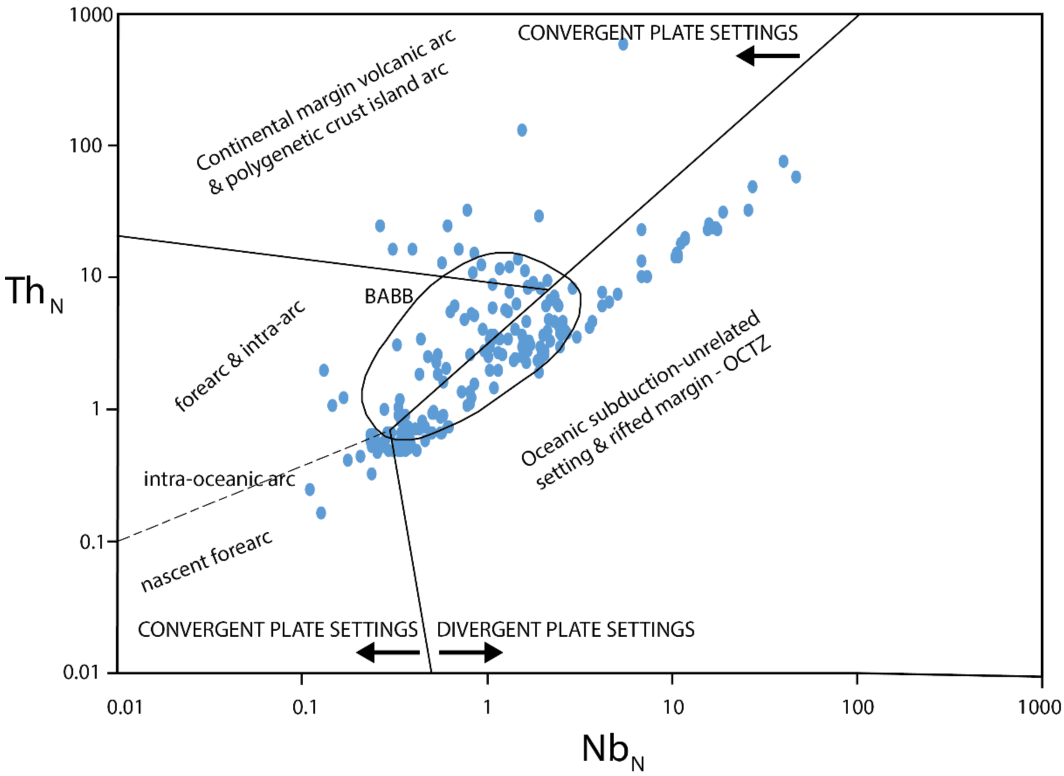

Figure 4.15. Samples of back-arc settings plotted on Saccani (2015) diagram

When these diagrams are evaluated, it can be seen that decision trees are more successful than the traditional diagrams on the discrimination between subduction and non-subduction settings, within subduction settings (between arc and back-arc settings).

4.4. Recommended Decision Trees for Discriminations

4.4.1. Recommended Decision Trees for Discrimination between Subduction and Non-Subduction

One decision stump (single-level decision tree) and two decision trees are constructed for discrimination between subduction and non-subduction. The decision tree cannot be longer simplified as it has only one level. It is also not necessary to simplify the third (alternative) decision tree as it has only two levels and both levels are necessary.

The second decision tree, on the other hand, can be simplified to the second level (Figure 4.16).

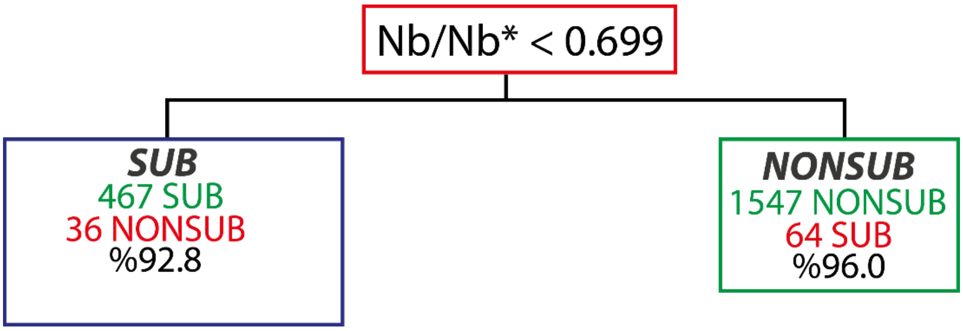

Figure 4.16. Recommended simplified version of the first decision tree for the discrimination between subduction and non-subduction

With the simplification in the second decision tree, the success ratio decreases by 0.15% and increase in misclassifications by 4. Therefore, it can be considered that the simplified version of the first decision tree can also be used with losing an insignificant rate of success in the discrimination between subduction and non-subduction settings.

4.4.2. Recommended Decision Trees for Discrimination between Arc and Back-arc

Simplified versions for both decision trees constructed for the discrimination between arc and back-arc settings are proposed.

The decision trees are simplified to the second level of the original decision tree, with a decrease in success ratio of 0.89% for the first decision tree (Figure 4.17) and 0.75% for the second decision tree (Figure 4.18) with an increase in misclassifications by 6 and 5, with respectively.

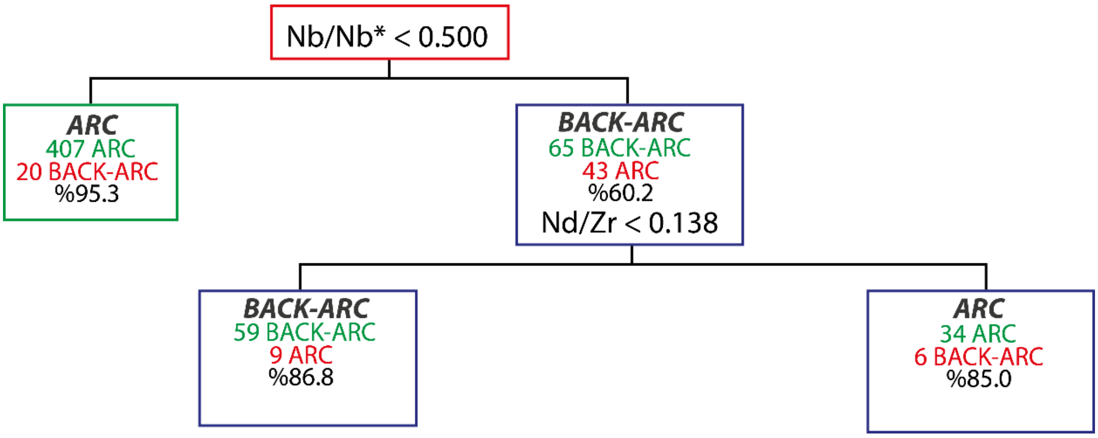

Figure 4.17. Recommended simplified version of the first decision tree for the discrimination between arc and back-arc settings

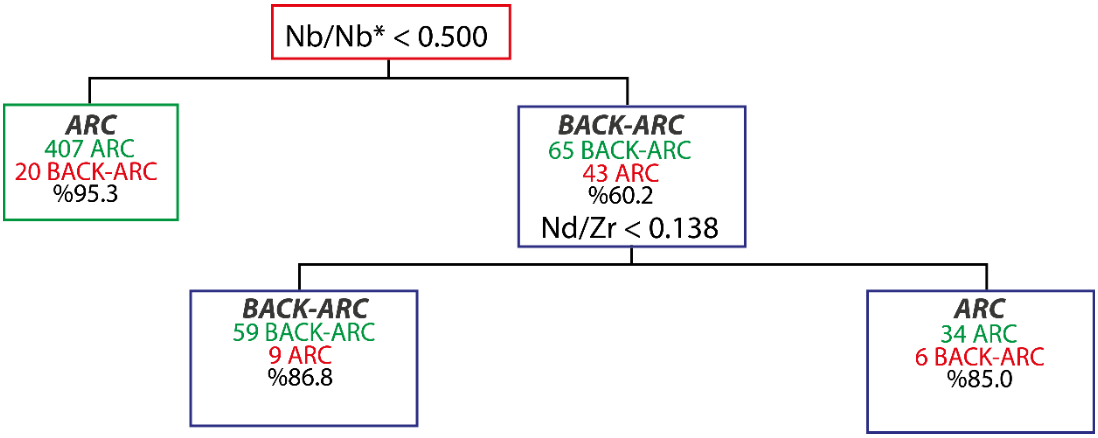

Figure 4.18. Recommended simplified version of the alternative decision tree for the discrimination between arc and back-arc settings

Therefore, it can be considered that the simplified version of both decision trees can also be used with losing an insignificant rate of success in the discrimination between arc and back-arc settings.

4.4.3. Recommended Decision Trees for Discrimination between Oceanic Arc and Continental Arc

Simplified versions for both decision tree constructed for the discrimination between oceanic arc and continental arc settings are proposed. The decision trees are simplified with a decrease in success ratio of 2.66% for the first decision tree (Figure 4.19) and 8.90% for the second decision tree (**Error! Reference source not found.**) with an i ncrease in misclassifications by 15 and 50, with respectively.

Therefore, it can be considered that the simplified version of both decision trees can also be used with losing a relatively insignificant rate of success in the discrimination between oceanic arc and continental arc settings.

4.4.4. Recommended Decision Trees for Discrimination between Oceanic and Continental Settings

Simplified versions for both decision trees constructed for the discrimination between arc and back-arc settings are proposed. The decision trees are simplified with a decrease in success ratio of 7.03% for the first decision tree (Figure 4.21) and 6.28% for the second decision tree (Figure 4.22) with an increase in misclassifications by 47 and 42, with respectively.

Therefore, it can be considered that the simplified version of both decision trees can also be used with losing a relatively insignificant rate of success in the discrimination between oceanic arc and continental arc settings.

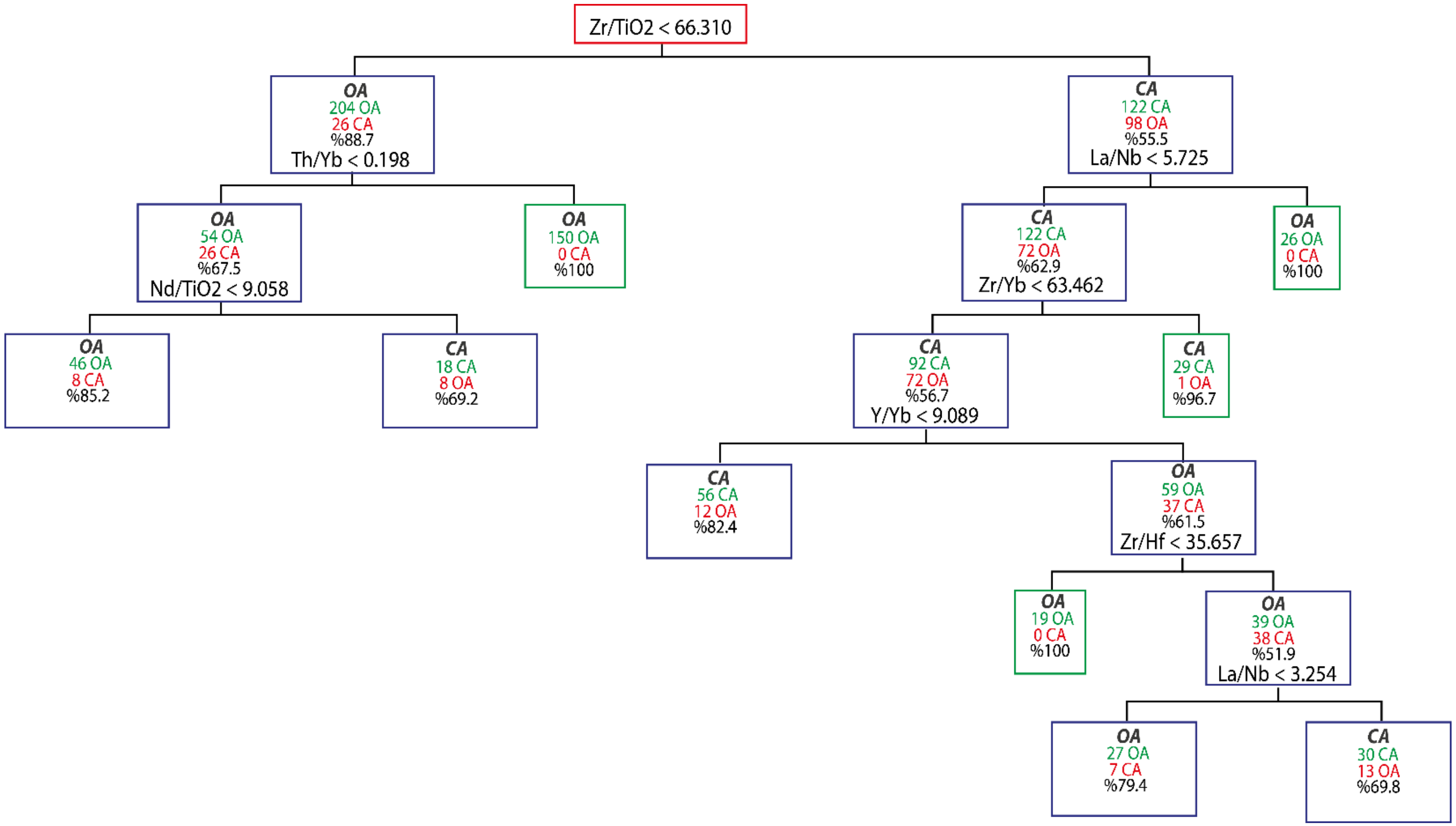

Figure 4.19. Recommended simplified version of the first decision tree for the discrimination between Oceanic Arc and Continental Arc

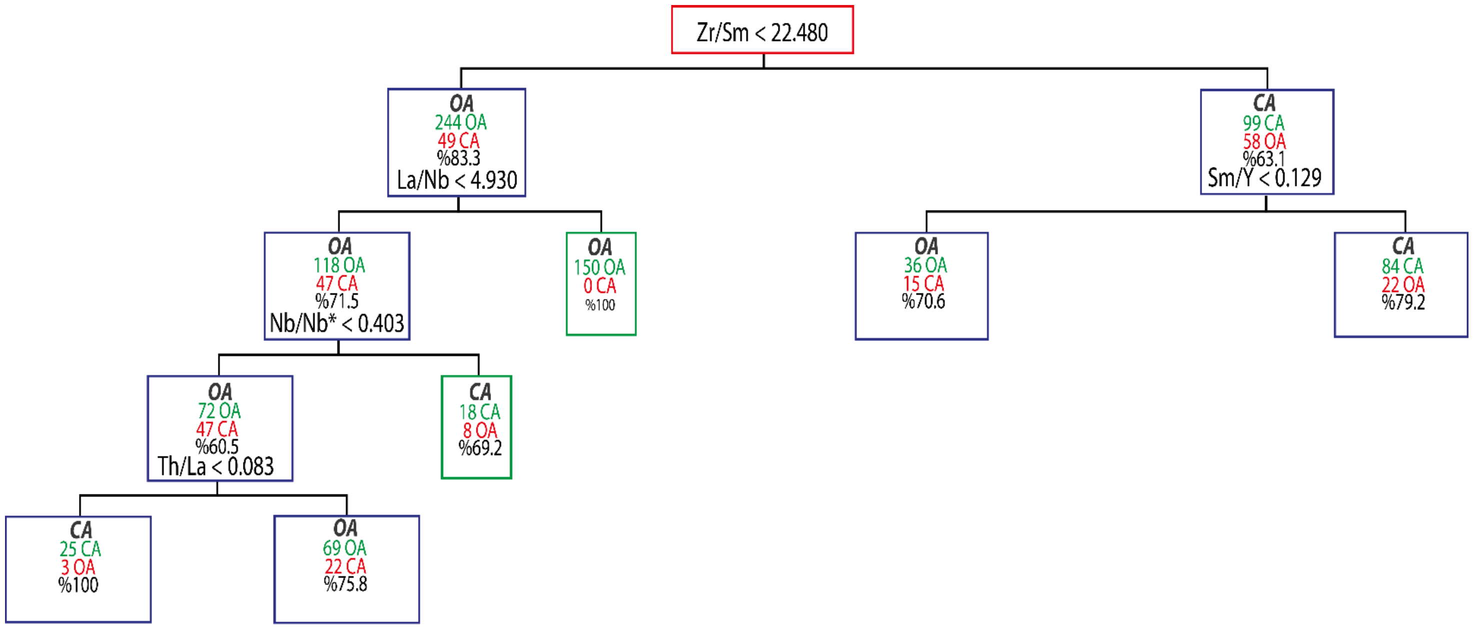

Figure 4.20. Recommended simplified version of the second decision tree for the discrimination between Oceanic Arc and Continental Arc

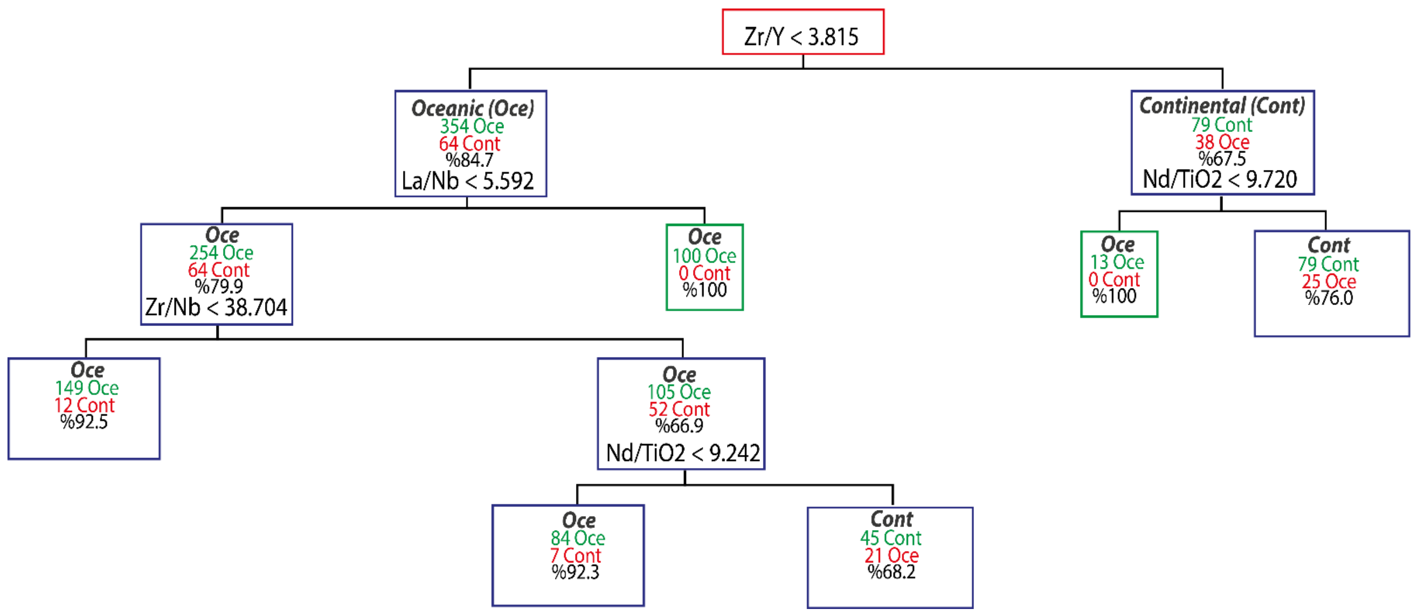

Figure 4.21. Recommended simplified version of the first decision tree for the discrimination between oceanic and continental settings

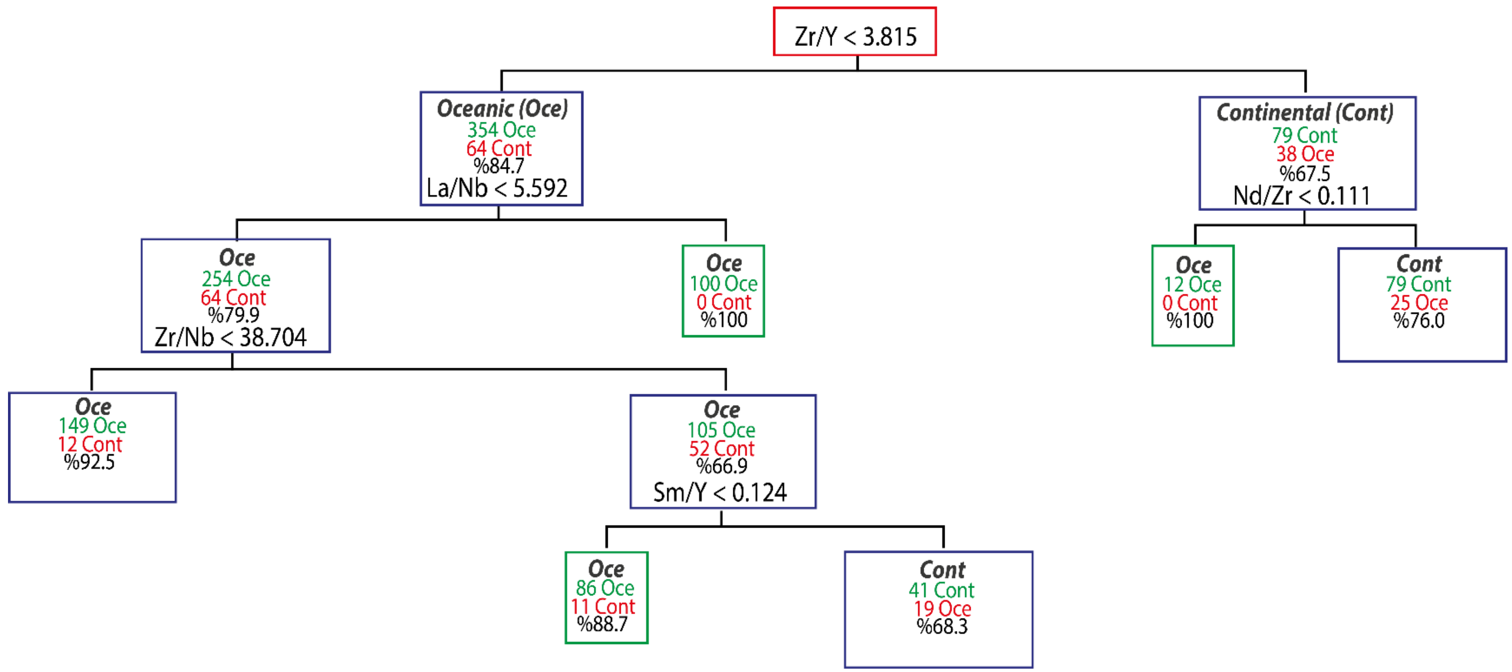

Figure 4.22. Recommended simplified version of the second decision tree for the discrimination between oceanic and continental settings

4.4.5. Recommended Decision Trees for Discrimination between Oceanic Arc and Back-arc

Only one simplified version for both decision tree (Figure 4.23) constructed for the discrimination between oceanic arc and oceanic back-arc settings is proposed.

The decision tree is simplified with a decrease in success ratio of 7.39% for both decision trees with an increase in misclassifications by 36.

Therefore, it can be considered that the simplified version of both decision trees can also be used with losing a relatively insignificant rate of success in the discrimination between oceanic and settings.

4.4.6. Recommended Decision Trees for Discrimination between Group 1 and Group 2 of Non-Subduction Settings

Only one simplified version for both decision tree (Figure 4.24) constructed for the discrimination between MOR+OP (Group 1) and OI+CWP (Group 2) is proposed.

The decision tree is simplified with a decrease in success ratio of 2.93% for both decision trees with an increase in misclassifications by 58.

Therefore, it can be considered that the simplified version can also be used with losing an insignificant rate of success in the discrimination between MOR+OP and OI+CWP.

4.4.7. Recommended Decision Trees for Discrimination between Mid-Ocean Ridges and Oceanic Plateaus

Simplified versions for both decision trees constructed for the discrimination between MOR and OP are proposed.

The decision trees are simplified with a decrease in success ratio of 1.96% for the first decision tree (Figure 4.26) and 3.92% for the second decision tree (Figure 4.28) with an increase in misclassifications by 22 and 44, with respectively.

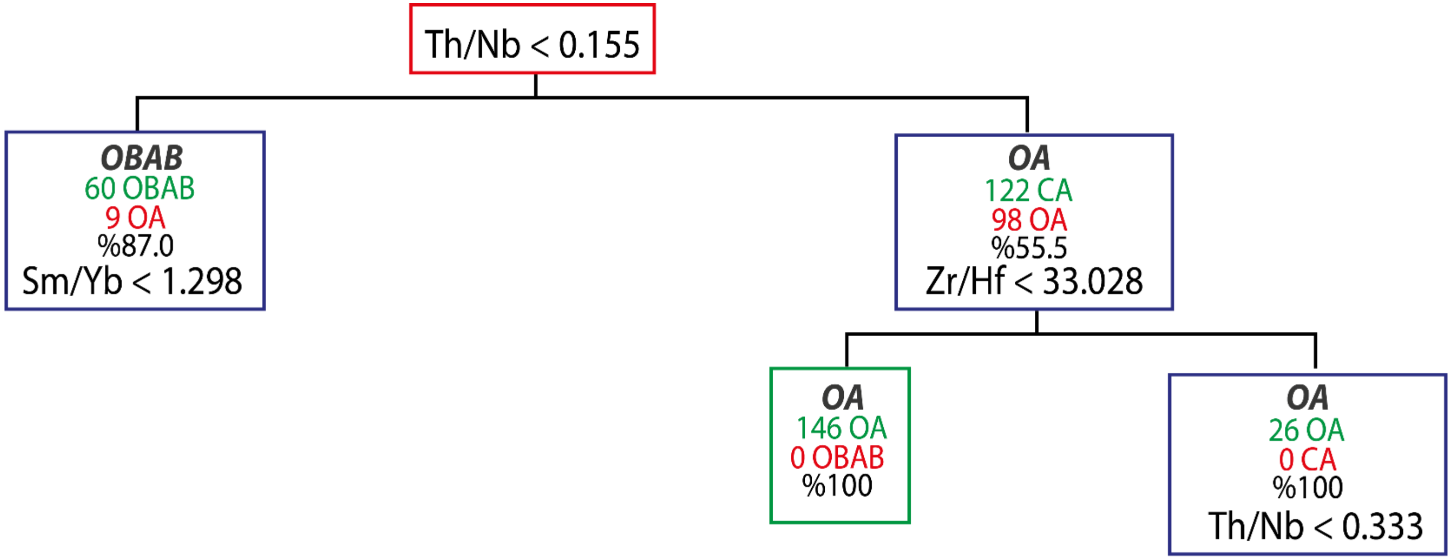

Figure 4.23. Recommended simplified version for the discrimination between oceanic arc and back-arc basin settings

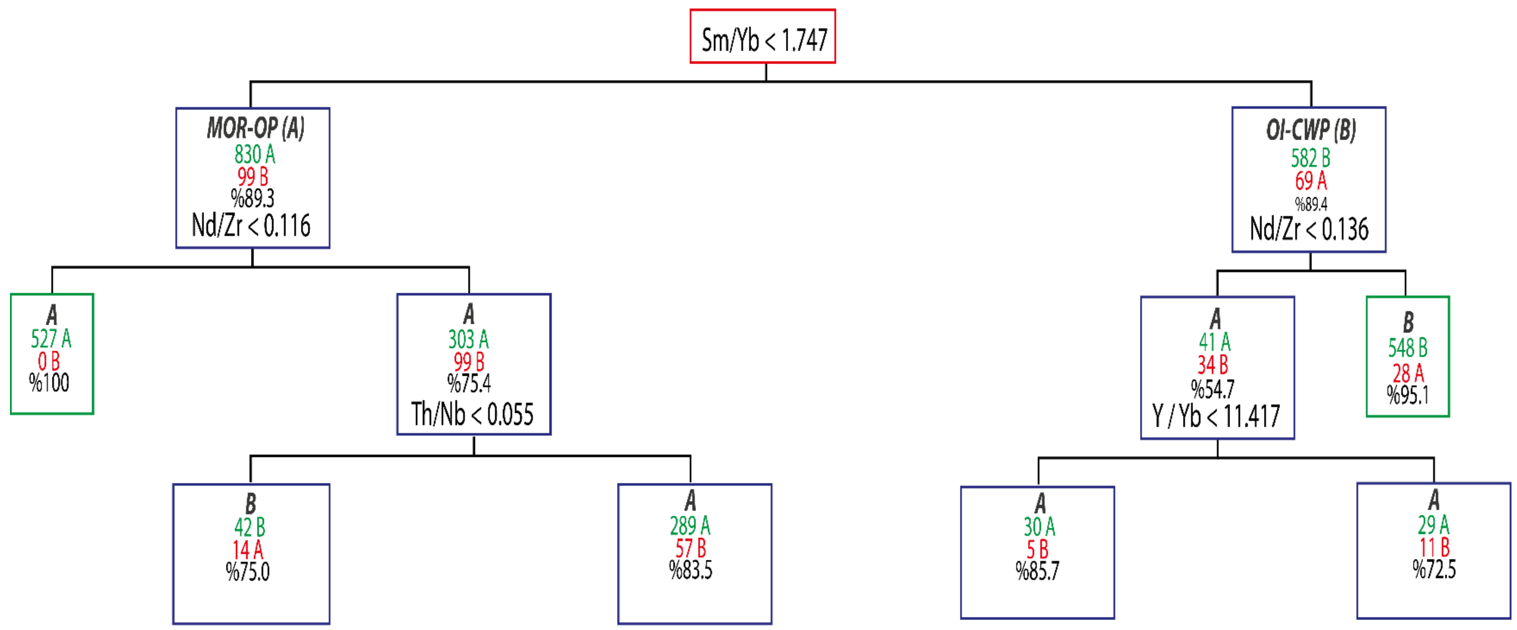

Figure 4.24. Recommended simplified version of the first decision tree for the discrimination MOR+OP and OI+CWP

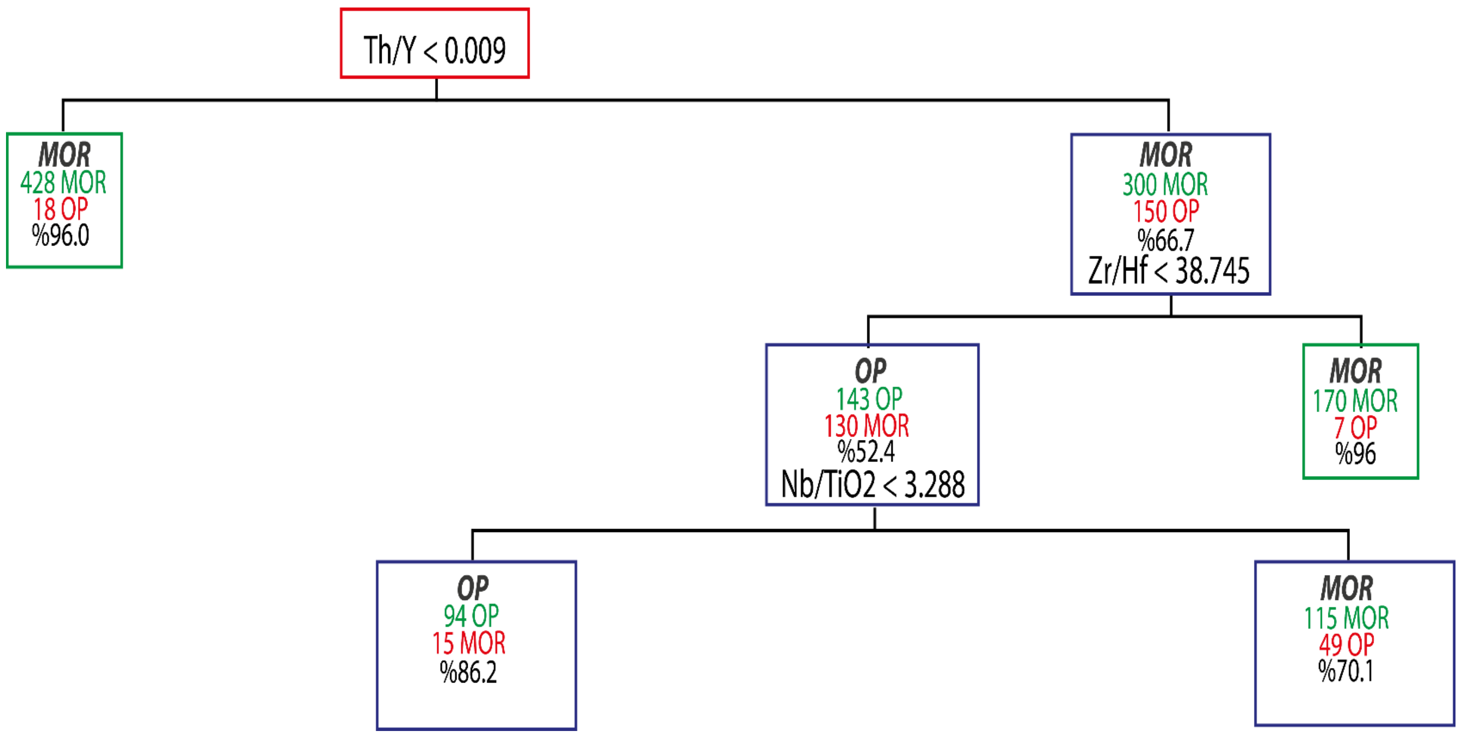

Figure 4.25. Recommended simplified version of the first decision tree for the discrimination between MOR and OP

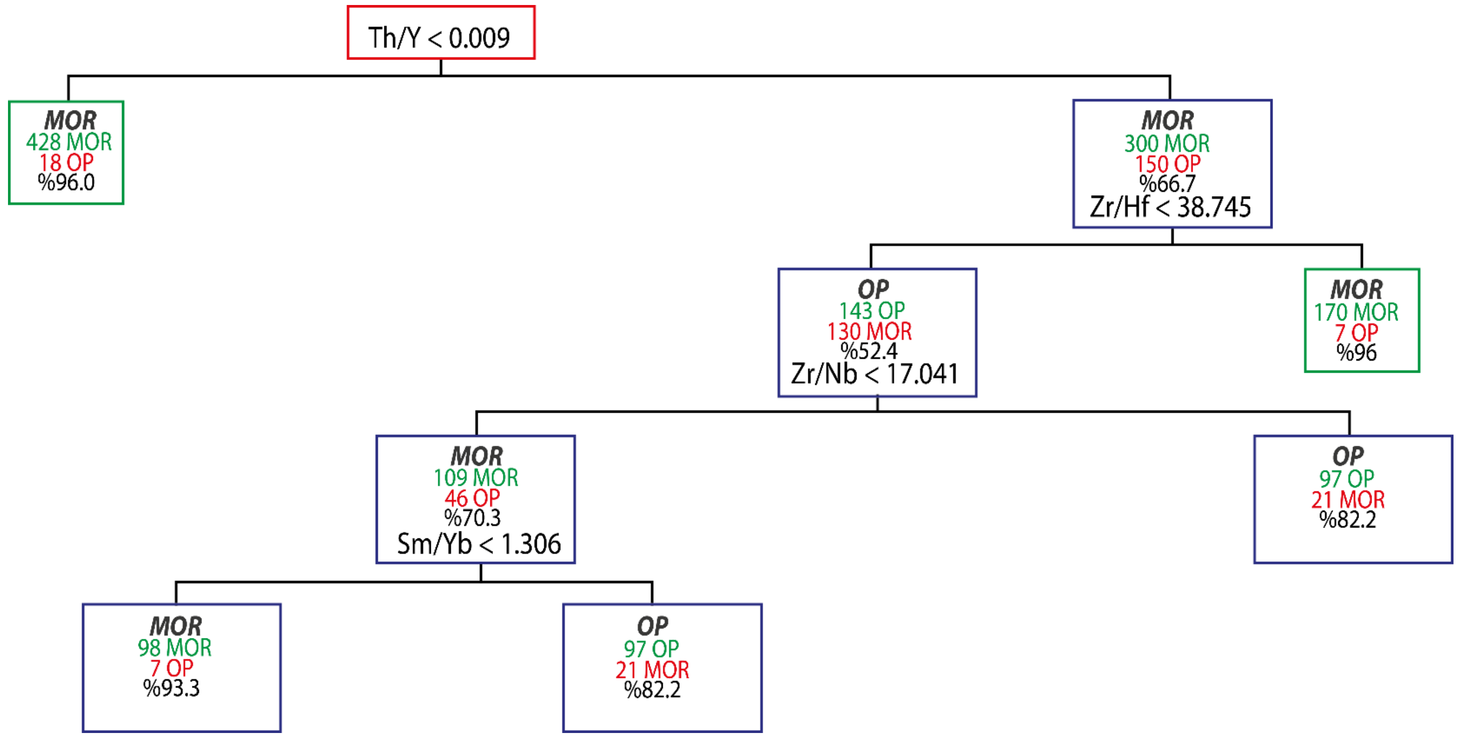

Figure 4.27. Recommended simplified version of the alternative decision tree for the discrimination between MOR and OP

Therefore, it can be considered that the simplified version of both decision trees can also be used with losing a relatively insignificant rate of success in the discrimination between MOR and OP.

4.4.8. Recommended Decision Trees for Discrimination between Oceanic Islands and Continental Within-Plates

Simplified versions for both decision trees constructed for the discrimination between OI and CWP are proposed.

The decision trees are simplified with a decrease in success ratio of 4.68% for the first decision tree (Figure 4.30) and 5.26% for the second decision tree (Figure 4.31) with an increase in misclassifications by 40 and 45, with respectively.

Therefore, it can be considered that the simplified version of both decision trees can also be used with losing a relatively insignificant rate of success in the discrimination between OI and CWP.

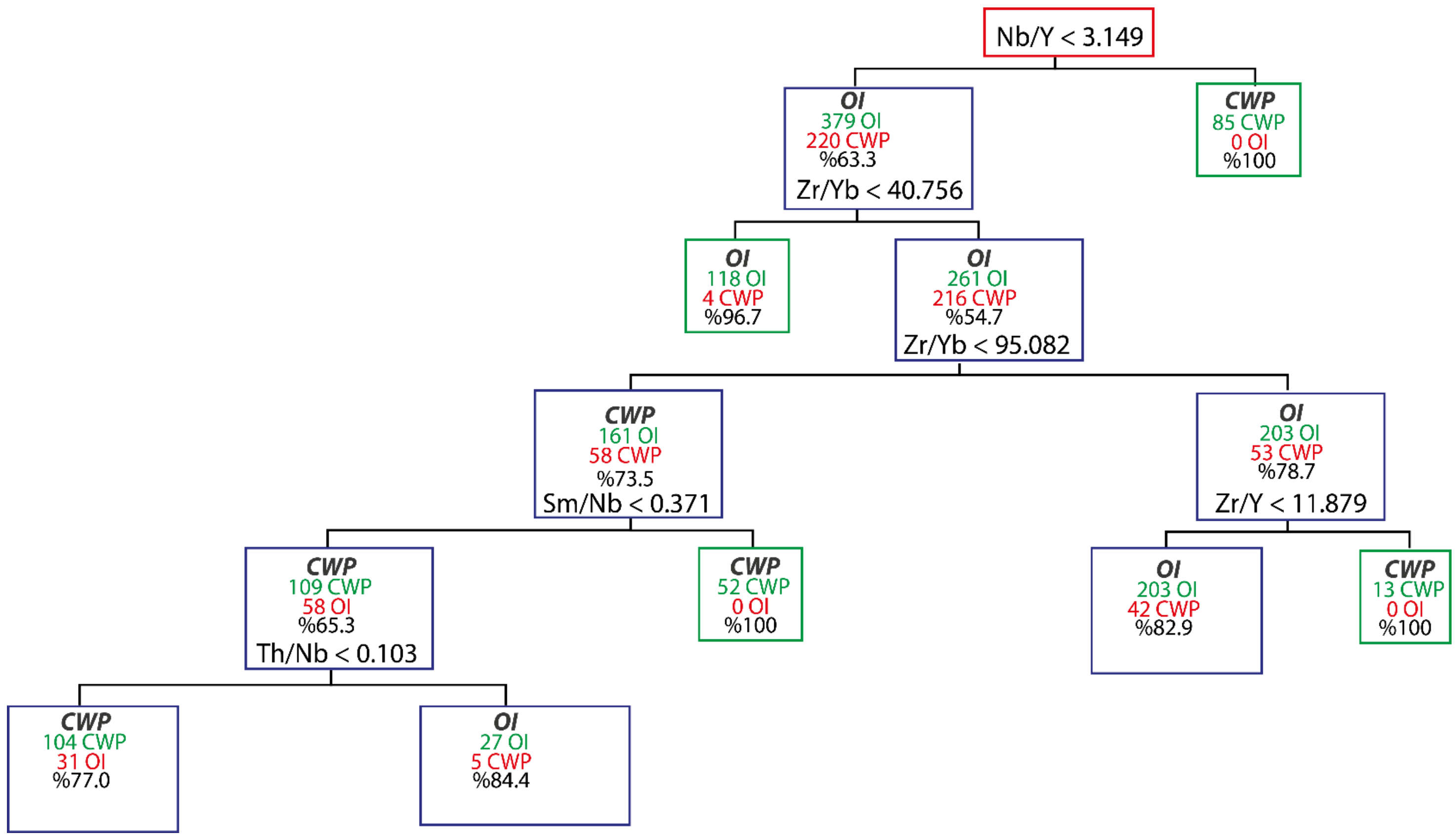

Figure 4.29. Recommended simplified version of the first decision tree for the discrimination between Ocean Islands and Continental Within-Plate

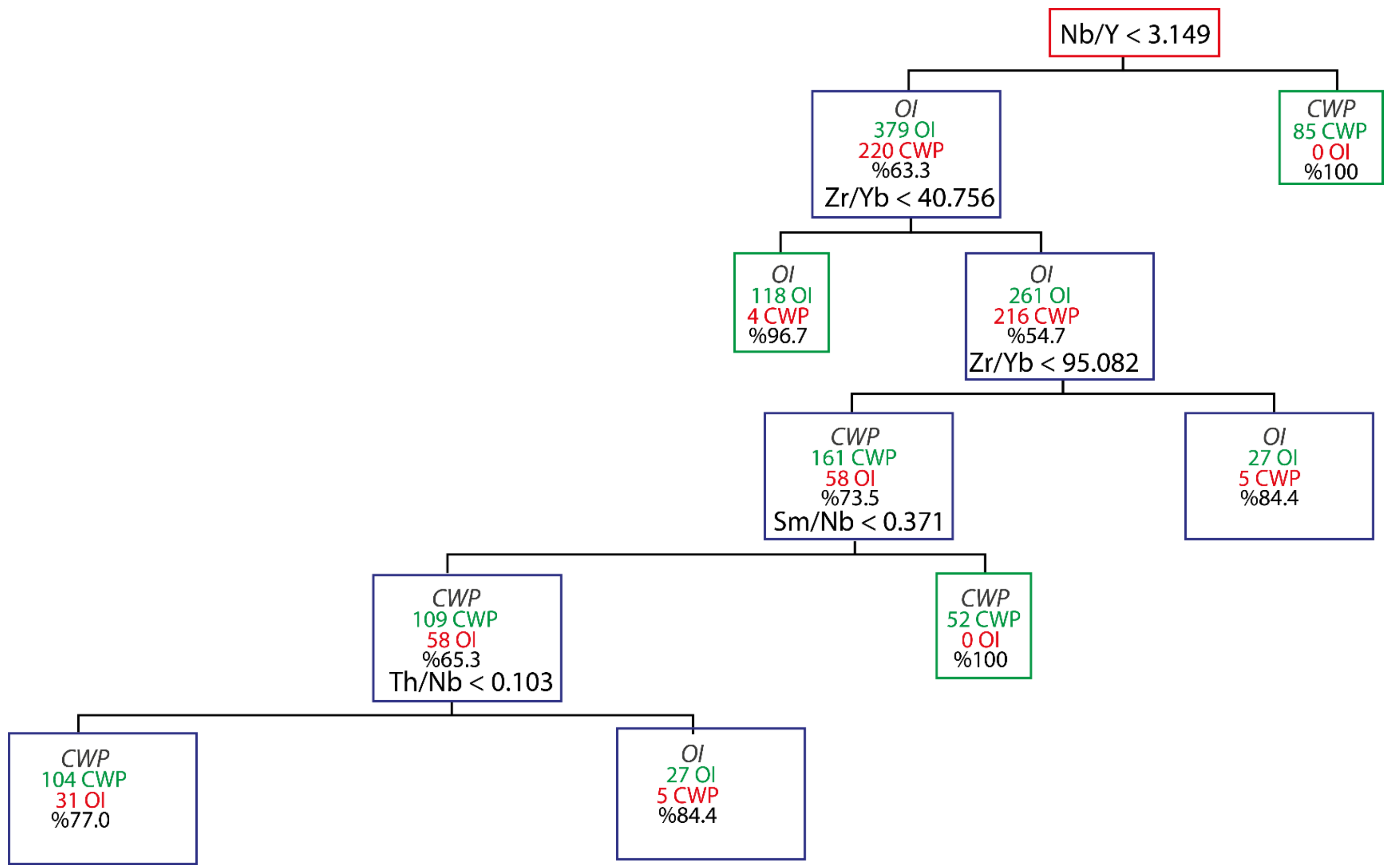

Figure 4.28. Recommended simplified version of the alternative decision tree for the discrimination between Ocean Islands and Continental Within-Plate

CHAPTER 5

CONCLUSIONS

Decision trees are constructed for the tectono-magmatic discrimination of mafic igneous rocks in order to discriminate between (1) subduction and non-subduction settings, (2) arc-related and back-arc-related settings within subduction settings, (3) oceanic arc and continental arc within arc-related settings, (4) oceanic and continental settings within subduction settings, (5) oceanic arc and oceanic back-arc within subduction-related oceanic settings, (6) mid-oceanic ridge + oceanic plateau and oceanic island + continental within-plate within non-subduction settings, (7) mid-oceanic ridge and oceanic plateau within non-subduction settings and (8) oceanic island and continental within-plate within non-subduction settings.

For the discrimination between subduction and non-subduction settings, one decision stump and two decision trees are constructed. The decision trees have 4 and 2 levels of depth, with respectively. The element ratios used in these trees are Th/Nb, Nb/Nb*, TiO_2/Yb, Zr/Nb, La/Nb and Nb/Y. All decision trees discriminated successfully with a success ratio of 97-99% for non-subduction and 86-88% for subduction settings. Most journals in the dataset are correctly classified with 100% success ratio.

Within subduction settings, for discrimination between arc and back-arc-related settings, two decision trees are constructed. The decision trees have 5 levels of depth. The element ratios used in these trees are Nb/Nb*, Nd/Zr, TiO_2/Y, Nd/TiO_2, Y/Yb, Zr/Hf, Zr/Nb, Zr/Y and Y/Yb. All decision trees discriminated successfully with a success ratio of 98% for arc and 83-86% for back-arc-related settings. There is no difference between two decision trees for the discrimination for arc-related settings.

Within arc-related settings, for discrimination between oceanic arcs and continental arcs, two decision trees are constructed. The decision trees have 7 levels of depth. The element ratios used in these trees are Zr/TiO_2, Th/Nb, La/Nb, Nd/TiO_2, Zr/Yb, La/Yb, Y/Yb, Sm/Hf, Zr/Hf, Nb/Nb*, Zr/Sm, La/Nb, Nb/Y, Th/Y, Sm/Y, Th/La, Zr/Y, La/Y, Sm/Nd and Zr/Nb. All decision trees discriminated successfully with a success ratio of 97-98% for continental arcs and 92-94% for oceanic arcs.

Within subduction settings, for discrimination between oceanic and continental settings, two decision trees are constructed. The decision trees have 6 levels of depth. The element ratios used in these trees are Zr/Y, La/Nb, Nd/TiO_2, Zr/Nb, Y/Yb, TiO_2/Y, Nb/Nb*, Zr/Hf, Sm/Hf, La/Yb, Nd/Zr and Sm/Y. All decision trees discriminated successfully with a success ratio of 95-96% for oceanic and 83-90% for continental settings. The second decision tree is weaker at discrimination of continental settings.

Within subduction-related oceanic settings, for discrimination between oceanic arc and oceanic back arcs, two decision trees are constructed. The decision trees have 6 levels of depth. The element ratios used in these trees are Th/Nb, Sm/Yb, Zr/Hf, La/Nb, Nb/Nb*, Nd/Zr, TiO_2/Yb, Y/Yb, Nb/Yb, La/Sm and Sm/Y. All decision trees discriminated successfully with a success ratio of 99% for oceanic arcs and 92-93% for oceanic back arcs.

Within non-subduction settings, for the discriminaton of mid-oceanic ridge and oceanic plateau (group 1) from oceanic island and continental within-plate (group 2), two decision trees are constructed. The decision trees have 7 levels of depth. The element ratios used in these trees are Sm/Yb, Nd/Zr, Th/Nb, Y/Yb, Zr/TiO_2, La/Nb, Nb/Nb*, La/Sm, Nb/Yb, TiO_2/Y, Zr/Hf, Th/La, Sm/Hf, Nb/Y. All decision trees discriminated successfully with a success ratio of 96% for group 1 and 95% for group 2.

Within non-subduction settings, for the discriminaton of mid-ocean ridge and oceanic plateau, two decision trees are constructed. The decision trees have 6 and 7 levels of depth, with respectively. The element ratios used in these trees are Th/Y, Zr/Hf, Nb/TiO_2, Zr/Y, Zr/Nb, Th/La, Nb/Nb*, Sm/Yb, Sm/Y, La/Nb, Y/Yb and La/Y. All decision trees discriminated successfully with a success ratio of 83% for oceanic plateaus and 99% for mid-oceanic ridges. The decision trees are much more successful for discrimination of mid-oceanic ridges.

Within non-subduction settings, for the discriminaton of oceanic island and continental within-plate, two decision trees are constructed. The decision trees have 8 levels of depth. The element ratios used in these trees are Nb/Y, Zr/Yb, Sm/Nb, Zr/Y, Th/Nb, TiO_2/Y, Nb/TiO_2, Y/Yb, Zr/Hf, Sm/Nd, Th/La, Sm/Yb, La/Y, Zr/Nb, La/Sm, Y/Yb and Nb/Yb. All decision trees discriminated successfully with a success ratio of 90% for oceanic islands and 91% for continental within-plate.

The success ratios for external datasets are also similar to the training set for nearly all decision trees, avoiding any risk of underfitting and overfitting. The decision trees only fail in external datasets for the discrimination of oceanic plateau from mid-ocean ridge (54%) and for the discrimination of continental within-plate from oceanic island (26%). In these discriminations, two tectonic settings (oceanic plateaus and continental within-plates) cannot be discriminated in external datasets.

A final recommendation for the decision trees is made by simplifying decision trees to a certain level of depth in a cost of an ignorable loss in success ratio.

There are no traditional discrimination methods available in literature to discriminate all tectonic settings included in this study. There are few diagrams discriminating subduction settings from non-subduction settings and discriminating within subduction setting between arc and back-arc settings. The decision trees constructed in this study are more successful when compared to traditional methods. Discrimination methods constructed with decision tree can only classify three tectonic settings. Decision trees constructed using other modern methods such as support vector machines or random forests tend to memorize the datasets achieving high success ratio but tend to overfit and fail at external datasets, with different characteristics related to training set. All modern methods use online databases such as GeoRoc or PetDB. They also use mobile elements, isotope ratios and absolute values of elements. Therefore, their success falls drastically in external datasets.

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