A FUZZY SOFTWARE PROTOTYPE FOR SPATIAL PHENOMENA: CASE STUDY PRECIPITATION DISTRIBUTION

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TAHSİN ALP YANAR

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ABSTRACT

A FUZZY SOFTWARE PROTOTYPE FOR SPATIAL PHENOMENA: CASE STUDY PRECIPITATION DISTRIBUTION

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As the complexity of a spatial phenomenon increases, traditional modeling becomes impractical. Alternatively, data-driven modeling, which is based on the analysis of data characterizing the phenomena, can be used. In this thesis, the generation of understandable and reliable spatial models using observational data is addressed. An interpretability oriented data-driven fuzzy modeling approach is proposed. The methodology is based on construction of fuzzy models from data, tuning and fuzzy model simplification. Mamdani type fuzzy models with triangular membership functions are considered. Fuzzy models are constructed using fuzzy clustering algorithms and simulated annealing metaheuristic is adapted for the tuning step. To obtain compact and interpretable fuzzy models a simplification methodology is proposed. The simplification methodology reduced the number of fuzzy sets for each variable and simplified the rule base. Prototype software is developed and mean annual precipitation data of Turkey is examined as case study to assess the results of the approach in terms of both precision and interpretability. In the first step of the approach, in which fuzzy models are constructed from data, "Fuzzy Clustering and Data Analysis Toolbox", which is developed for use with MATLAB®, is used. For the other steps, the optimization of obtained fuzzy models from data using adapted simulated annealing algorithm step and the generation of compact and interpretable fuzzy models by simplification algorithm step, developed prototype software is used. If accuracy is the primary objective then the proposed approach can produce more accurate solutions for training data than the geographically weighted regression method. The minimum training error

value produced by the proposed approach is 74.82 mm while the error obtained by geographically weighted regression method is 106.78 mm. The minimum error value on test data is 202.93 mm. An understandable fuzzy model for annual precipitation is generated with only 12 membership functions and 8 fuzzy rules. Furthermore, more interpretable fuzzy models are obtained when Gath-Geva fuzzy clustering algorithms are used during fuzzy model construction.

Keywords: Spatial modeling, Data-driven fuzzy modeling, Fuzzy clustering algorithms, Simulated annealing, Fuzzy model tuning, Interpretability, Precipitation

ÖZ

MEKÂNSAL FENOMENLER İÇİN BULANIK YAZILIM PROTOTİPİ: YAĞIŞ DAĞILIMI ÖRNEK OLAYI İNCELEMESİ

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Mekânsal fenomenlerin karmaşıklığı arttıkça geleneksel yöntemler ile modellenmesi pratikliğini yitirmektedir. Bu durumlarda, fenomeni niteleyen verilerin analiz edilmesine dayanan veri güdümlü modelleme yaklaşımı kullanılabilir. Bu tezde, anlaşılabilir ve güvenilir mekânsal modellerin gözlemsel veriler kullanılarak oluşturulması ele alınmıştır. Tezde, anlaşılabilir bulanık modellerin veriler kullanılarak oluşturulması (veri güdümlü) yöntemi sunulmuştur. Yöntem, bulanık modellerin verilerden oluşturulması, optimize edilmesi ve sadeleştirilmesi adımlarından oluşmaktadır ve Mamdani tipinde bulanık modeller ile üçgensel aitlik fonksiyonları için oluşturulmuştur. Bulanık modeller, bulanık kümeleme algoritmaları kullanılarak oluşturulmuştur ve optimizasyon adımı için benzetimli tavlama yöntemi uyarlanmıştır. Küçük ve anlaşılabilir bulanık modelleri elde edebilmek için bir sadeleştirme yöntemi önerilmiştir. Sadeleştirme yönteminde her bir dilsel değişkenin kullandığı bulanık küme sayısı azaltılmış ve kural tabanı basitleştirilmiştir. Yöntemin ürettiği sonuçların doğruluk ve anlaşılabilirlik açısından değerlendirilebilmesi için bir prototip yazılım geliştirilmiştir ve Türkiye'nin ortalama yıllık yağış verisi örnek olay olarak incelenmiştir. Yöntemin ilk adımı olan bulanık modellerin verilerden üretilmesi adımında MATLAB® için geliştirilmiş olan "Fuzzy Clustering and Data Analysis Toolbox" aracı kullanılmıştır. Elde edilen bulanık modellerin benzetimli tavlama yöntemi ile optimize edilmesi, sadeleştirilerek küçük ve anlaşılabilir bulanık modellerin oluşturulması adımları için ise geliştirilmiş olan prototip

yazılım kullanılmıştır. Birinci öncelikli amaç doğruluk olduğunda sunulan yaklaşım ile coğrafi ağırlıklandırılmış regresyon yöntemine göre daha iyi sonuçlar elde edilmiştir. Sunulan yaklaşım ile eğitim verisi için bulunan minimum hata 74.82 milimetreyken coğrafi ağırlıklandırılmış regresyon yönteminde eğitim verisi hatası 106.78 milimetre olmuştur. Sunulan yaklaşım ile test verisi için bulunan minimum hata ise 202.93 milimetredir. Yıllık yağış için sadece 12 aitlik fonksiyonu ve 8 kural içeren anlaşılır bir bulanık model oluşturulmuştur. Buna ilâveten, Gath-Geva bulanık kümeleme yöntemi ile oluşturulan bulanık modeller kullanılarak daha anlaşılabilir bulanık modeller elde edilmiştir.

Anahtar Kelimeler: Mekânsal modelleme, Veri güdümlü bulanık modelleme, Bulanık kümeleme algoritmaları, Benzetimli tavlama, Bulanık model en iyileme, Anlaşılabilirlik, Yağış

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During my graduate studies, I worked as a full time computer engineer in Savunma Teknolojileri ve Mühendislik A.Ş. and I would like to thank my company and my colleagues for their support.

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To My Family

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CHAPTER 1

INTRODUCTION

A spatial model represents an object or behavior of a phenomenon that exist in the real world (Aronoff, 1989). The development of reliable and understandable spatial models is very important to comprehend and work on natural phenomena. In traditional modeling, also known as white-box modeling, the parameters characterizing the phenomenon have clear and interpretable physical meanings and they are derived using geological, physical, biological laws. However, as the complexity of spatial phenomenon increases traditional modeling becomes impractical. Examples of such complex spatial phenomena are hydrologic systems, mineral prospectivity, seismic activities, groundwater vulnerability, landslide susceptibility, etc. Due to advances in data acquisition technology, it has been possible to collect large volumes of data associated with these spatial phenomena. Thus, spatial phenomenon can be modeled fully based on observational data without any need to prior knowledge with data-driven modeling techniques. This strategy is called black-box modeling. Although black-box modeling can generate a model which represents natural phenomenon reliably and precisely, the model structure and parameters usually give no explicit explanation about the behaviors of the phenomenon. Alternatively, the third modeling strategy seeks a balance between precision and understandability which are two conflicting modeling objectives. In this approach, models are generated using relationships between inputs and outputs but the primary objective is not the accuracy itself. Precise and understandable models give some explanation about the complex phenomena. These models can be a good starting point for better understanding of the nature and behavior of the phenomena and for further analysis.

Fuzzy set theory is a generalization to classical set theory to allow objects to take partial degrees between zero and one. A fuzzy model is a set of fuzzy if-then rules that maps inputs to outputs where a fuzzy rule establishes logical relation between

variables, by relating qualitative value of the input variable to qualitative value of the output variable. Fuzzy models are able to perform non-linear mappings between inputs and outputs and they are also able to handle linguistic knowledge in addition to numerical data. Therefore, fuzzy models can formulate the spatial phenomenon in interpretable fuzzy if-then rules.

FuzzyCell (Yanar, 2003) is a fuzzy processing software for raster data analyses. It incorporates human knowledge and experience in the form of linguistically defined variables into raster based GIS through the use of fuzzy set theory. The main purpose of the FuzzyCell is to assist a GIS user to make decisions using experts' experiences in decision-making processes. Experts' experiences described in natural language are captured by fuzzy if-then rules. Created fuzzy if-then rules are used to generate solutions to decision-making problems. According to feedbacks from FuzzyCell software users, they have some difficulties in the conversion of experts' experiences into fuzzy if-then rules. In addition to this, experts and users need some guidance while selecting membership function parameters and deciding on fuzzy rules. Therefore, before constructing fuzzy if-then rules, an initially created interpretable fuzzy model can assist experts and FuzzyCell users and simplify the fuzzy rule creation process.

The basic problem is the generation of understandable and reliable spatial models using observational data. Specifically, the problem is to construct interpretable and accurate fuzzy models using relationships between inputs and outputs.

1.1 Contributions

In this thesis, an interpretability oriented data-driven fuzzy modeling methodology is proposed. A software prototype is implemented for the proposed methodology. Mean annual precipitation data of Turkey is used as a case study to demonstrate the use of the proposed approach and to test its accuracy and interpretability.

Due to its rule structure, Mamdani type fuzzy model offers a more understandable model than a Takagi-Sugeno type fuzzy model. For data-driven Mamdani type fuzzy model construction, three fuzzy clustering algorithms namely fuzzy c-means, Gustafson-Kessel and Gath-Geva clustering algorithms are used. Fuzzy clustering algorithms are applied on both original spatial data and processed data. Processed data are obtained by applying Box-Cox power transformation to original data and then

scaling of data into the range $[0, 1]$. Cluster validity indices with accuracy measures are used to determine the cluster count and initial fuzzy models are created by using fuzzy partition matrix for fuzzy c-means algorithm and fuzzy covariance matrix for Gustafson-Kessel and Gath-Geva clustering algorithms.

- Results have proven the claim that data scale influences the performance of the clustering algorithms. The use of the processed data in the fuzzy clustering process makes fuzzy clustering algorithms more stable and improves their accuracies.

After initial fuzzy model construction, simulated annealing algorithm is adapted for tuning Mamdani type fuzzy models with triangular membership functions.

- In the disturbance mechanism of the adapted simulated annealing algorithm, transitions of each parameter of triangular membership function are decreased as temperature decreases. Therefore, at high temperatures each parameter has wider allowable change interval.

- A rule based disturbance mechanism is defined. Instead of modifying all or a number of randomly selected parameters, only parameters associated with a randomly selected rule are modified.

The computing time is decreased by adding constraints on temperature stage.

- After the tuning process, obtained model error on training data (74.82 mm) is reduced more than geographically weighted regression method (106.78 mm). Moreover, obtained model error on test data is 202.93 mm.

Since accuracy is the primary objective while tuning fuzzy models, at the end of the tuning process obtained membership functions have high degree of overlapping. Thus, the optimized fuzzy models are not interpretable. An algorithm is proposed to obtain compact and interpretable fuzzy models. The algorithm has two simplification phases and tuning phases. In a simplification phase, the number of fuzzy sets for each linguistic variable is reduced using similarity among fuzzy sets. Moreover, rule base simplification is performed.

- In the simplification algorithm, the degree of subset measure is defined to measure the degree of subset a fuzzy set is inside other fuzzy set.

- In the simplification algorithm, a combination measure is defined to detect cases where similarity between the fuzzy sets is low but they are indistinguishable because of the closeness of their centers.
- The results show that, simplified fuzzy models obtained by the simplification algorithm satisfy most of the interpretability criteria.
- Fuzzy models constructed by Gath-Geva clustering algorithms are simplified more.
- An interpretable fuzzy model for estimating mean annual precipitation of Turkey is generated only with 12 membership functions and 8 rules.
- A software prototype is implemented for the proposed methodology. The software is able to tune Mamdani type fuzzy models with triangular membership functions using the adapted simulated annealing algorithm. And it can simplify fuzzy models using the simplification methods to obtain interpretable fuzzy models.

1.2 Organization

The organization of the thesis is as follows: the next chapter, Chapter 2, describes the details of the mean annual precipitation data of Turkey. Properties of the precipitation data are described and information on some methods that can be used for precipitation modeling problem are given.

Chapter 3 presents detailed information about the clustering analysis of mean annual precipitation data. The results of the clustering analysis and discussion on these results are given.

Chapter 4 describes the adapted simulated annealing algorithm which is used to tune Mamdani type fuzzy models with triangular membership functions. And the results of the tuning process are given in this chapter.

Chapter 5 begins with the detailed information about the simplification methods for Mamdani type fuzzy models. After presenting simplification methods, the proposed simplification algorithm and the results of the application of the presented simplification algorithm to mean annual precipitation data are given.

Chapter 6 concludes and gives some future directions on the thesis.

CHAPTER 2

IDENTIFICATION OF ILL-DEFINED SPATIAL PHENOMENA

In Geographic Information System (GIS), a spatial model represents an object or behavior of a phenomenon that exists in the real world (Aronoff, 1989). Models are presented as mathematical descriptions. In most cases, however, the derivation of mathematical descriptions by geological, biological, or physical laws is not easy, time consuming and involves many unknown parameters (Nayak and Sudheer, 2008). In traditional approach, modeling spatial phenomena like hydrologic systems, mineral prospectivity, seismic activities, rainfall, groundwater vulnerability, landslide susceptibility, surface air temperature etc. not only requires deep understanding of the nature and behavior of the phenomena, but also requires knowledge on mathematical methods for developing such models (Nayak and Sudheer, 2008). Alternatively, data-driven modeling which is based on the analysis of data characterizing the phenomena can be used. Data-driven modeling uses connections in input data (e.g. data generated by input variables) and output data (e.g. data generated by output variables) to establish qualitative relationships among the variables of the phenomena. Therefore, data-driven modeling can be used only when at least some of the variables characterizing the phenomena have been measured and there is enough data to establish relationships among the variables of the phenomena. Data-driven modeling is an interdisciplinary field. It is related with fields such as data mining, artificial intelligence, machine learning, soft computing, pattern recognition and statistics.

The remainder of this chapter is organized as follows. In the first section, the detailed information about modeling annual precipitation of Turkey is given. In the next section, properties of the precipitation data are described. In the third section, information on some methods that can be used for precipitation modeling problem

Table 2.1: Input variables.

Variable	**Description**
Latitude	Latitude of the observation station (or point) (°)
Longitude	Longitude of the observation station (or point) (°)
Altitude	Height of the observation station (or point) (m)
SdGrid	Standard deviation of elevation in local 5 km × 5 km grid, local roughness value (m)

is given. In the last section, validation of the derived models are described and brief information about comparison metrics which are used to compare the models are given.

2.1 Modeling Annual Precipitation of Turkey

In this thesis, a data-driven modeling approach is proposed. Mean annual precipitation data is used to demonstrate the use of the proposed approach and to test its accuracy. A model which explains precipitation characteristics of Turkey is generated by using the data. While generating the precipitation model of Turkey, ancillary variables namely longitude, latitude, altitude, standard deviation of elevation in local 5 km × 5 km grid are used. A total of four geographical variables are included in the analyses (Bostan and Akyürek, 2007). The variable set is given in Table 2.1.

Precipitation is the condensation of atmospheric water vapor into liquid or solid phase aqueous particles which fall to the surface of the Earth. The main forms of precipitation include rain, freezing rain, sleet, snow, ice pellets and hail. It is usually expressed in terms of millimeters of depth of the water substance that has fallen at a given point (e.g., rain gauge) over a specified period of time. Although there are many forms of precipitation, only rainfall is considered in this thesis. Throughout the thesis the term precipitation is used to refer rainfall.

Note that values of the variables can be obtained or calculated for all geographical locations in Turkey easily without requiring any measurement. In addition to these variables, all meteorological observations obtained at each station can be used in the analysis and can increase the accuracy of the model. Precipitations at all locations in Turkey (1 km resolution) is estimated using the proposed model and an estimation of

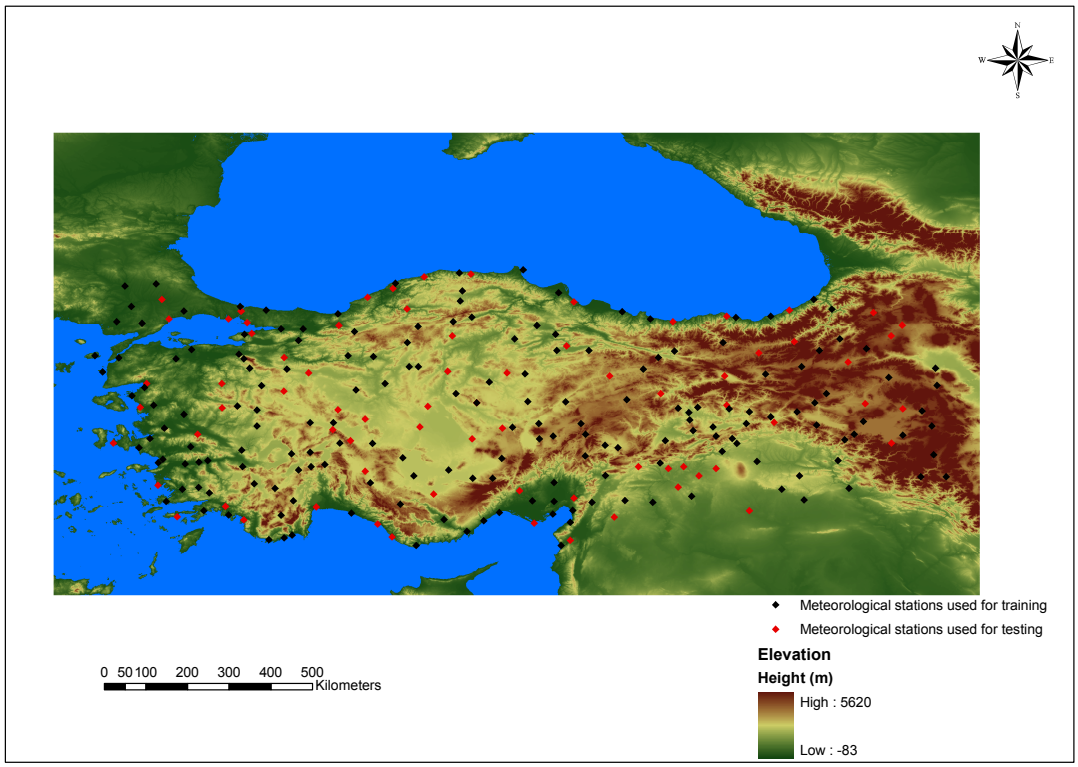


Figure 2.1: Meteorological stations used in the analyses.

long term mean annual precipitation map for Turkey is prepared (Figure 4.9).

2.2 Mean Annual Precipitation Data

Mean annual precipitation data measured at meteorological stations given in Figure 2.1 are used to model the annual precipitation of Turkey. Precipitation data is taken from the study of Bostan and Akyürek (2007). Data consist of precipitation observations measured at 254 meteorological stations over Turkey between the years 1970 and 2008. Mean monthly precipitation data are converted to annual average precipitation. Spatial distribution of meteorological stations is illustrated in Figure 2.1. Average precipitation data for meteorological stations over Turkey are given in Appendix A.

Latitude values of meteorological stations, which precipitation measurements are made, constitutes "latitude" input variable. Histogram of input variable "latitude" for the 254 stations is given in Figure 2.2a. Mean value of the variable is 38.9773° and the standard deviation is 1.5309°.

"Latitude" variable has a low degree of skewness 0.0681, the mode is very close,

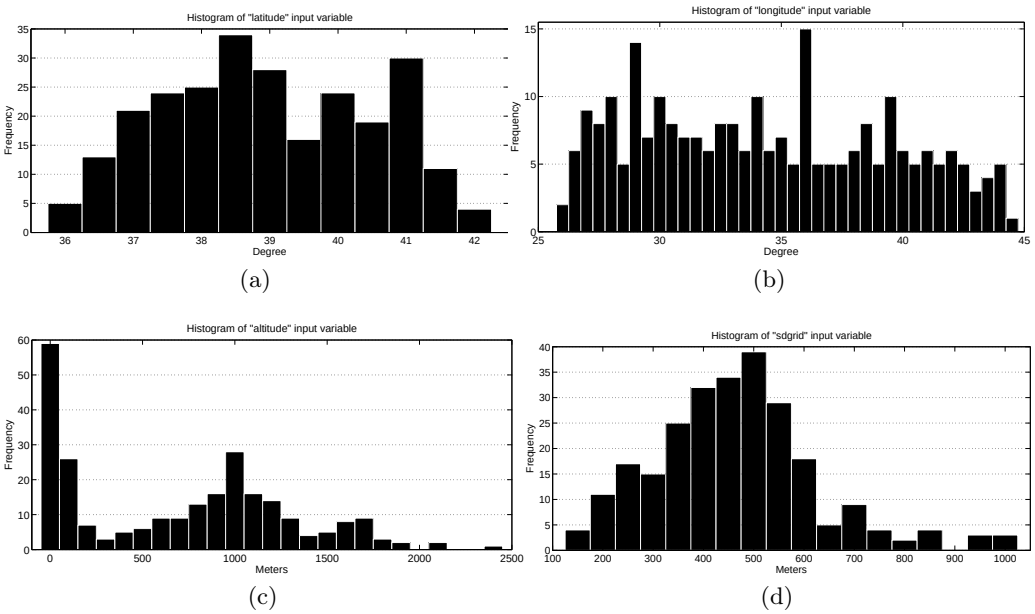


Figure 2.2: Histograms for each of the four input variables based on all 254 meteorological stations located over Turkey.

Table 2.2: Descriptive statistics of input variables are calculated using 254 meteorological stations.

Variable	**Mean**	**Standard deviation**	**Skewness**	**Kurtosis**
Latitude	38.9773	1.5309	0.0681	1.9607
Longitude	34.3572	5.0723	0.1880	1.8857
Altitude	702.6142	585.2418	0.3037	2.0663
SdGrid	463.5106	163.6029	0.7304	4.0975

or even coincides with, the mean. Moreover, "latitude" variable can be considered as a flat or platykurtic distribution, since it has low kurtosis value, 1.9607. Note that a normal distribution has a skewness of zero and a kurtosis of 3.0. Low kurtosis is one sign that "latitude" variable is not normally distributed.

The Q-Q plot is a graphical method for comparing two sample data sets (Aster et al., 2005). If the two data sets come from the same distribution, the plot will be linear. The Q-Q plot for the "latitude" variable is given in Figure 2.3a. The Q-Q plot for "latitude" data shows deviations from normality. Furthermore, Lilliefors test is used to statistically test for normality. The test is used to evaluate the null hypothesis that data have a normal distribution with unspecified mean and variance. The alternative

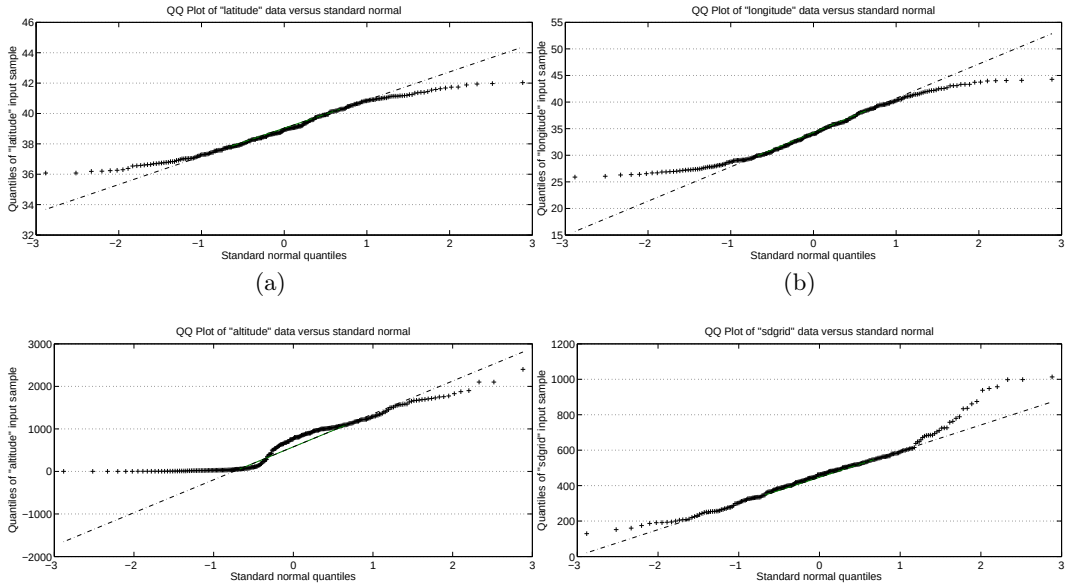


Figure 2.3: Q-Q plots for the input variables.

hypothesis states that data do not have a normal distribution (Lilliefors, 1967). Since Lilliefors test statistic is 0.0617 and the p-value is 0.0234, the hypothesis that "latitude" variable has a normal distribution can be rejected at the 5% significance level.

"Longitude" input variable is composed of longitude values of meteorological stations. Histogram of the variable is illustrated in Figure 2.2b. Descriptive statistics are given in Table 2.2. Mean value of the variable is 34.3572° and the standard deviation is 5.0723°. Unlike "latitude" variable "longitude" variable has a high skewness of 0.1880. "Longitude" variable can also be considered as a flat distribution with low kurtosis value of 1.8857. The Q-Q plot for "longitude" data in Figure 2.3b shows deviations from normality. Indeed, Lilliefors test statistic is calculated as 0.0800 but since the value of Lilliefors test statistic is outside the range of the Lilliefors table, the p-value could not be computed. The hypothesis that "longitude" variable has a normal distribution can be rejected at the 5% significance level.

"Altitude" input variable is composed of height values of meteorological stations. Histogram of the variable is illustrated in Figure 2.2c and the descriptive statistics of the variable are given in Table 2.2. "Altitude" variable has a high skewness of 0.3037 and low kurtosis value of 2.0663. The Q-Q plot for "altitude" data in Figure 2.3c clearly shows deviations from normality. Lilliefors test statistic is 0.1670; therefore the

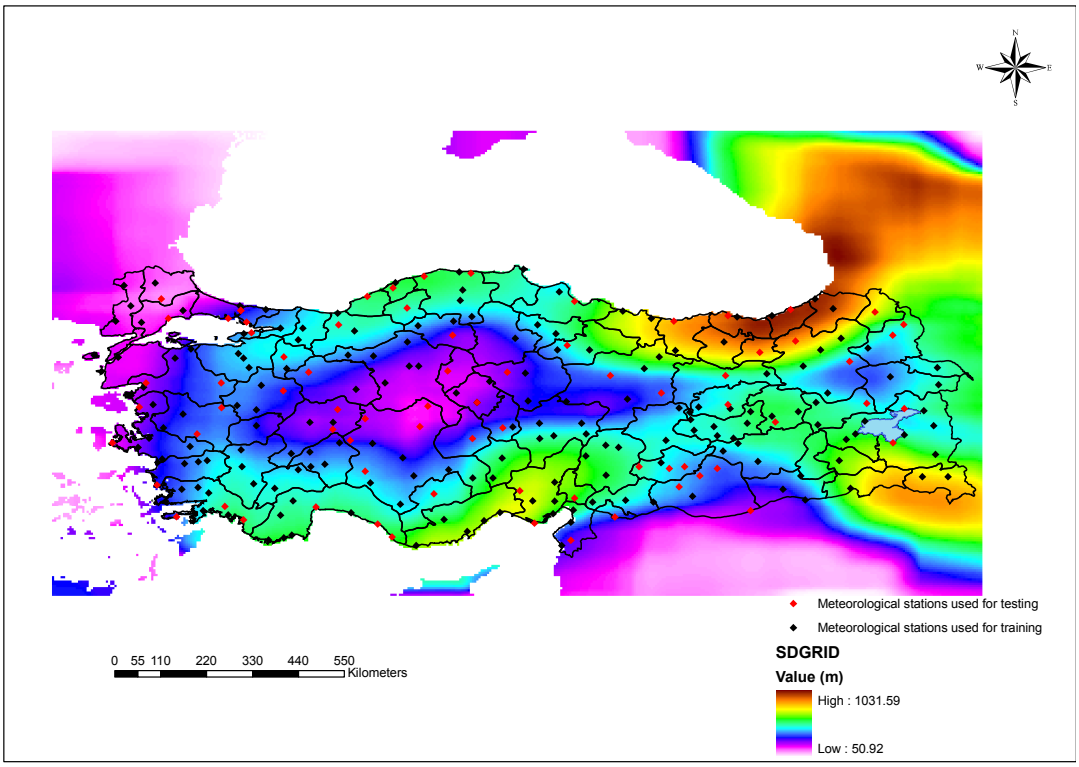


Figure 2.4: Standard deviation of elevation in local 5 km × 5 km grid, local roughness over Turkey.

hypothesis of normality can be rejected at the 5% significance level.

Essentially, violation of the normality for the input variables "latitude", "longitude" and "altitude" is not unexpected. Because, these variables are the components of the locations of meteorological stations, which were located based on some specified rules and regulations, in order to measure meteorological variables such as rainfall, temperature, humidity, wind speed and wind direction.

Local roughness (SdGrid) variable is derived by calculating standard deviation of elevation in local 5 km × 5 km grid. Derived SdGrid map of Turkey is illustrated in Figure 2.4. Digital elevation data which is provided by the NASA Shuttle Radar Topographic Mission (SRTM) is used. The spatial resolution of SRTM data is 3 arc seconds (approximately 90 m resolution) and the vertical error of the SRTM data is less than 16 m (Jarvis et al., 2008).

Histogram of the "SdGrid" variable is illustrated in Figure 2.2d and the descriptive statistics are given in Table 2.2. "SdGrid" variable has a high skewness of 0.7304 and also high kurtosis value of 4.0975. The Q-Q plot for "SdGrid" data in Figure 2.3d shows

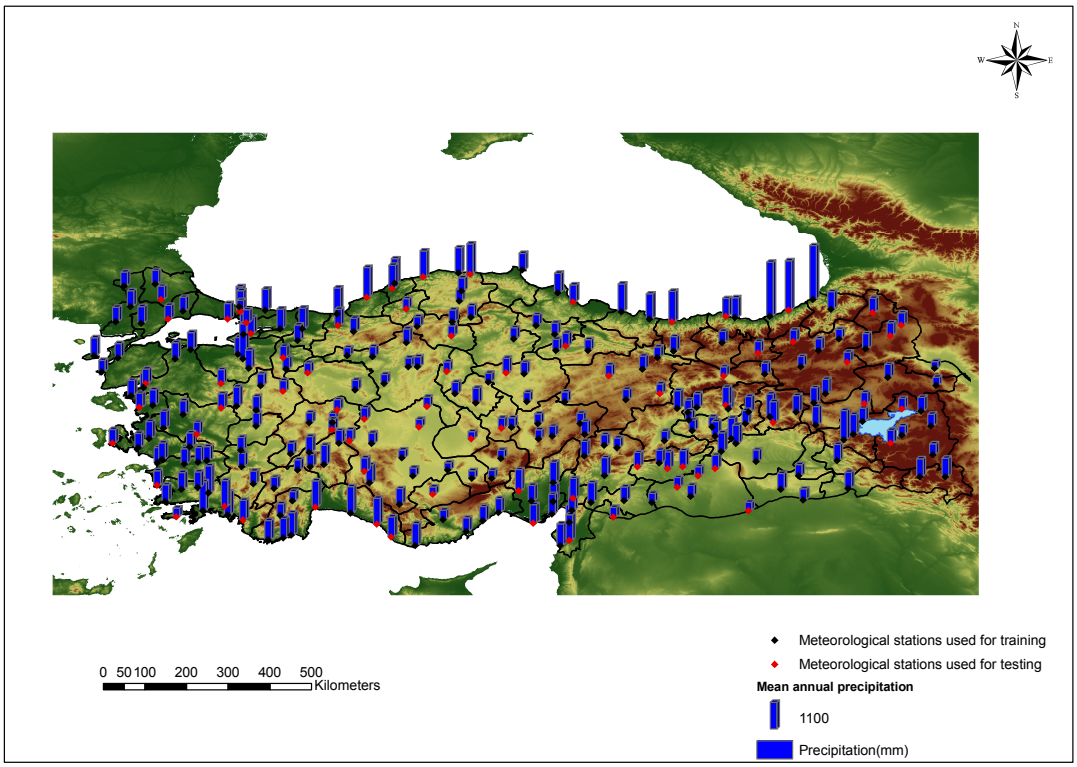


Figure 2.5: Mean annual precipitation values for meteorological stations over Turkey.

deviations from normality. Lilliefors test statistic is 0.0725; therefore the hypothesis of normality can be rejected at the 5% significance level.

Output variable contains annual average precipitation values obtained from meteorological stations over Turkey. Mean annual precipitation values calculated for 254 meteorological stations are shown in Figure 2.5.

Histogram of the output variable "precipitation" for 254 stations is given in Figure 2.6. Mean value of the output variable is 611.0961 mm and the standard deviation is 275.9812 mm.

"Precipitation" variable has a high degree of skewness 2.5942 the mode is very far from the mean. Since it also has a very high kurtosis value, 13.9359, output variable can be considered as a very peaky or leptokurtic distribution. "Precipitation" variable has a highly skewed and very peaky distribution. This indicates that the variable is not normally distributed. Descriptive statistics for the output variable are given in Table 2.3.

The Q-Q plot for the "precipitation" variable is illustrated in Figure 2.7. The Q-Q plot for "precipitation" data shows deviations from normality. Moreover, three values

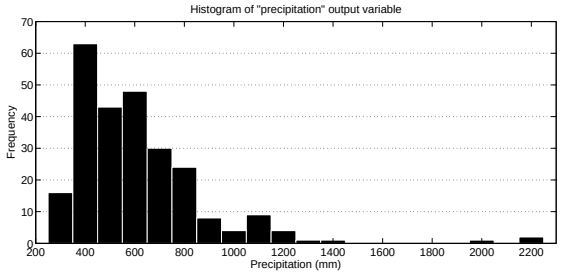


Figure 2.6: Histogram of the output variable "precipitation" based on all 254 meteorological stations located over Turkey.

Table 2.3: Descriptive statistics of output variable are calculated using 255 meteorological stations.

Variable	**Mean**	**Standard deviation**	**Skewness**	**Kurtosis**
Precipitation	611.0961	275.9812	2.5942	13.9359

in the plot are very far from the other values. These stations are located at Rize, Pazar (Rize) and Hopa. Actually, according to the annual precipitation values, this region which is at the north-east cost of Turkey, has the most rainfall in Turkey. Since Lilliefors test statistic is 0.1263, the hypothesis of normality can be rejected at the 5% significance level.

Bivariate scatter plots are constructed (Figure 2.8) between output variable and the input variables to examine the nature and the strength or degree of any relationship revealed by the data. Bivariate scatter plots suggested slight linear relationships between "precipitation" and "altitude" and "precipitation" and "sdgrid". The strength of the correlations between the variables are calculated using the Pearson's correlation coefficient, Table 2.4.

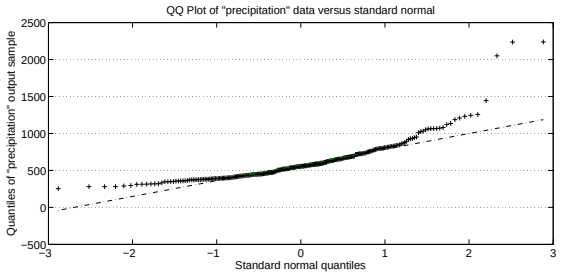


Figure 2.7: Q-Q plot for the output variable.

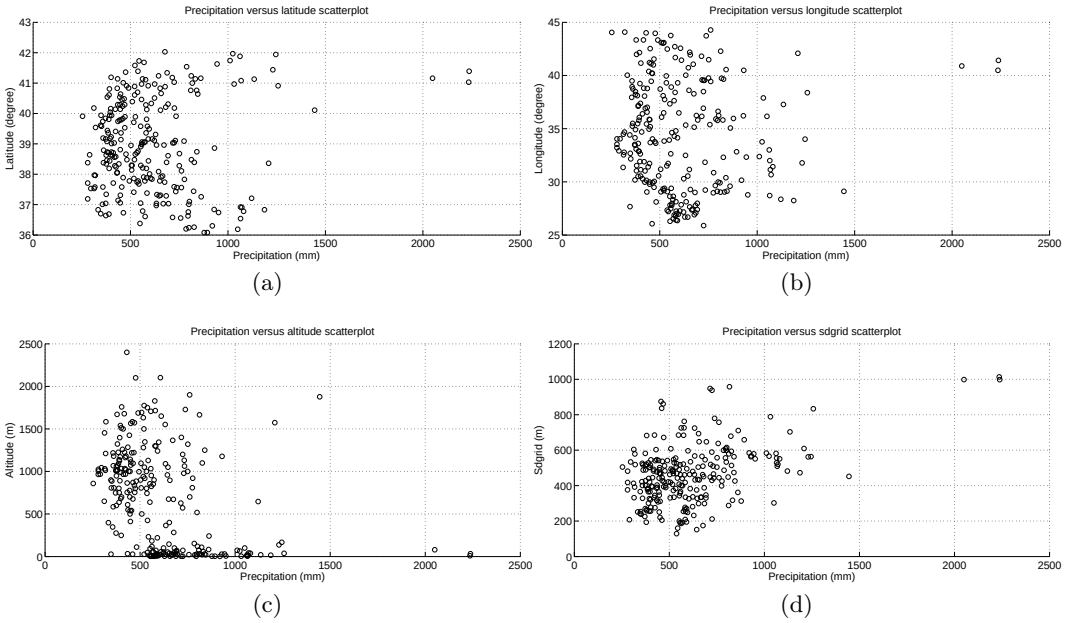


Figure 2.8: Bivariate scatter plots between precipitation and the input variables.

Table 2.4: The correlation coefficients calculated between the variables.

	Longitude	**Latitude**	**Altitude**	**SdGrid**	**Precipitation**
Longitude	1.0000	-0.0144	0.6005	0.5480	-0.0057
Latitude	-0.0144	1.0000	-0.0179	-0.0265	0.1052
Altitude	0.6005	-0.0179	1.0000	0.0883	-0.3856
SdGrid	0.5480	-0.0265	0.0883	1.0000	0.4481
Precipitation	-0.0057	0.1052	-0.3856	0.4481	1.0000

Matrix of p-values for testing the hypothesis of no correlation is given in Table 2.5. Results suggest that there is a negative correlation (-0.3856) between "precipitation" and "altitude", and a positive relationship (0.4481) between "precipitation" and "sdgrid".

Data are divided into training and test sets. The training data set is used for learning and test data set is used for measuring the predictive capability of the learned model. 218 meteorological stations have observations for more than 20 years. From this set, 180 meteorological stations (e.g. 70% of the total data set) are selected randomly by using MATLAB® "randperm" command then training data set is generated by using precipitation data measured at these stations. Test data set is generated by

Table 2.5: p-values for correlation coefficients.

	Longitude	**Latitude**	**Altitude**	**SdGrid**	**Precipitation**
Longitude	1.0000	0.8199	0.0000	0.0000	0.9275
Latitude	0.8199	1.0000	0.7765	0.6746	0.0944
Altitude	0.0000	0.7765	1.0000	0.1605	0.0000
SdGrid	0.0000	0.6746	0.1605	1.0000	0.0000
Precipitation	0.9275	0.0944	0.0000	0.0000	1.0000

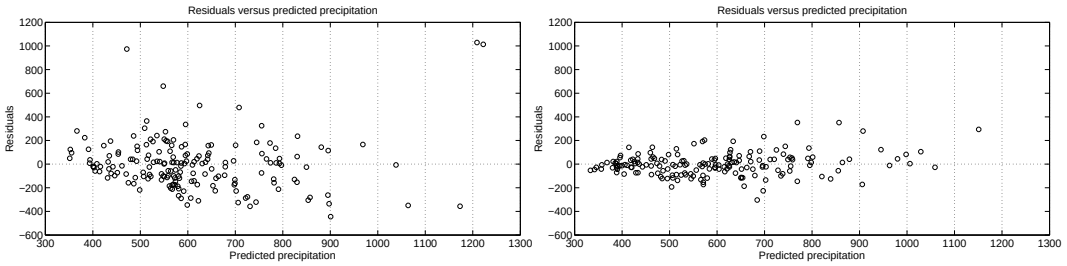
data obtained from the remaining 74 meteorological stations. Therefore, test data set contains 38 stations which have observations for more than 20 years and 36 stations which have shorter observations.

2.3 Some Methods Used in Data-Driven Modeling

In this section, information on some methods that can be used for precipitation modeling problem is given. These methods are linear regression, artificial neural networks, neuro-fuzzy systems and fuzzy systems. Although linear regression method can only be used for linear problems or problems which can be linearized with some transformations, artificial neural networks, fuzzy systems and neuro-fuzzy systems can be used for both linear and non-linear problems. Many other methods exist in addition to these methods.

2.3.1 Linear Regression

Regression analysis is used for the identification of relationships between variables. The values of dependent variable are to be predicted or explained using the values of the independent variables. In our case, dependent variable is precipitation and the independent variables are longitude, latitude, altitude and sdgrid. Linear regression is used to explain variation in precipitation with these four variables. It is found that 34.29 percent of the variation in precipitation is explained by the four input variables. The root mean squared error is calculated as 217.50 mm for the training data and 207.80 mm for the test data. The equation is given in Equation 2.1.



(a) (b)

Figure 2.9: Residuals versus predicted precipitation (a) linear regression, (b) geographically weighted regression.

$$\begin{aligned} \text{Precipitation} = \quad & -468.0335 - 5.044 \times \mathit{Longitude} + 24.6842 \times \mathit{Latitude} \\ & -0.1584 \times \mathit{Altitude} + 0.8713 \times \mathit{SdGrid} \end{aligned} \tag{2.1}$$

If this regression is to successfully explain the variation in the precipitation then no systematic variation should exist in the residuals (Ebdon, 1977). In other words, there should be no serial correlation or autocorrelation. To test whether residuals are autocorrelated Durbin-Watson test (Draper and Smith, 1981) is used. Durbin-Watson test tests if the residuals are independent. A Durbin-Watson test statistic lies between 0 and 4.0 with 2.0 indicates no autocorrelation. While values less than 2.0 indicate positive autocorrelation, values greater than 2.0 indicate negative correlation.

Durbin-Watson test statistic is computed as 1.66 which indicates low positive serial correlation. Residuals versus precipitation plot (Figure 2.9a) supports this result. Moreover, no spatial autocorrelation should exist in the residuals for a successful regression. Therefore, to see if there is any spatial autocorrelation in the residuals global Moran's I index is used. Global Moran's I index (Moran, 1950) is a measure of spatial autocorrelation and ranges between -1.0 (negative spatial autocorrelation) and 1.0 (positive spatial autocorrelation). As value of index approaches 1.0 similar values tend to cluster in geographic space, as the value of index approaches -1.0 dissimilar values tend to cluster in geographic space, and as the value of index approaches $-1/(n-1)$, where n is the number of observations, values are randomly scattered over the space. For linear regression, global Moran's I index values are given in Table 2.6.

In linear regression, only a small portion of the variation in precipitation is explained and also residuals are spatially autocorrelated. Therefore, linear regression

Table 2.6: Moran's I index measuring the spatial autocorrelation in residuals of linear regression.

Data	**Moran's I index**	**Expected value**	**Z-Score**	**In 5% significance level**
Training Data	0.035294	-0.005587	4.414005	Clustered
Testing Data	-0.055449	-0.013699	-2.067710	Dispersed

did not explain precipitation sufficiently.

A basic assumption in fitting a linear regression is that observations are independent, which is very unlikely in geographical data, and the structure of the model, i.e. regression equation, remains constant over the whole study area, no local variations are allowed. Geographically weighted regression (Fotheringham et al., 2002) is a technique which permits the parameter estimates to vary locally. This is accomplished by a weighting scheme such that observations near the point in space where the parameter estimates are desired have more influence on the result than the observations further away. Geographically weighted regression is applied on training data and better results are obtained than linear regression. The coefficient of determination is calculated as 0.8416 which means that the model can explain 84.16 percent of the variation in precipitation. The root mean squared error is calculated as 106.78 mm for the training data which is half of the error obtained with linear regression and all the parameters are significant at 5% level.

As in the linear regression case, residuals are tested whether they are autocorrelated or not by Durbin-Watson test. The Durbin-Watson test statistic is calculated as 2.15 indicating almost no serial correlation. Residuals versus the predicted precipitation values are plotted on Figure 2.9b. Morans'I index values between the residuals of geographically weighted regression are given in Table 2.7.

2.3.2 Artificial neural networks

Artificial neural networks (ANNs) are originally motivated by the biological structures in the brains of human and animals, which are powerful for such tasks as information processing, learning and adaptation (Nelles, 2000). ANNs are composed of a set of connected nodes or units where each connection has a weight associated with it. ANNs

Table 2.7: Moran's I index measuring the spatial autocorrelation in residuals of geographically weighted regression.

Data	**Moran's I index**	**Expected value**	**Z-Score**	**In 5% significance level**
Training Data	-0.023052	-0.005587	-1.873512	Random
Testing Data	-	-0.013699	-	-

can "learn" from prior applications. During the learning phase, the network learns by adjusting the weights. If a poor solution to the problem is made, the network is modified to produce a better solution by changing its weights.

ANNs provide a mechanism for learning from data and mapping of data. These properties make neural networks a powerful tool for modeling nonlinear systems. Therefore, neural networks can be trained to provide an alternative approach for problems that are difficult to solve such as decision-making problems in GIS (Yanar and Akyürek, 2007).

Although, ANNs learn well, they have a long training time (time required for learning phase). Also, there are no clear rules to build network structure (Han and Kamber, 2001). Network design is a trial-and-error process which may affect accuracy of the result and there is no guarantee that the selected network is the best network structure. Another major drawback in the use of ANNs is their poor interpretability (Yen and Langari, 1999).

On the other hand, neural network's tolerance to noisy data is high and they are robust against the failure of single units. Like all statistical models, ANNs are subject to overfitting when the neural network is trained to fit one set of data almost exactly (Russell and Norvig, 2003; Dunham, 2003). When training error associated with the training data is quite small, but error for new data is very large, generalization set is used. Also, to avoid overfitting, smaller neural networks are advisable (Dunham, 2003).

An example for the use of ANNs for a decision-making problem in GIS and comparison between the accuracies of models obtained by using ANNs and linear time-invariant systems are given in Appendix B.

2.3.3 Fuzzy Systems

Fuzzy logic (Zadeh, 1965) generalizes crisp logic to allow truth-values to take partial degrees. Since bivalent membership functions of crisp logic are replaced by fuzzy membership functions, the degree of truth-values in fuzzy logic becomes a matter of degree, which is a number between zero and one. Fuzzy logic is unique in that it provides a formal framework to process linguistic knowledge and its corresponding numerical data through membership functions (Zadeh, 1973). The linguistic knowledge is used to summarize information about a complex phenomenon and is used to express concepts and knowledge in human communication, whereas numerical data is used for processing (Zadeh, 1973; Mendel, 1995). An important advantage of using fuzzy models is that they are capable of incorporating knowledge from human experts naturally and conveniently, while traditional models fail to do so (Yen and Langari, 1999). Other important properties of fuzzy models are their ability to handle nonlinearity and interpretability feature of the models (Yen and Langari, 1999).

Fuzzy logic offers a way to represent and handle uncertainty present in the continuous real world. Using fuzzy logic continuous nature of landscape can be modeled appropriately. The use of fuzzy logic in GIS has become an active field in recent years. Fuzzy set theory has been widely used for many different problems in GIS including soil classification (Lark and Bolam, 1997; Zhu et al., 1996), crop-land suitability analysis (Ahamed et al., 2000), identifying and ranking burned forests to evaluate risk of desertification (Sasikala and Petrou, 2001), estimating forest fire risky areas (Akyürek and Yanar, 2005), classifying and assessing natural phenomena (Kollias and Kalivas, 1998; Benedikt et al., 2002), and classifying slope and aspect maps into linguistically defined classes (Yanar, 2003). Moreover, fuzzy logic can be used for decision-making in GIS. Fuzzy decision-making can be used for different kinds of purposes such as selecting suitable sites for industrial development (Yanar and Akyürek, 2006), seeking the optimum locations for real estate (Zeng and Zhou, 2001), assessing vulnerability to natural hazards (Rashed and Weeks, 2003; Martino et al., 2005), or estimating risk (Sadiq and Husain, 2005; Chen et al., 2001; Iliadis, 2005).

In this thesis, an approach for building optimal and interpretable fuzzy systems for GIS applications using relationships in spatial data is proposed. In general, the proposed approach has three stages:

1. Building fuzzy models from spatial data,

2. Optimizing fuzzy models, and

3. Enhancing interpretability of the driven fuzzy models.

Details of the proposed approach are given in Chapters 3, 4 and 5, respectively.

2.3.4 Neuro-Fuzzy Systems

The underlying rational behind the neuro-fuzzy systems is to generate a fuzzy system from data or to enhance a fuzzy system by learning from examples (Nauck and Kruse, 1999; Nauck, 2003a; Jang, 1993). Learning methods are obtained from neural networks. Since neural network learning algorithms are usually based on gradient descent methods, the application of neural networks to fuzzy system needs some modifications on the fuzzy inference procedure such as selecting differentiable functions. For example in Adaptive-Network-based Fuzzy Inference System (ANFIS) a Sugeno-type fuzzy system (Takagi and Sugeno, 1985) is implemented in neural network structure and differentiable t-norm and membership functions are selected. On the other hand, NEFCON (Nauck, 1994), NEFCLASS and NEFPROX systems can also implement Mamdani-type fuzzy systems (Mamdani and Assilian, 1975) and do not use a gradient-based learning algorithm but uses a heuristic learning algorithm in which semantics and interpretability of the fuzzy system are retained (Nauck and Kruse, 1999).

Dixon (2005) integrated GIS and neuro-fuzzy techniques to predict groundwater vulnerability and examined sensitivity of neuro-fuzzy models. For hydro geologic applications, Dixon (2005) shows that neuro-fuzzy models are sensitive to model parameters which are used during learning and validation steps. Vasilakos and Stathakis (2005) show that granular neural network (Bortolan, 1998), which is based on the selection of fuzzy sets that represent data, are suited to model the inherent uncertainty of geographical phenomena. Both studies use neuro-fuzzy classification software, NEFCLASS, with geographic data.

An example for the use of neuro-fuzzy systems for a decision-making problem in GIS is given in Appendix C.

Adaptive-Network-Based Fuzzy Inference System

ANFIS (Jang, 1993) is one of the first hybrid neuro-fuzzy systems for function approximation. ANFIS implements the Sugeno-type (Takagi and Sugeno, 1985) fuzzy system, which has a functional form (linear combination of input variables) of the consequent part. This system uses differentiable membership functions and a differentiable t-norm operator. Since ANFIS does not have an algorithm for structure learning (rule generation), the rule base must be known in advance.

The architecture is five-layer feed-forward network, where the first layer contains elements which realize the membership functions in the antecedent part of the IF-THEN rules. The second layer corresponds to calculation of firing strengths of each rule. Next layers correspond to the consequent part of the rules (Rutkowska, 2002). The structure of ANFIS is assumed to be fixed and the parameter identification is solved through the hybrid learning rule. However, since there is no structure identification, the number of rules, number of membership functions assigned to each input and initial step size, which is the length of each gradient transition in the parameter space (used to change the speed of convergence), have to be given by the user (see Table 2.8).

Neuro-Fuzzy Function Approximator

NEuro-Fuzzy function apPROXimator (Nauck and Kruse, 1999) (NEFPROX) can be applied to function approximation. The system is based on a generic fuzzy perceptron. A generic fuzzy perceptron is designed as a three-layer neural network, it has special activation and propagation functions and uses fuzzy sets as weights. The fuzzy perceptron provides a framework for learning algorithm to be interpreted as a system of linguistic rules and enables to use prior knowledge in the form of fuzzy IF-THEN rules (Rutkowska, 2002). The architecture of fuzzy perceptron is a three-layer feed-forward network. The units of input layer represent the input variables. The hidden layer is composed of units representing fuzzy rules. And the units of the output layer represent output variables which compute crisp output values by defuzzification. The connections between input units (neurons) and hidden units are labeled with linguistic terms corresponding to the antecedent fuzzy sets and the connection between hidden neurons and output neurons are labeled with linguistic terms corresponding to consequent

Table 2.8: Major inputs and outputs of ANFIS and NEFPROX systems.

Neuro-Fuzzy System	**Inputs**	**Outputs**
ANFIS	number of rules number of membership functions assigned to each input initial step size	fuzzy if-then rules (rule base) learned membership functions [a]
NEFPROX	initial fuzzy partitions for input and output type of membership functions t-norm operators t-conorm operators defuzzification procedure initialization parameters learning restrictions	fuzzy if-then rules (rule base) learned membership functions [a]

[a] Log files, statistics, membership function plots, etc. are also obtained.

fuzzy sets.

The learning of NEFPROX system consists of two steps: structure learning (learning of rule base) and parameter learning (learning of fuzzy sets). In this system, some rules can be given a priori and the remaining rules may be found by learning. Moreover, NEFPROX can generate the whole rule base by the rule learning algorithm, which each fuzzy rule is based on a predefined partition of the input space (Rutkowska, 2002; Nauck and Kruse, 1999). Parameter learning procedure (learning of fuzzy sets) is a simple heuristic. For details, see (Nauck and Kruse, 1999). Initial fuzzy partitions for input and output variables, type of membership functions, t-norm and t-conorm operators, defuzzification procedure, initialization parameters and learning restrictions are given to the system by user.

2.4 Model Comparisons

Comparative statistics and error metrics are used to assess the accuracy of the models build using relationships in data. These metrics also allow to make comparisons between the models according to their prediction accuracies. These metrics are as follows:

1. The product-moment correlation coefficient or Pearson's correlation coefficient,
2. Root mean squared error (RMSE).

First metric provides statistical measures of the strength of the relationship between the target output and predicted output. Second metric measures the amount by which

predicted output differs from the target output.

The product-moment correlation coefficient or Pearson's correlation coefficient measures the association or correlation between two variables. To calculate product-moment correlation coefficient, data must be measured on an interval or ratio scale. It is also assumed that both variables have come from normally distributed populations and they have a linear relationship (McGrew and Monroe, 2000). The product-moment correlation coefficient for two variables x_1 and x_2 is calculated by following equation:

$$\mathrm{r} = \frac{\left[\sum (x_1 - \bar{x_1})(x_2 - \bar{x_2})\right]/N}{S_{x_1} * S_{x_2}} \tag{2.2}$$

where r is the product-moment correlation coefficient or Pearson's correlation coefficient, $\bar{x_1}$, $\bar{x_2}$ are the mean of variables x_1 and x_2, N is the number of paired data values and S_{x_1} and S_{x_2} are the standard deviations of x_1 and x_2. r values can vary between -1.0 and 1.0 with 0.0 indicating no association, 1.0 and -1.0 indicating perfect positive and negative relationships, respectively.

RMSE is computed by taking square root of average of the squared differences between each computed value ($\hat{x_i}$) and its corresponding correct value (x_i). Root mean squared error formula is given below:

$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_i - \hat{x_i})^2} \tag{2.3}$$

CHAPTER 3

BUILDING FUZZY MODELS

A fuzzy model is a set of fuzzy if-then rules that maps inputs to outputs. A fuzzy if-then rule describe relationships between variables such as

If the precipitation is high then the landslide risk will be high. (3.1)

This rule establishes logical relation between variables by relating qualitative value of the input variable (precipitation is high) to qualitative value of the output variable (landslide risk will be high). The qualitative values, such as in the above example are called linguistic terms or linguistic values. The symbolic knowledge is used to summarize information about a phenomenon and to express concepts and knowledge in a clear linguistic interpretation, whereas numerical data is used for processing. A fuzzy model integrates numerical data and symbolic knowledge into one common framework by means of linguistic variables (Babuška, 1998; Mendel, 1995).

Fuzzy models can be created from expert knowledge by translating linguistic information obtained from human experts into fuzzy rules. Then, parameters of the fuzzy model (membership functions, weights of rules, etc.) can be fine tuned using available input-output data (Babuška, 1998). However, no standard method exists for transforming experts' knowledge into fuzzy rules (Jang, 1993; Yen and Langari, 1999; Yanar, 2003). Moreover, expert knowledge is not sufficient to define complex partially unknown systems satisfactorily (Guillaume and Charnomordic, 2004). In such cases, fuzzy models can be constructed by using numerical data (Jang, 1993; Guillaume and Charnomordic, 2004; Yen and Wang, 1998; Emami et al., 1998; Wang and Mendel, 1992; Shi and Mizumoto, 2000; Chen and Linkens, 2004; Jin, 2000; Nauck and Kruse, 1999; Guély et al., 1999).

In this study, clustering is used in learning fuzzy rules from data. In fuzzy clustering, space partitioning is derived from data partitioning and rules are associated

to each clusters. To completely define rules, clustering is applied in the Cartesian product-space of inputs and outputs where premise part of a fuzzy if-then rule corresponds to the input part and consequent corresponds to the output part (Babuška, 1998; Guillaume, 2001; Sugeno and Yasukawa, 1993). To find the optimum number of clusters fuzzy cluster validation indices are used.

The remainder of this chapter is organized as follows. In the first section, brief information about the related work done in this area is given. The detailed information about the clustering analysis of mean annual precipitation data are given in the second section. The results of the clustering analysis and discussion on these results are given in the third section. Information about the fuzzy model construction using results of the fuzzy clustering algorithms is given in the forth section. In the next section, performances of the constructed fuzzy models are given. Discussions are provided in the last section.

3.1 Related Work

The most remarkable step during a fuzzy modeling procedure is to detect the underlying data structure and to transform it into a collection of fuzzy rules (Delgado et al., 1996; Sugeno and Yasukawa, 1993; Yoshinari et al., 1993; Pedrycz, 2005). For data-driven fuzzy modeling, there are three kinds of methods:

The first kind partitions each variable domain into a given number of intervals without considering any physical meaning and distribution in data. In the grid partitioning approach all possible combinations of the fuzzy sets are used during rule generation. For example, a Mamdani type fuzzy model with five variables (four input variables and an output) and three membership functions on each variable would result in $3^5 = 243$ fuzzy rules. Ruspini-type partition (Ruspini, 1970) arranges membership functions such that the sum of the membership degrees equal to one. These techniques create interpretable fuzzy rules and the rule base generation is easy. However, these techniques suffer from the curse of dimensionality problem.

The second kind tries to gather data into homogeneous groups to create rules where a rule is associated to each group. The clustering technique can be hard or fuzzy. In hard or crisp clustering algorithm each pattern belongs to a single specific cluster. For example, the Isodata (k-means or c-means) is one of the most famous and

well-known algorithm of this type (Duda et al., 2001). A fuzzy clustering algorithm assigns a pattern to a specific cluster up to a certain degree. Different fuzzy clustering techniques have been used to drive fuzzy models from data (Chiu, 1994; Wong and Chen, 1999; Yao et al., 2000; Angelov, 2004; Panella and Gallo, 2005). The fuzzy c-means or fuzzy k-means (Dunn, 1973) is the most widely used clustering approach in fuzzy modeling. Together with fuzzy c-means, the Gustafson-Kessel (Gustafson and Kessel, 1978) and Gath-Geva (Gath and Geva, 1989) clustering algorithms are also used in fuzzy modeling (Ansari et al., 2009; Nayak and Sudheer, 2008; Vernieuwe et al., 2006, 2007). The fuzzy c-means (FCM), Gustafson-Kessel (GK) and Gath-Geva (GG) clustering algorithms are based on a cost function optimization technique. All these clustering algorithms are derived by minimizing a cost function of the form

$$J_m(Q,U) = \sum_{i=1}^{N}\sum_{j=1}^{c} u_j(x_i)^m * d(x_i, q_j) \tag{3.2}$$

with respect to Q and U, subject to the constraints

$$\sum_{j=1}^{c} u_j(x_i) = 1, \qquad i = 1 \ldots N \tag{3.3}$$

where

$$u_j(x_i) \in [0,1], \qquad i = 1 \ldots N, \qquad j = 1 \ldots c \tag{3.4}$$

$$0 < \sum_{i=1}^{N} u_j(x_i) < N, \qquad j = 1 \ldots c \tag{3.5}$$

and $Q = [q_1, q_2, \ldots, q_c], q_i \in \Re^n$ is a matrix of cluster prototypes (centers), U is $N * c$ matrix whose (i,j) element equals $u_j(x_i)$ the membership degree of data vector x to cluster Q_j and U is called a fuzzy partition matrix, $d(x_i, Q_j)$ is a dissimilarity measure between data vector x_i and cluster center q_j. The exponent $m \in [1, \infty)$, called fuzzifier, is a weighting exponent which determines the fuzziness of the resulting clusters. Commonly, the fuzzifier is chosen as $m = 2$ (Babuška, 1998; Vernieuwe et al., 2006) and this value is used in the experiments. To obtain estimates for U and Q, these clustering algorithms employ an iterative algorithm which its outline is shown in Algorithm 1.

As the termination criterion, a tolerance value epsilon may be chosen for the maximal difference between partition matrices of the previous and the current iteration. If the difference between the partition matrices $\left\|U^{(t)} - U^{(t-1)}\right\| < \epsilon$, then the iteration ends. The difference between these clustering techniques is in the use of different

Algorithm 1 Generalized Fuzzy Clustering Algorithmic Scheme (adapted from (Duda et al., 2001))

Require: The data set X, number of clusters $1 < c < N$, fuzziness $m > 1$ and termination tolerance $\epsilon > 0$.

1: Initialize partition matrix, $U^{(0)}$
2: $t = 0$
3: **repeat**
4: Compute cluster prototypes, $q_i^{(t)}$
5: Compute dissimilarity measure between data points x_i and cluster centers q_j
6: Update partition matrix, $U^{(t)}$
7: $t = t + 1$
8: **until** a termination criterion is met

dissimilarity measures. While the FCM uses Euclidean distance, GK clustering algorithm uses covariance matrices for the calculation of the distance between cluster centers and data points. Therefore, GK algorithm uses an adaptive distance norm to detect clusters of different geometrical shapes (Gustafson and Kessel, 1978). Contrary to the GK algorithm, GG algorithm uses cluster covariance matrix in conjunction with an "exponential" distance.

The FCM algorithm is suitable for recovering well-separated, compact clusters and it imposes a circular shape. The FCM depends on the initialization of the iteration (Tsekouras, 2007; Abonyi and Feil, 2007) and it is sensitive to the scaling (normalization) of data. The GK algorithm can detect clusters with different geometrical shapes in data as it can adapt the distance norm to the underlying distribution of data. It can recover clusters with ellipsoidal shape, but it cannot reflect the different size of the clusters (Abonyi and Feil, 2007). As the FCM algorithm, resulting clusters obtained by the GK algorithm can be significantly changed by different initial states. The GK algorithm is not so sensitive to the normalization of data as it is based on an adaptive distance measure (Babuška, 1998). The GG algorithm is able to detect clusters of varying shapes and varying volumes as contrary to the GK algorithm (Babuška, 1998). However, it is very sensitive to the initial conditions due to the exponential distance measure (Babuška, 1998; Abonyi and Feil, 2007).

The third kind is based on ad hoc data-driven methods (Wang and Mendel, 1992;

Casillas et al., 2002; Nozaki et al., 1997; Higgins and Goodman, 1994). These are the efficient and simple methods. They are easily understandable, implementable and suitable to be used as a first stage of modeling process because they are very fast, computationally inexpensive algorithms. They can be used if data contains numeric and non-numeric attributes and if the data contains missing values. One of the most widely used methods is the Wang and Mendel's method (Wang and Mendel, 1992). In this method, all variables are partitioned by equidistant overlapping triangular or trapezoidal membership functions. Rules are generated by using these partitions and input-output data pairs. Each rule is assigned a weight to solve conflicts among the generated rules. This method is designed to create fuzzy systems for function approximation.

Fuzzy clustering has been used in many different GIS problems. For instance, Tütmez (2009) used FCM algorithm to initially create structure of a neuro-fuzzy system then after learning of the neuro-fuzzy inference system is done, it is used for estimation of mineral resource parameters such as grade and thickness. Tütmez et al. (2007) also employed possibilistic fuzzy clustering algorithm in fuzzy modeling for reserve estimation. Xiong et al. (2001) used a first order Takagi-Sugeno fuzzy model combined with FCM clustering algorithm for flood forecasting, Chang and Chang (2001) used subtractive clustering while developing reservoir operation model, Hong et al. (2002) used the GK algorithm in forecasting ground water levels, Ansari et al. (2009) employed GG algorithm to create a non-subjective seismic catalog of Iran for helping in better seismological interpretations and seismic zoning. Nayak and Sudheer (2008) analyzed the relative performance of two clustering techniques, i.e., the GK and subtractive clustering in reservoir inflow forecasting. Vernieuwe et al. (2006) used different clustering algorithms (FCM, GK, GG, simplified GK, simplified GG, modified GG and subtractive clustering) to identify Takagi-Sugeno models for unsaturated groundwater flow. Then, they compared the complexity and accuracy by using this hydrological case study. Similarly, a comparison of clustering techniques can be found in (Vernieuwe et al., 2007) and (Agarwal et al., 2005).

3.2 Clustering Analysis of the Mean Annual Precipitation Data

FCM, GK and GG clustering algorithms are used to construct fuzzy models from data. To completely define rules, clustering is applied in the Cartesian product space of inputs and outputs. Before fuzzy clustering can be applied, the number of clusters must be specified. Partition coefficient, fuzzy hypervolume and partition density cluster validity indices are used to determine an appropriate number of clusters in the data set. The partition coefficient (PC) measures the amount of overlapping between clusters. The index is defined as (Bezdek, 1981)

$$V_{PC} = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{c} (u_j(x_i))^2 \tag{3.6}$$

where $u_j(x_i)$ is the membership of data point i in cluster j. The index values range in $[1/c, 1]$ where c is the number of clusters. The optimal number of clusters is at the maximum value. Gath and Geva (1989) proposed the fuzzy hypervolume (FHV) and the partition density (PD) indices. The FHV is defined by

$$V_{FHV} = \sum_{i=1}^{c} [det(F_i)]^2 \tag{3.7}$$

where the matrix F_i denotes the fuzzy covariance matrix of cluster i. A good fuzzy partition is indicated by small values of V_{FHV}. The PD is defined as

$$V_{PD} = \frac{\sum_{i=1}^{c} S_i}{V_{FHV}} \tag{3.8}$$

where S_i is the sum of membership degrees of data that are within a pre-specified region around cluster centroid. Large values of V_{PD} indicate good partitions.

The range of the number of clusters is selected as $c_{min} = 2$ and $c_{max} = 16$. Then, cluster validity analysis are performed by running the fuzzy cluster algorithms for different values of c in the range $[c_{min}, c_{max}]$. Furthermore, clustering is performed 20 times for each c with a different initialization, since these clustering algorithms are sensitive to the initialization. Clustering is performed with the Fuzzy Clustering and Data Analysis Toolbox (Balasko et al., 2005) which is a collection of MATLAB® functions. For cluster validity indices FHV and PD, MATLAB® functions are written.

FCM is initialized randomly (Table 3.1). For GK clustering algorithm, two approaches are applied. First, GK is initialized randomly (this procedure is named as

Table 3.1: Initialization methods applied to clustering algorithms.

Clustering algorithm	**Initialization method**	**Abbreviation of the algorithm**
Fuzzy c-means	Random	FCM_1
Gustafson-Kessel	Random	GK_1
Gustafson-Kessel	Fuzzy c-means	GK_2
Gath-Geva	Gustafson-Kessel	GG_3

GK_1). Second, the results of the FCM are used to initialize GK (GK_2). The initialization of GG clustering is done with GK, since GG is very sensitive to initial solution.

The data scale may have an influence on the performance of the clustering algorithms (Babuška, 1998; Vernieuwe et al., 2006). Moreover, according to Sudheer et al. (2003) the performance of soft computing-based models can be improved by following the guidelines which are used in traditional statistical modeling. In the previous chapter it is noticed that variables related with the annual precipitation are not normally distributed. Therefore, Box-Cox power transformations (Box and Cox, 1964) are applied to the data. Box-Cox power transformation transforms non-normally distributed data to a set of data that has approximately normal distribution. The transformation is defined as

$$x^* = \begin{cases} \frac{x^\lambda - 1}{\lambda} & if \lambda \neq 0 \\ \ln(x) & if \lambda = 0 \end{cases} \tag{3.9}$$

with x is the data and λ is a scalar called power parameter. Power parameters used in the transformations are listed in Table 3.2. After Box-Cox transformations the variables are scaled to fall between 0 and 1. Hence, two training data sets namely original and processed set are used.

Errors on original data set for linear regression and geographically weighted regression are given in Section 2.3.1. On processed data set, errors associated with these methods are as follows: For linear regression, the RMSE is calculated as 208.79 mm for the training data and 226.53 mm for the test data. For geographically weighted regression, the RMSE is calculated as 255.77 mm for the training data.

Table 3.2: Power parameters for training and testing data. λ values that maximize the logarithm of the likelihood function are calculated for training and testing data respectively.

Variable	**λ values for training data**	**λ values for testing data**
Longitude	0.07475000	-0.24143750
Latitude	-1.25018750	2.80850000
Altitude	0.43081250	0.28187500
SdGrid	0.47031250	0.25187500
Precipitation	-0.53293750	-0.68568750

3.3 Clustering Analysis Results and Discussion

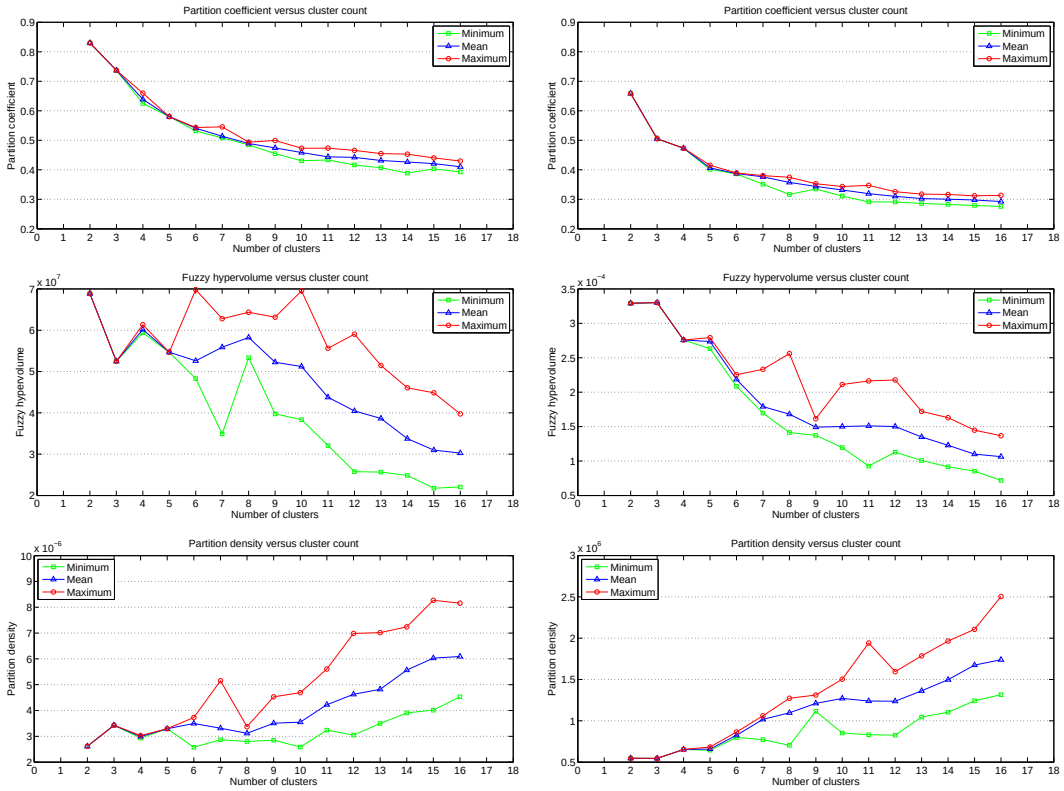
The cluster validity indices for the clusters obtained by FCM, GK and GG clustering algorithms for original and processed data sets are given in Figure 3.1, Figure 3.2, Figure 3.3 and Figure 3.4. Note that for each cluster c, clustering is performed 20 times with different initial conditions. In these figures in addition to the mean values minimum and maximum values for each cluster are also provided.

The PC value for FCM clustering in Figure 3.1 is, in this case, monotonic for both data sets and choosing appropriate cluster count was not possible using only PC value. Actually, the main drawback of PC is its monotonic decreasing behavior with c and the lack of direct connection with data (Abonyi and Feil, 2007; Tsekouras, 2007).

The FHV index value decreases suddenly at $c = 6$. Although it seems the FHV index has local minima at 6 clusters, as the number of cluster increases FHV values decreases for both training data sets. The minimum value is at $c = 16$.

The PD index is also monotonic for this case. While PD index values gradually increases after $c = 11$ for original data set, for processed data set this value is $c = 5$. The maximum value is at $c = 16$ for both data sets.

Although PC index monotonically decreases with increasing number of clusters, PC index values for GK_1, GK_2 and GG_3 initially decreases up to a point (8 clusters for GK_1 and GK_2, 4 clusters for GG_3) and then increases. PC index value for GG_3 reaches to almost its theoretical maximum value at $c = 16$. Also, note that index value for GG_3 for both data sets, maximum increase in index values is at $c = 5$.



(a) (b)

Figure 3.1: Plots of the minimum, mean and maximum values of the validity indices for clusters detected by FCM_1 (a) original data, (b) processed data.

The FHV index decreases monotonically for three of the clustering algorithms GK_1, GK_2 and GG_3. The minimum and maximum values of FHV index for these algorithms are closer than in the FCM_1 case. The minimum values are at $c = 16$.

The PD increases monotonically for GK_1, GK_2 and GG_3. As in the FHV index, the differences between minimum and maximum values are lower than the FCM_1 case. The maximum values are at $c = 16$.

For both training data sets, as cluster count increases validity indices indicate better clustering. Cluster validity indices measured for processed data behave similar to the validity indices of original data. Sudden increases or decreases are at the same cluster counts. On the other hand, the differences between minimum and maximum values of the validity indices are lower than that of the original data. Clustering algorithms become more stable when transformed data are used.

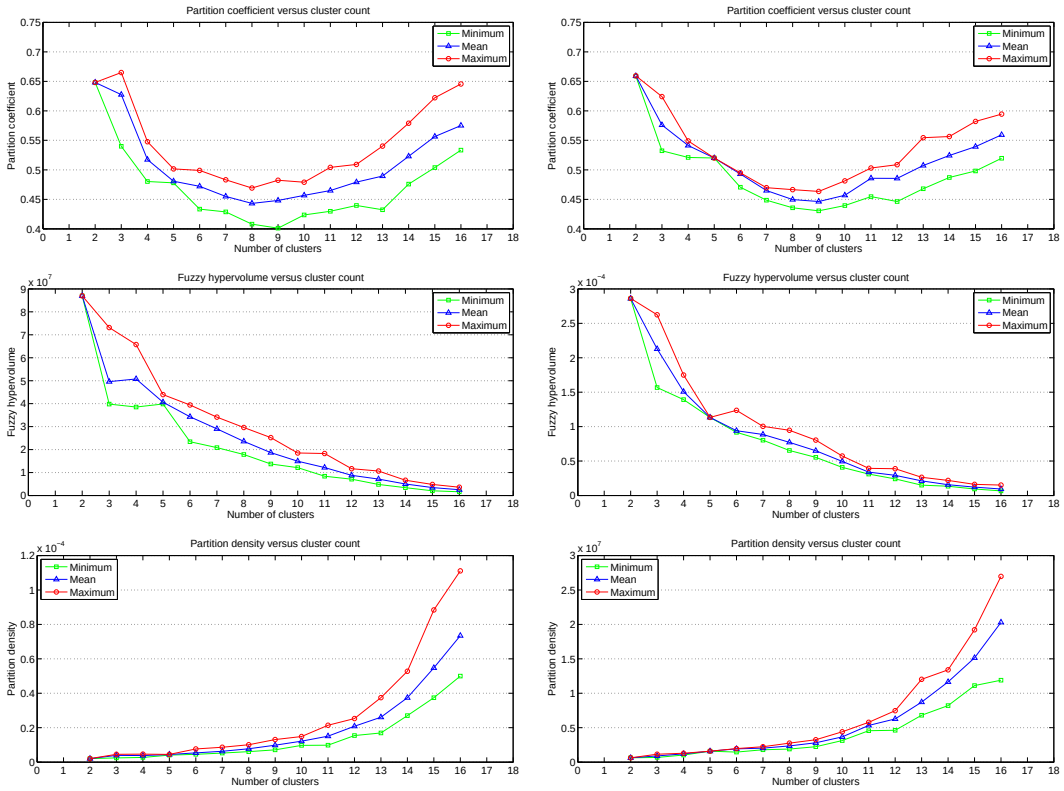
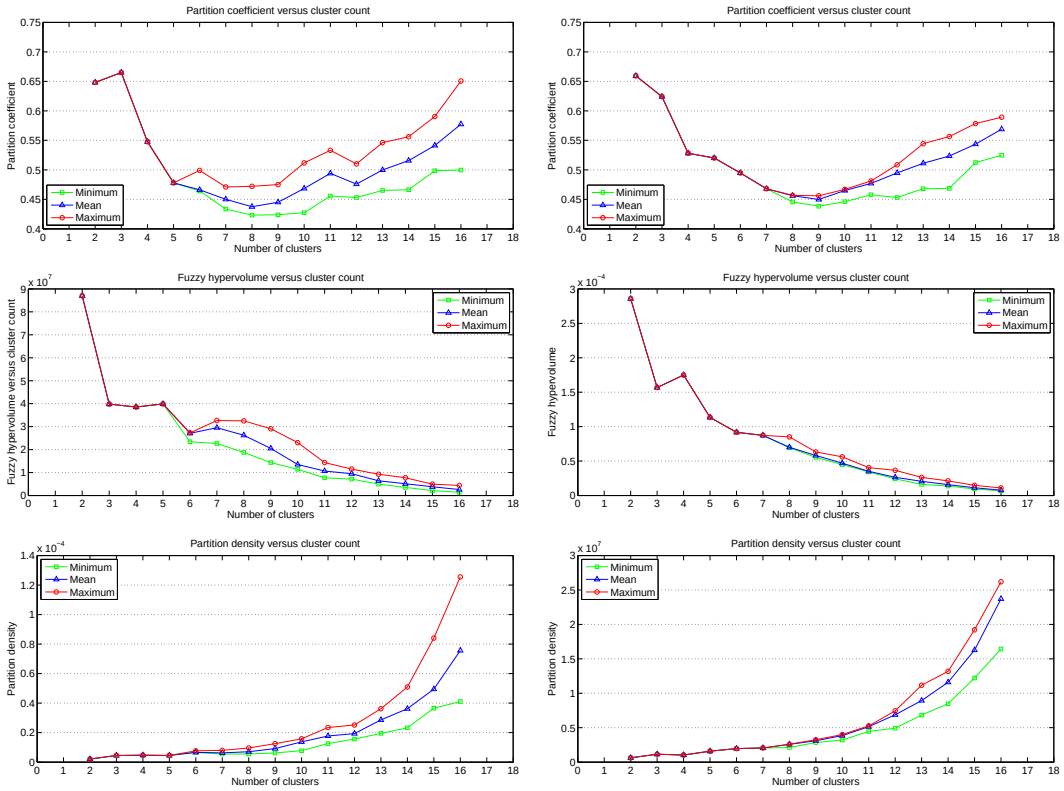


Figure 3.2: Plots of the minimum, mean and maximum values of the validity indices for clusters detected by GK_1 (a) original data, (b) processed data.

3.4 Construction of Fuzzy Models

FCM, GK and GG clustering algorithms are applied on the original and processed training data sets. After obtaining fuzzy partitions from the input-output product space clustering, fuzzy rule-based models are constructed from these partitions. Each partition (cluster) obtained by product space clustering of the training data is associated with a multidimensional membership functions as shown in Figure 3.5.

In order to obtain one-dimensional membership functions, the clusters are projected onto the variable axes. The center of a membership function is the cluster center and width of the membership function is computed using fuzzy partition matrix for FCM algorithm or using fuzzy covariance matrix for GK and GG clustering algorithms. The resulting fuzzy sets are usually difficult to interpret (Guillaume, 2001; Babuška, 1998; Abonyi and Feil, 2007; Tsekouras, 2007). Rules of the fuzzy models are associated to each cluster. Membership functions of variables "altitude" and "precipitation" for a



(a) (b)

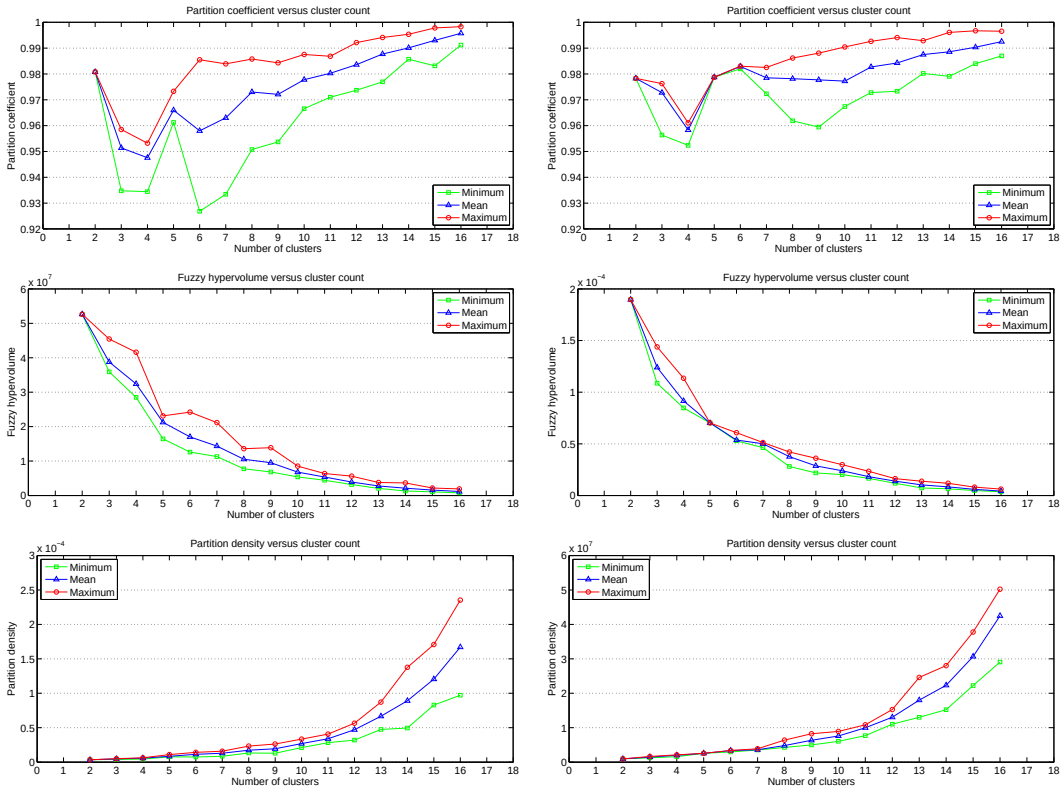
Figure 3.3: Plots of the minimum, mean and maximum values of the validity indices for clusters detected by GK_2 (a) original data, (b) processed data.

fuzzy model constructed from data is given in Figure 3.6.

3.5 Fuzzy Models

Fuzzy models are created for all iterations. In order to compare performance of fuzzy models, RMSE and the product moment correlation coefficient values are calculated. The results are illustrated in Figure 3.7, Figure 3.8, Figure 3.9 and Figure 3.10.

Although, cluster validity indices indicate better clustering for increasing number of clusters, the RMSE and the product moment correlation coefficient values for fuzzy models created using original data set do not support this outcome. Surprisingly, increase in the cluster count (increase in complexity) also increases error and reduces correlation between predicted and the original data values. On the other hand, as cluster validity indices suggested increasing the number of clusters decreases error obtained from the fuzzy models constructed with the processed data set.



(a) (b)

Figure 3.4: Plots of the minimum, mean and maximum values of the validity indices for clusters detected by GG_3 (a) original data, (b) processed data.

The difference between upper and lower bounds of the error measures are listed in Table 3.3. The subscript p refers to the results obtained with models identified on the processed data set.

With increasing the number of clusters fuzzy clustering algorithms may provide different solutions. The deviation between the different solutions is high when original data set is used to create fuzzy models as oppose to the processed data set. Therefore, transformations made on the original data set to produce processed data set improved clustering results in two ways: it improves the performance of the fuzzy models obtained from data and it provides clustering algorithms to be less affected from the initialization. On the other hand, this conclusion is specific to the precipitation case study and cannot be generalized to all other data sets.

For these reasons, fuzzy models constructed with processed data are used for further analysis. In addition, cluster count is selected using, firstly cluster validity indices

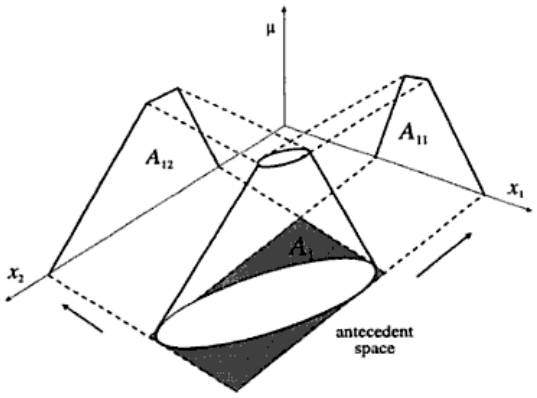
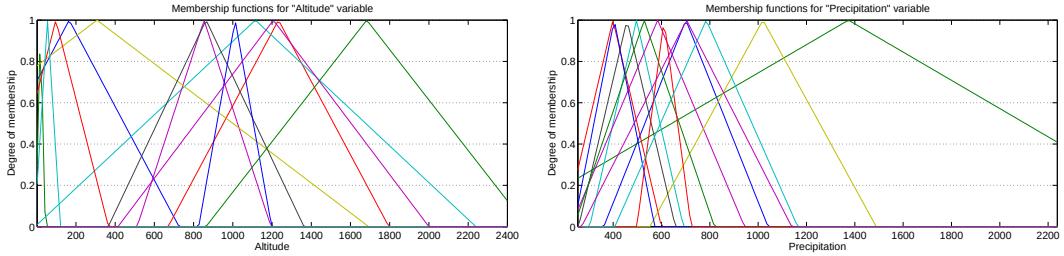


Figure 3.5: An example of multidimensional membership functions (adapted from (Babuška, 1998)).



(a) (b)

Figure 3.6: An example of membership functions identified from original training data set (a) membership functions for "altitude" variable, (b) membership functions for "precipitation" variable.

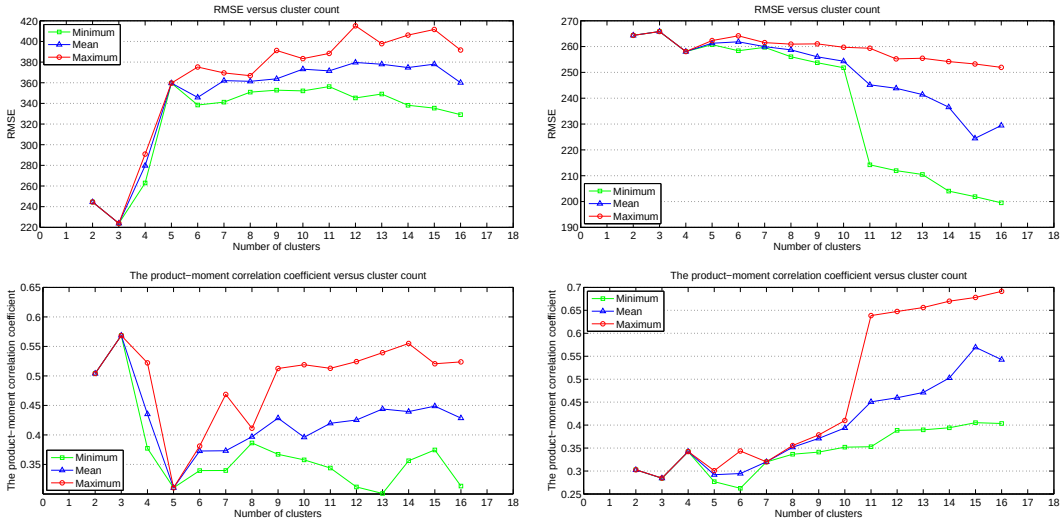
and secondly using global error measures (RMSE and product moment correlation coefficient values). If cluster validity indices impose a cluster count, then it is selected. But if indices do not clearly specify a cluster count such as if they are monotonically increasing or decreasing with c, then the global error measures are used to select the cluster count. The selected cluster counts and their associated indices and error measures are listed in Table 3.4. In Table 3.4, iteration numbers at which indices and error measures are calculated are given.

Table 3.3: The difference between upper and lower bounds of the error measures for original and processed training data sets. The subscript p refers to the results obtained with models identified on the processed data set.

	RMSE		**Product moment correlation coefficient**	
Algorithms	**Cluster Number**	**Difference**	**Cluster Number**	**Difference**
FCM_1	15	76.1600	13	0.2385
FCM_{1p}	16	52.4451	16	0.2879
GK_1	16	437.5250	12	0.6222
GK_{1p}	11	44.9843	11	0.2636
GK_2	12	492.4061	13	0.6856
GK_{2p}	15	20.0169	15	0.0991
GG_3	12	439.6502	6	0.6520
GG_{3p}	16	52.0668	16	0.3094

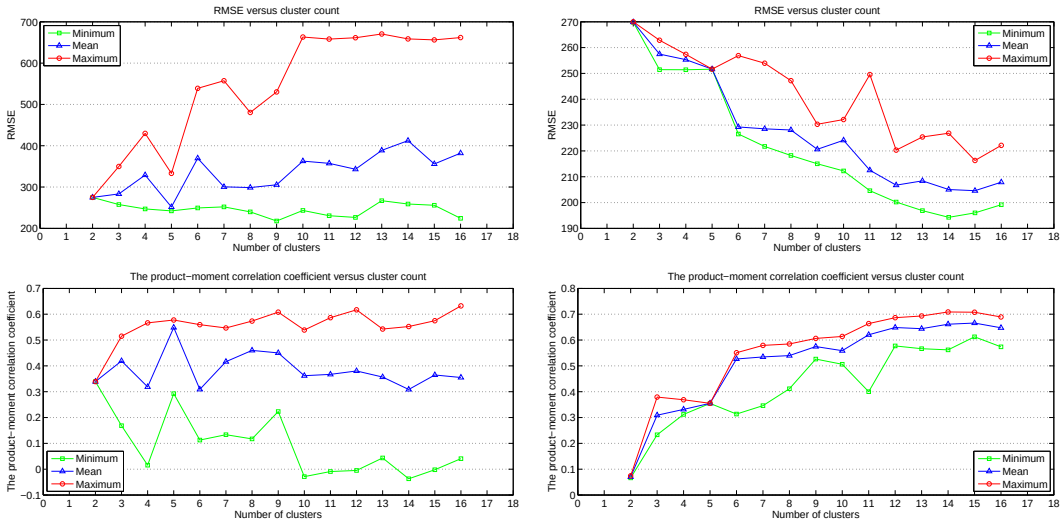
Table 3.4: Selected cluster counts and their associated indices and error measures for training data. The subscript p refers to the results obtained with models identified on the processed data set. PMCC refers to the product moment correlation coefficient.

Measures	FCM_{1p}	GK_{1p}	GK_{2p}	GG_{3p}
Cluster Count	16	14	14	14
Iteration	6	18	15	10
PC	0.3057	0.4870	0.4685	0.9876
FHV	$0.84 * 10^{-4}$	$0.20 * 10^{-4}$	$0.21 * 10^{-4}$	$0.08 * 10^{-4}$
PD	$2.14 * 10^{6}$	$0.91 * 10^{7}$	$0.85 * 10^{7}$	$2.33 * 10^{7}$
RMSE	199.5172	194.2788	194.8994	199.9073
PMCC	0.6914	0.7088	0.7022	0.7002



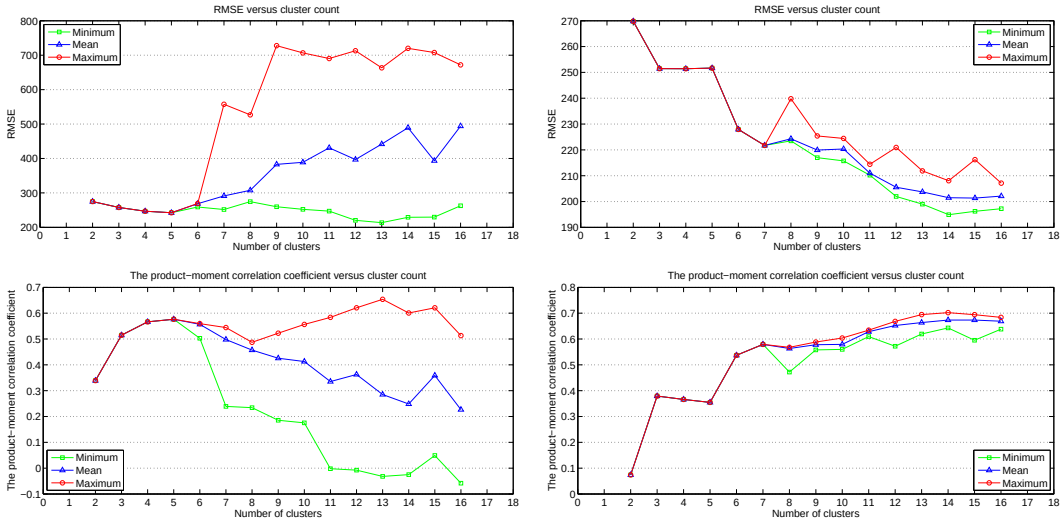
(a) (b)

Figure 3.7: Plots of the minimum, mean and maximum values of the error measures for fuzzy models constructed using FCM_1 (a) original data, (b) processed data. The constructed fuzzy models use triangular type membership functions.



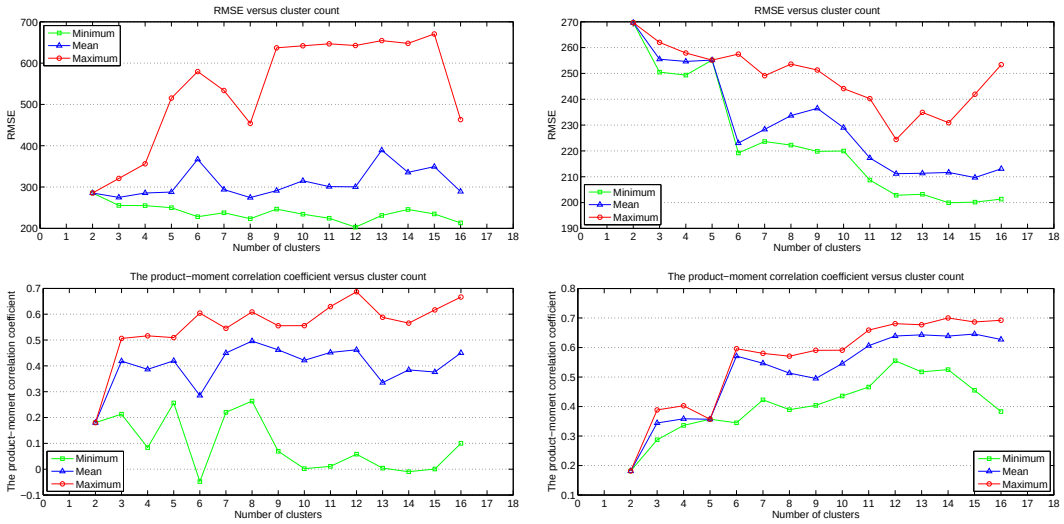
(a) (b)

Figure 3.8: Plots of the minimum, mean and maximum values of the error measures for fuzzy models constructed using GK_1 (a) original data, (b) processed data. The constructed fuzzy models use triangular type membership functions.



(a) (b)

Figure 3.9: Plots of the minimum, mean and maximum values of the error measures for fuzzy models constructed using GK_2 (a) original data, (b) processed data. The constructed fuzzy models use triangular type membership functions.



(a) (b)

Figure 3.10: Plots of the minimum, mean and maximum values of the error measures for fuzzy models constructed using GG_3 (a) original data, (b) processed data. The constructed fuzzy models use triangular type membership functions.

3.6 Discussion

Fuzzy models can be created from expert knowledge. However, when no experts are available or expert knowledge is not sufficient to define complex partially unknown systems fuzzy models can be constructed by using available data. For data-driven fuzzy model construction fuzzy clustering algorithms are most widely used. Three of the fuzzy clustering algorithms namely fuzzy c-means, Gustafson-Kessel and Gath-Geva clustering algorithms are used. However, the implementation of all these clustering algorithms suffers from three major problems:

1. Before fuzzy clustering can be applied, the number of clusters must be known a priori. To resolve this problem either cluster validity indices or optimal fuzzy clustering algorithms can be applied. According to the first approach, clustering is applied in an iterative fashion. In each of the iteration, the complexity of the model is increased by increasing cluster count (this also increases rule count) and the goodness of the obtained partitions are measured by validity measures. This iteration is repeated until a predefined criterion. Three of the cluster validity indices partition coefficient, fuzzy hypervolume and partition density are used. Unfortunately, none of the indices specify cluster count clearly. Wang and Zhang (2007) conducted extensive comparisons on a large number of cluster validity indices with fuzzy c-means clustering algorithm on a number of widely used data sets and conclude that none of the tested cluster validity indices correctly recognized optimal cluster count.

2. The fuzzy clustering algorithms are sensitive to the initialization. The resulting clusters obtained by fuzzy clustering algorithms (fuzzy c-means, Gustafson-Kessel and Gath-Geva) can be significantly changed by different initial states. For each of these fuzzy clustering algorithms, clustering is performed 20 times for each cluster count with different initialization. Clustering results support this statement. Performance of the obtained fuzzy models constructed by using identified clusters significantly changed by different initial states (Table 3.3). Fortunately, when the processed data are used, which is produced by Box-Cox power transformation to normality and then scaling is applied, the effect of initialization is lowered. Using the processed data in the fuzzy clustering process

makes fuzzy clustering algorithms more stable and performances of the fuzzy models are also improved.

3. After obtaining fuzzy partitions from data partitioning, fuzzy rule based models are constructed from these partitions. However, the obtained fuzzy models are usually difficult to interpret (Figure E.7, Figure E.9, Figure E.11 and Figure 4.11a). Obtained fuzzy models need further processing for interpretability.

After obtaining fuzzy models using available data, the accuracies of the fuzzy models are further increased by tuning membership function parameters using simulated annealing. The details of the optimization of parameters of fuzzy models are given in the next chapter. Moreover, while tuning parameters of the membership functions interpretability is also enhanced by analyzing fuzzy sets and rules in the fuzzy models. The details of the proposed approach are given in Chapter 5.

CHAPTER 4

FUZZY MODEL TUNING

Fuzzy systems based on fuzzy if-then rules are being used successfully for modeling of nonlinear, uncertain and complex systems. Fuzzy rules can be obtained from experts' knowledge. However, there is no standard method available for transforming experts' knowledge into the database of fuzzy systems (Jang, 1993; Yen and Langari, 1999; Yanar, 2003). In addition, expert rules are not sufficient to define complex partially unknown systems satisfactorily (Guillaume and Charnomordic, 2004). Therefore, various methods have been applied to fuzzy systems for automatically generating and adjusting if-then rules (Jang, 1993; Guillaume and Charnomordic, 2004; Yen and Wang, 1998; Emami et al., 1998; Wang and Mendel, 1992; Shi and Mizumoto, 2000; Chen and Linkens, 2004; Jin, 2000; Nauck and Kruse, 1999; Guély et al., 1999).

Among the data driven, automatic fuzzy rule generation and tuning methods there are local optimization methods such as gradient descent algorithm and global optimization methods such as simulated annealing and genetic algorithms. Simulated annealing is an iterative search method inspired by the annealing of metals (Kirkpatrick et al., 1983; Cerny, 1985). It simulates the annealing of metal where annealing is a strategy to find optimum state by controlling the temperature. The technique starts with heating a metal to a temperature near its melting point and then the metal is cooled slowly by keeping at each stage temperature in sufficient duration. The method of controlling the temperature decrease leads to a stable crystallized solid state which corresponds to an obsolete minimum of energy. Simulated annealing introduces a control parameter, temperature, in optimization and searches for global optimum by gradually decreasing the temperature similar to real annealing technique. Simulated annealing has two advantages over gradient descent algorithms: simulated annealing is able to find the global minimum of the function under certain conditions (Aarts and Laarhoven, 1985; Hajek, 1988; Hajek and Sasaki, 1989; Kan and Timmer, 1987a,b) and it can handle

any cost function. However its convergence speed is low unlike gradient descent. Moreover, since gradient descent based algorithms use derivatives they are mostly applied to Sugeno (Takagi and Sugeno, 1985) type fuzzy systems. These models are not as interpretable as Mamdani (Mamdani and Assilian, 1975) type fuzzy models since they use rules with linear models as consequents. For learning and tuning of fuzzy models global optimization methods such as simulated annealing (Mohamadi et al., 2008; Ghazanfari et al., 2007; Cordón et al., 2000; Liu and Yang, 2000; Cheng and Chen, 1997) and genetic algorithms (Antonelli et al., 2009; Marquez et al., 2007; Cordón and Herrera, 2001; Cordón et al., 2001; Roubos and Setnes, 2001; Setnes and Roubos, 2000) are also used. On the other hand, simulated annealing convergence has been demonstrated under more general assumptions than genetic algorithm (Aarts and Laarhoven, 1985) and genetic algorithm convergence depends on the way of coding parameters into genes.

In this study, simulated annealing algorithm was used to fine-tune Mamdani type fuzzy models which were constructed by using fuzzy clustering approach presented in the previous chapter.

The remaining of this chapter is organized as follows. In the first section, brief information on the related work done in this area is given. The detailed information about the proposed algorithm for Mamdani type fuzzy model tuning using simulated annealing is given in the second section. In the third section, the results of the tuning process are given. Discussions are provided in the last section.

4.1 Related Work

Simulated annealing (SA) is considered as a metaheuristic. It does not guarantee finding an optimal solution. However, under certain constraints (Aarts and Laarhoven, 1985; Hajek, 1988; Hajek and Sasaki, 1989; Kan and Timmer, 1987a,b) SA probably converges towards a global optimum (Dreo et al., 2006). The SA algorithm is given in Algorithm 2.

SA starts with an initial solution at high temperature. Initial solution can be a randomly selected point within the search space of all the possible solutions. Current solution in search space is evaluated by an objective function. Objective function (evaluation function) measures the energy of the current solution (in the algorithm

Algorithm 2 Simulated Annealing Algorithm

Require: The initial temperature T_0 and an initial solution X.

repeat
  repeat
    Generate a new solution Y, near to X
    if $E(Y) < E(X)$ **then**
      Accept new solution, $X = Y$
    else if $MetropolisAcceptance(E(Y), E(X), T_k) == true$ **then** {use Metropolis Acceptance Rule (Algorithm 3) for decision}
      Accept new solution, $X = Y$
    end if
  until temperature stage length is reached
  Reduce the temperature, $T_{k+1} = \alpha * T_k$
until $T_{k+1} \geq T_{final}$

energy of the solution is indicated by $E()$). New solution near to the current solution is selected from the search space using disturbance mechanism. If energy of the newly selected solution is less than the current solution, then newly selected solution is accepted as the current solution. On the contrary, if energy of the newly selected solution is higher than the energy of the current solution, SA does not automatically reject new candidate solution. Instead, it uses Metropolis Acceptance Criterion (Metropolis et al., 1953). Metropolis Acceptance Criterion will accept the new solution on a probabilistic basis. Bad moves in the search space are accepted with probability $p(T)$.

$$p(T) = e^{-\Delta E/T} \tag{4.1}$$

ΔE is the change in energy and T defines the temperature of the current configuration. Metropolis acceptance rule is given in Algorithm 3. According to the algorithm, change in the energy, ΔE, is calculated using the current and new solution. A real number is randomly selected from the interval $[0, 1]$. New solution is accepted if the randomly selected number is lower than $p(T)$. At high temperature probability of accepting bad configurations $p(T)$ is high, close to 1, therefore most of the moves are accepted. At low temperature, $p(T)$ is low, close to 0, majority of the bad moves are rejected.

At each temperature SA performs selected number of iterations (i.e., temperature

Algorithm 3 Metropolis Acceptance Rule

Require: The energy of the new solution E_{new}, the energy of the current solution E_{cur} and the current temperature T.

1: Calculate change in energy, $\Delta E = E_{new} - E_{cur}$
2: Calculate acceptance probability, $p(T) = e^{-\Delta E/T}$
3: **if** $Random(0,1) < p(T)$ **then**
4: **return** true {accept solution}
5: **end if**
6: **return** false {reject solution}

stage length) to allow the algorithm to settle into a balanced state. Then, the temperature is reduced according to the selected cooling schedule. Annealing process is repeated until the current temperature reaches the final temperature as in the Algorithm 2 or any termination criteria have been met. For example, three successive temperature stages without any acceptance or a time limit for the execution of the algorithm may also be stopping criterion.

Guély et al. (1999) use SA to optimize the membership functions of Takagi-Sugeno rules with constant output functions. The membership functions in this study are symmetric triangular membership functions. Therefore, the optimization problem consists of tuning the parameters of symmetric triangular membership functions (center and width) and the constant value for output. They compare SA results with gradient descent optimization results and state that SA enables to obtain better results when the number of membership functions and rules is as small as possible.

Chen and Linkens (2004) propose a hybrid fuzzy modeling approach using a self organizing map and SA for self constructing and optimizing Takagi-Sugeno type fuzzy rule-based models. The fuzzy rule-based model is generated by a self-organizing map (SOM) and the parameters of the membership functions (parameter learning) are performed with SA. Similarly, Liu and Yang (2000) use SA for learning parameters of Takagi-Sugeno fuzzy model. In their work, the structure of the fuzzy model and the initial membership function parameters are given.

Cheng and Chen (1997) combine fuzzy sets and SA in processing image brightness values. They represent brightness of gray levels in an image by S-type membership

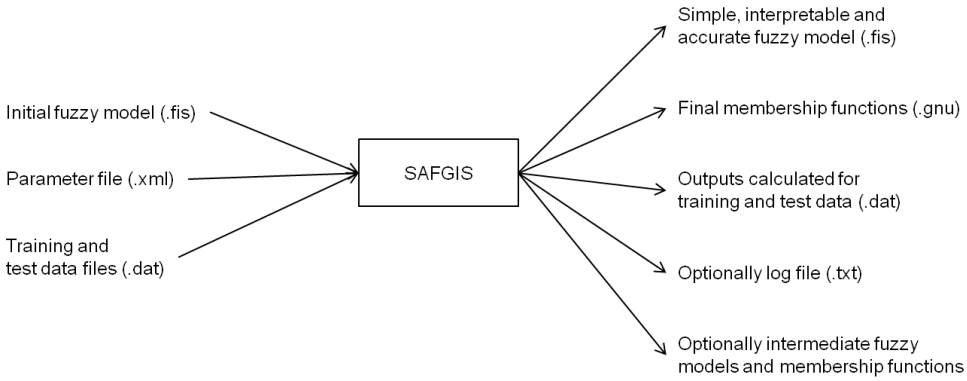


Figure 4.1: Workflow of prototype software, SAFGIS.

function and try to find an optimum or near optimum parameters for each gray level in the image. Mohamadi et al. (2008) use SA for constructing a fuzzy classification system and compare the approach with several well-known classification algorithms. Youssef et al. (2001) compare general iterative algorithms namely genetic algorithms, simulated annealing and tabu search on the same optimization problem and compare these techniques with respect to 1) quality of the best solution identified, 2) progress of the search from initial solutions to the end, 3) time (iteration count) needed to find best solution, and 4) the number solutions found at successive iterations.

4.2 Fuzzy Software Prototype

Prototype software, SAFGIS (Simulated Annealing Fuzzy Geographic Information Systems), is implemented for the interpretability oriented data-driven fuzzy modeling approach, which is presented throughout the thesis. SAFGIS can optimize a fuzzy model using adapted SA algorithm, whose details are given in Section 4.3, and generate compact and interpretable fuzzy model using simplification algorithm presented in Section 5.2. The general workflow of the software is shown in Figure 4.1.

An initial fuzzy model, a parameter file, training and test data files are given as inputs to the software. Initial fuzzy model generation from data is given in the previous chapter. SAFGIS is loosely coupled with MATLAB® and accepts initial fuzzy model in MATLAB® FIS file format, which has .fis suffix. Parameter file is an XML (eXtensible Markup Language) file and defines initial fuzzy model, training and test data file paths, user preferences and thresholds for adapted SA algorithm and simplification algorithm.

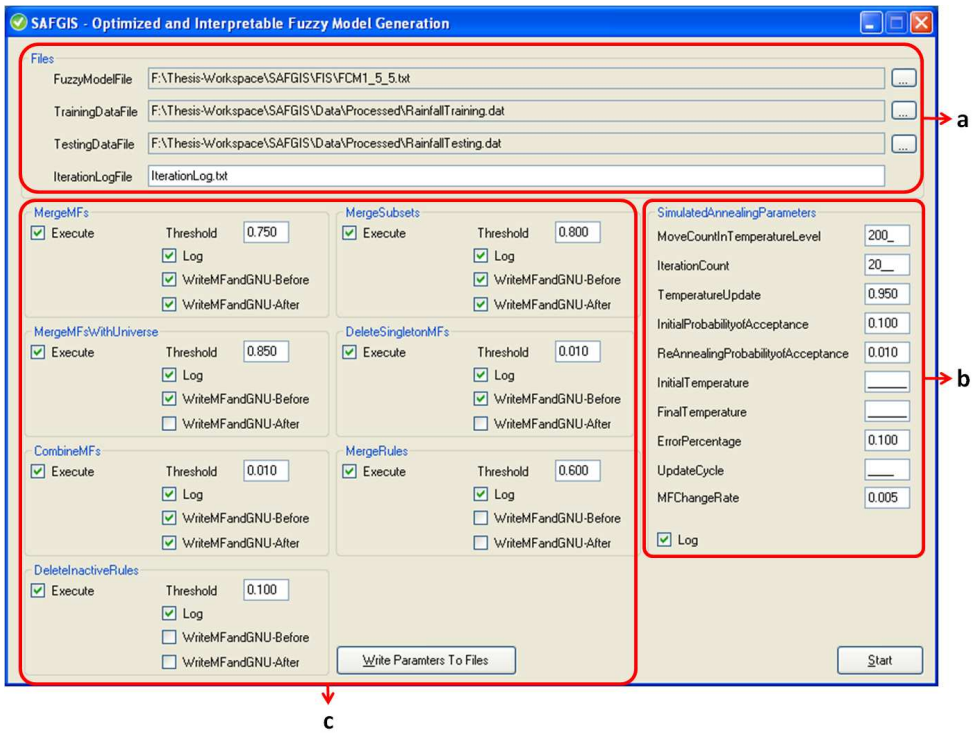


Figure 4.2: SAFGIS graphical user interface. (a) Files required for execution, initial fuzzy model file, training and test data files, (b) thresholds used in the adapted SA algorithm, and (c) thresholds used in the simplification algorithm.

SAFGIS has two operation modes; it can be run from command prompt or can be run as Windows® application. In command prompt mode, the usage of SAFGIS software is defined as follows:

$$\text{SAFGIS parameter\_file\_name} \tag{4.2}$$

In this mode, the software takes one parameter. The parameter defines name and full path of the parameter file. In Windows® application mode, when the software is started, graphical user interface (GUI) shown in Figure 4.2 is opened. User can enter initial fuzzy model, training and test data files and thresholds for adapted SA algorithm and simplification algorithm. Therefore, in this mode, there is no need to prepare parameter file manually, parameter file can be prepared using GUI. After specifying parameters using GUI in Windows® application mode or by parameter file in command prompt mode, running the software generates accurate and interpretable fuzzy model using adapted SA algorithm (given in Section 4.3), simplification algorithm (given in Section 5.2) and the given thresholds.

Accuracy and interpretability are two conflicting objectives. User can control the balance using the parameters. When the software finishes its execution, generated fuzzy model in FIS file format, final membership functions in GNU file format, outputs calculated for training and test data files, optionally a log file, which contains information about execution, other optional intermediate fuzzy model files and membership function files are written in a newly generated folder. SAFGIS is also integrated with GNUPLOT software and generates membership function plots in GNU file format.

SAFGIS software is implemented using Microsoft Visual C# 2005© and Microsoft .NET Framework Version 2.0.50727 SP2©. It has three modules; one module is for making inferences from a fuzzy model, second module is for optimization of fuzzy model using adapted SA algorithm which is presented in the next section and the other module is for simplifying fuzzy model using simplification methods described in Section 5.2.

4.3 Parameter Tuning Using Simulated Annealing

Mamdani type fuzzy models were constructed from input and output data using fuzzy clustering approach. FCM, GK and GG clustering algorithms were employed on the training data. After obtaining fuzzy partitions from input-output product space clustering, Mamdani type fuzzy rule-based models were generated from these partitions. And, a fuzzy model was selected for each fuzzy clustering algorithm (FCM_1, GK_1, GK_2 and GG_3) for further analysis. The details of this approach are given in the previous chapter. The accuracy of constructed fuzzy models was increased by tuning parameters using SA. Each rule in Mamdani fuzzy models has the following properties:

$$R_i : \begin{cases} If & V_{Longitude} \; is \; mf_{i1} \; and \; V_{Latitude} \; is \; mf_{i2} \; and \\ & V_{Altitude} \; is \; mf_{i3} \; and \; V_{SdGrid} \; is \; mf_{i4} \\ then & V_{Rainfall} \; is \; mf_{i5} \end{cases} \tag{4.3}$$

where $V_{Longitude}$, $V_{Latitude}$, $V_{Altitude}$ and V_{SdGrid} define values for each variable, mf_{ij} is the membership function of the ith rule associated with jth variable. Triangular membership functions were used in the fuzzy models and three parameters (a, b, c) were

Table 4.1: Properties of initial solutions (fuzzy models).

Name	Rule Count	Parameter Count	Training Error	Test Error
FCM_{1p}	16	240	199.5172	235.0664
GK_{1p}	14	210	194.2788	232.5839
GK_{2p}	14	210	194.8994	263.5563
GG_{3p}	14	210	199.9073	245.9093

used to define membership functions. Triangular membership functions are defined as

$$triangle(x : a, b, c) = \begin{cases} 0 & x < a \\ (x-a)/(b-a) & a \leq x \leq b \\ (c-x)/(c-b) & b \leq x \leq c \\ 0 & x > c \end{cases} \tag{4.4}$$

The parameters a and c locate the "feet" of the triangle and the parameter b locates the "peak". Therefore, the optimization problem contains tuning of the parameters a_{ij}, b_{ij} and c_{ij}.

Outline of the proposed approach for parameter tuning using SA is presented as follows (Algorithm 4):

Initial Solution: SA starts with an initial solution which was obtained from fuzzy clustering. Initial configuration which contains fuzzy if-then rules and initial membership function parameters for Mamdani fuzzy model was automatically generated from input-output data using fuzzy clustering approach. This structure learning method provides a good starting point for SA. Properties of initial fuzzy models are given in Table 4.1. All fuzzy models have four input variables and an output variable. FCM_{1p} contains 16 rules and has 240 parameters (i.e., $16 \times 5 \times 3$), other fuzzy models contain 14 rules and has 210 parameters (i.e., $14 \times 5 \times 3$).

Initial Temperature (Step 3): Initial temperature was calculated using the method described by Wong and Liu (1986). According to the Metropolis rule of acceptance SA accepts an energy rise (worse solution), h, with probability $p(T)$ given in Equation 4.1 where T is the current temperature. The initial temperature, T_0, can be calculated from mean energy rises, h_{mean}, during the initialization. Before the start of the actual SA algorithm, a number of moves (i.e., temperature stage length) in the neighborhood of the initial rule base were made and created new solutions were evaluated using

Algorithm 4 Adapted Simulated Annealing Algorithm for Fuzzy Model Tuning

Require: Initial fuzzy model FM_0, initial probability of acceptance P_0, the percentage of transition parameter ξ, temperature update parameter α.

Set iteration count and iterations without improvement count to zero, $k = 0, IWI = 0$
Set initial solution as current and the best solution, $S_{best} = FM_0, S_{cur} = FM_0$
$T_0 = InitialTemperature(S_{cur}, P_0, \xi)$
while $((k < 100)\&(IWI < N))$ **do**
  Set accepted good moves count to zero, $AGM = 0$
  Set move in temperature stage count to zero, $MITS = 0$
  Set best improvement flag to false, $BIF = false$
  while $((MITS < 500N)\&(AGM < 32N))$ **do**
    $S_{new} = DisturbanceMechanism(S_{cur}, \xi, T_o, T_k)$
    if $E(S_{new}) < E(S_{cur})$ **then** {good move}
      $S_{cur} = S_{new}$ {Set new solution as current solution}
      if $E(S_{new}) < E(S_{best})$ **then** {best solution}
        $S_{best} = S_{new}$ {Set new solution as best solution}
        $BIF = true$
      end if
      $AGM = AGM + 1$
    else if $MetropolisAcceptance(E(S_{new}), E(S_{cur}), T_k) == true$ **then**
      $S_{cur} = S_{new}$ {bad move but accepted}
    end if
    $MITS = MITS + 1$
  end while
  Decrease temperature, $T_{k+1} = \alpha T_k$ {cooling procedure}
  if $BIF == false$ **then**
    $IWI = IWI + 1$
  else
    $IWI = 0$
  end if
  $k = k + 1$
end while

objective function. During the initialization, mean value of energy rises, h_{mean}, was calculated using the formula given by Equation 4.5.

$$h_{mean} = \frac{1}{M_{bad}} \sum_{i=1}^{M_{bad}} \Delta Error_{bad} \tag{4.5}$$

where $\Delta Error_{bad}$ defines the energy rise of a bad move and M_{bad} is the number of bad moves made. Then, initial temperature T_0 was calculated using the following formula. The formula was derived from the Metropolis function.

$$T_0 = \frac{-h_{mean}}{In(P_0)} \tag{4.6}$$

Selecting the initial probability, P_0, near to 1 allows SA to start with a high temperature and accepting worse solutions with high probability. If the initial probability, P_0, is adjusted near to 0 then SA starts with a low temperature which accepts worse solutions with low probability.

The initial solution was obtained from structure learning algorithms described in the previous chapter and we did not want to alter this initial knowledge too much therefore we wish to keep the initial probability, P_0, of accepting worse solutions low (Guély et al., 1999). Throughout the tuning process, $P_0 = 0.25$ was used.

Objective Function: Output calculated from the tuned fuzzy model at current temperature can be evaluated using RMSE. Therefore, the objective function was minimizing the RMSE. Since, SA can use any cost function, any function measuring error between calculated output and target values can be used. However, evaluation function calculation must be direct and rapid to increase SA convergence speed and to decrease CPU consumption.

Disturbance Mechanism (Step 9): Instead of modifying all the parameters of a fuzzy model (i.e., 240 parameters for FCM_{1p} and 210 parameters for the other models) for selecting a new solution near to the current solution in the search space, only parameters associated with a randomly selected rule were modified. A rule was randomly selected from the rule base. Then, parameters of membership functions associated with this rule were modified. To update a parameter of a triangular membership function, a change interval was introduced. Change interval defines allowable minimum and maximum percentage of transitions that can be made to each parameter (a_{ij}, b_{ij}, c_{ij}). At each move, each parameter was updated proportional to the change rate randomly chosen in the interval $[-maxchangerate, +maxchangerate]$, where $maxchangerate$ was

calculated based on the current temperature. An update for a parameter is calculated using a random value which is drawn between $[-0.5, +0.5]$, percentage of transition parameter, ξ, which is given by the user as an optimization parameter and the current temperature as given in Equation 4.7.

$$\tau_{ij} = Random(-0.5, +0.5) * \xi * \frac{T_{current}}{T_{initial}} \tag{4.7}$$

where τ_{ij} is the update calculated for jth membership function of ith variable. Then, new parameter was calculated by adding update to the parameter.

$$a_{ij}^{new} = a_{ij}^{cur} * \tau_{ij} \tag{4.8}$$

Updates for each parameter of a fuzzy set were calculated separately. Therefore, transitions made to the parameters of a fuzzy set were not equal. At high temperatures each parameter has wider allowable change interval. As the temperature decreases, change in parameters decreases proportional to the temperature decrease.

Decrease of the Temperature (Step 22): The geometrical law of decrease $T_{k+1} = \alpha T_k$, where k defines temperature stage number and α is a constant between 0 and 1, was used to perform temperature decrease. Temperature update parameter was chosen as $\alpha = 0.99$.

Temperature Stage Length (Step 8): The number of iterations performed at each temperature stage is called temperature stage length. Adaptive temperature stage length was used in the analysis. Temperature stage was changed when one of the two following conditions was satisfied:

1. $32 \times N$ perturbations accepted
2. $500 \times N$ perturbations attempted

N indicates the number of variables used. In mean annual precipitation problem $N = 5$. After performing iterations at each temperature stage, temperature was decreased according to the cooling strategy.

Termination of SA algorithm (Step 4): SA algorithm was terminated after N successive temperature stages without any global improvement or the maximum number of temperature stages was reached. The maximum number of temperature stages was chosen as 100.

Table 4.2: Simulated annealing parameters used in the analysis.

Parameter	**Value**	**Allowable Range**
Initial probability of acceptance, P_0	0.25	$0 < P_0 < 1$
The percentage of transition parameter, ξ	0.10	$0 < \xi \leq 1$
Temperature update parameter, α	0.99	$0 < \alpha < 1$

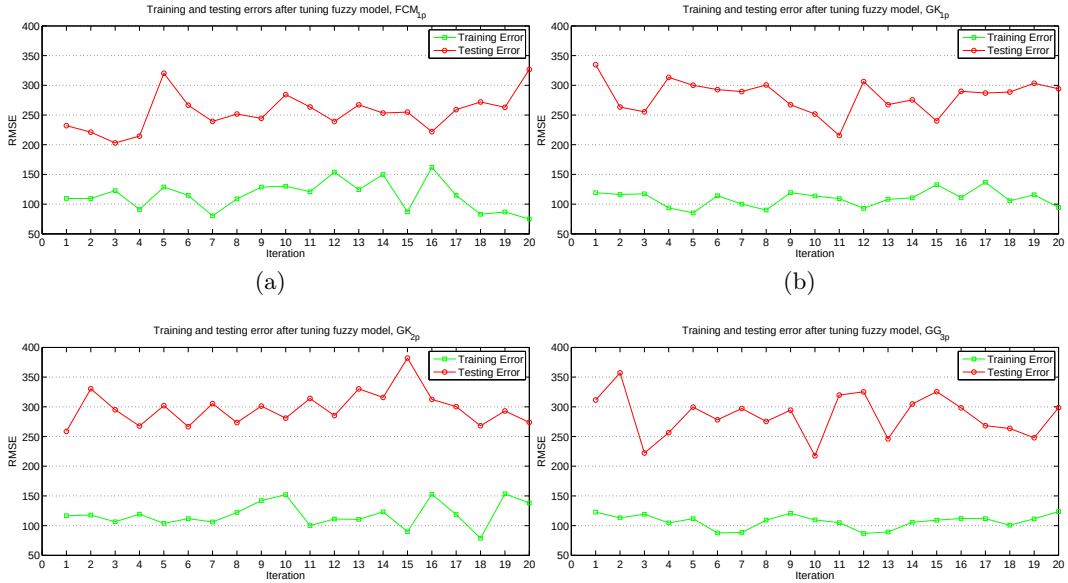


Figure 4.3: Training and testing errors after tuning fuzzy models.

4.4 Results

Fuzzy models learned from data were used as initial solution for SA algorithm to optimize. Optimization starts with the calculation of the initial error and the initial temperature. To calculate initial temperature specified number of moves (i.e., temperature stage length, $500 \times N$) was made and the mean value of energy rises was estimated for each fuzzy models. Then, initial temperature T_0 was calculated with the selected initial probability, P_0. Initial probability was chosen near to zero not to alter initial solution too much. The percentage of transition parameter ξ for membership functions was selected as 10%, temperature update coefficient was chosen as $\alpha = 0.99$. SA parameters used in the analysis are summarized in Table 4.2.

In the disturbance mechanism of the adapted SA algorithm, only parameters associated with a randomly chosen rule are modified. And the modifications on the

Table 4.3: Properties of training errors obtained after tuning fuzzy models.

Fuzzy Model	**Min.**	**Max.**	**Mean**	**Mean Difference**	**Mean (%) Difference**	**Standard Deviation**
FCM_{1p}	74.8169	162.0107	114.0498	−85.4671	−42.84	24.9373
GK_{1p}	85.1901	136.8754	109.3118	−84.9670	−43.73	13.5764
GK_{2p}	78.7496	153.5968	118.7519	−76.1475	−39.07	20.4463
GG_{3p}	86.7839	123.7203	107.1306	−92.7767	−46.41	11.4663

Table 4.4: Properties of testing errors obtained after tuning fuzzy models.

Fuzzy Model	**Min.**	**Max.**	**Mean**	**Mean Difference**	**Mean (%) Difference**	**Standard Deviation**
FCM_{1p}	202.9307	326.6135	254.8912	+19.8248	+8.43	31.3841
GK_{1p}	215.5814	334.7319	281.8435	+49.2603	+21.18	27.6830
GK_{2p}	258.6844	382.1230	297.8304	+34.7241	+13.17	29.0666
GG_{3p}	217.5669	357.1768	285.3823	+39.4730	+16.05	36.0128

membership functions are based on randomly chosen rate in an interval which is calculated using a given parameter and the current temperature. In addition to these probabilistic behaviors, SA algorithm uses Metropolis Acceptance Criterion which accepts worse solutions on a probabilistic basis. Therefore, results obtained from the algorithm may vary when the algorithm is executed several times with different seed value. Seed values are used in the random number generation process. For this reason, tuning of each initial fuzzy model was repeated 20 times with a different seed value. Training and test data errors after tuning fuzzy models $FCM_{1p}, GK_{1p}, GK_{2p}$ and GG_{3p} are shown in Figure 4.3. Properties of training and test data errors are listed in Table 4.3 and Table 4.4.

Besides the stochastic behavior of the algorithm, the deviations of error on training data were low especially for GG_{3p} and GK_{1p} fuzzy models. Yet the algorithm must be run several times before making a decision.

After the tuning process, error on training data reduced approximately 43%. On the other hand, error on test data increased only about 15%. Even in some iterations both training and test data errors decreased. For example, at the fourth iteration

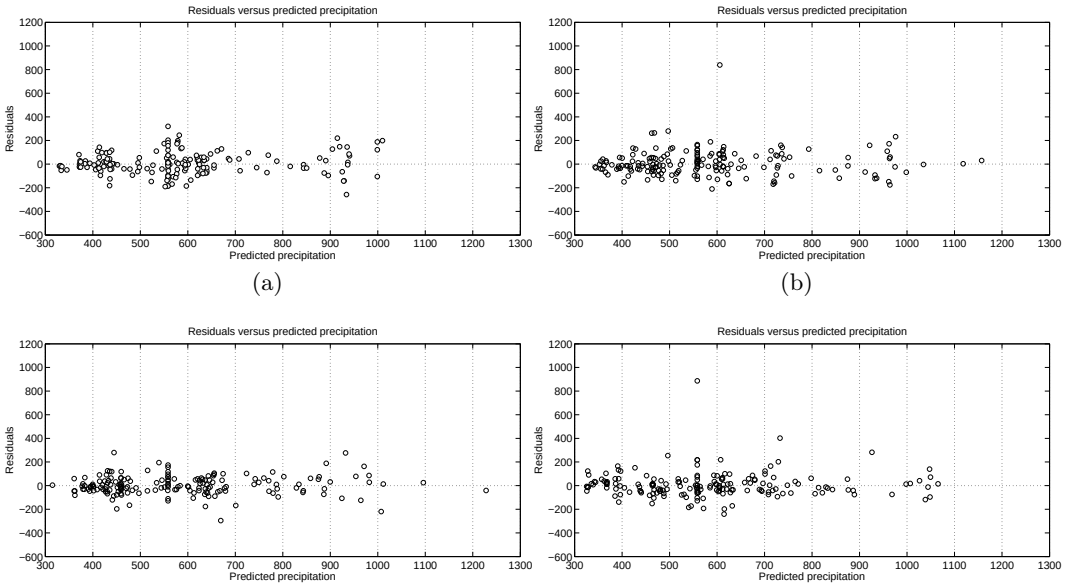


Figure 4.4: Residuals versus predicted precipitation for tuned fuzzy models (a) FCM_{1p}, (b) GK_{1p}, (c) GK_{2p}, (d) GG_{3p}.

(Figure 4.3a) the adapted SA algorithm tuned FCM_{1p} fuzzy model such that error on training data is 90.9208 mm and error on test data is 214.4794 mm.

A tuned fuzzy model was selected for each tuning session (FCM_{1p}, GK_{1p}, GK_{2p} and GG_{3p}) to analyze its residuals and visualize errors obtained for each meteorological station on map. Selected tuned fuzzy models are:

- for FCM_{1p}, fuzzy model obtained at the 4th iteration,
- for GK_{1p}, fuzzy model obtained at the 11th iteration,
- for GK_{2p}, fuzzy model obtained at the 18th iteration,
- for GG_{3p}, fuzzy model obtained at the 10th iteration.

Selection was based on both training and test data errors; fuzzy model which minimized the sum of training and test data errors most was selected. Residuals versus predicted precipitation values are plotted on Figure 4.4.

The residuals are tested for autocorrelation using Durbin-Watson test. The Durbin-Watson test statistics are 2.20 (FCM_{1p}), 2.05 (GK_{1p}), 2.35 (GK_{2p}) and 2.12 (GG_{3p}). The Durbin-Watson test statistic for GK_{2p} indicates low negative autocorrelation.

Table 4.5: Moran's I index measuring the spatial autocorrelation in residuals of tuned fuzzy models.

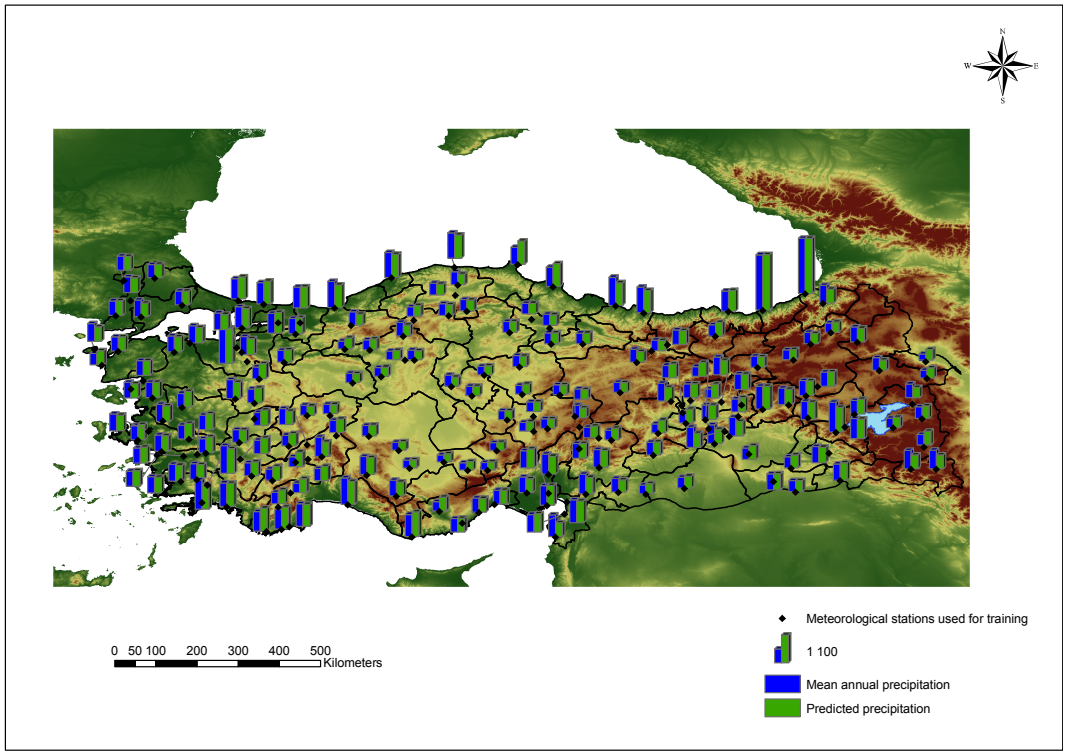
Fuzzy model	**Data**	**Moran's I index**	**Expected value**	**Z-Score**	**In 5% significance level**
FCM_{1p}	Training Data	0.006819	-0.005587	1.318221	Random
FCM_{1p}	Testing Data	-0.041939	-0.013699	-1.391968	Random
GK_{1p}	Training Data	0.015554	-0.005587	2.361172	Clustered
GK_{1p}	Testing Data	-0.015849	-0.013699	-0.105874	Random
GK_{2p}	Training Data	-0.015753	-0.005587	-1.084701	Random
GK_{2p}	Testing Data	-0.024197	-0.013699	-0.536431	Random
GG_{3p}	Training Data	0.017959	-0.005587	2.675365	Clustered
GG_{3p}	Testing Data	-0.034016	-0.013699	-1.002188	Random

For the other fuzzy models, test statistics indicate no autocorrelation. Moreover, the degree of spatial autocorrelation in the residuals was measured using global Moran's I index and the results are listed in Table 4.5. No spatial autocorrelation should exist in the residuals for a successful model. Only residuals of training data for GK_{1p} and GG_{3p} show spatial autocorrelation (marked as "Clustered" in Table 4.5). Predictions made by the selected tuned fuzzy models for meteorological stations are mapped in Figure 4.5, Figure 4.6, Figure 4.7 and Figure 4.8.

Predictions of FCM_{1p} (Figure 4.5) model for training data are accurate and there are no remarkable errors. For test data, FCM_{1p} fuzzy model underestimates precipitation on the northwestern Anatolia region especially the cities Zonguldak, Bartın and Kastamonu. On the other hand, model overestimates precipitation remarkably for the cities Aksaray, Tokat and Erzincan. Predictions of GK_{1p} (Figure 4.6) model for training data exhibit a considerable error for meteorological station located at Uludağ (peak). Most of the error on training data is due to the error for this station. Actually, mean precipitation for this station is considerably higher than the mean precipitations of surrounding stations. In spite of this, prediction errors of FCM_{1p} and GK_{2p} models for this station are low, 11.3 mm and 34.0 mm respectively. For the test data, like FCM_{1p} models GK_{1p} fuzzy model underestimates precipitation on the northwestern Anatolia region especially the cities Zonguldak, Bartın and Kastamonu

and overestimates precipitation remarkably for the cities Konya, Aksaray and Erzincan. GK_{2p} (Figure 4.7) model seems over fitted on training data, while prediction error on training data is very low, error on test data is high. GK_{2p} fuzzy model underestimates precipitation on the northwestern Anatolia region cities Zonguldak, Bartın, Kastamonu and northeast Anatolian city Giresun. Moreover, the model considerably overestimates precipitation for the cities Kütahya, Bilecik, Aksaray, Tokat, Erzincan, Trabzon and Şanlıurfa. Prediction error for Trabzon Akçaabat meteorological station is -1300 mm. Like the GK_{1p} model, most of the error on training data for GG_{3p} fuzzy model (Figure 4.8) is due to error for meteorological station located at Uludağ (peak). On the test data, GG_{3p} model underestimates precipitation for the cities Zonguldak, Bartın, Kastamonu and Giresun and overestimates precipitation for the cities Kütahya, Aksaray and Erzincan.

Although prediction errors associated with the cities Zonguldak, Aksaray and Erzincan are high for all the models, these cities have few meteorological stations. For example, there is only one meteorological station for Zonguldak and Aksaray and this station is included in the test data set. For Erzincan, there are two meteorological stations, one station is included in the training data set and the other is included in the test data set by chance.



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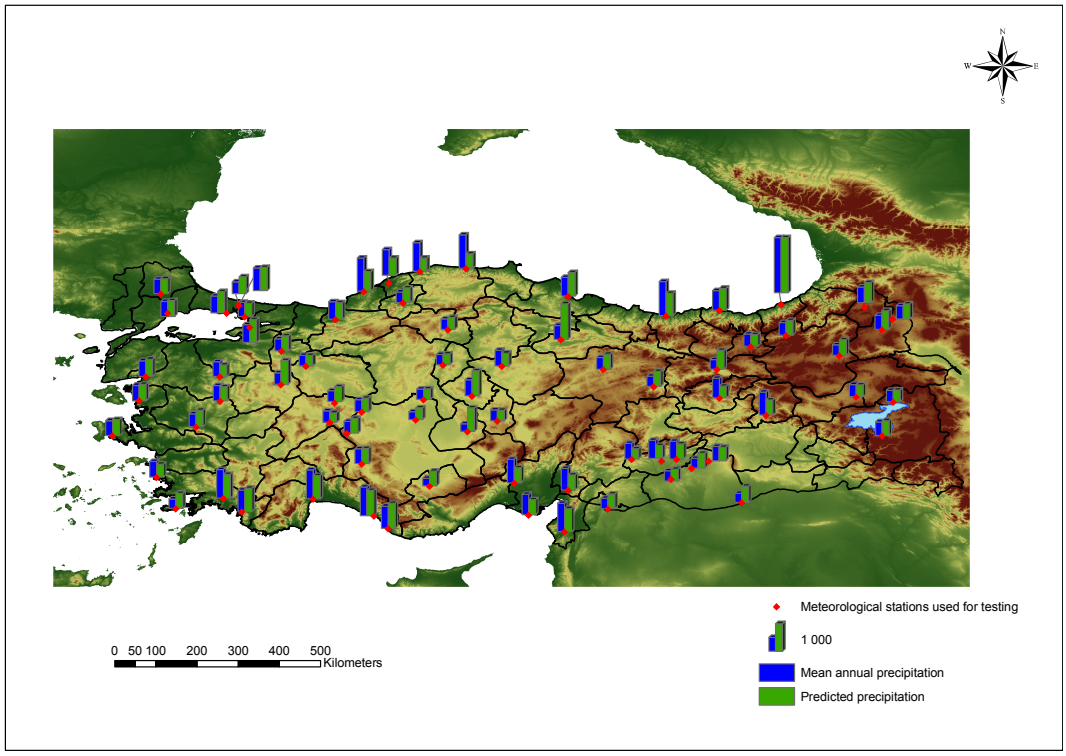
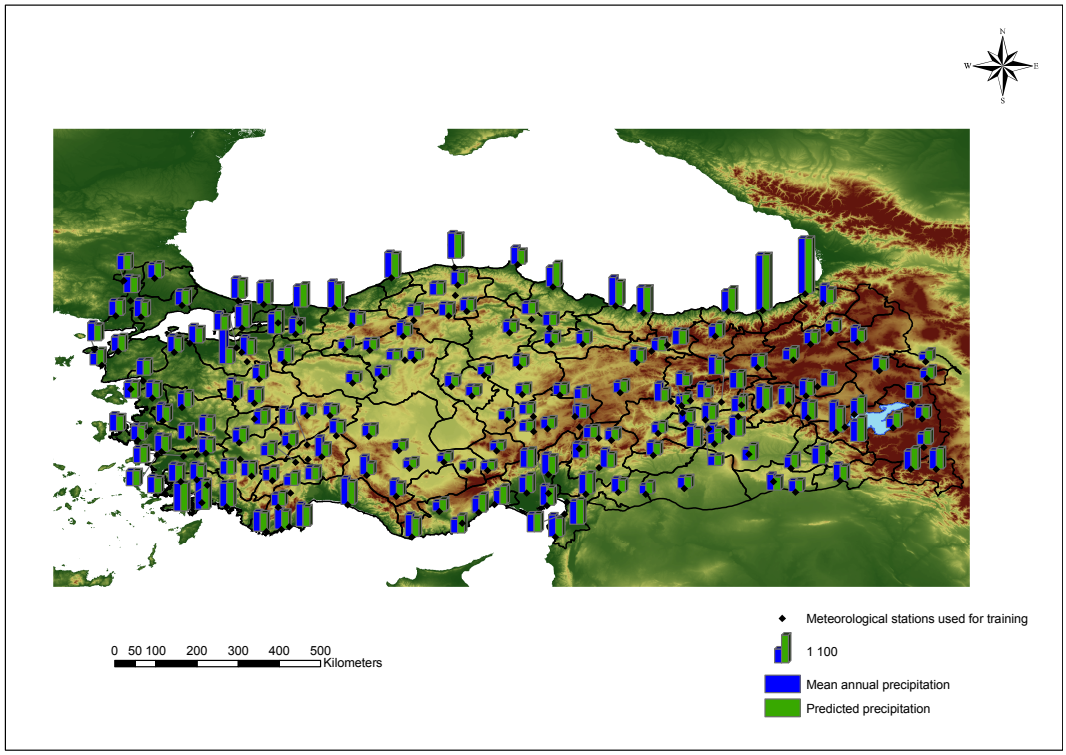


(b)

Figure 4.5: Predictions of the tuned FCM_{1p} fuzzy model. (a) Predictions of the tuned FCM_{1p} fuzzy model for training data. Training error is 90.9208 mm. (b) Predictions of the tuned FCM_{1p} fuzzy model for testing data. Testing error is 214.4794 mm.



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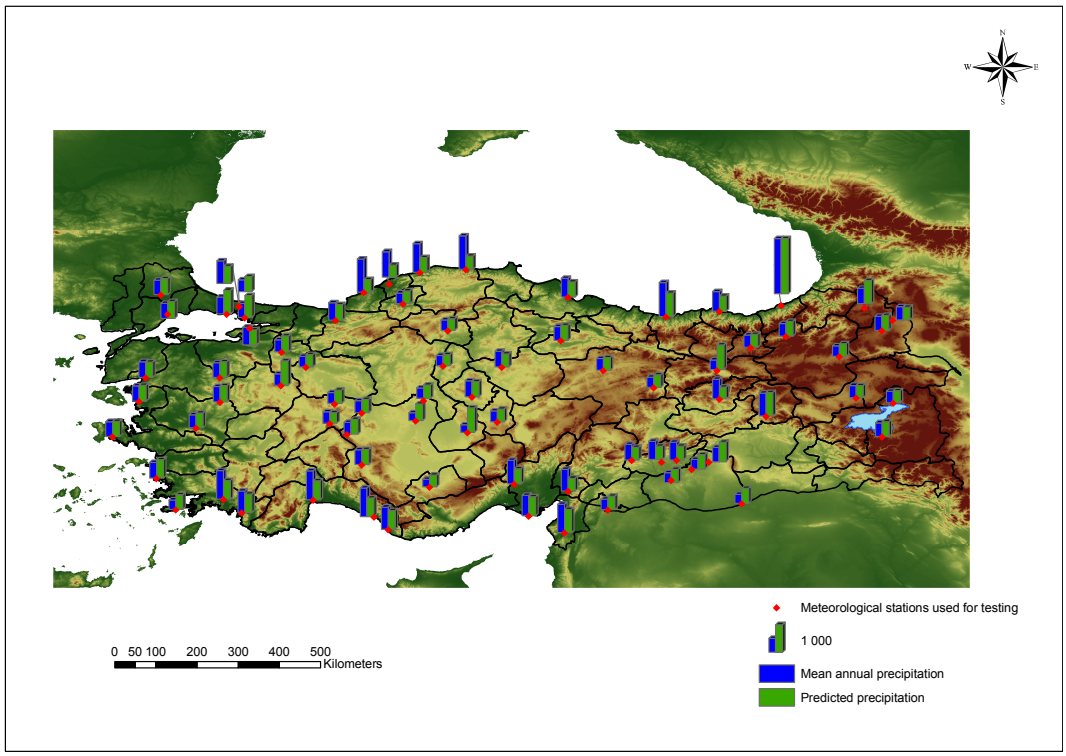
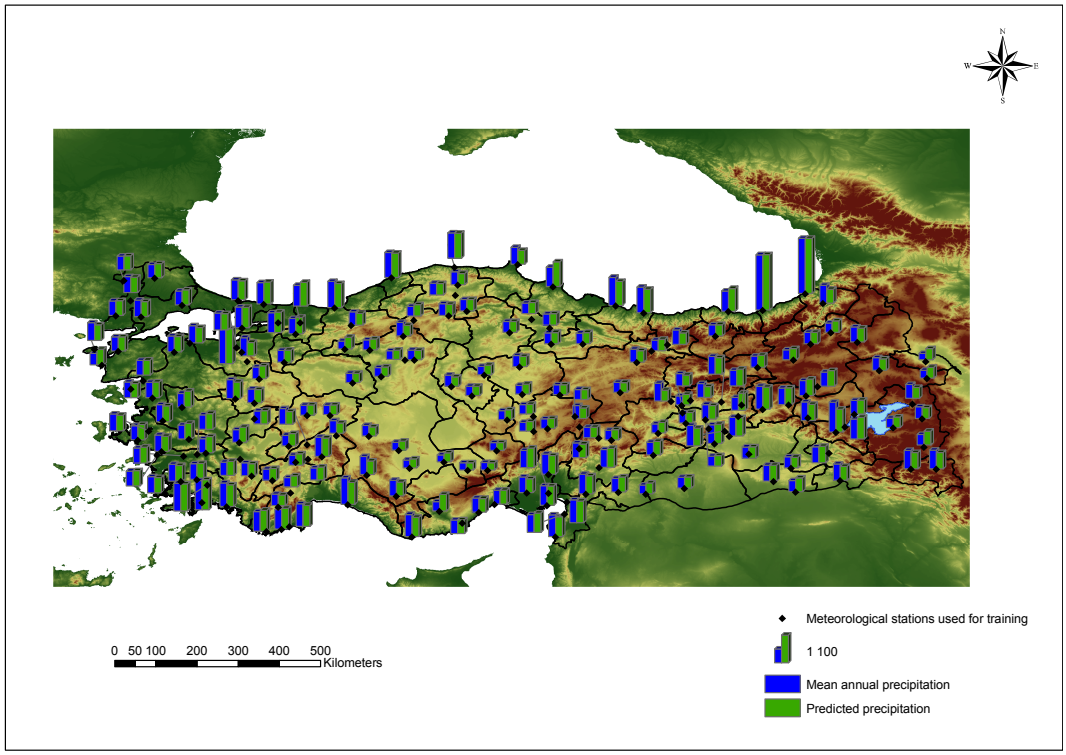


(b)

Figure 4.6: Predictions of the tuned GK_{1p} fuzzy model. (a) Predictions of the tuned GK_{1p} fuzzy model for training data. Training error is 109.3242 mm. (b) Predictions of the tuned GK_{1p} fuzzy model for testing data. Testing error is 215.5814 mm.



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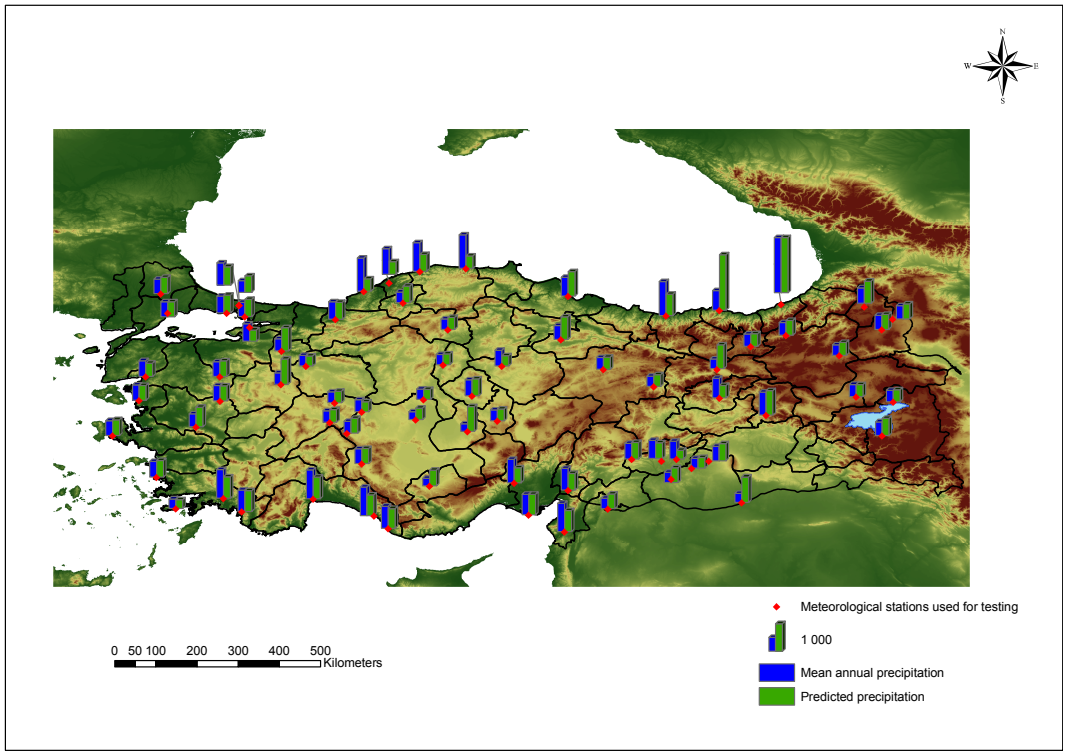
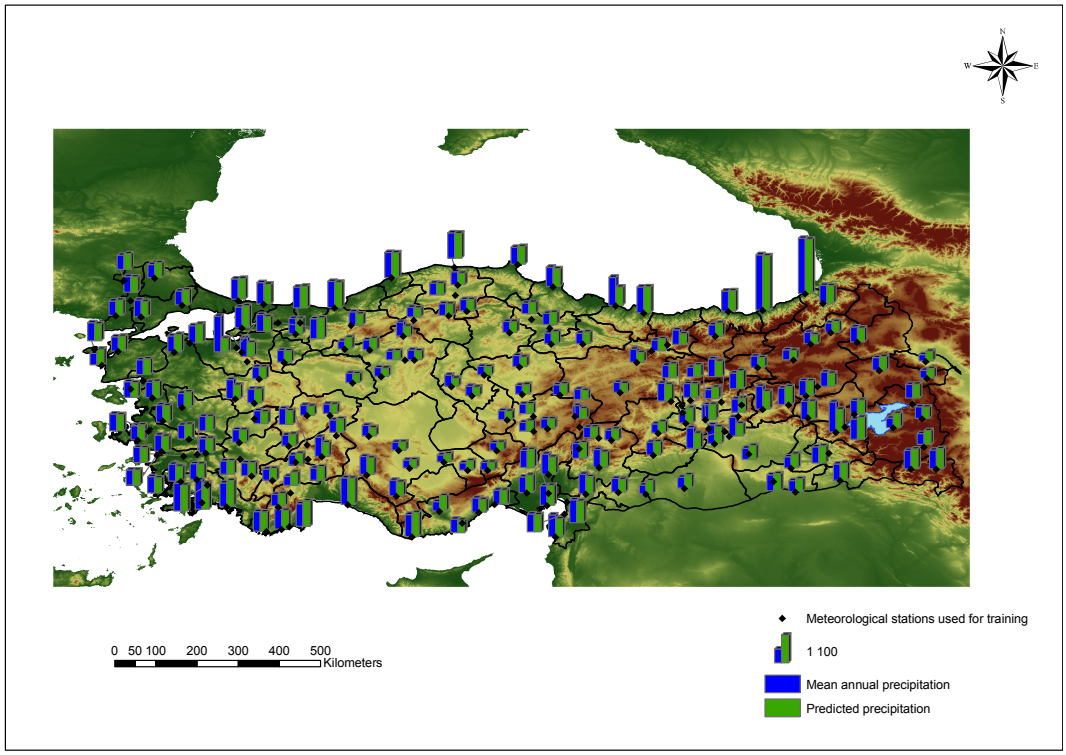


(b)

Figure 4.7: Predictions of the tuned GK_{2p} fuzzy model. (a) Predictions of the tuned GK_{2p} fuzzy model for training data. Training error is 78.7496 mm. (b) Predictions of the tuned GK_{2p} fuzzy model for testing data. Testing error is 268.1016 mm.



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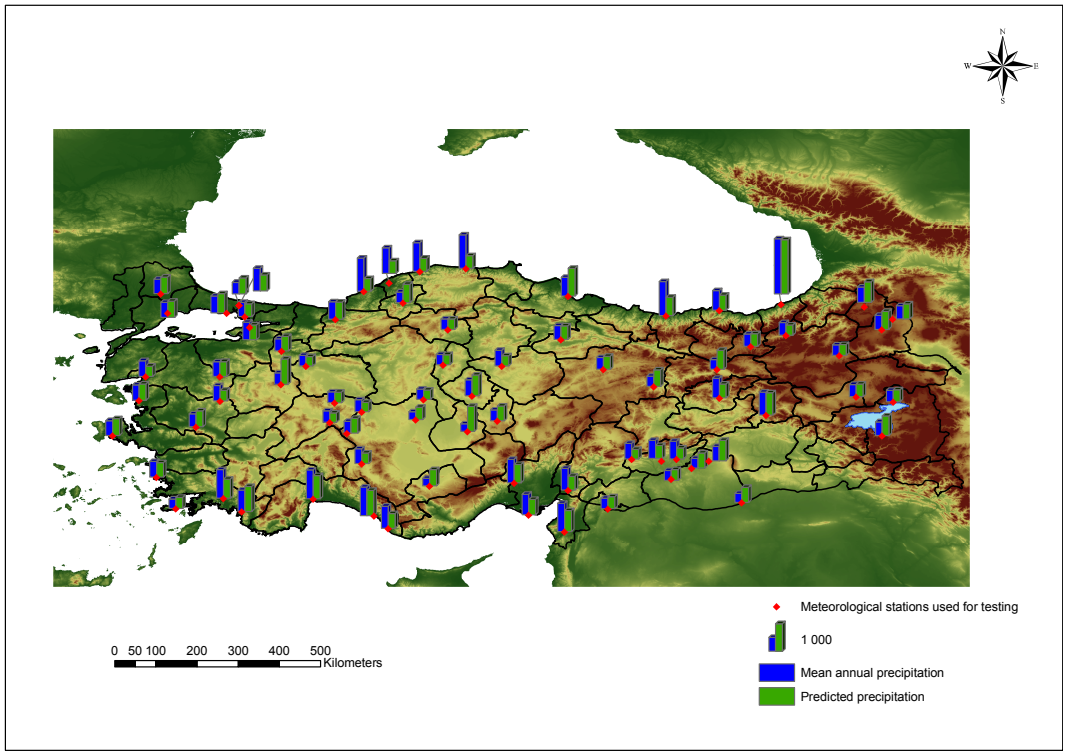

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Figure 4.8: Predictions of the tuned GG_{3p} fuzzy model. (a) Predictions of the tuned GG_{3p} fuzzy model for training data. Training error is 109.5233 mm. (b) Predictions of the tuned GG_{3p} fuzzy model for testing data. Testing error is 217.5669 mm.

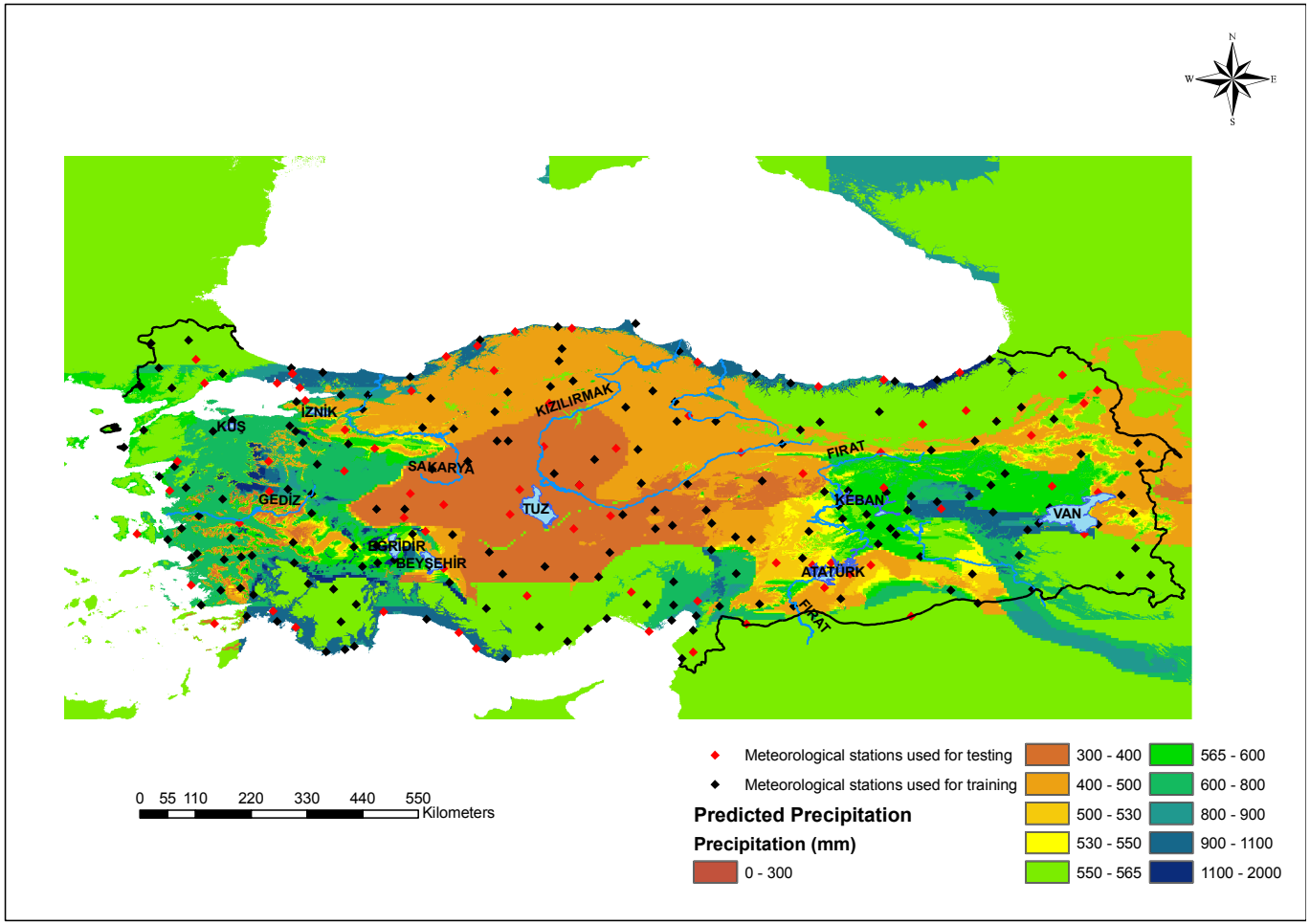


Figure 4.9: Predicted precipitation map for Turkey generated using the model FCM_{1p}. Training error is 90.9208 mm and testing error is 214.4794 mm.

Fuzzy models created and tuned using data-driven approach can be used not only for data related with the meteorological stations but also for the whole Turkey. An example of such precipitation prediction map (Figure 4.9) for Turkey is generated using the FCM_{1p} fuzzy model which is selected for the above residual analysis. The precipitation values of all locations of Turkey in 1 km resolution are estimated using the model. According to the prediction map, northeastern coast of Turkey (especially the cities Trabzon, Rize and Artvin) has the highest precipitation values. As it is moved away from the coast, precipitation decreases. Other wet cities and regions are Giresun, Ordu, Central Black Sea region (Samsun and Sinop), West Black Sea region (Bartın, Zonguldak and Sakarya), Kocaeli, İstanbul, Balıkesir (especially the region among the borders of Manisa, Bursa and Kütahya), southwestern cost of Turkey (Muğla and Antalya), Bingöl and Bitlis. In addition to these Çukurova region has also high precipitation value and this region gets more rainfall than its surrounding region. The central Anatolia has the least precipitation. Most or all parts of the cities in this region (Afyon, Konya, Eskişehir, Ankara, Kırıkkale, Kırşehir, Aksaray, Nevşehir, Niğde, Kayseri and Çorum) are the driest regions according to the prediction map. Southeastern Anatolia has relatively higher precipitation than the central Anatolia.

Since the model is generated using data obtained from the meteorological stations covering Turkey, the model is only valid for Turkey. Although the model is also used to estimate the surrounding locations of Turkey, they may contain quite large errors. On the other hand, models for any region of the earth can be generated using data related with the region.

The average computing time was about 25 minutes (1477.183 seconds) on a notebook which contains an Intel® 1.83 GHz Core™ Duo processor (T2400), 1 GB RAM and Microsoft® Windows® Home Edition Version 2002 with Service Pack 3.

In addition to the fuzzy models tuned above, which are selected among the others in Section 3.5, fuzzy models constructed with five clusters are also tuned. Same SA parameters are used as in the previous tuning process. These parameters are given in Table 4.2. Training and test errors after tuning fuzzy models are shown in Figure 4.10. Properties of training and test data errors are listed in Table 4.6 and Table 4.7.

According to the results, training errors obtained after tuning fuzzy models which are constructed with five clusters are approximately 37% worse. On the other hand, testing errors obtained for the second tuning process (tuning of fuzzy models which

Table 4.6: Properties of training errors obtained after tuning fuzzy models which are constructed with five clusters.

Fuzzy Model	**Min.**	**Max.**	**Mean**	**Mean Difference**	**Mean (%) Difference**	**Standard Deviation**
FCM_{1p}	137.0620	208.9881	187.8785	−72.8498	−27.94	14.6928
GK_{1p}	124.4373	186.8453	162.7168	−88.9155	−35.34	18.5641
GK_{2p}	129.1925	196.1799	160.7316	−90.9372	−36.13	17.2777
GG_{3p}	115.5658	182.9143	162.3836	−92.7979	−36.37	21.1890

Table 4.7: Properties of testing errors obtained after tuning fuzzy models which are constructed with five clusters.

Fuzzy Model	**Min.**	**Max.**	**Mean**	**Mean Difference**	**Mean (%) Difference**	**Standard Deviation**
FCM_{1p}	222.9331	319.2139	272.6508	−7.8922	−2.81	20.1023
GK_{1p}	211.6637	316.0900	255.4841	−6.4650	−2.47	28.1635
GK_{2p}	219.8441	309.2197	266.1297	+4.0828	+1.62	24.7084
GG_{3p}	218.7518	378.9263	266.9077	−12.1857	−4.78	37.0660

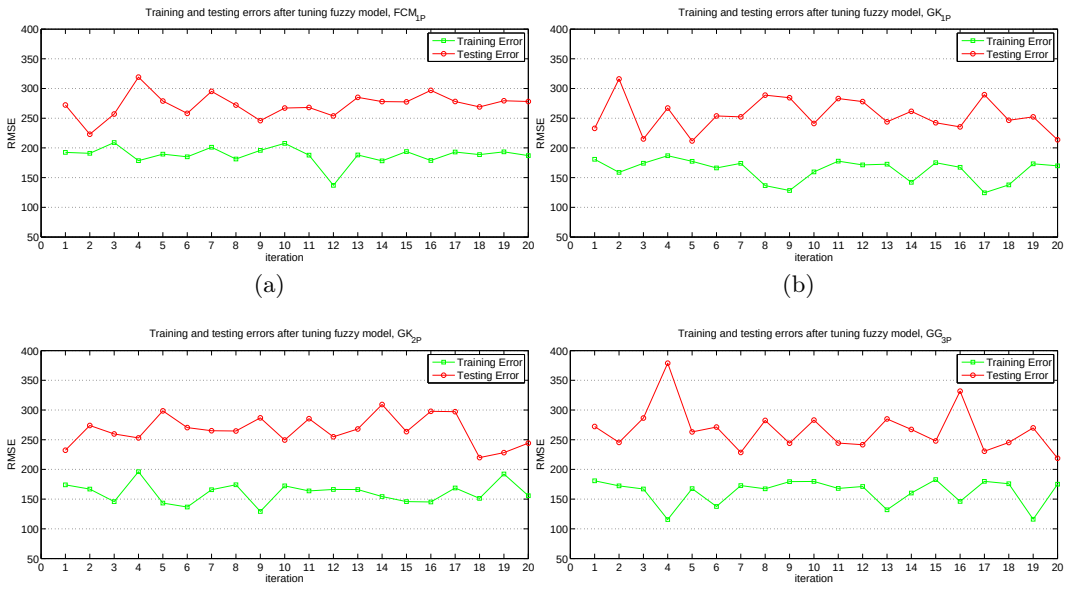


Figure 4.10: Training and testing errors after tuning fuzzy models which are constructed with five clusters.

are constructed with five clusters) are only approximately 6% better. The average computing time for the second tuning process was about 8 minutes (484.72 seconds) on the same configuration given above.

4.5 Discussion

The aim of this study was to introduce a simulated annealing algorithm for tuning Mamdani type fuzzy models with triangular membership functions. The tuning of the membership functions is a complex problem, because the cost function to be optimized is not derivable everywhere and when the membership functions do not overlap it is not continuous everywhere (Guély et al., 1999). Furthermore, the parameters to optimize are numerous, in the mean annual precipitation case there were more than 200 parameters.

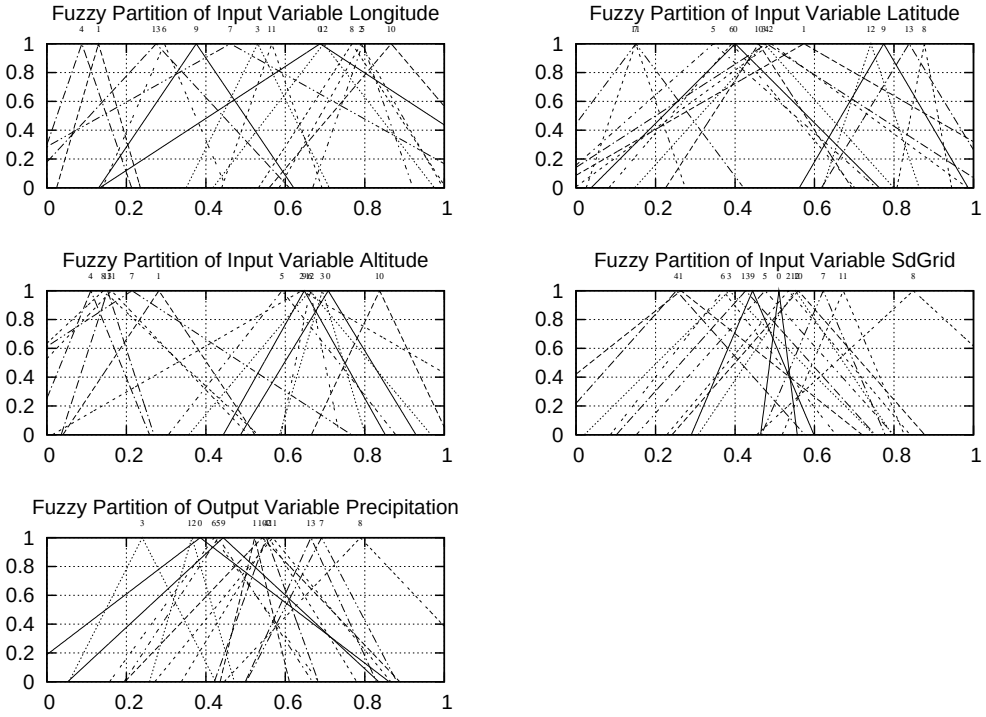
Simulated annealing is a general method, it is easy to understand and implement and can use any cost function. Unlike gradient descent methods simulated annealing can use any type of membership functions and it does not depend on fuzzy logic operators, implication or defuzzification functions, etc.

Simulated annealing can be used to solve many combinatorial optimization prob-

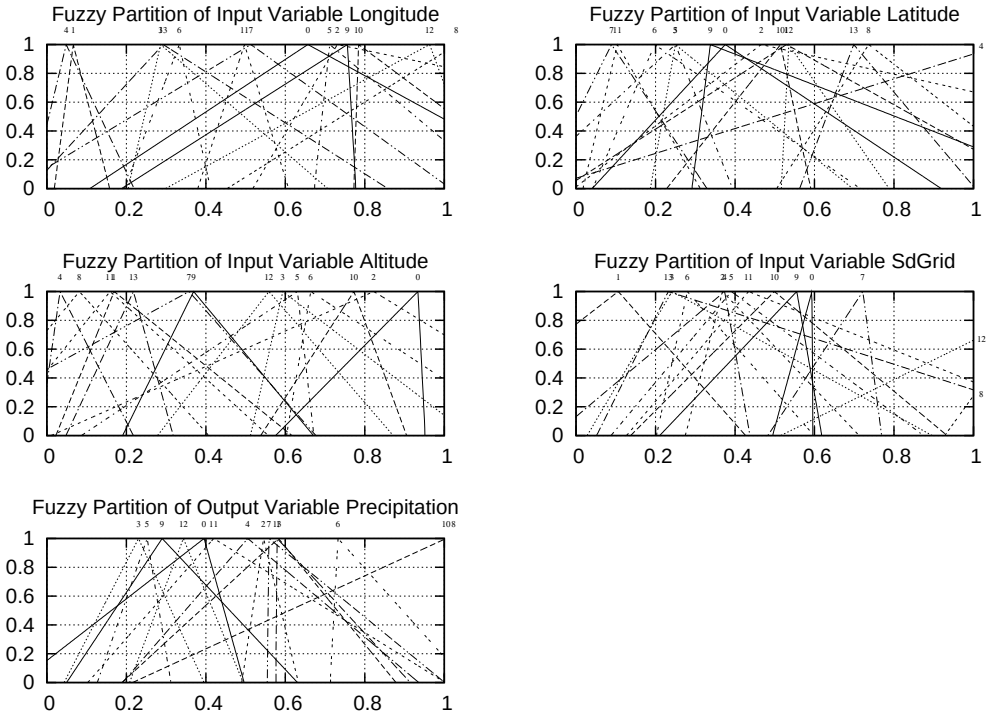
lems and some continuous variable problems (Bonomi and Lutton, 1984). Optimizing the parameters of membership functions is a continuous variable problem. Therefore, a specific method was needed for discretization of each parameter. In the disturbance mechanism of the adapted simulated annealing algorithm, transitions of each parameter of triangular membership functions were calculated based on randomly chosen rate in an interval which was calculated using a given parameter and the current temperature. Moreover, instead of modifying all the parameters in a fuzzy model only parameters associated with a randomly selected rule were modified. Therefore, the tuning process was based on the selection of parameters of the rule that decrease the overall cost function.

Simulated annealing involves many parameters such as initial temperature, the rate of decrease of temperature, length of the temperature stages, termination criteria, etc. Although there are some methods to obtain them, generally they depend on the problem therefore finding appropriate simulated annealing parameters requires empirical testing. Such an approach was used in Appendix D to find simulated annealing parameters for fuzzy models which were built using Mackey-Glass time series data. The second disadvantage of the simulated annealing is the computing time. The computing time was decreased by adding a limit on iterations in a temperature stage. In the adapted algorithm, the number of accepted perturbations was limited to $32 \times N$.

Interpretability of a fuzzy model was not considered while tuning a fuzzy model using simulated annealing. In Figure 4.11a, membership functions of an initial fuzzy model GG_{3p} is shown and the tuned fuzzy model is given in Figure 4.11b. From both figures, it is clear that the fuzzy models before and after the tuning process are not interpretable. In the next chapter, an approach for enhancing interpretability of a fuzzy model by analyzing fuzzy sets and rules in the fuzzy models while tuning is introduced.



(a)



(b)

Figure 4.11: Membership functions of fuzzy model GG_{3p} before and after tuning. (a) Membership functions of initial fuzzy model GG_{3p} before tuning. (b) Membership functions of fuzzy model after tuning process.

CHAPTER 5

INTERPRETABILITY ENHANCEMENT

Fuzzy models are able to perform nonlinear mappings between inputs and outputs, as they are universal approximators (Kosko, 1994; Buckley, 1993). On the other hand, fuzzy models are also able to handle linguistic knowledge. Due to the use of linguistic knowledge fuzzy models are assumed to be interpretable. However, this assumption is not true when data-driven fuzzy modeling methods are used to build fuzzy models or adaptive learning methods are used to tune fuzzy models. One strength of fuzzy models, interpretability, is lost with the use of automatic fuzzy rule generation and tuning methods, since the primary objective of these methods is the highest possible accuracy.

Model interpretability and accuracy are two conflicting modeling objectives, as improving interpretability of fuzzy models generally degrades accuracy, and vice versa (Zhou and Gan, 2008; Antonelli et al., 2010; Guillaume and Charnomordic, 2004; Paiva and Dourado, 2004; Nauck and Kruse, 1999; Bersini and Bontempi, 1997; Mencar and Fanelli, 2008; Mencar et al., 2007). There is a trade-off between model interpretability and accuracy. An interpretable and accurate fuzzy model is expected to have high interpretability and at the same time can provide as much accuracy as possible (Zhou and Gan, 2008; de Oliveira, 1999; Ishibuchi and Nojima, 2007).

In the previous chapters, fuzzy models are initially created by clustering techniques, and then constructed fuzzy models are tuned using simulated annealing. Structure learning by means of clustering techniques and optimization lead to a set of membership functions with a high degree of overlapping. Thus, the models are not interpretable. Simplification methods based on similarity among the fuzzy sets are used to reduce the number of fuzzy sets. In addition to decreasing the number of fuzzy sets, redundant

and inconsistent rules are detected and eliminated. When the number of fuzzy sets and the number of rules in a fuzzy model are decreased the interpretability of the model is improved, since the complexity of a fuzzy model increases with the number of fuzzy sets per linguistic variable and the number of rules. The aim is to obtain more compact and interpretable fuzzy models while preserving accuracy of the models.

This chapter is organized as follows. In the first section, brief information on the related work done in this area is given. The detailed information about the simplification methods for Mamdani type fuzzy model is given in the second section. In the third section, results of the application of the presented simplification method to mean annual precipitation data are shown. Discussions are provided in the last section.

5.1 Related Work

The interpretability or transparency of fuzzy models excessively depends on human's prior knowledge (Furuhashi, 2002; Furuhashi and Suzuki, 2001; Zhou and Gan, 2008). Although there are some formalized definitions for interpretability of fuzzy models (Bodenhofer and Bauer, 2000, 2003; Riid, 2002; Riid et al., 2001), it is highly subjective (Cordón and Herrera, 2003; Mikut et al., 2005). Furuhashi (2002) proposed low-level and high-level interpretability concepts for fuzzy models. The low-level interpretability of fuzzy models refers to interpretability achieved on fuzzy set level by optimizing membership functions in terms of the semantic criteria on membership functions. The high-level interpretability refers to interpretability of fuzzy models which is obtained on fuzzy rule level by performing overall complexity reduction considering coverage, completeness and consistency of the rules.

Some criteria for fuzzy set interpretability are (Mencar and Fanelli, 2008; Furuhashi, 2002; de Oliveira, 1999):

1. Normality, each membership function of a linguistic variable should be normal such that there exist one data point in universe of discourse with full membership. A normal membership function can represent a linguistic term with a clear semantic meaning.

2. Moderate number of membership functions, the number of membership functions in a linguistic variable should not be too high. Considering Miller (1956)'s work,

a linguistic variable is suggested to contain 7 ± 2 membership functions for a human to efficiently handle this linguistic variable.

3. Distinguishability, each membership function of a linguistic variable should be distinct enough from each other to represent clear semantic meaning to avoid inconsistencies and to reduce redundancy and complexity. Figure 4.11b shows an example of indistinguishable membership functions. Disjoint membership functions are maximum distinguishable. On the other hand, other interpretability criteria for fuzzy sets suggest some degree of overlapping. Therefore, distinguishability should be balanced with other constraints.

4. Completeness, every data point in universe of discourse should be covered by a membership function of the linguistic variable.

Some criteria for fuzzy model interpretability are (Mencar and Fanelli, 2008; Zhou and Gan, 2008):

1. The number of rules (compactness), the total number of rules in a rule base should be as small as possible.

2. Rule readability, the antecedent part of the rule should preferably contain 7 ± 2 distinct conditions.

3. Consistency, if antecedents of rules are similar then consequent part of the rules should be similar. Violating this constraint leads to contradictions in rule base.

4. Completeness, for each input there should be at least one rule with non-zero activation. However, very low activation strength of a rule may decrease interpretability of the fuzzy model also. Moreover, over fitting on data may lead to incomplete fuzzy models (Jin et al., 1999).

5. Number of variables, the number of input and output variables should be as small as possible.

Other than the above constraints there are many other constraints for fuzzy set and fuzzy model interpretability (Mencar and Fanelli, 2008; Zhou and Gan, 2008).

To develop interpretable and accurate fuzzy models, Xing et al. (2006), Ishibuchi and Nojima (2007), González et al. (2007), Antonelli et al. (2009) and Gacto et al.

(2010) used multiobjective optimization techniques. They try to optimize both global fuzzy model accuracy and interpretability using evolutionary algorithms while generating fuzzy models.

Paiva and Dourado (2004) defined a set of constraints on parameters of fuzzy model for interpretability and try to optimize accuracy subject to these constraints. The locations of membership functions are limited during learning. In addition to the constraints, they merged similar fuzzy sets by using similarity measure which is defined by Setnes et al. (1998).

Setnes et al. (1998) proposed a rule base simplification method to reduce the number of fuzzy sets in a fuzzy model by using similarity measures. The rule base is simplified by merging similar fuzzy sets and redundant rules. Using the proposed method compact fuzzy models with distinguishable membership functions are obtained. Similarity between two fuzzy sets A and B is measured by

$$sim(A, B) = \frac{|A \cap B|}{|A \cup B|} \tag{5.1}$$

where $|.|$ denotes the cardinality of a set and $\cap$ and $\cup$ operators represent the intersection and union respectively. In the proposed algorithm if similarity measure between two fuzzy sets A and B is greater than a given threshold then they are merged. This merging process is repeated until there are no similar fuzzy sets. Finally fuzzy sets that are close to universal set are removed.

Since interpretability of a fuzzy model is highly subjective and excessively depends on human's prior knowledge, some researches allow users to get involved in the fuzzy model generation process to use human subjective evaluation. For example, NEFCLASS model developed by Nauck (2003a) allows users to supervise the fuzzy model generation process. Users can interactively delete fuzzy sets and change parameters of heuristic learning process. However, deleting fuzzy sets can lead to inconsistent rule base. Moreover, finding a good trade-off between accuracy and interpretability and selecting the best model requires many trials.

Similar to the NEFCLASS model, Alonso et al. (2008) designed the High Interpretable Linguistic Knowledge (HILK) fuzzy modeling methodology which offers an integration framework for combining both expert knowledge and knowledge extracted from data. And they pointed out that the combination of expert and induced knowledge yields compact and robust systems.

Alonso and Magdalena (2010) upgraded HILK to deal with automatic learning from data and presented methodology HILK++ for building interpretable fuzzy classification systems. HILK++ uses the general framework provided by HILK and enhances it with new functionalities such as feature selection, interpretability guided simplification, etc. to get comprehensible fuzzy rule based classifier.

For evaluating the interpretability of fuzzy models interpretability indices are defined. For example, similarity measure defined by Equation 5.1 is an interpretability index which is mainly used for merging similar fuzzy sets to obtain distinguishable membership functions. Interpretability indices which evaluate the similarity, distinguishability, coverage, overlapping, etc. (Botta et al., 2009; Jin et al., 1999; Mencar, 2007; Setnes et al., 1998) are usually considered to preserve the readability of fuzzy models automatically generated from data. They are used in tuning algorithms to preserve interpretability while improving accuracy. On the other hand, some indices are used as a criterion to maximize interpretability while generating fuzzy models by multiobjective optimization techniques (Antonelli et al., 2009; Gacto et al., 2010; Ishibuchi and Nojima, 2007). There are some indices which cover several interpretability constraints and used globally to assess transparency of the whole fuzzy model (Nauck, 2003b; Alonso et al., 2008). Alonso et al. (2009) compared global interpretability indices quantitatively and qualitatively.

5.2 Simplification of Fuzzy Models

In the previous chapters, Mamdani type fuzzy models were initially created by fuzzy clustering techniques, then initial fuzzy models were tuned using simulated annealing to improve accuracy of the models. Although very high accuracies were obtained, interpretability of the tuned fuzzy models were poor. Since accuracy was the primary objective, interpretability was not considered during the tuning process. On the other hand, one of the important purposes of using fuzzy sets for modeling complex systems is their transparency. To maintain interpretability of the fuzzy models, an algorithm is developed which has two major parts. In the first part, interpretability at the fuzzy set level is achieved by using similarity measures. In the second part, fuzzy model interpretability is considered by merging similar redundant fuzzy rules, eliminating inconsistent rules from the rule base and deleting rules which have low influence on

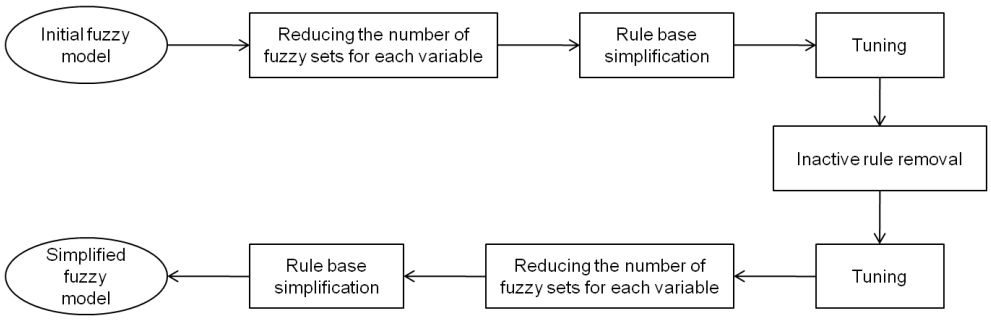


Figure 5.1: Overview of the simplification algorithm.

the fuzzy model (i.e., rules with low activation strength). Overview of the algorithm is given in Figure 5.1.

After rule base simplification, fuzzy model is tuned using simulated annealing. Since primary objective is not the accuracy and to keep changes in parameters of simplified fuzzy model as small as possible, simulated annealing is initialized with low temperature and the other parameters are also designed for that purpose. At the end of the tuning, rules with low activation strengths are removed. Then, tuning is performed again to allow fuzzy models to adapt the remaining rules for this removal. In the second tuning process, initial temperature is lower than the first tuning step. Although tuning algorithms are designed as not to change simplified fuzzy models much, interpretability of the fuzzy models might decrease. Therefore, interpretability operations on fuzzy sets and rule base simplification are repeated after tuning process. The details of the algorithm are given in the next sections.

5.2.1 Reducing the Number of Fuzzy Sets for Each Variable

Initial fuzzy models created by the fuzzy clustering algorithms may contain fuzzy sets that are close to universal set. A fuzzy set A, is close to universal set U if $\mu_A(x) \approx 1,\ \forall x \in A$. The similarity $sim(A, U)$ is calculated using Equation 5.1. If $sim(A, U) > \lambda_r$ then the fuzzy set A is removed from the rule where $\lambda_r \in (0, 1)$ is the threshold for removing fuzzy sets similar to universal set. In the algorithm fuzzy sets similar to U are removed first, because these fuzzy sets dominate the merging process and excessively merged with other membership functions which reduce both accuracy and transparency. The threshold $\lambda_r = 0.85$ is used in the analysis.

Fuzzy sets that are similar to singleton are also removed from the rules. A fuzzy

set A is close to a singleton function if $\mu_A(x) \approx 0,\ \forall x \in A$. If a fuzzy set is similar to a singleton, then $sim(A, U) \approx 0$. Therefore, if $sim(A, U) < \lambda_s$ then fuzzy set A is removed from the rule, where $\lambda_s \in (0, 1)$ is the threshold for removing singleton fuzzy sets. Removing singleton fuzzy sets from rules decrease accuracy much, because these kinds of rules represent exceptions exist in data. On the other hand, removing such fuzzy sets increases model generalization ability. For the threshold, $\lambda_s = 0.01$ is used.

After removing fuzzy sets, similar fuzzy sets are merged. Similarity of fuzzy sets A and B is calculated using Equation 5.1. If $sim(A, B) > \lambda_m$ then fuzzy sets A and B are merged into a new fuzzy set C, where $\lambda_m \in (0, 1)$ is the threshold for similar fuzzy set merging. The support of the new fuzzy set is taken as the support of the $A \cup B$ to preserve the coverage of A and B. The center of the new fuzzy set is calculated by averaging the centers of the original functions. Fuzzy set merging is repeated until no more pairs satisfy the merging threshold. The new fuzzy set created after merging is also used in the following iterations. Fuzzy sets created by merging are given stronger weight in the merging process. Two similar triangular membership functions A and B defined by parameters (a_1, b_1, c_1) and (a_2, b_2, c_2) are merged to create a new fuzzy set C defined with parameters (a_3, b_3, c_3) as follows (Setnes et al., 1998; Paiva and Dourado, 2004):

$$a_3 = min(a_1, a_2) \tag{5.2}$$

$$b_3 = \frac{n_a b_1 + n_b b_2}{n_a + n_b} \tag{5.3}$$

$$c_3 = max(c_1, c_2) \tag{5.4}$$

The center of the newly created membership function C is calculated by weighted mean of the centers of the parameters of original membership functions where n_a and n_b represent the number of pairs of functions merged before A and B were created. The threshold λ_m influence model interpretability and also accuracy significantly. Small values of λ_m produce few fuzzy sets and simpler fuzzy models with low accuracy. The threshold $\lambda_m = 0.75$ is used in the analysis.

Fuzzy set merging using Equation 5.1 cannot solve subsets (fuzzy sets inside other fuzzy sets) or functions passing through other functions (Paiva and Dourado, 2004). To detect such cases, Equation 5.1 is used as in the following: if $A \subseteq B$ then $A \cap B = A$ and $A \cup B = B$. Let $A \cap B = D$, if support of B includes support of A and $sim(A, D) > \lambda_i$ then fuzzy set A and B are merged where $\lambda_i \in (0, 1)$ is the threshold for inclusion

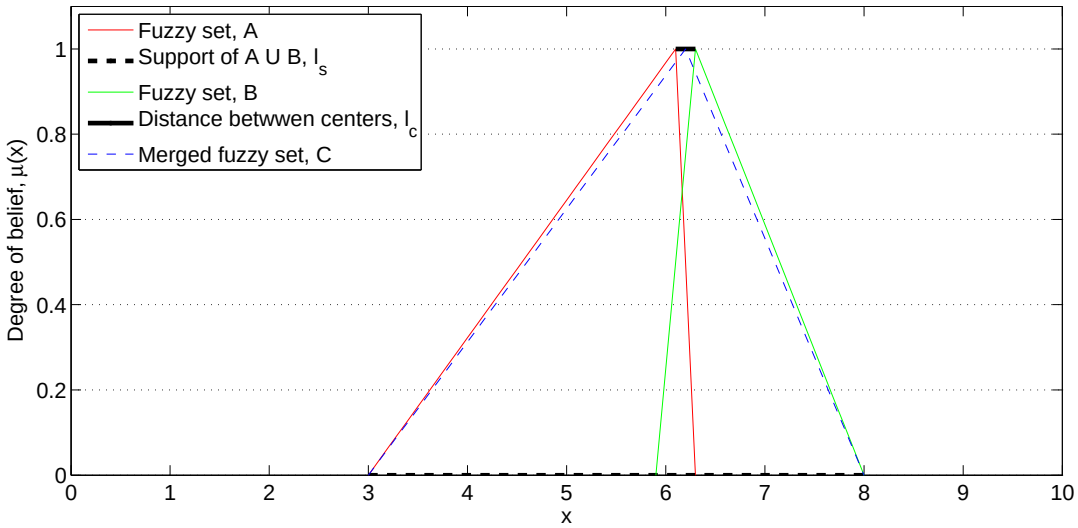


Figure 5.2: Similarity measure between fuzzy sets A and B is low, $sim(A, B) = 0.05$. Since their centers are too close, they are not distinguishable. l_c/l_s measure is an indication for this case. In the figure, merging fuzzy sets A and B results in fuzzy set C.

case. The threshold $\lambda_i = 0.80$ is used.

There are rarely some cases where similarity of fuzzy sets is low but their centers are too close. Figure 5.2 depicts this case. When the centers of the fuzzy sets are too close then giving names to fuzzy sets A and B are difficult, because the fuzzy sets A and B are actually not distinguishable enough. These cases are detected by calculating the proportion of the length between centers to the length of the support of $A \cup B$. If the proportion $|b_2 - b_1| \,/\, |c_2 - a_1| > \lambda_c$ then fuzzy sets A and B are merged. $\lambda_c \in (0, 1)$ is the threshold for detecting such cases. The threshold $\lambda_c = 0.01$ is used.

Outline of the interpretability operations on fuzzy sets is presented in Algorithm 5. After removing fuzzy sets, merging similar function pairs etc. the rule base is updated.

5.2.2 Rule Base Simplification

The interpretability operations on fuzzy sets may produce similar rules. Redundancy or inconsistency in a rule base decrease interpretability of the fuzzy model. Similarity of rules R_i and R_j is calculated using

$$simP(R_i, R_j) = min_{k=1}^{n} sim(A_{ik}, A_{jk}) \tag{5.5}$$

Algorithm 5 Reducing the Number of Fuzzy Sets for Each Variable

Require: Initial fuzzy model FM_0, threshold for removing fuzzy sets similar to universal set λ_r, threshold for removing singleton fuzzy sets λ_s, threshold for similar fuzzy set merging λ_m, threshold for function inclusion λ_i, threshold for combine λ_c.

1: **for all** fuzzy sets, $f_i \in$ fuzzy model FM_0 **do**
2: **if** $(sim(f_i, U) > \lambda_r)$ or $(sim(f_i, U) < \lambda_s)$ **then** {fuzzy set f_i is similar to U or a singleton}
3: Delete fuzzy set f_i
4: Update rule base
5: **end if**
6: **end for**
7: **for all** fuzzy sets, f_i and $f_j \in$ fuzzy model FM_0 **do**
8: **if** $(sim(f_i, f_j) > \lambda_m)$ or $(sim(f_i, f_i \cap f_j) > \lambda_i)$ or $((|b_j - b_i| \,/\, |c_j - a_i|) < \lambda_c)$ **then** {fuzzy sets are similar or $f_i \subseteq f_j$ or their centers are close}
9: Merge fuzzy sets f_i and f_j
10: Update rule base
11: **end if**
12: **end for**

where A_{ik} are antecedent fuzzy sets of rule R_i and A_{jk} are antecedent fuzzy sets of rule R_j. If similarity between premises of the two rules is high, $simP(R_i, R_j) > \gamma_{sp}$, where $\gamma_{sp} \in (0, 1)$ is a threshold for rule premise similarity, then similarity between the consequents are computed. For multiple input single output (MISO) systems similarity of rule consequents is calculated by

$$simC(R_i, R_j) = sim(B_i, B_j) \tag{5.6}$$

where B_i and B_j are consequent fuzzy sets of R_i and R_j respectively. The degree of consistency of fuzzy rules R_i and R_j is calculated using Equation 5.7 (Jin et al., 1999).

$$Cons(R_i, R_j) = e^{-\frac{(\frac{simP(R_i,R_j)}{simC(R_i,R_j)}-1)^2}{(\frac{1}{simP(R_i,R_j)})^2}} \tag{5.7}$$

This index ranges between 0 and 1.0. High values indicate consistency. If consistency degree between similar rules R_i and R_j is low such that $Cons(R_i, R_j) < \gamma_c$, where $\gamma_c \in (0, 1)$ is a threshold for rule consistency then these rules are inconsistent. To solve inconsistency in the rule base, the rule with high activation strength is kept in the rule base and the other rule is deleted. On the other hand, if the rules are consistent, $Cons(R_i, R_j) \geq \gamma_c$ and the similarity between the consequent fuzzy sets is high, $simC(R_i, R_j) > \gamma_{sc}$, where γ_{sc} is a threshold for similarity between rule consequents, then one of these rules is redundant. R_i and R_j are merged to create a new rule according to the merging process described in the previous section. The thresholds are selected as $\gamma_{sp} = 0.60$, $\gamma_c = 0.50$ and $\gamma_{sc} = 0.70$.

After detecting and solving inconsistencies and redundancies, fuzzy model is tuned with very low temperature and without changing membership function parameters much. At the end of this tuning, activation strength of each rule and the total activation is computed. If all rules are equally contributed to the outputs of a fuzzy model then activation strength of each rule would be the average, $\frac{totalactivationstrength}{rulecount}$. If activation strength of a rule is less than τ_a percent of the average then rule is removed. $\tau_a \in (0, 1)$ is the threshold for inactive rule removal and represents percentage of average activation strength a rule must have. $\tau_a = 0.1$ (i.e., 10% of the average activation strength) is used.

Outline of the rule base simplification is presented in Algorithm 6.

Algorithm 6 Rule Base Simplification

Require: Fuzzy model FM, threshold for rule premise similarity γ_{sp}, threshold for rule consistency γ_c, threshold for similarity between rule consequents γ_{sc}, threshold for inactive rule removal τ_a.

1: **for all** rules R_i and R_j **do**
2: **if** $(simP(R_i, R_j) > \gamma_{sp})$ **then** {premises of the rules are similar}
3: **if** $(Cons(R_i, R_j) > \gamma_c)$ **then** {rules are consistent}
4: **if** $(simC(R_i, R_j) > \gamma_{sc})$ **then** {consequents of the rules are similar}
5: Merge rules R_i and R_j
6: **end if**
7: **else**
8: Remove inconsistent rule R_i or R_j
9: **end if**
10: **end if**
11: **end for**
12: Tune fuzzy model
13: Calculate activation strengths of the rules and total activation strength
14: Set rule deletion flag to false, $isRuleRemoved = false$
15: **for all** rules $R_i \in$ fuzzy model FM **do**
16: **if** (activation strength of rule $R_i < \tau_a$) **then** {activation strength of R_i is low}
17: Remove rule R_i from rule base
18: $isRuleRemoved = true$
19: **end if**
20: **end for**
21: **if** $isRuleRemoved == true$ **then**
22: Tune fuzzy model with very low temperature
23: **end if**

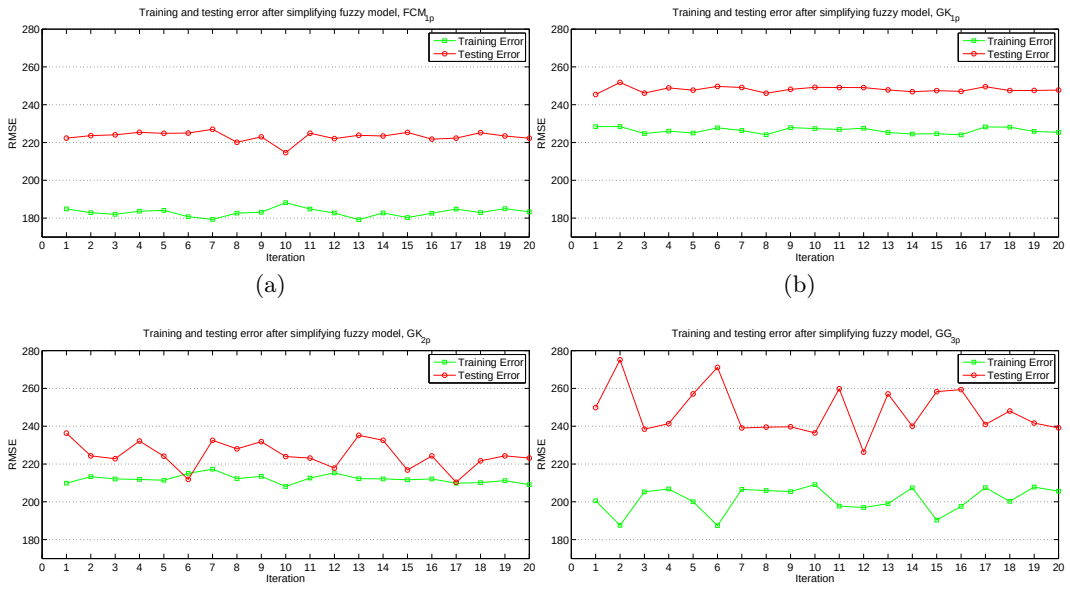


Figure 5.3: Training and testing errors of simplified fuzzy models.

5.3 Results

Fuzzy models learned from data were used as initial solution for simplification algorithm. The algorithm starts with reducing the number of fuzzy sets for each variable then rule base simplification is performed. After rule base simplification, simplified model is tuned without changing fuzzy model much. Next, rules with low activation strength are removed from the rule base. Since tuning mechanism is based on a probabilistic function, results obtained from the simplification algorithm may vary, when the algorithm is executed several times with different seed value. Therefore, simplification algorithm was repeated 20 times with different seed values. The thresholds and simulated annealing parameters used in the simplification algorithm are given in Table 5.1.

Training and test data errors of simplified fuzzy models FCM_{1p}, GK_{1p}, GK_{2p} and GG_{3p} are shown in Figure 5.3. Properties of training and test data errors are listed in Table 5.2 and Table 5.3.

Simplification algorithm reduced the number of fuzzy sets used for linguistic variables using similarity measures and simplified the rule base of fuzzy models either by removing inconsistent rules or by merging redundant ones. GG_{3p} fuzzy models were simplified more than the other fuzzy models. Figure 5.4 depicts a simplified GG_{3p}

Table 5.1: The thresholds and tuning parameters used in the simplification algorithm.

Parameter	**Value**	**Allowable Range**
Fuzzy Set Simplification		
Similarity with U, α_r	0.85	$0 < \alpha_r < 1$
Similarity to a singleton, α_s	0.01	$0 < \alpha_s < 1$
Merging similar functions, α_m	0.75	$0 < \alpha_m < 1$
Inclusion, α_i	0.80	$0 < \alpha_i < 1$
Consistency, α_c	0.01	$0 < \alpha_c < 1$
Rule Base Simplification		
Similarity of rule premise, γ_{sp}	0.60	$0 < \gamma_{sp} < 1$
Similarity of rule consequent, γ_{sc}	0.70	$0 < \gamma_{sc} < 1$
Consistency, γ_c	0.50	$0 < \gamma_c < 1$
Tuning Parameters - 1		
Initial probability of acceptance, P_0	0.10	$0 < P_0 < 1$
The percentage of transition parameter, ξ	0.005	$0 < \xi \leq 1$
Temperature update parameter, α	0.95	$0 < \alpha < 1$
Tuning Parameters - 2		
Initial probability of acceptance, P_0	0.01	$0 < P_0 < 1$
The percentage of transition parameter, ξ	0.005	$0 < \xi \leq 1$
Temperature update parameter, α	0.95	$0 < \alpha < 1$

Table 5.2: Properties of training errors obtained after simplifying fuzzy models.

Fuzzy Model	**Min.**	**Max.**	**Mean**	**Mean Difference**	**Mean (%) Difference**	**Standard Deviation**
FCM_{1p}	179.1740	188.1766	182.9947	−16.5247	−8.28	2.1094
GK_{1p}	224.0958	228.4579	226.3449	+32.0661	+16.51	1.5456
GK_{2p}	208.1055	217.2496	212.0530	+17.1536	+8.80	2.1736
GG_{3p}	187.4285	209.1155	201.2518	+1.3445	+0.67	6.7542

Table 5.3: Properties of testing errors obtained after simplifying fuzzy models.

Fuzzy Model	**Min.**	**Max.**	**Mean**	**Mean Difference**	**Mean (%) Difference**	**Standard Deviation**
FCM_{1p}	214.6314	226.9859	223.2313	−11.8351	−5.03	2.5799
GK_{1p}	245.3889	251.8004	248.0863	+15.5024	+6.67	1.4954
GK_{2p}	210.3524	236.3316	224.8523	−38.7040	−14.69	7.1921
GG_{3p}	226.2879	275.1404	247.9185	+2.0092	+0.82	12.5833

fuzzy model where associated initial fuzzy model is shown in Figure 4.11a and the tuned one is shown in Figure 4.11b. Both the initial and tuned fuzzy models are not interpretable, since membership functions are indistinguishable and the number of membership functions is more than the number generally suggested in the literature (ie., 7 ± 2 membership functions). For both the initial and tuned fuzzy model, it is not easy to name fuzzy sets and to obtain understandable rule base. On the other hand, simplified fuzzy model given in Figure 5.4 is interpretable.

It has three membership functions for linguistic variables "longitude" and "latitude" and two membership functions for linguistic variables "altitude", "sdgrid" and "precipitation". All membership functions are distinguishable. All linguistic variables are complete i.e., every data point in universe of discourse is covered by a membership function. Each fuzzy set was given a name based on its position. The rules in the rule base are given as follows:

R_1 : If longitude is near-west and latitude is near-north and altitude is low and sdgrid is medium then precipitation is medium.

R_2 : If longitude is east and latitude is near-north and altitude is high and sdgrid is medium then precipitation is medium.

R_3 : If longitude is west and latitude is near-north and altitude is low and sdgrid is medium then precipitation is medium.

R_4 : If longitude is near-west and latitude is near-north and altitude is high and sdgrid is medium then precipitation is medium.

R_5 : If longitude is near-west and latitude is south and altitude is low

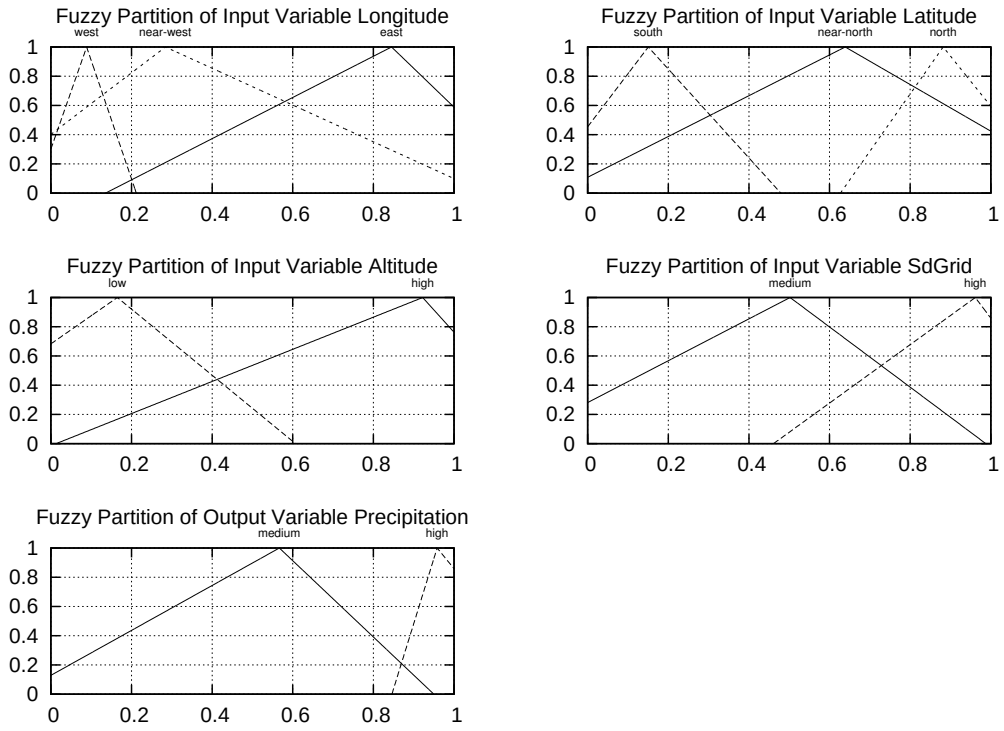


Figure 5.4: Membership functions of simplified GG_{3p} fuzzy model.

and sdgrid is medium then precipitation is high.

R_6 : If longitude is east and latitude is north and altitude is low and sdgrid is high then precipitation is high.

R_7 : If longitude is east and latitude is south and altitude is low and sdgrid is medium then precipitation is medium.

R_8 : If longitude is near-west and latitude is north and altitude is low and sdgrid is medium then precipitation is high.

The rule base is compact and every rule is readable and consistent with the other rules. In order to increase comprehensibility of each rule, centers of the triangular membership functions for linguistic variables "longitude" and "latitude" are drawn on map of Turkey (Figure 5.5) and effectiveness of these triangular membership functions are also given in Figure E.1, Figure E.2, Figure E.3, Figure E.4, Figure E.5 and Figure E.6.

The average computing time was about 3 minutes (177.094 seconds) on a notebook which contains an Intel® 1.83 GHz Core^{TM} Duo processor (T2400), 1 GB RAM and

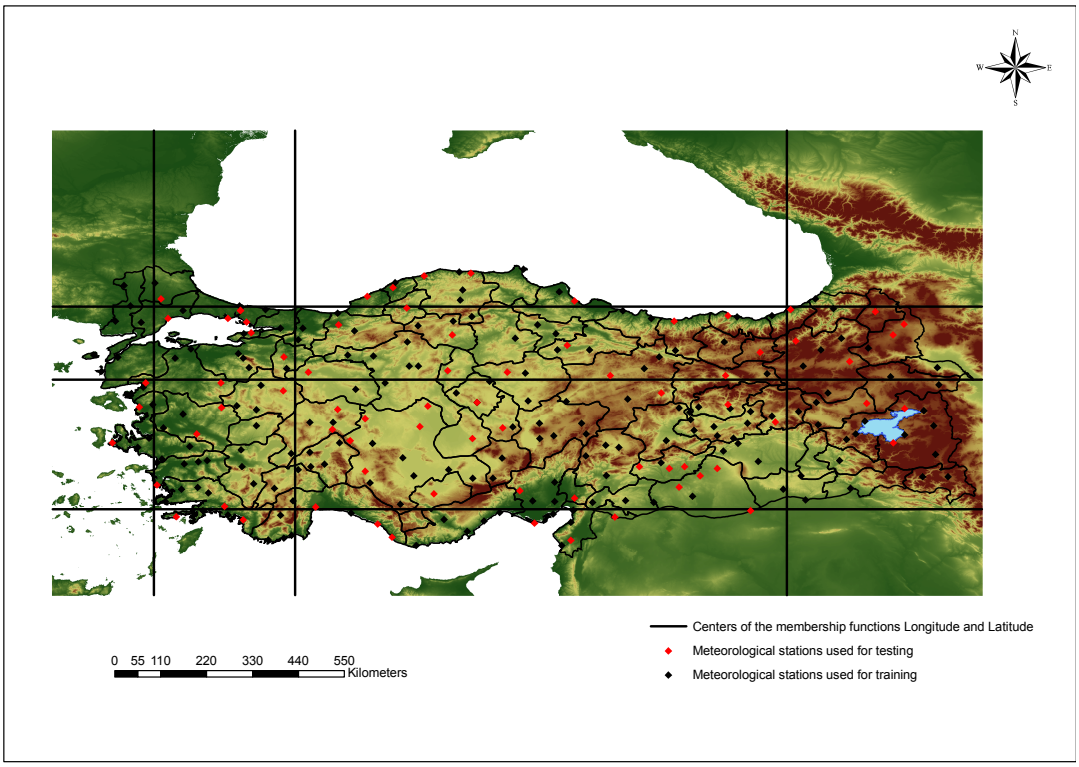


Figure 5.5: The centers of the triangular membership functions for linguistic variables "longitude" and "latitude".

Microsoft® Windows® Home Edition Version 2002 with Service Pack 3.

As in the previous chapter, in addition to the fuzzy models simplified above, fuzzy models constructed with five clusters are also simplified. Same thresholds and SA parameters are used in the simplification process. These thresholds and parameters are given in Table 5.1. Training and test data errors of simplified fuzzy models are depicted in Figure 5.6. Properties of training and test data errors are listed in Table 5.4 and Table 5.5.

According to the results, training errors obtained after simplifying fuzzy models which are constructed with five clusters are approximately 13% worse. Testing errors obtained for the second tuning process (tuning of fuzzy models which are constructed with five clusters) are also approximately 10% worse. Initial and simplified fuzzy models are given in Figure E.13, Figure E.14, Figure E.15, Figure E.16, Figure E.17, Figure E.18, Figure E.19 and Figure E.20. The average computing time for the second simplification process was about 1.5 minutes (95.25 seconds) on the same configuration given above.

Table 5.4: Properties of training errors obtained after simplifying fuzzy models which are constructed with five clusters.

Fuzzy Model	**Min.**	**Max.**	**Mean**	**Mean Difference**	**Mean (%) Difference**	**Standard Deviation**
FCM_{1p}	252.1641	262.2974	255.1242	−5.6041	−2.15	2.5640
GK_{1p}	228.5758	233.1885	231.2684	−20.3640	−8.09	0.9933
GK_{2p}	228.1740	233.1526	231.1777	−20.4911	−8.14	1.3257
GG_{3p}	224.5395	254.0930	232.6494	−22.5322	−8.83	12.4164

Table 5.5: Properties of testing errors obtained after simplifying fuzzy models which are constructed with five clusters.

Fuzzy Model	**Min.**	**Max.**	**Mean**	**Mean Difference**	**Mean (%) Difference**	**Standard Deviation**
FCM_{1p}	273.8001	288.4236	279.4921	−1.0510	−0.37	3.4087
GK_{1p}	258.8537	261.6111	259.7090	−2.2400	−0.86	0.7874
GK_{2p}	255.9232	270.5631	260.6076	−1.4393	−0.55	3.6975
GG_{3p}	248.0283	276.1197	255.4549	−23.6385	−8.47	11.5646

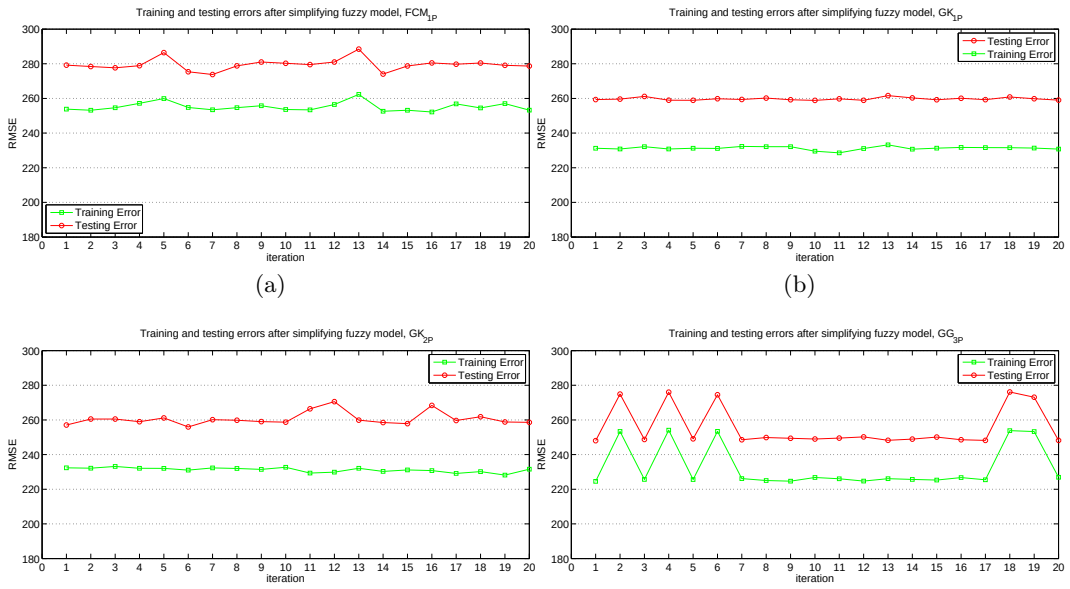


Figure 5.6: Training and testing errors of simplified fuzzy models. Initial fuzzy models are constructed with five clusters.

5.4 Discussion

Fuzzy models can be constructed by expert knowledge. When expert knowledge is not available then data-driven modeling techniques can be used to automatically construct fuzzy models. However, interpretability of fuzzy models is lost with the use of automatic data-driven techniques, since the primary objective of these methods is the highest possible accuracy. Interpretability of fuzzy models can be maintained while generating fuzzy models from data or by applying simplification techniques. In this study, a simplification algorithm is proposed to obtain more compact and interpretable fuzzy models.

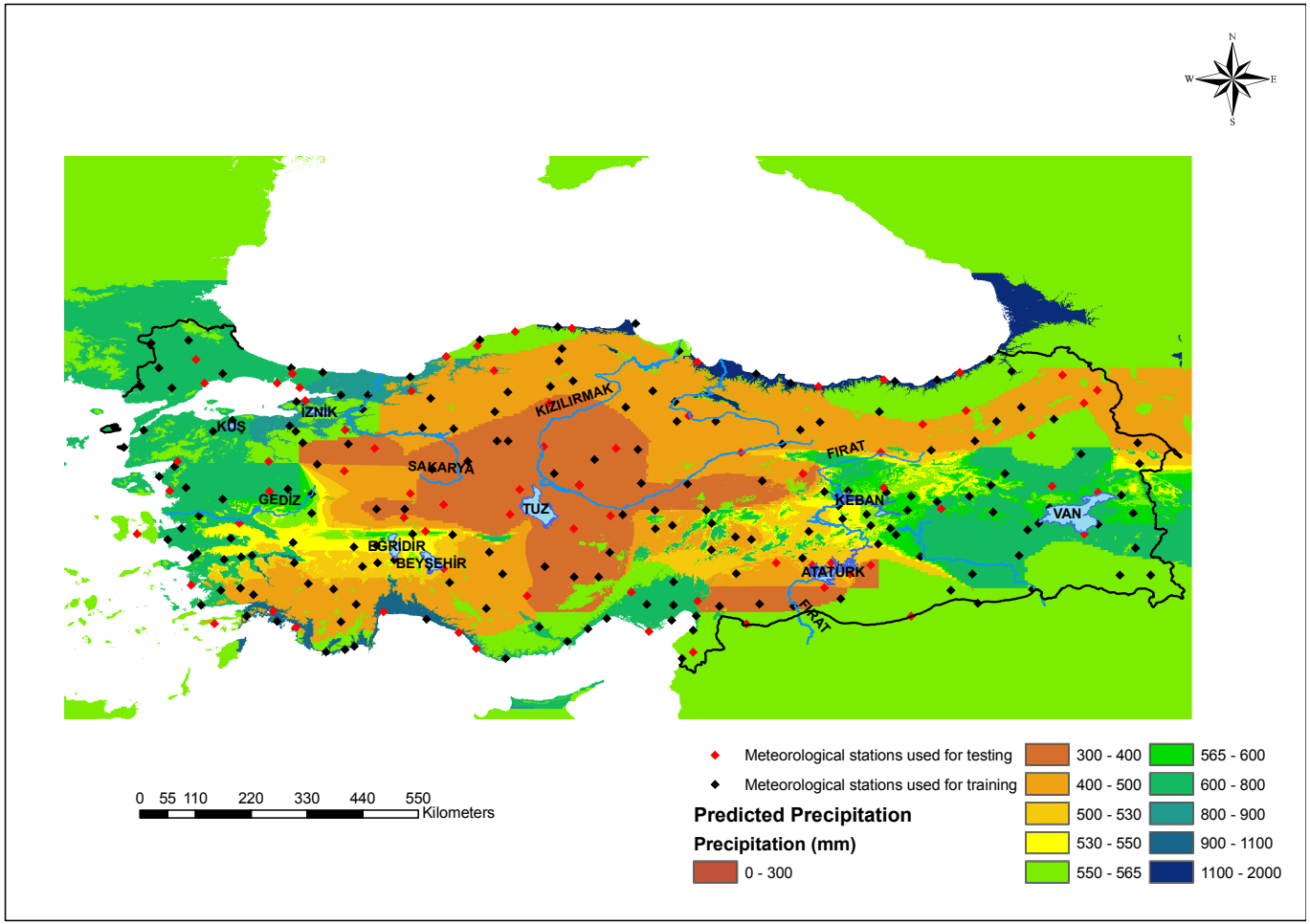


Figure 5.7: Predicted precipitation map for Turkey generated using simplified FCM_{1p} model. Training error is 188.1766 mm and testing error is 214.6314 mm.

Examples of the simplified fuzzy models obtained from the algorithm are given in Figure 5.4, Figure E.8, Figure E.10 and Figure E.12. Although interpretability of fuzzy models is a subjective concept, obtained simplified fuzzy models satisfy most of the interpretability criteria given in the previous sections. A precipitation prediction map for the whole Turkey is generated using simplified FCM_{1p} fuzzy model (Figure 5.7). The precipitation values of all locations of Turkey in 1 km resolution are estimated using the simplified model.

Simplification algorithm simplified GG_{3p} fuzzy models more than the others. On the other hand, FCM_{1p} fuzzy models are simplified less. Additionally interpretability of simplified FCM_{1p} fuzzy models are not good enough. However, it is possible to obtain more interpretable results for FCM_{1p} models by changing the thresholds. In Table 5.6, error values obtained by different methods are listed. As discussed in Chapter 2, linear regression technique assumes that observations are independent which is very unlikely in geographical data. The regression equation fitted on data remains constant over the whole study area and no local variations are allowed. Linear regression was used to model mean annual precipitation. Residuals obtained from linear regression model were spatially autocorrelated and interpretability of the regression equation was low. Better result was obtained using geographically weighted regression (GWR). Error on training data was reduced and the residuals of GWR were not spatially autocorrelated. To model variation in data GWR estimates parameters associated with the (training) data. However, interpretability of these parameters and the model are very low and application of the obtained model to data, other than the training data, for testing and prediction is difficult. The proposed approach can produce accurate and interpretable solutions. If the accuracy is the primary objective then the proposed approach can produce more accurate solutions for training data. The minimum training error value obtained is 30 percent less than the error obtained by GWR method (tuned fuzzy model in Table 5.6). However, interpretability of the accurate solutions was low. Furthermore, the proposed approach can generate interpretable solutions by decreasing the complexity of the fuzzy models (and also the accuracy). Interpretability and accuracy are conflicting modeling objectives. Although the simplified fuzzy modes are more interpretable than the tuned fuzzy models, their accuracies are lower. For the simplified fuzzy models, average error on training data is increased (Table 4.3 and Table 5.2), but average error on test data is decreased (Table 4.4 and Table 5.3).

Table 5.6: Error values for linear regression, GWR and the proposed approach.

Method	**Training Error (mm)**	**Testing Error (mm)**
Linear Regression	217.50	207.80
Linear Regression[a]	208.79	226.53
GWR	106.78	-
GWR[a]	255.77	-
Tuned Fuzzy Model[b]	74.82	326.61
Simplified Fuzzy Model[b]	179.17	223.81
Tuned Fuzzy Model[c]	122.70	202.93
Simplified Fuzzy Model[c]	209.85	210.35

[a] Error values on processed data set.

[b] Error values are associated with the fuzzy model which has minimum error value on training data.

[c] Error values are associated with the fuzzy model which has minimum error value on testing data.

Thus, simplification algorithm produced not only interpretable but also more generalized fuzzy models. In addition to these, after the model is built, it can be easily applied to test data set and it can be used for prediction purposes.

Moreover, simplification algorithm produced simplified fuzzy models for more than eight times faster than the tuning algorithm whose primary objective is the accuracy.

Simplification algorithm involves many thresholds. Interpretability and accuracy of the final fuzzy model can be adjusted by changing the values of these thresholds.

CHAPTER 6

CONCLUSION

In traditional modeling, the development of spatial models not only requires deep understanding of the nature and behavior of the phenomena but also requires knowledge on mathematical methods. Therefore, as the complexity of the spatial phenomenon increases traditional modeling becomes impractical. Alternatively, data-driven modeling which is based on the analysis of data characterizing the phenomena can be used. Since the development of reliable and understandable spatial models is crucial to comprehend and work on natural phenomena, both precision and understandability have to be considered in the data-driven modeling techniques. In this thesis, the primary motivation is the generation of understandable and reliable spatial models using observational data. In the scope of this thesis, an interpretability oriented data-driven fuzzy modeling approach is proposed, a prototype software is developed for the proposed approach and mean annual precipitation data of Turkey is used as case study to assess obtained fuzzy models in terms of both accuracy and transparency.

Results show that data scale influences the performance of the methods. Therefore, before using the proposed approach, it is important to apply proper transformations and scaling to original data. Mamdani type fuzzy models with triangular membership functions are generated using fuzzy clustering techniques. Simulated annealing algorithm is adapted to tune Mamdani type fuzzy models with triangular membership functions. After the initial fuzzy model construction, fuzzy models are tuned using the adapted simulated annealing algorithm by considering only the accuracy to show its optimization capability. According to the results adapted simulated annealing algorithm is able to optimize fuzzy models such that error on training data is 30 percent less than the error obtained by geographically weighed regression model (Table 5.6). However, tuned fuzzy models are not interpretable, because accuracy is the primary objective and interpretability is not considered while tuning.

To obtain compact and interpretable fuzzy models, a simplification methodology is proposed. Together with the tuning process, simplification methodology produced simplified fuzzy models which satisfy most of the interpretability criteria. Furthermore, more interpretable fuzzy models are obtained when Gath-Geva fuzzy clustering algorithms are used during fuzzy model construction.

An interpretable fuzzy model for estimating mean annual precipitation of Turkey is generated only with 12 membership functions and 8 rules.

GIS is an interdisciplinary field. It is related with fields such as geodesy, geography, surveying, cartography, remote sensing, computer science, statistics and etc. Recently, the use of soft computing approaches especially fuzzy logic in GIS has become an active field. Since the underlying logic in conventional GIS software systems is crisp logic, continuous nature of landscape cannot be modeled appropriately. Because the real physical world is gray but crisp logic is black and white. Therefore, fuzzy logic offers a way to represent and handle uncertainty present in the continuous real world. Most of the researches primarily focus on the use of fuzzy logic in classifying the continuum of the landscape. In addition to the classification, fuzzy logic is also used for decision-making and modeling purposes. The development of reliable and understandable spatial models, classification and decision rules requires knowledge on the phenomena which is working on. Fuzzy rules and models can be created from expert knowledge by translating linguistic information obtained from human experts. However, there is no standard method exist for transforming experts' knowledge into fuzzy rules. Moreover, expert knowledge is not sufficient to define complex partially unknown systems satisfactorily. In such cases, fuzzy models can be constructed by using numerical data. Using the proposed methodology in this thesis, interpretable and accurate fuzzy models can be constructed using relationships between inputs and outputs. Fuzzy models constructed using the proposed methodology can be used in three different ways:

1. As a starting point for the further analysis,
2. If interpretability is the primary objective while fuzzy model generation then constructed models present valuable information about the phenomenon being modeled and may help in understanding the phenomenon,
3. To generate prediction maps where the phenomenon is not measured before.

With the increase in the use fuzzy logic in GIS, automatic generation of reliable and interpretable fuzzy models (fuzzy rules, membership functions) from input and output data becomes a valuable tool for GIS users. Input and output data are prepared in GIS software and used in the fuzzy model creation process. After constructing a fuzzy model, it can be used for other regions to generate prediction map for that region. The prediction maps are generated by running the model with the input data for the region. These maps can be not only visualized but also analyzed further using the GIS software.

Prototype software can be extended such that initial fuzzy model can be generated from data using fuzzy clustering techniques. In such a case, it will no longer need any other software. Moreover, if the use of the software is increased, then the proposed methodology can be added to GIS software as an add-on package. Although the average computing time for the generation of interpretable (simplified) fuzzy models is about 3 minutes on a standard notebook, it takes approximately 25 minutes for the generation of accurate fuzzy models. Most of the execution time is spent for the calculation of objective function while optimizing the fuzzy models using simulated annealing. Therefore, objective function calculation must be direct and rapid to increase simulated annealing convergence speed and to decrease CPU consumption. This is the key point to decrease the execution time.

Future directions for this study can be summarized as follows:

- Fuzzy c-means, Gustafson-Kessel and Gath-Geva fuzzy clustering algorithms are used to construct fuzzy models from data. These clustering algorithms require a priori knowledge of the number of clusters. Although, cluster validity indices are used to determine an appropriate number of clusters in the data sets, none of the indices clearly specify the cluster count and usually they are not in agreement. Alternatively, fuzzy clustering techniques which do not require cluster count can be used as a future work. Examples of such algorithms are hierarchical clustering, weighted fuzzy c-means, subtractive clustering, compatible cluster merging, etc.

- In the scope of this thesis, Mamdani type fuzzy models with triangular membership functions are considered. Mamdani type fuzzy models are selected because they offer more understandable models than Takagi-Sugeno fuzzy models. On the other hand, different types of membership functions can be used instead of

triangular membership functions. Fuzzy model construction, adapted simulated annealing algorithm and simplification methodology can be extended to work on other types of membership functions such as gaussian, trapezoidal, bell-shaped, etc.

- Simulated annealing is adapted for tuning Mamdani type fuzzy models with triangular membership functions. Other global optimization methods such as evolutionary algorithms can be used instead of simulated annealing as a future work.

- New similarity measure and interpretability constraints can be added to the simplification methodology. For example, feature selection can be added to the methodology.

- Adapted simulated annealing algorithm and proposed simplification methodology involve many parameters and thresholds which is very difficult to estimate them. Therefore, automatic estimation of parameters and thresholds from data can be specified as a future work.

- To find the right balance between model accuracy and fuzzy model interpretability, global interpretability indices can be used while tuning fuzzy models. Adapted simulated annealing algorithm can be extended such that tuning is based on both accuracy and interpretability (i.e., multi-objective optimization).

- The primary objective while tuning fuzzy models is the accuracy, error on training data. Therefore, adapted simulated annealing algorithm optimizes fuzzy models for this criterion. Although, accuracy of the fuzzy models on training data is the main objective, generalization ability of the fuzzy models is also important. Adapted simulated annealing algorithm can be extended such that it presents not only the best solution but also a specified number of solutions before the best solution. Therefore, user can prefer any solution from the solution set by looking errors on both training and test data sets.

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APPENDIX A

MEAN ANNUAL PRECIPITATION DATA

Table A.1: Training data.

Station Name	**Longitude (°)**	**Latitude (°)**	**Altitude (m)**	**SdGrid (m)**	**Rainfall (mm)**
INEBOLU	33.76	41.97	64	566.4	1024.8
SINOP	35.14	42.03	42	509.9	676.4
ORDU	37.89	40.97	4	788.4	1031.7
TRABZON	39.74	41	30	957.6	816.7
RIZE	40.49	41.03	9	1013.3	2235.3
HOPA	41.42	41.39	33	997.7	2237.8
ARTVIN	41.81	41.18	628	947.8	714.2
EDIRNE	26.54	41.68	51	191.2	569.3
KIRKLARELI	27.21	41.73	232	160.4	543.8
CORLU	27.81	41.14	183	186.8	561.9
KUMKOY-KILYOS	29.03	41.24	30	287.8	811.6
KOCAELI	29.91	40.76	76	448.2	809.4
SAKARYA	30.39	40.76	30	473.9	839.6
BOLU	31.5	40.7	743	504.2	536.3
KASTAMONU	33.78	41.36	800	511.8	474.6
MERZIFON	35.44	40.83	755	477.8	431.9
CORUM	34.96	40.54	776	364.0	445.3
AMASYA	35.84	40.64	412	501.1	448.8
TOKAT	36.56	40.29	608	546.4	434.7
GUMUSHANE	39.46	40.46	1219	874.9	456.5

Table A.1: Cont'd

Station Name	**Longitude (°)**	**Latitude (°)**	**Altitude (m)**	**SdGrid (m)**	**Rainfall (mm)**
ERZURUM	41.16	39.94	1758	545.6	403.0
AGRI	43.04	39.71	1632	406.9	516.7
IGDIR	44.05	39.91	858	505.0	253.6
GOKCEADA	25.89	40.18	72	211.6	725.1
BOZCAADA	26.06	39.83	28	205.5	460.6
CANAKKALE	26.41	40.13	6	209.0	583.5
BANDIRMA	27.98	40.31	58	347.1	692.3
BURSA	29	40.21	100	451.0	680.5
ETIMESGUT	32.68	39.94	806	253.5	348.7
ANKARA	32.88	39.94	891	256.1	393.7
KIRSEHIR	34.14	39.16	1007	270.1	372.9
GEMEREK	36.06	39.18	1171	326.2	395.2
VAN	43.34	38.46	1671	520.6	378.9
AYVALIK	26.69	39.31	4	232.0	628.6
AKHISAR	27.81	38.91	93	343.1	552.6
MANISA	27.39	38.61	71	330.5	692.3
USAK	29.39	38.66	919	334.6	524.5
AFYON	30.54	38.73	1034	256.2	401.5
KAYSERI	35.48	38.71	1093	384.4	386.4
MALATYA	38.21	38.34	948	488.7	375.6
ELAZIG	39.24	38.64	990	503.6	398.1
BINGOL	40.49	38.86	1177	568.0	931.2
MUS	41.48	38.68	1320	557.5	751.3
TATVAN	42.29	38.48	1665	579.0	812.7
SIIRT	41.94	37.91	896	648.0	656.5
IZMIR	27.08	38.39	29	298.9	684.9
KUSADASI	27.26	37.87	22	325.9	603.0
AYDIN	27.84	37.84	56	382.8	609.8
DENIZLI	29.08	37.78	425	469.3	539.2

Table A.1: Cont'd

Station Name	**Longitude (°)**	**Latitude (°)**	**Altitude (m)**	**SdGrid (m)**	**Rainfall (mm)**
BURDUR	30.29	37.71	967	445.1	411.6
ISPARTA	30.56	37.78	997	420.8	494.0
KONYA	32.54	37.97	1031	332.0	314.5
EREGLI-KONYA	34.05	37.53	1044	533.4	296.3
NIGDE	34.68	37.96	1211	578.6	318.9
KAHRAMANMARAS	36.92	37.59	572	589.2	723.6
GAZIANTEP	37.34	37.05	855	490.6	551.8
SANLIURFA	38.78	37.14	549	390.2	436.2
MARDIN	40.73	37.29	1050	328.1	646.7
DIYARBAKIR	40.19	37.89	677	444.7	462.3
BATMAN	41.11	37.58	540	465.9	454.9
HAKKARI	43.73	37.56	1728	779.9	738.1
BODRUM	27.43	37.03	26	334.6	668.2
MUGLA	28.36	37.21	646	481.9	1121.1
DALAMAN	28.78	36.74	6	551.4	951.7
MARMARIS	28.24	36.83	16	472.8	1187.3
ANAMUR	32.83	36.08	4	658.6	894.0
SILIFKE	33.93	36.38	15	685.3	548.5
MERSIN	34.63	36.79	3	725.9	562.2
ADANA	35.34	37.04	27	724.4	632.8
ISKENDERUN	36.16	36.58	4	447.8	715.5
FINIKE	30.15	36.3	2	584.5	919.9
KAS	29.65	36.2	153	599.4	785.1
AMASRA	32.38	41.74	73	583.3	1010.6
UZUNKOPRU	26.68	41.24	52	152.0	644.0
SILE	29.59	41.16	83	361.7	860.5
AKCAKOCA	31.14	41.08	10	509.3	1067.5
DEVREKANI	33.83	41.58	1050	547.0	522.4
BAFRA	35.91	41.54	20	486.6	788.0

Table A.1: Cont'd

Station Name	**Longitude (°)**	**Latitude (°)**	**Altitude (m)**	**SdGrid (m)**	**Rainfall (mm)**
UNYE	37.28	41.13	20	703.1	1134.4
IPSALA	26.36	40.91	10	195.1	590.3
MALKARA	26.91	40.88	283	174.9	677.2
CERKES	32.87	40.81	1126	440.6	391.5
ILGAZ	33.63	40.91	885	400.2	479.7
TOSYA	34.03	41.01	870	428.2	462.6
CINARCIK	29.12	40.64	20	425.8	845.1
GEYVE	30.29	40.51	100	480.2	623.3
KIZILCAHAMAM	32.64	40.46	1033	358.2	556.5
OLTU	41.98	40.54	1322	682.5	380.7
GONEN	27.64	40.11	37	299.0	653.9
ULUDAG ZIRVE	29.11	40.11	1877	451.9	1445.0
NALLIHAN	31.36	40.18	650	412.9	311.7
BEYPAZARI	31.91	40.16	682	365.9	398.3
ZILE	35.87	40.29	700	442.2	446.1
SEBINKARAHISAR	38.41	40.28	1300	762.6	578.5
SUSEHRI	38.06	40.14	1163	685.3	422.0
TORTUM	41.54	40.29	1572	671.6	470.1
SARIKAMIS	42.56	40.33	2102	462.9	606.8
KELES	29.23	39.91	1063	442.7	733.8
BOZUYUK	30.04	39.89	754	421.8	471.7
TAVSANLI	29.49	39.53	833	393.9	470.5
SORGUN	35.18	39.79	1110	311.5	451.3
ZARA	37.74	39.89	1347	529.6	525.0
TERCAN	40.38	39.78	1425	541.8	443.6
DOGUBEYAZIT	44.08	39.54	1584	518.3	320.4
BURHANIYE	26.96	39.49	10	249.1	595.5
SIVRIHISAR	31.53	39.44	1070	258.1	381.4
POLATLI	32.16	39.58	886	238.5	351.2

Table A.1: Cont'd

Station Name	**Longitude (°)**	**Latitude (°)**	**Altitude (m)**	**SdGrid (m)**	**Rainfall (mm)**
CICEKDAGI	34.41	39.61	900	242.7	346.6
MAZGIRT	39.59	39.03	1400	519.7	717.3
HINIS	41.69	39.36	1715	460.9	579.5
BERGAMA	27.16	39.11	53	281.4	622.3
SIMAV	28.97	39.09	809	398.6	774.7
GEDIZ	29.39	39	825	366.9	558.9
KAMAN	33.69	39.36	1075	220.5	451.0
BOGAZLIYAN	35.24	39.19	1067	328.4	359.1
KANGAL	37.38	39.23	1512	320.5	400.8
ARAPKIR	38.49	39.04	1200	429.8	724.2
AGIN	38.72	38.95	900	462.8	502.4
CEMISGEZEK	38.91	39.06	953	461.6	558.8
KARAKOCAN	40.03	38.96	1090	567.1	633.7
SOLHAN	41.06	38.96	1366	565.4	671.6
VARTO	41.44	39.16	1650	534.8	611.2
MURADIYE-VAN	43.76	38.98	1706	517.4	556.4
BOLVADIN	31.04	38.73	1018	264.7	380.6
PINARBASI-KAYSERI	36.39	38.71	1500	393.0	410.9
KEBAN	38.74	38.79	808	488.1	362.2
PALU	39.96	38.71	1000	555.2	533.2
AHLAT	42.49	38.76	1750	523.8	538.5
OZALP	43.97	38.66	2100	483.0	476.6
SEFERIHISAR	26.84	38.19	22	265.2	581.6
ODEMIS	27.96	38.21	117	400.5	562.2
GUNEY	29.06	38.14	806	418.9	505.9
SENIRKENT	30.54	38.09	959	375.5	643.8
YALVAC	31.18	38.29	1096	331.1	504.7
ILGIN	31.89	38.28	1034	333.0	419.8
URGUP	34.91	38.63	1060	399.4	375.4

Table A.1: Cont'd

Station Name	**Longitude (°)**	**Latitude (°)**	**Altitude (m)**	**SdGrid (m)**	**Rainfall (mm)**
DEVELI	35.49	38.38	1180	517.3	360.8
TOMARZA	35.79	38.44	1397	502.0	392.9
SARIZ	36.49	38.48	1500	481.4	520.3
BASKIL	38.81	38.56	1225	491.4	417.9
SIVRICE	39.31	38.44	1240	494.9	591.8
MADEN ELAZIG	39.66	38.39	1100	513.8	826.9
ERGANI	39.76	38.28	1000	504.5	750.0
BITLIS	42.09	38.36	1573	609.5	1208.5
SULTANHISAR	28.14	37.88	72	417.6	583.1
SELCUK	27.36	37.94	17	334.4	664.7
NAZILLI	28.33	37.91	60	440.5	567.6
DINAR	30.14	38.06	864	386.8	432.0
GOKSUN	36.48	38.01	1344	596.6	597.9
AFSIN	36.91	38.24	1180	540.8	425.7
ELBISTAN	37.19	38.19	1137	528.1	390.2
DOGANSEHIR	38.1	37.86	1280	482.8	517.2
CERMIK	39.44	38.11	700	444.9	761.4
BASKALE	44.01	38.04	2400	603.1	430.2
EGIRDIR	30.86	37.83	920	425.4	776.8
MILAS	27.78	37.29	52	387.6	683.1
YATAGAN	28.13	37.33	365	432.3	635.2
ACIPAYAM	29.33	37.41	941	488.5	516.7
TEFENNI	29.78	37.31	1142	489.6	448.0
SEYDISEHIR	31.84	37.43	1131	465.3	732.2
CUMRA	32.78	37.58	1013	391.6	317.3
KARAPINAR	33.53	37.71	1004	418.0	280.4
ULUKISLA	34.48	37.53	1453	604.2	313.2
KOZAN	35.81	37.44	109	678.9	823.8
YUKSEKOVA	44.28	37.56	1900	757.4	760.8

Table A.1: Cont'd

Station Name	**Longitude (°)**	**Latitude (°)**	**Altitude (m)**	**SdGrid (m)**	**Rainfall (mm)**
KORKUTELI	30.18	37.04	1014	513.7	372.8
HADIM	32.49	36.97	1552	462.0	632.0
NUSAYBIN	41.21	37.06	500	346.1	446.9
CIZRE	42.18	37.31	400	693.3	654.0
ELMALI	29.91	36.73	1095	537.3	463.3
MANAVGAT	31.43	36.78	38	551.2	1080.2
MUT	33.43	36.64	275	581.7	373.5
ALATA-ERDEMLI	34.29	36.61	9	684.1	575.1
CEYHAN	35.81	37.03	30	647.3	695.0
DORTYOL	36.21	36.84	28	563.3	929.1
ISLAHIYE	36.63	37.01	518	532.9	799.4
BIRECIK	37.94	37.01	347	422.5	355.8
KALE-DEMRE	29.98	36.24	25	598.8	799.5
YUMURTALIK	35.78	36.76	27	609.9	796.6
SAMANDAG	35.96	36.08	4	313.1	878.1

Table A.2: Testing data.

Station Name	**Longitude (°)**	**Latitude (°)**	**Altitude (m)**	**SdGrid (m)**	**Rainfall (mm)**
ZONGULDAK	31.78	41.44	137	561.9	1230.5
SAMSUN	36.24	41.34	4	545.9	688.0
GIRESUN	38.38	40.91	37	833.7	1257.4
TEKIRDAG	27.49	40.97	3	190.6	556.3
KIRECBURNU	29.05	41.14	58	317.3	832.5
CANKIRI	33.61	40.61	751	300.8	390.0
SIVAS	37.01	39.74	1285	403.3	435.6
KIRIKKALE	33.51	39.84	748	225.7	371.2
YOZGAT	34.79	39.81	1298	276.8	582.5
DIKILI	26.87	39.06	3	254.6	573.9
NEVSEHIR	34.69	38.61	1260	397.2	407.5
CESME	26.29	38.29	5	200.2	552.6
ADIYAMAN	38.28	37.74	672	462.0	675.1
FETHIYE	29.11	36.63	3	556.5	795.0
ANTALYA	30.67	36.91	42	520.0	1071.2
ALANYA	32	36.54	6	555.2	1064.5
BOZKURT	34.01	41.94	167	563.5	1245.4
AKCAABAT	39.54	41.03	3	937.9	724.4
PAZAR-RIZE	40.89	41.16	79	998.2	2049.8
FLORYA	28.78	40.97	36	336.5	623.7
ARPACAY	43.33	40.84	1687	541.7	489.9
ISPIR	41	40.48	1222	861.1	467.2
HORASAN	42.16	40.04	1540	420.4	396.1
DURSUNBEY	28.63	39.58	639	408.5	551.6
DIVRIGI	38.11	39.36	1225	377.5	385.3
EMIRDAG	31.14	39.01	700	277.4	402.4
KULU	33.08	39.08	1010	193.4	379.0
MALAZGIRT	42.53	39.14	1565	469.2	450.9
ERCIS	43.34	39.03	1678	482.5	416.4

Table A.2: Cont'd

Station Name	**Longitude (°)**	**Latitude (°)**	**Altitude (m)**	**SdGrid (m)**	**Rainfall (mm)**
SALIHLI	28.11	38.48	111	389.3	481.5
YUNAK	31.73	38.81	1000	251.2	447.3
GENC	40.56	38.74	1250	562.9	840.3
GEVAS	43.1	38.29	1694	608.0	508.0
SIVEREK	39.31	37.74	801	383.5	533.8
KOYCEGIZ	28.71	36.92	24	529.0	1064.3
KARAISALI	35.06	37.26	241	710.6	862.6
GAZIPASA	32.31	36.26	21	594.0	826.1
KARATAS	35.38	36.56	22	637.7	757.1
BARTIN	32.33	41.63	30	579.0	944.4
ARDAHAN	42.71	41.11	1829	726.1	577.1
GOZTEPE-ISTANBUL	29.05	41.14	33	317.3	433.8
KARTAL	29.18	40.89	27	372.6	521.2
DUZCE	31.16	40.83	146	504.2	652.1
KARABUK	32.63	41.19	248	516.1	400.4
BAYBURT	40.23	40.24	1584	836.4	459.5
ERZINCAN	39.49	39.74	1218	525.6	357.6
KARS	43.09	40.61	1775	468.3	521.0
YENISEHIR	34.14	39.16	220	270.1	590.9
YALOVA	29.28	40.66	4	432.1	657.1
BILECIK	29.98	40.14	539	470.9	447.4
ESKISEHIR	30.51	39.81	801	381.6	388.4
EDREMIT	27.01	39.58	21	254.1	586.7
KUTAHYA	29.97	39.41	969	344.5	423.3
TUNCELI	39.54	39.11	978	510.1	729.6
CIHANBEYLI	32.91	38.64	968	207.7	290.1
AKSARAY	34.04	38.38	965	376.3	280.3
DIDIM	27.25	37.38	33	334.7	584.5
AKSEHIR	31.41	38.34	1002	308.3	440.4

Table A.2: Cont'd

Station Name	**Longitude (°)**	**Latitude (°)**	**Altitude (m)**	**SdGrid (m)**	**Rainfall (mm)**
KARAMAN	33.21	37.19	1025	481.4	280.4
KILIS	37.11	36.69	638	365.5	389.4
DATCA	27.67	36.7	28	366.5	347.1
OSMANIYE	36.24	37.1	120	615.3	802.1
ANTAKYA	36.16	36.19	100	302.6	1050.1
CIDE	33	41.88	10	581.9	1061.6
LULEBURGAZ	27.34	41.39	46	128.9	537.9
CEYLANPINAR	40.03	36.83	398	251.7	333.4
TURHAL	36.08	40.39	500	493.4	509.2
DEMIRCI-MANISA	28.64	39.05	851	399.5	569.2
CAY	31.03	38.58	1020	275.3	424.3
GOLBASI	37.63	37.78	900	521.6	573.4
BEYSEHIR	31.73	37.68	1129	442.8	542.6
KAHTA	38.61	37.78	675	434.9	649.8
HILVAN	38.94	37.58	585	400.7	358.4
BOZOVA-URFA	38.49	37.34	600	428.0	375.2

APPENDIX B

COMPARING MODEL ESTIMATION ACCURACIES OF LINEAR TIME INVARIANT MODELS AND ARTIFICIAL NEURAL NETWORKS FOR SPATIAL DECISION-MAKING

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B.1 Abstract

Building spatial analyses rules for a spatial decision-making problem is difficult if the decision problem to be modeled is high dimensional. If the spatial nature of the phenomena is not entirely known by the user, then it is quite difficult to adequately describe the solution steps. In such cases, decision models can be estimated using observed input-output data for the phenomena. In this paper, we used linear time-invariant systems and artificial neural networks to acquire knowledge about spatial analysis tasks using input-output relationship in data. Then, we examined the use of linear time-invariant systems and artificial neural networks by measuring their prediction accuracies and time required for learning and prediction. For linear time-invariant systems, ARX, ARMAX and state-space model structures, for artificial neural networks, feed forward backpropagation neural networks were used. To compare methods two-sample Kolmogorov-Simirnov test, root mean square error value and time required for training (learning) and prediction were used. Experiments were performed with two disjoint geographical regions which have different characteristics. The results indicate that linear time-invariant systems perform better predictions and require less training time compared to artificial neural networks and models trained with data which have higher Moran's I values performed better predictions.

Keywords: GIS, Spatial decision-making, Linear time-invariant systems, Artificial neural networks, Inverse problems, Site

B.2 Introduction

Spatial decision-making is one of the primary uses of geographic information systems (GIS). Although the developments in GIS have led to significant improvements in decision-making, the rate of data acquisition far exceeds the analytical ability of humans (Clementini et al., 2000). Increase in both amount and complexity of data points an intelligent assistant. This concerns the extraction of useful information from vast amount of data for decision-making.

Geographic knowledge discovery (GKD) (Li and Cheng, 1994; Miller and Han, 2001) process extracts useful, interesting and non-trivial information from geo-referenced data. These learned useful concepts, relationships and rules characterizing knowledge in data can guide spatial decision-making (Lee and Kerschberg, 1998; Berdard et al., 2003; Somodevilla et al., 2002; Han et al., 2004; Sester, 2000; Bui et al., 2006; Santos and Amaral, 2004; Eklund et al., 1998; Qi and Zhu, 2003). The decision-making is affected by many factors and sometimes needs many criteria. In numerous situations involving a large set of feasible alternatives and multiple, conflicting and incommensurate criteria, it is difficult to state and measure these factors and criteria (Malczewski, 1996). Although knowledge discovery methods soften these problems and assist decision-makers in their analysis, it is very difficult for human experts to build spatial analysis rules if the decision problem to be modeled is high dimensional. Even in some cases, it is quite difficult to adequately describe the solution steps, especially when the spatial nature of the phenomena is not entirely known. In such cases, based on observed input-output data for the phenomena decision models can be estimated.

The problem of building mathematical models of systems based on observed data from the systems is known as system identification (Ljung, 1987). Linear time-invariant systems (LTIS) and artificial neural networks (ANNs) are the two examples of the theories and techniques used in the system identification field.

LTIS can be used to model systems by using input-output relationships. Unless time-invariant linear systems represent idealizations of the processes encountered in real life, the approximations involved are often justified and design considerations based on linear theory lead to good results in many cases (Ljung, 1987). The response of time-invariant systems to a certain input does not depend on absolute time. The output response of linear systems to a linear combination of inputs is the same linear combination of the output responses of individual inputs (Ljung, 1987).

ANNs provide a mechanism for learning from data and mapping of data. They can solve complex problems and can "learn" from prior applications. These properties make neural networks a powerful tool for modeling nonlinear systems. Therefore, neural networks can be trained to provide an alternative approach for problems that are difficult to solve such as decision-making problems in GIS.

Identifying models using input-output data has been extensively studied in the control field and has been successfully applied to modeling of complex systems. System identification methods and tools, such as LTIS and ANNs, are also applied to GIS (Kanevski et al., 2004; Almasri and Kaluarachchi, 2005; Taylor et al., 2007; Sousa et al., 2007). In GIS, attributes of the neighbors of some object of interest may have an influence on the object and therefore have to be considered as well (Ester et al., 1997). This is also the main difference between knowledge discovery in databases for relational database systems and in spatial database systems (Ester et al., 1997).

The aim of this study is to compare model estimation accuracies of the two of the system identification tools, LTIS and ANNs, for ill-defined spatial decision-making problem. In this perspective, FuzzyCell (Yanar and Akyurek, 2006) was used to model a site selection problem by capturing rules from human experts using its natural language interfaces. Then, FuzzyCell converts these rules to fuzzy if-then rules. Application of these fuzzy rules to input data layers produces sites with degree of satisfaction depending on the searching criteria. If LTIS and ANNs are trained by the obtained data defining suitable sites against input data, then these systems can produce models for the decision-making problem. The comparison of the LTIS and ANNs for spatial decision-making problems in GIS is done by measuring their prediction accuracies and time required for learning and prediction.

The paper is organized as follows. A brief description of the system identification process from GIS perspective is given in Section B.3. Section B.4 introduces methods, linear time-invariant systems and artificial neural networks. In Section B.5, decision-making problem, data used in the analyses, performance metrics used to compare methods are given and experiment results are reported. Discussions and conclusions are given in Sections B.6 and B.7.

B.3 System Identification from GIS Perspective

The system identification is a general term used to describe set of tools and algorithms to estimate a model of a system based on the observed input-output data (Ljung, 1987). Estimating a model of a system from observed input-output data involves three basic steps; (Ljung, 1987)

1. Input and output data
2. Model structure
3. Identification method (i.e., a criterion to select a particular model in the set)

From the GIS perspective;

1. The data collections may consist of maps, imagery, sensor data, in situ measurements which are in various forms (e.g., raster, vector, text, etc.) and formats. In order to obtain successful estimations it will be necessary to access such large and heterogeneous data collection.
2. Determining the model structure is the most important and the most difficult part of the system identification procedure. There are so many techniques defined. For example, fuzzy set theory (Yen and Langari, 1999; Takagi and Sugeno, 1985; Emami et al., 1998; Grisales et al., 2005), statistical methods (Fukunaga, 1990; Kohonen, 1990; Anderberg, 1971), unsupervised learning techniques (Fukunaga, 1990; Kohonen, 1990; Anderberg, 1971) followed by supervised learning techniques, decision trees (e.g., ID3 (Quinlan, 1986) and C4.5 (Quinlan, 1993)), neural networks (Haykin, 1994), genetic algorithms (Holland, 1975; Kristinsson and Dumont, 1992), etc. and hybrid systems which are the combination of more than one technique (Takagi and Hayashi, 1991; Lee and Takagi, 1993; Takagi, 1993).

   Despite there is no fuzzy model identification example (i.e., system identification from input-output data using fuzzy models) in GIS, plenty of research investigated the identification of

membership function parameters for geo-referenced data. One approach in obtaining membership function parameters and rules is using users' own experience or throughout the consultation with experts in the related field (Yanar and Akyurek, 2006; Zhu et al., 1996; Sasikala and Petrou, 2001; Jiang and Eastman, 2000; Dragicevic and Marceau, 2000; Kollias and Kalivas, 1998; Zeng and Zhou, 2001; Benedikt et al., 2002). Other approaches rely on the numerical processing of data. For example, Ahamed et al. (2000) used Euclidean distance based measure to determine membership degree of soil in soil erosion classes. Eigenvector method is also used to determine membership function parameters and weights (Chen et al., 2001). It is based on the computation of pairwise comparison matrices for evaluating the relative importance of criteria where the importance weights for criteria are given by two decision groups. K-means clustering (Iliadis, 2005) and analytical hierarchy process (Sadiq and Husain, 2005) are other examples for determining membership function parameters and weights. Determination of membership function parameters i.e., parameter estimation is only a part of the sub problem of fuzzy system identification.

Other methods that can be used for system identification than fuzzy logic are also used extensively in GIS but largely for knowledge discovery processes. Such as, Lee and Kerschberg (1998) integrate two types of learning, unsupervised Bayesian classification and supervised inductive learning to discover useful concepts, relationships and rules that characterize knowledge in precision agriculture data space. Sester (2000) also used supervised learning for interpretation of 2D map data and discover structural models. Rough sets concept and GIS data attributes are also used for knowledge discovery from geographic information (Han et al., 2004). In the proposed work, experts provide condition attributes, decision attributes, parameters, minimum-maximum values of the domain and linguistic values for each attribute. Bell shaped membership function is used assuming that data is normally distributed and membership function parameters are calculated based on data distribution, user entered values and parameters. A decision table is constructed to get a reduction of attributes and to reduce every rule. Finally, the most concise rules are determined by building and training a neural network with reduced rule set.

3. To identify the best available model in the set, performances of the models are evaluated for unseen data (i.e., validation or testing data set). Dividing the available training data into an estimation subset and a validation subset to result in spatially disjoint sets may provide better evaluation results (Lazarevic et al., 2000).

B.4 Methods and Tools

In broad terms, an object in which variables of different kinds interact and produce observable output data is called a system (Ljung, 1987). External influences that can be manipulated by the observer are called input. Determining relations between the measurements of the behavior of the system (outputs of the system) and the external influences (inputs to the system) without going into the details of what actually happening inside the system is known as system identification.

In linear system, behavior of the resulting system subjected to a complex input can be described as sum of responses to simpler inputs. On the other hand, in nonlinear system, behavior of the system is not expressible as sum of the behaviors of its descriptors.

In this work, LTIS and ANNs were used to identify ill-defined spatial decision-making problems. LTIS were selected because of their high prediction accuracies. And, ANNs were selected since they are frequently used in problems of GIS.

B.4.1 Models of Linear Time-Invariant Systems

A linear time-invariant (LTI) system investigates the response of a linear and time-invariant system to an arbitrary input. LTI system is identified by its linearity and time invariance properties. In linear systems, the output response to a linear combination of inputs is the same linear combination of the output responses of individual inputs. Time invariance property means that system's response to a certain input does not depend on absolute time (Ljung, 1987).

A simple input-output relationship can be obtained by describing it as a linear difference equation (Equation B.1).

$$\begin{aligned} y(t) + a_1 y(t-1) + a_2 y(t-2) + \ldots + a_{n_a} y(t-n_a) &= \\ b_1 u(t-1) + b_2 u(t-2) + \ldots + b_{n_b} u(t-n_b) + e(t) & \end{aligned} \tag{B.1}$$

which relates the current output $y(t)$ to a finite number of past outputs $y(t-k)$ and inputs $u(t-k)$. $a_1, \ldots, a_{n_a}, b_1, \ldots, b_{n_b}$ are the system coefficients. If we define backward shift operator q^{-1} as $q^{-1}u(t) = u(t-1)$ then Equation B.1 becomes

$$A(q)y(t) = B(q)u(t) + e(t) \tag{B.2}$$

where

$$\begin{aligned} A(q) &= 1 + a_1 q^{-1} + a_2 q^{-2} + \ldots + a_{n_a} q^{-n_a} \\ B(q) &= b_1 q^{-1} + b_2 q^{-2} + \ldots + b_{n_b} q^{-n_b} \end{aligned} \tag{B.3}$$

Equation B.3 is called an ARX model where AR refers to autoregressive part $A(q)y(t)$ and X to the extra input $B(q)u(t)$ part.

Unlike the ARX model, the ARMAX model structure includes disturbance dynamics. Error is described by a moving average of white noise. The ARMAX model has more flexibility in the handling of disturbance modeling than the ARX model. The ARMAX model is given in Equation B.4.

$$A(q)y(t) = B(q)u(t) + C(q)e(t) \tag{B.4}$$

A state-space model provides a more complete representation of the system than parametric models like ARX and ARMAX. A state-space model represents a system as a set of input, output and state variables with related first-order differential equations. The model is written in the following form

$$\begin{aligned} x(t+1) &= Ax(t) + Bu(t) + Ke(t) \\ y(t) &= Cx(t) + Du(t) + e(t) \end{aligned} \tag{B.5}$$

$x(t)$ is the state vector, $y(t)$ is the system output, $u(t)$ is the system input and $e(t)$ is the error. A, B, C, D and K are the system matrices.

B.4.2 Artificial Neural Networks

Artificial neural networks are originally motivated by the biological structures in the brains of human and animals, which are powerful for such tasks as information processing, learning and adaptation (Nelles, 2000). ANNs are composed of a set of connected nodes or units where each connection has a weight associated with it. ANNs can "learn" from prior applications. During the learning phase, the network learns by adjusting the weights. If a poor solution to the problem is made, the network is modified to produce a better solution by adjusting its weights.

Although, ANNs learn well, they have a long training time (time required for learning phase). Also, there are no clear rules to build network structure (Han and Kamber, 2001). Network design is a trial-and-error process which may affect accuracy of the result and there is no guarantee that the selected network is the best network structure. Another major drawback to the use of ANNs is their poor interpretability (Yen and Langari, 1999).

On the other hand, neural network's tolerance to noisy data is high and they are robust against the failure of single units. Like all statistical models, ANNs are subject to overfitting when the ANN is trained to fit one set of data almost exactly (Russell and Norvig, 2003; Dunham, 2003). When training error associated with the training data is quite small, but error for new data is very large, generalization set is used. Also, to avoid overfitting, smaller neural networks are advisable (Dunham, 2003).

B.5 Application

Decision-making problem, used in the analysis and tests, was taken from the study of Yanar and Akyurek (2006). According to the decision problem, suitable sites for industrial development are selected using the criteria "if site has flat or gentle slope and if site is close to roads and town then site is suitable for industrial development". For humans it is simple to comprehend and make decisions based on these vague terms. Conventional GIS, which is based on crisp logic, cannot evaluate such vague statements. On the other hand, FuzzyCell can be used to model the decision problem by using its natural language interfaces and find fuzzy answer to site selection problem. The decision-making problem was modeled by using FuzzyCell and named as FuzzyCellModel. This model, which involves fuzzy rules and membership functions, was captured from human experts using FuzzyCell. This model has two fuzzy rules given in Rules B.6 and B.7.

Rule 1. IF	Slope is flat and	
	Distance to road is close and	
	Distance to town is close	
THEN	Suitability is good.	(B.6)

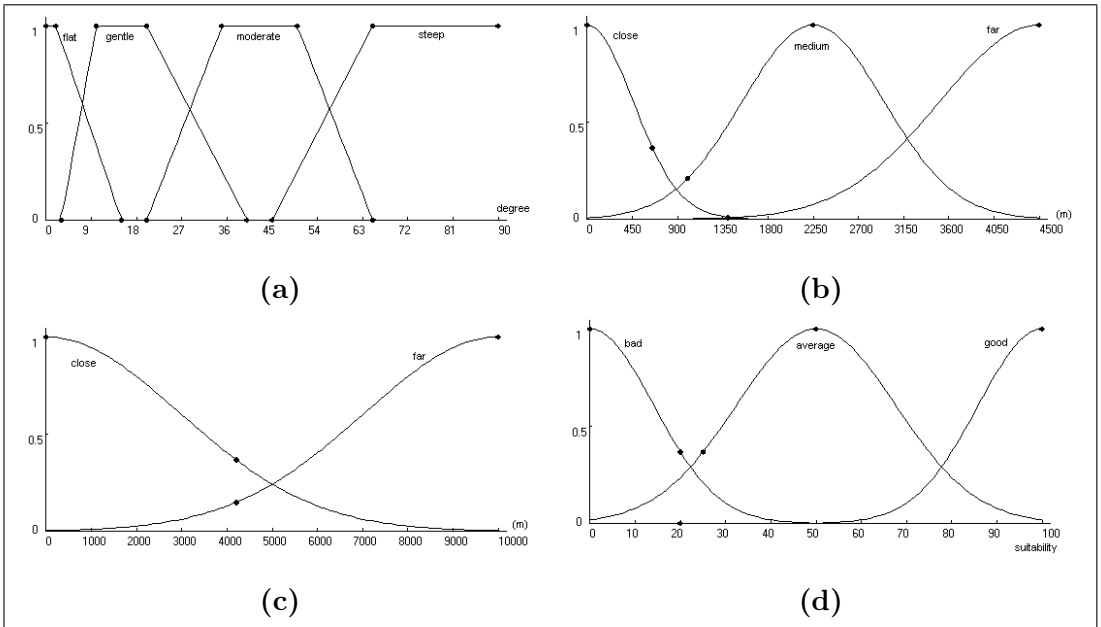


Figure B.1: Membership functions for (a) Slope, (b) Distance to road, (c) Distance to town, and (d) Suitability.

Rule 2. IF Slope is gentle and
Distance to road is close and
Distance to town is close
THEN Suitability is good. (B.7)

Membership functions for linguistic terms constructed based on expert knowledge are depicted in Figure B.1.

Membership functions can be chosen by the experts arbitrarily based on experts' experiences on the problem domain. Hence, membership functions for two experts could be quite different upon their experiences and perspectives. Both membership function types and parameters shown in Figure B.1 were given by experts. It has to be also noted that linguistic term "close" was used twice, one stands for "distance to road" and the other stands for "distance to town" and two different membership functions were defined for this linguistic term. This illustrates the fact that membership functions can be quite context dependent.

B.5.1 Data

FuzzyCellModel, which was built depending on expert knowledge, uses slope, closeness to roads and closeness to town maps as input. Output data were generated by using FuzzyCell applying the constructed model to input data layers and define suitability values for industrial development sites.

Two different data sets belonging to two geographically disjoint regions were used. One data set

Table B.1: Minimum and maximum values of the DataSet1 and DataSet2

Layer Name	Minimum Value	Maximum Value
DataSet1 (Birecik region)		
Slope	0	44.9880
Distance to Road	0	4371.1440
Distance to Town	0	9798.4453
Output Suitability	50	96.5000
DataSet2 (Bartın region)		
Slope	0	73.9123
Distance to Road	0	3802.6824
Distance to Town	0	11344.0928
Output Suitability	50	93.0000

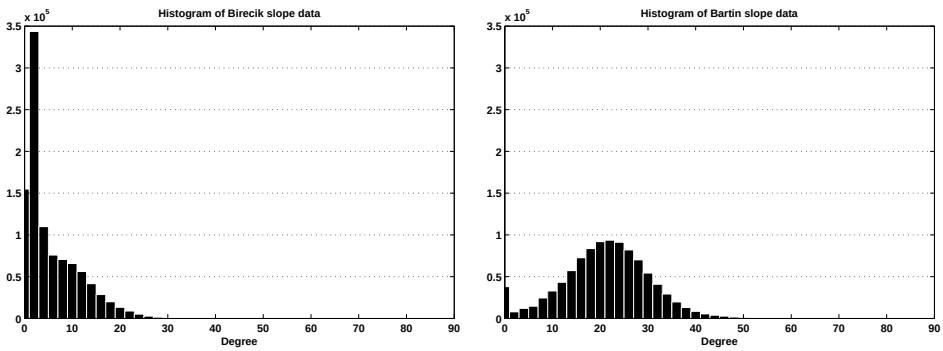
was taken from Birecik region (DataSet1) and the second data set was from Bartın region (DataSet2). Each data set includes three input maps (i.e., slope, closeness to roads and closeness to town) and one calculated map (i.e., suitability map). All input and output maps have the same cell size and the same coordinate system. Dimensions of all the maps are 1000-by-1000 pixels. Histograms of the data layers used are given in Figure B.2 and minimum and maximum values of the data layers are listed in Table B.1.

Input and target values of Birecik and Bartın zone were mapped into the interval $[-1, +1]$ by using formula given in Equation B.8 to simplify the problem.

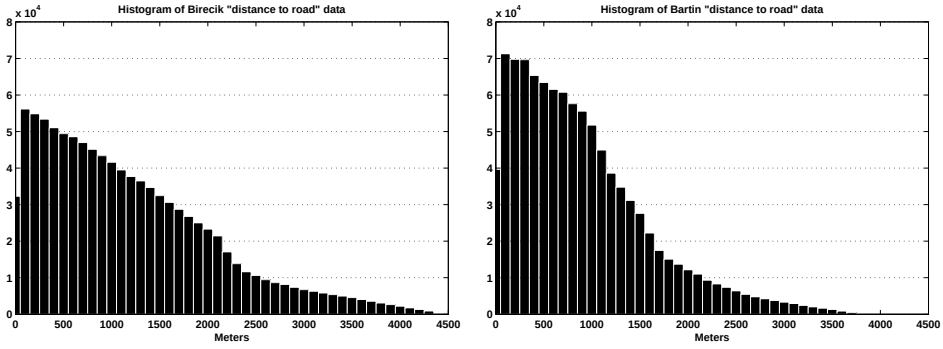
$$y = \frac{(y_{max} - y_{min}) \times (x - x_{min})}{(x_{max} - x_{min})} + y_{min} \tag{B.8}$$

Equation B.8 processes matrix x by normalizing the minimum (x_{min}) and maximum (x_{max}) values to $[y_{min}, y_{max}]$ and produces a normalized matrix y.

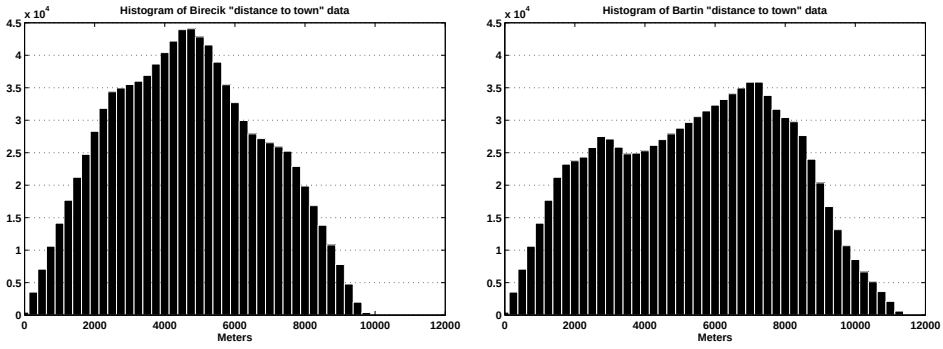
It also ensures that target values fall into the range that new neural networks can reproduce. Lastly, the data were divided into training, generalization and test sets for ANNs. The training set was used for training the network. Generalization set was used to validate network performance during training so that training stopped early if it attempted to overfit the training data. Test set was used for an independent measure of how the network might be expected to perform on data it was not trained on. 20% of data (i.e., 200000 cells) was selected for generalization set and 20% for the test set (i.e., 200000 cells), remaining 60% of data (i.e., 600000 cells) was selected for training set. For LTIS, the data were divided into training and test sets. The training set was used for estimation of model parameters. And test set was used for an independent measure of how the identified model might be expected to perform on data it was not trained on. 40% of data (i.e., 400000 cells) was selected for test set and remaining 60% of data (i.e., 600000 cells) was selected for training set.



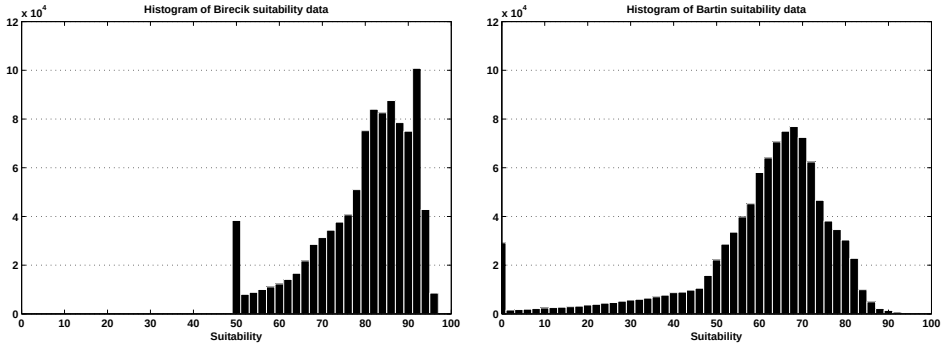
(1) Slope



(2) Distance to road



(3) Distance to town



(a) **(b)**

(4) Suitability

Figure B.2: Histograms of the data layers belonging to (a) DataSet1 and (b) DataSet2.

B.5.2 Performance Metrics

The goal of this study was to compare models identified by LTIS and ANNs, in defining the ill-defined GIS based decision-making problems. As discussed in the Section B.5, the problem "selection of suitable sites for industrial development" was modeled by using FuzzyCell with the help of expert judgments. Model of this decision problem includes rule base (Rules 1 and 2) and membership function parameters (Figure B.1). Output was generated by applying these rule base and membership functions to input data. Calculated output data (i.e., suitability map) using the constructed model (i.e., rule base, membership function parameters and output) was taken as reference.

The reference output and the predictions made with LTIS and ANNs were compared using two performance metrics;

1. Two-sample Kolmogorov-Simirnov (KS) test statistic, and
2. Root mean square error (RMSE).

These metrics specify error and similarity between the reference and the predicted outputs. These metrics compare predicted data set with target data set and give lower results when predicted data and target data are more similar.

Two-sample KS test is a non-parametric test for ratio scale data. The two-sample KS test statistic compares the distribution of values in the two sample data vectors representing random samples from some underlying distributions (McKillup, 2006). The objective is to determine if these two data sets have been drawn from identical population distribution functions. Therefore, null hypothesis for this test is whether the two sample data vectors are drawn from the same continuous distribution. The alternative hypothesis is that they are drawn from different continuous distributions. To compare the distributions of the values in the two data vectors x_1 and x_2, the test statistic is computed by:

$$\text{KSStatistic} = max\left(|F_1(x) - F_2(x)|\right) \tag{B.9}$$

where $F_1(x)$ is the proportion of x_1 values less than or equal to x and $F_2(x)$ is the proportion of x_2 values less than or equal to x.

RMSE is computed by taking square root of average of the squared differences between each computed value ($\hat{x_i}$) and its corresponding correct value (x_i). Root mean square error formula is given below:

$$\text{RMSE} = \left(\frac{1}{n}\sum_{i=1}^{n}(x_i - \hat{x_i})^2\right)^{1/2} \tag{B.10}$$

Since input and target values were mapped into the interval $[-1, +1]$, before calculating two-sample KS test statistic and RMSE the predictions made with LTIS and ANNs were mapped back into their original scale. Furthermore, for two-sample KS test, significance level was set to 5%.

In addition to the prediction accuracy, training time and time needed to accomplish the application of identified model to input data from geographically different regions were also used to compare run-time efficiency of the LTIS and ANNs. The configuration of the dedicated workstation was Intel® Xeon® 3.20GHz Dual CPU with 1GB RAM and operating system was Microsoft® Windows® XP Professional Version 2002 with Service Pack 2.

B.5.3 Site Selection Example

LTIS

MATLAB® System Identification Toolbox™ was used for modeling linear time-invariant systems. In the System Identification Toolbox™ input and output data are represented as column vectors. If the system has several input layers, the input data is represented by a matrix, where the columns are the input data in different layers. The same holds for systems with several output layers.

$$\text{Input Column Vector, } u = [u_{road}\ u_{town}\ u_{slope}] \tag{B.11}$$

$$\text{Output Column Vector, } y = [y_{suitability}] \tag{B.12}$$

Estimation of parametric models in this study involves AutoRegressive with eXternal input (ARX), AutoRegressive Moving Average with eXternal input (ARMAX) and state-space models. Best models for each type of parametric models were investigated and selected based on their prediction performances. All models require some parameters (coefficients of polynomials) for system definitions. These parameters and model structure together identify a linear time-invariant model. Therefore, it is the main idea to find parameters such that the prediction performance of the whole model is the highest.

ARX model has an advantage that many models (10000 models in this study) can be estimated simultaneously. According to the estimation results, models with highest fitness values were further investigated and best model is selected.

ARMAX models are the elaborations of the basic ARX model where different disturbance models are introduced. The reason for introducing all these model variants is to provide for flexibility in the disturbance description and to allow for common or different dynamics (poles) for different inputs (Ljung, 1987). Unfortunately, it is not possible to estimate many different structures simultaneously for input-output models. For these models, parameters of the systems were investigated by taking ARX model parameters as reference and performing trials. Models, which gave the smallest error value, were chosen.

As in ARX models, parameterization of state-space models were performed by estimating many models simultaneously and selecting the one with the highest fitness value. There are two basic methods for estimation of parameters in state-space models:

1. PEM: Prediction error/maximum likelihood method, based on iterative minimization of a criterion.
2. N4sid: Subspace based method that does not use iterative search.

In this work, both methods were used for state-space models.

Input and output vectors for the analyses were prepared by transforming input and output matrices with two different methods.

1. Column tracing: Each column of matrices was added back to back to form vector structure.

2. Row tracing: First row was converted to column vector, second row was reverted and then converted to column vector and added to the first column vector. Other rows were processed according to this rule.

For example, assume that we are given matrix A.

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix} \tag{B.13}$$

The column vector, A_{column}, after performing column tracing process is shown in Equation B.14.

$$A_{column} = \begin{bmatrix} 1 \\ 4 \\ 7 \\ 2 \\ 5 \\ 8 \\ 3 \\ 6 \\ 9 \end{bmatrix} \tag{B.14}$$

and column vector after performing row tracing rule is shown in Equation B.15.

$$A_{row} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 6 \\ 5 \\ 4 \\ 7 \\ 8 \\ 9 \end{bmatrix} \tag{B.15}$$

Both methods preserve neighborhood relation in only one direction. To evaluate global spatial autocorrelation in input and output data for adjacencies defined by column tracing and row tracing, Moran's I measure was calculated and given in Table B.2.

Moran's I values range from -1 (indicating perfect dispersion) to $+1$ (perfect correlation). A zero value indicates a random spatial pattern. All values in Table B.2 indicate near perfect correlation. In addition, for DataSet1, Moran's I values of layers for row tracing method (left-right adjacency) are slightly higher than values for column tracing method (top-down adjacency). Since spatial autocorrelation in DataSet1 for row tracing method is slightly higher than column tracing method, we may expect slightly better accuracies from the models identified using row tracing data for DataSet1.

Experiment-1 Results Constructed models are listed in Table B.3. Prediction performance comparison tables for Birecik and Bartın zones for both column and row tracing methods are given

Table B.2: Moran's I measures for DataSet1 and DataSet2

Layer Name	**Top-Bottom Adjacency**[1]	**Left-Right Adjacency**[2]
	DataSet1	
Slope	0.9779	0.9824
Distance to Road	0.9962	0.9980
Distance to Town	0.9955	0.9980
Output Suitability	0.9956	0.9977
	DataSet2	
Slope	0.9561	0.9528
Distance to Road	0.9975	0.9979
Distance to Town	0.9964	0.9980
Output Suitability	0.9318	0.9247

[1] Column tracing method.

[2] Row tracing method.

in Table B.4, Table B.5, Table B.6 and Table B.7. Prediction accuracy measures were calculated for test sets.

Since input and output data are represented as column vectors, we used two different methods to transform input and output matrix data into vector form as discussed in Section B.5.3. According to KS statistics, models trained and tested with row tracing method performed better predictions than models trained and tested with column tracing method for both data sets DataSet1 and DataSet2. For DataSet1, models constructed with row tracing method also produced smaller RMSE values. Therefore, for DataSet1, models constructed with row tracing method are better as expected since spatial autocorrelation in DataSet1 for row tracing method was slightly higher than column tracing method. According to RMSE statistics, models for DataSet1 performed better predictions than models built for DataSet2. In addition, Arx models required less training times than other methods require.

ANNs

MATLAB® Neural Network Toolbox™ was used for identifying neural network prediction performance trained with geographic data. In the Neural Network Toolbox™ input and output (target) data are represented as row vectors. If the system has several input layers, the input data is represented by a matrix, where the rows are the input data in different layers. Similar convention is used for output with more than one layer; which is not very common.

$$\text{Input Row Vector, } p = \begin{bmatrix} p_{road} \\ p_{town} \\ p_{slope} \end{bmatrix} \tag{B.16}$$

$$\text{Output Row Vector, } t = [t_{suitability}] \tag{B.17}$$

Table B.3: Constructed models

Region	**Vectorization Method**	**Model Name**	**Model Type**
Birecik (DataSet1)	Column tracing	Birecik-LTIM-C1	ARX
		Birecik-LTIM-C2	ARMAX
		Birecik-LTIM-C3	N4sid
		Birecik-LTIM-C4	PEM
	Row tracing	Birecik-LTIM-R1	ARX
		Birecik-LTIM-R2	ARMAX
		Birecik-LTIM-R3	N4sid
		Birecik-LTIM-R4	PEM
Birecik (DataSet2)	Column tracing	Bartın-LTIM-C1	ARX
		Bartın-LTIM-C2	ARMAX
		Bartın-LTIM-C3	N4SID
		Bartın-LTIM-C4	PEM
	Row tracing	Bartın-LTIM-R1	ARX
		Bartın-LTIM-R2	ARMAX
		Bartın-LTIM-R3	N4sid
		Bartın-LTIM-R4	PEM

Table B.4: Model prediction accuracies for DataSet1 (column tracing)

Model	**KS**	**RMSE**	**Training Time (sec.)**
Birecik-LTIM-C1	0.0327	0.6667	11
Birecik-LTIM-C2	0.0306	0.6638	114
Birecik-LTIM-C3	0.0336	0.6807	109
Birecik-LTIM-C4	0.0328	0.6679	335

Table B.5: Model prediction accuracies for DataSet1 (row tracing)

Model	**KS**	**RMSE**	**Training Time (sec.)**
Birecik-LTIM-R1	0.0191	0.2163	13
Birecik-LTIM-R2	0.0294	0.2149	60
Birecik-LTIM-R3	0.0291	0.2193	54
Birecik-LTIM-R4	0.0196	0.2232	133

Table B.6: Model prediction accuracies for DataSet2 (column tracing)

Model	**KS**	**RMSE**	**Training Time (sec.)**
Bartın-LTIM-C1	0.0291	5.3854	15
Bartın-LTIM-C2	0.0272	5.5070	180
Bartın-LTIM-C3	0.0298	5.3670	28
Bartın-LTIM-C4	0.0249	5.5618	28

Table B.7: Model prediction accuracies for DataSet2 (row tracing)

Model	**KS**	**RMSE**	**Training Time (sec.)**
Bartın-LTIM-R1	0.0284	5.4922	12
Bartın-LTIM-R2	0.0246	5.6192	35
Bartın-LTIM-R3	0.0286	5.4703	26
Bartın-LTIM-R4	0.0246	5.6191	180

Before using data layers with neural networks some pre-processing steps were taken for all input and output maps. Since neural networks use data vectors, two dimensional input and output maps were transformed to one dimensional column vectors. Data vectors for the analyses may be prepared by transforming data matrices with different methods such as column and row tracing as discussed previously. These methods preserve neighborhood relation in one dimension. Because multilayer feed-forward neural networks have no internal state other than the weights themselves (Russell and Norvig, 2003), vectorization process should not affect the performance. Therefore, in this work input and output column vectors were formed randomly, using MATLAB® "randperm" command. For example, assume that we are given matrix A as in Equation B.13. The column vector, A_{column}, after randomly selecting locations is shown in Equation B.18.

$$A_{column} = \begin{bmatrix} 8 \\ 2 \\ 7 \\ 4 \\ 3 \\ 6 \\ 9 \\ 5 \\ 1 \end{bmatrix} \tag{B.18}$$

Although there are plenty of network types that can be used for identifying models of unknown geographic phenomena, feed forward backpropagation networks were used in this work. Standard backpropagation is a gradient descent algorithm in which the network weights are moved along the negative of the gradient of the performance function (Demuth et al., 2006).

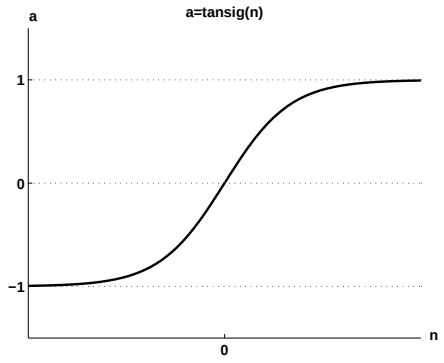


Figure B.3: Tan-sigmoid transfer function.

A multilayer network has multiple layers of neurons. Each layer plays different roles. A layer that produces the network output is called an output layer. All other layers are called hidden layers. Since there is only one target value associated with input vectors, all networks used in this study should have one output neuron. The number of hidden layers and the number of neurons used in each layer were changed to create different network structures. The aim was to find a network structure which gives the most similar values with output layer. Unfortunately, there are no clear rules to build appropriate network structure (Han and Kamber, 2001). Therefore, this step requires testing many different structures and there is no guarantee that the selected network which gives the most similar values is the best network structure among all alternatives. This is the main disadvantage of using neural networks.

Multiple layers of neurons with nonlinear transfer functions allow the network to learn nonlinear and linear relationships between input and output data. A linear transfer function in the output layer lets the network produce values outside the range -1 to $+1$. On the other hand, we want to constrain the outputs of a network between -1 and $+1$ therefore in the output layer we used tan-sigmoid transfer function. For all networks tan-sigmoid transfer function was used. Equation of the transfer function is given in Equation B.19 and the function is depicted in Figure B.3.

$$a = \text{tansig}(n) = \frac{2}{1 + e^{-2n}} - 1 \tag{B.19}$$

Once network weights and biases were initialized the network training began. All networks used Levenberg-Marquardt backpropagation algorithm for training and gradient descent with momentum weight and bias learning function. Mean squared error was used for network performance function which measures the network's performance according to the mean squared errors.

Experiment-2 Results Built networks and their properties are listed in Table B.8. Prediction performances of networks trained and tested with data from Birecik and Bartın zones are shown in Table B.9 and Table B.10.

According to RMSE test metrics network Birecik-ANN-5 trained and tested with DataSet1 was the best predictor. Network Birecik-ANN-5 contains one hidden layer with five nodes and one output layer with one node. KS statistics indicate network Birecik-ANN-8, which consists of two hidden layer

Table B.8: Trained feed forward neural networks for DataSet1 and DataSet2

Network Name	**Layer Count**	**Neuron Count Hidden Layer1**	**Neuron Count Hidden Layer2**	**Neuron Count Output Layer**
Birecik-ANN-1 & Bartın-ANN-1	2	1	NA	1
Birecik-ANN-2 & Bartın-ANN-2	2	2	NA	1
Birecik-ANN-3 & Bartın-ANN-3	2	3	NA	1
Birecik-ANN-4 & Bartın-ANN-4	2	4	NA	1
Birecik-ANN-5 & Bartın-ANN-5	2	5	NA	1
Birecik-ANN-6 & Bartın-ANN-6	3	1	1	1
Birecik-ANN-7 & Bartın-ANN-7	3	1	2	1
Birecik-ANN-8 & Bartın-ANN-8	3	2	2	1

Table B.9: Network prediction accuracies for DataSet1

Model	**KS**	**RMSE**	**Training Time (sec.)**
Birecik-ANN-1	0.1507	2.6199	1160
Birecik-ANN-2	0.0846	1.0971	1675
Birecik-ANN-3	0.0614	0.9763	2222
Birecik-ANN-4	0.0384	1.0597	3249
Birecik-ANN-5	0.0388	0.4821	1749
Birecik-ANN-6	0.1507	2.6183	1586
Birecik-ANN-7	0.1507	2.6200	1974
Birecik-ANN-8	0.0346	0.4937	2650

Table B.10: Network prediction accuracies for DataSet2

Model	KS	RMSE	Training Time (sec.)
Bartın-ANN-1	0.3014	11.9558	230
Bartın-ANN-2	0.0546	8.2210	1106
Bartın-ANN-3	0.0456	2.1163	736
Bartın-ANN-4	0.0458	1.9819	3220
Bartın-ANN-5	0.0329	1.7718	3570
Bartın-ANN-6	0.3645	11.8817	1570
Bartın-ANN-7	0.2895	11.6739	1995
Bartın-ANN-8	0.1671	6.6730	2669

with two nodes in both hidden layers and one output layer with one node, produced best prediction performance for DataSet1. For DataSet2, according to KS and RMSE statistics network Bartın-ANN-5 produced better prediction performances.

All identified linear time-invariant models using row tracing method performs better than neural networks according to both metrics. According to KS statistics, identified linear time-invariant models using column tracing method also performs better. For DataSet1, based on RMSE statistics LTIS generally performed better than ANN. In addition, linear tine-invariant models required less training times than ANNs require.

B.5.4 Testing Models with Different Geographical Region

LTIS and neural networks constructed for one region were used for other geographical region, to test their prediction performance. Geographical regions are disjoint and have different characteristics (see Figure B.2). The purpose of this test was to find the generic methods which give better prediction performances over different geographical regions. Models and networks trained with DataSet1 were tested with DataSet2 and models and networks trained with DataSet2 were tested with DataSet1.

LTIS

Experiment-3 Results Table B.11 and Table B.12 show test results obtained by testing trained models with unseen DataSet2. Times given in tables are the time needed to accomplish the application of trained model to input data from geographically separated (disjoint) region (i.e., DataSet2). Table B.13 and Table B.14 show results for linear time-invariant models constructed from DataSet2 and tested with DataSet1.

Models constructed using row tracing method performed better predictions for both data sets according to KS statistics. Based on RMSE test values, models constructed using DataSet2 are more general, since accuracies of the predictions made using DataSet2 models are higher than the accuracies of the predictions made using DataSet1 models. RMSE values obtained when models

Table B.11: Performance tests for LTIS constructed from DataSet1 and tested with DataSet2 (column tracing)

Model	**KS**	**RMSE**	**Prediction Time (sec.)**
Birecik-LTIM-C1	0.0321	5.5766	18.3
Birecik-LTIM-C2	0.0222	5.6105	30.6
Birecik-LTIM-C3	0.0279	5.7807	12.9
Birecik-LTIM-C4	0.0313	5.5765	26.9

Table B.12: Performance tests for LTIS constructed from DataSet1 and tested with DataSet2 (row tracing)

Model	**KS**	**RMSE**	**Prediction Time (sec.)**
Birecik-LTIM-R1	0.0216	5.5628	9.6
Birecik-LTIM-R2	0.0216	5.6584	55.6
Birecik-LTIM-R3	0.0220	6.0601	22.6
Birecik-LTIM-R4	0.0220	5.6050	7.9

Table B.13: Performance tests for LTIS constructed from DataSet2 and tested with DataSet1 (column tracing)

Model	**KS**	**RMSE**	**Prediction Time (sec.)**
Bartın-LTIM-C1	0.0345	0.7632	18.0
Bartın-LTIM-C2	0.0346	0.6828	80.4
Bartın-LTIM-C3	0.0343	0.7441	15.4
Bartın-LTIM-C4	0.0346	0.6710	6.2

Table B.14: Performance tests for LTIS constructed from DataSet2 and tested with DataSet1 (row tracing)

Model	**KS**	**RMSE**	**Prediction Time (sec.)**
Bartın-LTIM-R1	0.0313	0.3801	9.2
Bartın-LTIM-R2	0.0198	0.2211	9.1
Bartın-LTIM-R3	0.0201	0.3271	15.4
Bartın-LTIM-R4	0.0176	0.2219	17.8

Table B.15: Performance tests for ANNs constructed from DataSet1 and tested with data from DataSet2

Model	**KS**	**RMSE**	**Prediction Time (sec.)**
Birecik-ANN-1	0.2317	14.4030	6.4
Birecik-ANN-2	0.1572	13.0735	6.6
Birecik-ANN-3	0.1433	12.9009	6.9
Birecik-ANN-4	0.1374	13.5434	7.2
Birecik-ANN-5	0.1291	12.9502	7.5
Birecik-ANN-6	0.2311	14.3979	6.7
Birecik-ANN-7	0.2317	14.4029	7.0
Birecik-ANN-8	0.1180	13.3484	7.2

Table B.16: Performance tests for ANNs constructed from DataSet2 and tested with data from DataSet1

Model	**KS**	**RMSE**	**Prediction Time (sec.)**
Bartın-ANN-1	0.3934	6.1940	6.0
Bartın-ANN-2	0.2192	5.5380	6.4
Bartın-ANN-3	0.1530	3.9441	6.5
Bartın-ANN-4	0.1401	3.9198	6.8
Bartın-ANN-5	0.1205	3.9283	7.2
Bartın-ANN-6	0.4341	7.6215	6.4
Bartın-ANN-7	0.3934	8.3824	6.6
Bartın-ANN-8	0.3122	5.3134	7.0

constructed using DataSet2 were used to predict DataSet1 are in the range $[0.2211, 0.7632]$, while RMSE values obtained from the models constructed using DataSet1 are in the range $[5.5628, 6.0601]$. Also, generally models built with DataSet2 end the estimation in less time.

ANNs

Experiment-4 Results Results in Table B.15 shows test results obtained by testing trained networks with unseen DataSet2. Times given in table are the time needed to accomplish the application of trained network to input data from geographically separated (disjoint) region (i.e., DataSet2).

Table B.16 shows results for networks trained with DataSet2 and tested with DataSet1.

There is not much difference between accuracies for the models constructed from both data sets when they were tested on different geographic region when KS statistics are used for comparison. On the other hand, according to RMSE metric networks trained with DataSet2 produced better

predictions. While RMSE metrics for DataSet2 networks are in between 3.9198 and 8.3824, RMSE metrics for DataSet1 networks are in between 12.9009 and 14.4030. Although, the error on networks trained with DataSet1 were small than DataSet2 networks, when new data was presented to the networks the error was large for DataSet1 networks. Moreover, prediction times were in between 6.0 seconds and 7.5 seconds.

B.6 Discussion

In this work, LTIS and ANNs were used to model a spatial decision-making problem. Both methods can construct models and networks by using input-output data relationships. We used slope, distance to road and distance to town maps as input. Output data were the suitability map, which was calculated using FuzzyCell. We have two datasets which came from two disjoint regions. The characteristics of the regions were different as shown in Figure B.2. LTIS and ANNs were compared with different examples and results were given in the previous section. According to the results, linear time-invariant models and networks trained with DataSet1 seem overfitted to the data. While performances of the predictions on DataSet1 test data were very good, they did not achieve similar success when they used to predict DataSet2. On the other hand, linear time-invariant models and networks learned using DataSet2 were more general since they performed good predictions for DataSet1.

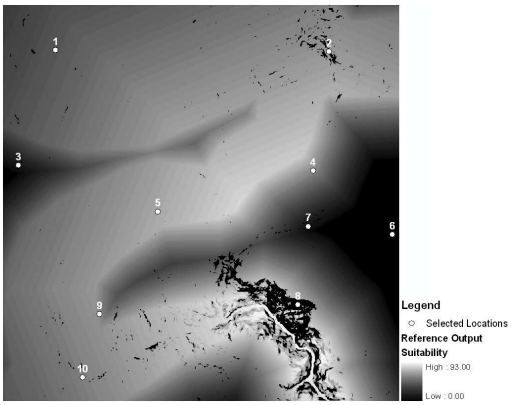
MATLAB® System Identification Toolbox™ and Neural Network Toolbox™ were used in the experiments. Since both toolboxes use data in vector form, input and output matrices were converted to vector form using column (top-bottom adjacency) and row tracing (left-right adjacency) methods. After conversion, spatial autocorrelation in data were calculated using Moran's I. According to the experiment results, models trained with data which have higher Moran's I values result in higher prediction accuracies. Moreover, LTIS performed better predictions than ANNs. They also required less training times than ANNs require. Although, learning of networks took much time, prediction times were as low as LTIS prediction times.

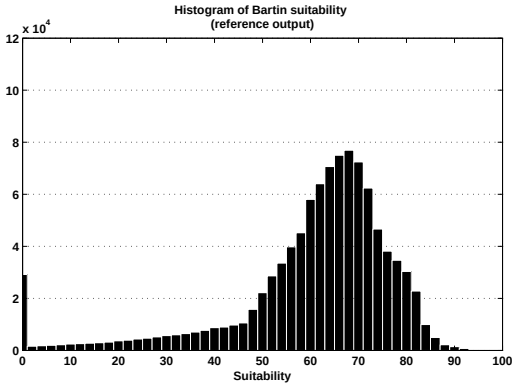
In Figure B.4, we illustrate predictions made on DataSet2 using linear time-invariant models and ANNs trained with DataSet1. Original output and outputs produced by best methods for LTIS and ANNs are given. To compare the values of reference output and outputs produced by best methods for LTIS and ANNs, ten locations were randomly selected and associated values are given in Table B.17.

B.7 Conclusion

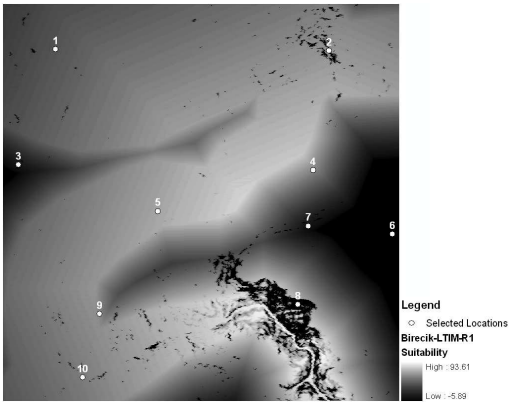
Building spatial analyses rules for a decision problem is difficult if the decision problem to be modeled is high dimensional. If the spatial nature of the phenomena is not entirely known by the user, then it is quite difficult to adequately describe the solution steps. In such cases, decision models can be estimated using observed input-output data for the phenomena.

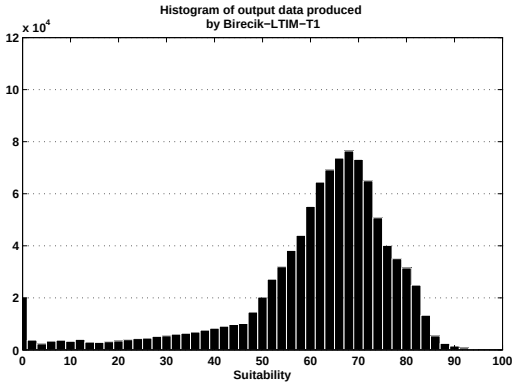
In this paper, we used linear time-invariant systems and feed forward backpropagation neural networks to acquire knowledge about unknown or unmanageable spatial analysis tasks using input-output relationship. To compare methods two metrics, two-sample KS test and RMSE value and



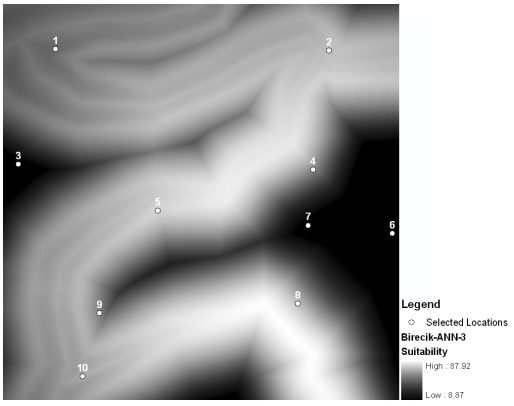


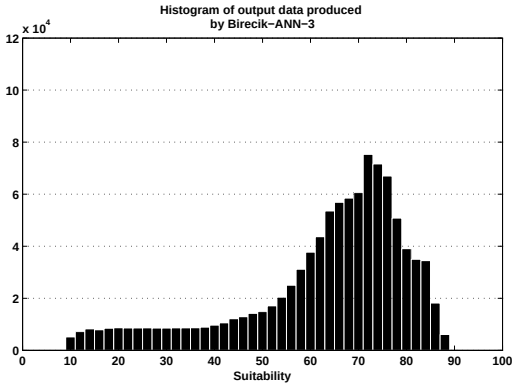
(a)





(b)





(c) **(d)**

Figure B.4: Graphs for (a) Bartın suitability (reference output), (b) Output data produced by Birecik-LTIM-R1, (c) Output data produced by Birecik-ANN-3, and (d) Histograms of output suitability values.

Table B.17: Selected output values

Point no	Reference output	Birecik-LTIM-R1 output	Birecik-ANN-3 output
1	55	55.05	58.61
2	0	11.42	76.14
3	33	32.95	22.66
4	68	68.07	65.78
5	75	74.92	80.07
6	0	0.13	10.77
7	32	31.15	23.78
8	0	-0.06	76.86
9	69	67.93	64.15
10	66	65.94	72.13

time required for training and prediction were used. It was seen that these metrics are not always in agreement. In addition to these, residual graphs may be used for comparing results of the models and networks.

The work examined the use of LTIS and ANNs for decision-making problems of GIS by measuring their prediction accuracies and time required for learning and prediction. For LTIS, ARX, ARMAX, and state-space model structures, for ANNs feed forward backpropagation networks were used. FuzzyCell was used to model site selection problems by capturing rules from human experts using its natural language interfaces. After capturing rules from human experts, FuzzyCell converted these rules to fuzzy if-then rules. Application of these fuzzy rules to input data layers produced sites with degree of satisfaction for searching criteria. LTIS and ANNs were trained with input-output data pairs where output data were calculated by GIS-based fuzzy inference system, FuzzyCell, as described above. In this work, it was tested that whether system identification models trained by data obtained from fuzzy models can produce reasonable guesses for locations other than training sites when compared to results obtained from fuzzy rule based system, FuzzyCell. Additionally, system identification models constructed from one geographical region were used for another geographical region to test their prediction performance. Geographical regions are disjoint and have different characteristics. The purpose of this test was to find the generic methods which give better prediction performances over different geographical regions. When models were tested with geographically separate region, LTIS produced better predictions. Also, in the experiments LTIS required less training times than ANNs. However, after learning was done, ANNs produced predictions in less time. LTIS perform better predictions and require less training time.

While identifying an unknown spatial phenomena using input-output data relationship, both prediction accuracy and interpretability of driven model are important. Despite higher prediction accuracies were obtained by both LTIS and ANNs, interpretability of driven models and networks were very difficult. Therefore, neither LTIS nor ANNs are convenient to acquire knowledge about

unknown or unmanageable spatial analysis tasks using input-output relationship. However, after learning both methods can be used to estimate decisions for new locations faster.

Building accurate interpretable models while identifying an unknown spatial phenomena using input-output data relationship can be addressed as a future work.

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APPENDIX C

THE USE OF NEURO-FUZZY SYSTEMS IN ILL-DEFINED DECISION MAKING PROBLEMS WITHIN GIS

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Submitted to Information Sciences

C.1 Abstract

Fuzzy set theory is introduced into GIS to obtain more flexibility and more effective capability of handling and processing imprecise information about the real world. Extending GIS operations with fuzzy logic methodologies not only offers a way to represent and handle uncertainty present in the continuous real world but also assist GIS user to make decisions using experts' experiences in decision-making process. Using fuzzy logic methodologies, the GIS user can approximate complex ill-defined problems in decision-making processes by capturing rules from experts' experiences in the form of fuzzy if-then rules. Fuzzy system consists of many properties such as fuzzy if-then rules, input and output linguistic variables, membership function types and membership function parameters. Suitable fuzzy systems for the decision problem can be identified by learning from data. In this study, the use of neuro-fuzzy systems, namely NEFPROX and ANFIS, which can construct a set of fuzzy if-then rules with appropriate membership functions using input-output pairs, for decision-making problems of GIS was examined by measuring their prediction accuracies and time required for learning and prediction. It was found that NEFPROX system provides more interpretable and manageable rule bases than ANFIS structure. Moreover, constructed rule bases still require human expert for further processing.

Keywords: Neuro-fuzzy systems, Function approximation, Fuzzy if-then rules, Decision-making, GIS

C.2 Introduction

One of the main tasks of Geographic Information Systems (GIS) is to support the decision-making process using information from different data sources. In GIS, decision-making based on conventional tools such as threshold modeling is not well suited for ill-defined problems. The incorporation of human knowledge and reasoning process through the use of fuzzy set theory into GIS provides an approximate and yet effective means of describing the ill-defined decision-making problems (Stefanakis et al., 1996; Yanar and Akyurek, 2006).

Fuzzy decision-making in GIS can be used for different kinds of purposes such as selecting suitable sites for industrial development (Yanar and Akyurek, 2006), seeking the optimum locations for real estates (Zeng and Zhou, 2001), assessing vulnerability to natural hazards (Rashed and Weeks, 2003; Martino et al., 2005), or estimating risk (Chen et al., 2001; Iliadis, 2005; Sadiq and Husain, 2005). Other than decision-making, fuzzy set theory has been widely used for many different problems in GIS including soil classification (Zhu et al., 1996; Lark and Bolam, 1997), crop-land suitability analysis (Ahamed et al., 2000), identifying and ranking burned forests to evaluate risk of desertification (Sasikala and Petrou, 2001), classifying and assessing natural phenomena (Kollias and Kalivas, 1998; Benedikt et al., 2002), and classifying slope and aspect maps into linguistically defined classes (Yanar, 2003). Enhancing GIS operations with fuzzy logic methodologies helps the GIS user to make decisions using experts' experiences in the decision-making process easier and fuzzy logic methodologies enable decision-makers to express imprecise concepts that are used with geographic data. Another advantage of fuzzy logic is that fuzzy result of a decision-making process provides a set of locations whose attribute values partially satisfy the constraints posed by the user (Yanar and Akyurek, 2006).

Despite the advantages of using fuzzy logic with GIS, no standard method exists for the identification of fuzzy if-then rules, which involves transforming experts' experiences into the database of fuzzy inference system or determining membership function parameters such as the choice of function types, estimating and tuning parameters and partitioning of input space (Jang, 1993; Yen and Langari, 1999; Yanar, 2003). In order to estimate parameters of membership functions, both linguistic information from human experts and numerical data (e.g. statistical data, data obtained from observations on the system) obtained from the actual physical system can be used (Yen and Langari, 1999). Plenty of research investigated the identification of membership function parameters for geo-referenced data. One approach in obtaining membership function parameters and rules is using users' own experience or throughout the consultation with experts in the related field (Zhu et al., 1996; Kollias and Kalivas, 1998; Dragicevic and Marceau, 2000; Jiang and Eastman, 2000; Sasikala and Petrou, 2001; Zeng and Zhou, 2001; Benedikt et al., 2002; Yanar and Akyurek, 2006). Other approaches rely on the numerical processing of data. For example, Ahamed et al. (2000) used Euclidean distance based measure to determine membership degree of soil in soil erosion classes. Eigenvector method is also used to determine membership function parameters and weights (Chen et al., 2001). It is based on the computation of pair wise comparison matrices for evaluating the relative importance of criteria, where weights representing the importance of the criteria are given by two decision groups. K-means clustering (Iliadis, 2005) and analytical hierarchy process (Sadiq and Husain, 2005) are other examples for determining membership function parameters and weights.

In addition to these, database of fuzzy if-then rules with appropriate membership function parameters can be estimated based on observed input-output data for the phenomena (Jang, 1993). Learning rule base (structure) and membership function parameters from input-output data pairs in fuzzy systems is most often implemented by learning techniques derived from neural networks (Nauck, 2003). The combinations of neural networks and fuzzy systems are referred as neuro-fuzzy systems. Such well-known neuro-fuzzy systems are Adaptive-Network-based Fuzzy Inference System (ANFIS) (Jang, 1993), Neuro-Fuzzy Function Approximation (NEFPROX) (Nauck and Kruse, 1999) and Neuro-Fuzzy Classification (NEFCLASS) (Nauck, 2003).

The aim of this study is to test whether neuro-fuzzy systems for function approximation, namely ANFIS and NEFPROX, can produce similar predictions for rule base (structure identification) and membership function parameters (parameter identification) for ill-defined decision-making problems, compared to actual fuzzy rule based system which is constructed by using FuzzyCell (Yanar and Akyurek, 2006) with the help of expert knowledge. The goal is to identify the structure (rule base) and parameters (membership function parameters) of the model of a GIS based decision problem by using neuro-fuzzy systems, which are used for function approximation, and to compare identified models with the reference model. Optimization of membership function parameters is not the aim of this study. Tuning of membership function shapes and membership function parameters with the use of neuro-fuzzy systems is not aimed. Moreover, the use of fuzzy logic in GIS is not presented. The use of fuzzy logic in GIS and the integration of fuzzy logic and GIS were discussed in Yanar (2003) and Yanar and Akyurek (2006). In this perspective, FuzzyCell was used to model site selection problems by capturing rules from human experts using its natural language interfaces. Then, FuzzyCell converts these rules to fuzzy if-then rules. Application of these fuzzy rules with the input data layers produces sites with degree of satisfaction depending on the searching criteria. If neuro-fuzzy systems for function approximation are trained by the obtained data defining suitable sites against input data, then these systems can produce rule base and membership function parameters for decision-making problem. The objective of this study is to examine the use of neuro-fuzzy systems for decision-making problems in GIS by measuring their prediction accuracies and time required for learning and prediction.

C.3 Methods and Tools

C.3.1 Fuzzy Set Theory

Fuzzy logic (Zadeh, 1965) generalizes crisp logic to allow truth-values to take partial degrees. Since bivalent membership functions of crisp logic are replaced by fuzzy membership functions, the degree of truth-values in fuzzy logic becomes a matter of degree, which is a number between zero and one. An important advantage of using fuzzy models is that they are capable of incorporating knowledge from human experts naturally and conveniently, while traditional models fail to do so (Yen and Langari, 1999). Other important properties of fuzzy models are their ability to handle nonlinearity and interpretability feature of the models (Yen and Langari, 1999).

In the decision analysis within GIS, FuzzyCell was used. FuzzyCell is a GIS-based fuzzy inference system and assists the GIS users in making decisions using experts' experiences in the decision-

making process. Users can approximate complex ill-defined problems in decision-making processes and classification by using FuzzyCell. FuzzyCell is a generic (not problem specific) module integrated into commercial GIS software (ArcMap®) which enables decision-makers to express their constraints and imprecise concepts that are used with geographic data through the use of natural language interfaces (Yanar and Akyurek, 2006).

C.3.2 Neuro-Fuzzy Systems

The underlying rational behind the neuro-fuzzy systems is to derive a fuzzy system from data or to enhance it by learning from examples (Jang, 1993; Nauck and Kruse, 1999; Nauck, 2003). Learning methods are obtained from neural networks. Since neural network learning algorithms are usually based on gradient descent methods, the application of neural networks to fuzzy system needs some modifications on the fuzzy inference procedure such as selecting differentiable functions. For example in ANFIS a Sugeno-type fuzzy system (Takagi and Sugeno, 1985) is implemented in neural network structure and differentiable t-norm and membership functions are selected. On the other hand, NEFCON (Nauck, 1994), NEFCLASS and NEFPROX systems can also implement Mamdani-type fuzzy systems (Mamdani and Assilian, 1975) and do not use a gradient-based learning algorithm but a restricted learning algorithm such that the semantics and interpretability of the represented fuzzy system are retained (Nauck and Kruse, 1999).

Dixon (2005) examined the sensitivity of neuro-fuzzy models used to predict groundwater vulnerability in a spatial context by integrating GIS and neuro-fuzzy techniques. The results show that the neuro-fuzzy models are sensitive to the model parameters used during learning and validation steps for hydro geologic applications (Dixon, 2005). Vasilakos and Stathakis (2005) show that granular neural network (Bortolan, 1998), which is based on the selection of fuzzy sets that represent data, are suited to model the inherent uncertainty of geographical phenomena. Both studies use neuro-fuzzy classification software, NEFCLASS, with geographic data.

Adaptive-Network-Based Fuzzy Inference System

ANFIS (Jang, 1993) (Adaptive-Network-based Fuzzy Inference System) is one of the first hybrid neuro-fuzzy systems for function approximation. ANFIS implements a Sugeno-type (Takagi and Sugeno, 1985) fuzzy system, which has a functional form (linear combination of input variables) in the consequent part of the fuzzy if-then rules. This system uses a differentiable t-norm and differentiable membership functions. Since ANFIS does not have an algorithm for structure learning (rule generation), the rule base must be known in advance.

The architecture is five-layer feed-forward network, where the first layer contains elements which realize the membership functions in the antecedent part of the if-then rules. The second layer corresponds to calculation of firing strengths of each rule. Next layers correspond to the consequent part of the rules (Rutkowska, 2002). The structure of ANFIS is assumed to be fixed and the parameter identification is solved through the hybrid learning rule. However, since there is no structure identification, the number of rules, number of membership functions assigned to each input and initial step

Table C.1: Major inputs and outputs of ANFIS and NEFPROX systems.

Neuro-Fuzzy System	**Inputs**	**Outputs**
ANFIS	number of rules number of membership functions assigned to each input initial step size	fuzzy if-then rules (rule base) learned membership functions [a]
NEFPROX	initial fuzzy partitions for input and output type of membership functions t-norm operators t-conorm operators defuzzification procedure initialization parameters learning restrictions	fuzzy if-then rules (rule base) learned membership functions [a]

[a] Log files, statistics, membership function plots, etc. are also obtained.

size, which is the length of each gradient transition in the parameter space (used to change the speed of convergence), have to be given by the user (see Table C.1).

Neuro-Fuzzy Function Approximator

Neuro-Fuzzy function apPROXimator (Nauck and Kruse, 1999) (NEFPROX) can be applied to function approximation. The system is based on a generic fuzzy perceptron, which is a three-layer neural network with special activation and propagation functions, and fuzzy sets as weights. The fuzzy perceptron provides a framework for learning algorithm to be interpreted as a system of linguistic rules and enables to use prior knowledge in the form of fuzzy if-then rules (Rutkowska, 2002). The architecture of fuzzy perceptron is a three-layer feed-forward network. The units of input layer represent the input variables. The hidden layer is composed of units representing fuzzy rules. And the units of the output layer represent output variables which compute crisp output values by a defuzzification procedure. The connections between input units (neurons) and hidden units are labeled with linguistic terms corresponding to the antecedent fuzzy sets and the connection between hidden neurons and output neurons are labeled with linguistic terms corresponding to consequent fuzzy sets.

The learning of NEFPROX system consists of two steps: structure learning (learning of rule base) and parameter learning (learning of fuzzy sets). In this system, some rules can be given a priori and the remaining rules may be found by learning. Moreover, NEFPROX can generate the whole rule base by the rule learning algorithm, which selects fuzzy rules based on a predefined partitioning of the input space (Nauck and Kruse, 1999; Rutkowska, 2002). Parameter learning procedure (learning of fuzzy sets) is a simple heuristic. For details, see (Nauck and Kruse, 1999).

Initial fuzzy partitions for input and output variables, type of membership functions, t-norm and t-conorm operators, defuzzification procedure, initialization parameters and learning restrictions are given to the system by user.

C.4 Application

Decision-making problem, used in the analysis and tests, was taken from the study of Yanar and Akyurek (2006). According to the decision problem, suitable sites for industrial development are selected using the criteria 'if site has flat or gentle slope and if site is close to roads and town then site is suitable for industrial development'. For humans it is simple to comprehend and make decisions based on these vague terms. Conventional GIS, which is based on crisp logic, cannot process such vague statements. On the other hand, FuzzyCell can be used to model the decision problem by using its natural language interfaces and find fuzzy answer to site selection problem. The model, which involves fuzzy rules and membership functions, was captured from human experts using FuzzyCell. This model has two fuzzy rules given in Rules C.1 and C.2.

IF Slope is flat and
Distance to road is close and
Distance to town is close
THEN Suitability is good. (C.1)

IF Slope is gentle and
Distance to road is close and
Distance to town is close
THEN Suitability is good. (C.2)

Membership functions for linguistic terms constructed based on expert knowledge are depicted in Figure C.1.

Membership functions can be chosen by the experts arbitrarily based on experts' experiences on the problem domain. Hence, membership functions for two experts could be quite different upon their experiences and perspectives. Both membership function types and parameters shown in Figure C.1 were given by experts. It has to be also noted that linguistic term 'close' was used twice, one stands for 'distance to road' and other stands for 'distance to town' and two different membership functions were defined for this linguistic term. This illustrates the fact that membership functions can be quite context dependent.

C.4.1 Data

The model, which was built depending on expert knowledge, uses slope, closeness to roads and closeness to town maps as input. Output data were generated by using FuzzyCell applying the constructed model to input data layers and define suitability values for industrial development sites. Two different data sets belonging to two geographically disjoint regions were used. One data set was taken from Birecik region and the second data set was from Bartın region. Each data set includes three input maps (i.e., slope, closeness to roads and closeness to town) and one calculated map (i.e., suitability

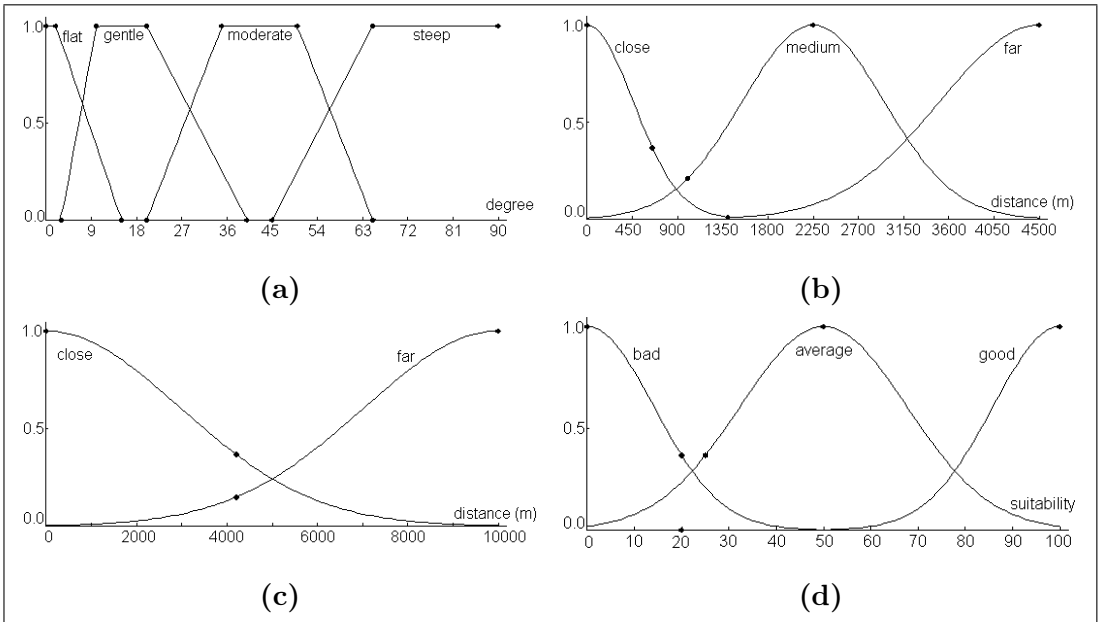


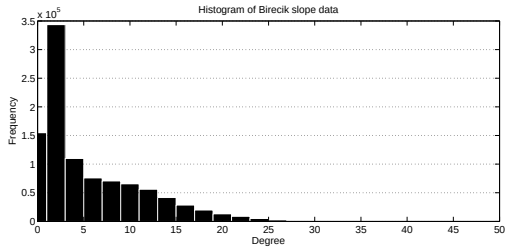
Figure C.1: Membership functions for (a) Slope, (b) Distance to road, (c) Distance to town, and (d) Suitability.

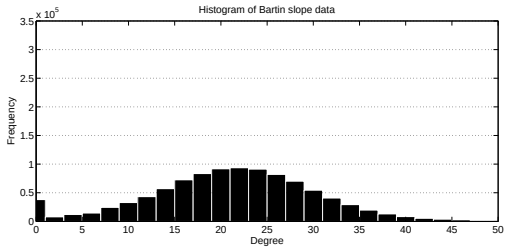
map). All input and output maps have the same cell size and the same coordinate system. Dimensions of all the maps are 1000-by-1000 pixels. Histograms of the data layers used are given in Figure C.2.

C.4.2 Comparison Methods and Tests

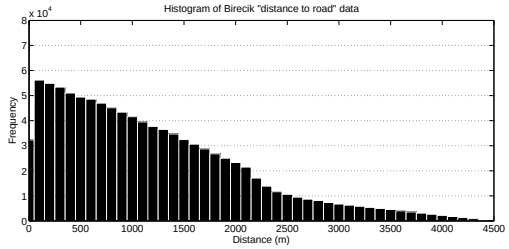
The goal of this study is to compare the use of neuro-fuzzy systems (namely ANFIS and NEFPROX), which are used for function approximation, in defining the ill-defined GIS based decision-making problems. As discussed in Section C.4 the problem 'selection of suitable sites for industrial development' was modeled by using FuzzyCell with the help of expert judgments. Model of this decision-making problem includes rule base (Rules C.1 and C.2), membership function parameters (Figure C.1) and output generated by applying these rule base and membership functions to input data. Constructed model (i.e., rule base, membership function parameters and output) by using expert knowledge was taken as reference. The comparison between the predicted decision models and reference model was made in two steps:

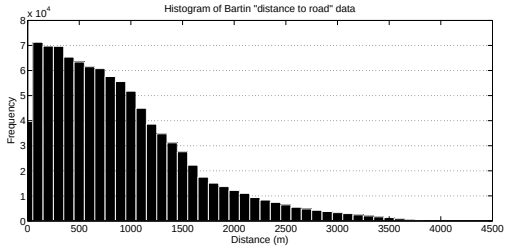
1. In the first step, performance metrics, root mean squared error and Kolmogorov-Smirnov test metrics were used to compare outputs generated by both neuro-fuzzy systems and reference output. These metrics specify error and similarity between the reference and the predicted outputs. These metrics compare predicted data set with target data set and give higher results when predicted data and target data are more similar. In this work, Kolmogorov-Smirnov statistics, which is a non-parametric test for ratio scale data, and root mean squared error value are used for comparison metric. The two-sample Kolmogorov-Smirnov test compares the distribution of values in the two sample data vectors representing random samples from some



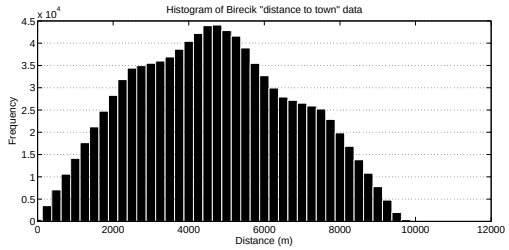


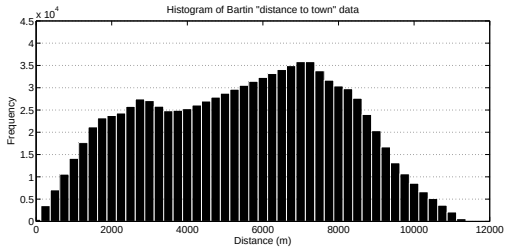
(1) Slope



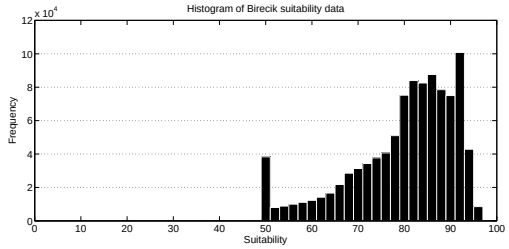


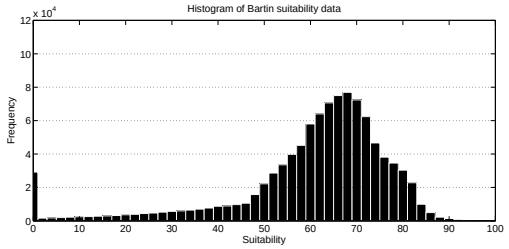
(2) Distance to road





(3) Distance to town





(a) **(b)**

(4) Suitability

Figure C.2: Histograms of the data layers belonging to (a) Birecik region, (b) Bartın region.

underlying distributions (McKillup, 2006). The objective is to determine if these two data sets have been drawn from identical population distribution functions. Therefore, null hypothesis for this test is whether the two sample data vectors are drawn from the same continuous distribution. The alternative hypothesis is that they are drawn from different continuous distributions. Root mean squared error is computed by taking square root of average of the squared differences between each computed value and its corresponding reference value.

2. Second step involves the comparison of the rule bases based on their interpretability. Comparison of the interpretation of the rule bases constructed by both neuro-fuzzy systems was intuitive.

Lastly, training time and time needed to accomplish the application of trained network for input data from geographically different regions were also used to compare run-time efficiency of neuro-fuzzy systems. The configuration of the dedicated workstation is Intel® Xeon™ 3.20 GHz Dual CPU, 1 GB RAM and operating system is Microsoft® Windows XP Professional™ Version 2002 with Service Pack 2.

C.4.3 Structure and Parameter Identification

As discussed in Section C.4.1 two different data sets, which come from two geographically disjoint regions, were used. One data set was taken from Birecik region and used to train neuro-fuzzy models to derive rule base and membership function parameters. Thus, the model of a GIS-based decision-making problem, which is given in Section C.4, was constructed by using Birecik data set. Constructed model includes rule base and membership function parameters. Moreover, output was produced by applying these rule base and membership functions to input data (slope, closeness to roads and closeness to town maps). Then, produced output compared with the reference output data using comparison tests given in Section C.4.2.

Before using data layers with neuro-fuzzy models some pre-processing steps were taken for all input and output maps. Since neuro-fuzzy models use data vectors, two dimensional input and output maps were transformed to one dimensional column vectors. Because ANFIS and NEFPROX neuro-fuzzy models use multilayer feed-forward neural networks, which have no internal state other than the weights themselves (Russell and Norvig, 2003), vectorization process does not affect the performance. Therefore, in this work input and output column vectors were formed randomly using MATLAB™ 'randperm' command. For example, assume that we are given matrix A.

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix} \tag{C.3}$$

The column vector, A_{column}, after randomly selecting locations is shown in Equ. C.4.

$$A_{column} = \begin{bmatrix} 8 \\ 2 \\ 7 \\ 4 \\ 3 \\ 6 \\ 9 \\ 5 \\ 1 \end{bmatrix} \tag{C.4}$$

Using these command indices were randomized and the same permutation indices were used for all the matrices. Furthermore, input and target values of Birecik zone were mapped into the interval $[-1, +1]$ by using formula given in Equ. C.5 to simplify the problem of network.

$$y = \frac{(y_{max} - y_{min}) * (x - x_{min})}{(x_{max} - x_{min})} + y_{min} \tag{C.5}$$

It also ensures that target values fall into the range that new network can reproduce. Third, the data were divided into training, generalization and test sets. The training set was used for training the network. Generalization set was used to validate network performance during training so that training stopped early if it attempted to over fit the training data. Test set was used for an independent measure of how the network might be expected to perform on data it was not trained on. 20% of data (i.e., 200000 cells) was selected for generalization set and 20% for the test set (i.e., 200000 cells), remaining 60% of data (i.e., 600000 cells) was selected for training set.

NEFPROX neuro-fuzzy tool for function approximation produced by Nauck and Kruse (1999) was used. NEFPROX can implement Mamdani-type fuzzy systems and also has ability to perform ANFIS architecture which is used to implement Sugeno-type fuzzy system that uses a differentiable t-norm and differentiable membership functions (Jang, 1993). NEFPROX can use either supervised learning, where the correct vector is known for each given input vector or prior knowledge if available. Prior to learning process initial fuzzy partitions for each input and output variables (i.e. number of fuzzy sets for input and output variables), type of membership functions, t-norm and t-conorm operators, defuzzification procedure, initialization parameters and learning restrictions are given to the system. System produces learned fuzzy rules, predicted output and performance measures for overall training, generalization and test patterns.

The initial conditions of the analyzed ANFIS and NEFPROX models were the same. Neuro-fuzzy model properties for neuro-fuzzy models are shown in Table C.2. For ANFIS system, parameters in the output layer are referred as consequent parameters. Therefore, numbers for the column 'Output membership function count' in Table C.2 represent consequent parameter count for ANFIS system.

Because actual fuzzy rule base is known previously (Rules C.1 and C.2), the number of fuzzy sets for input and output variables were selected based on prior knowledge. In fact, the optimum number of fuzzy sets for both input and output variables might have been found by performing many trials and selecting the configuration which gives the smallest error value. Initial guesses for fuzzy set count might begin with two. Learning algorithm was applied to triangular and Gaussian membership

Table C.2: The initial conditions of neuro-fuzzy models.

Model	Method	Fuzzy set count for input variables	Input mf type	Fuzzy set count for output variables	Output mf type
Model10	NEFPROX	2	Triangular	2	Triangular
Model11	ANFIS	2	Triangular	2[b]	-
Model12	NEFPROX	2	Gaussian	2	Gaussian
Model1	NEFPROX	4	Triangular	3	Triangular
Model2	ANFIS	4	Triangular	3[b]	-
Model3	NEFPROX	4	Gaussian	3	Gaussian
Model4	NEFPROX	3	Triangular	3	Triangular
Model5	ANFIS	3	Triangular	3[b]	-
Model6	NEFPROX	3	Gaussian	3	Gaussian
Model8	NEFPROX	$Road \rightarrow 3$ $Town \rightarrow 2$ $Slope \rightarrow 4$	Gaussian Gaussian Triangular	3	Gaussian
Model9	ANFIS	$Road \rightarrow 3$ $Town \rightarrow 2$ $Slope \rightarrow 4$	Gaussian Gaussian Triangular	3[b]	-

[b] Consequent parameter count.

Table C.3: Performance metrics for tested neuro-fuzzy models.

Model	Kolmogorov-Smirnov test (KSTAT)	RMSE	Generated rule counts	Training time (sec.)
Model10	0.632980	0.449468	2	292
Model11	0.115340	0.111423	8	652
Model12	0.229220	0.279462	4	116
Model1	0.322460	0.281184	10	130
Model2	0.074365	0.057002	48	593
Model3	0.087495	0.178551	11	755
Model4	0.569090	0.366189	5	234
Model5	0.092485	0.070755	23	354
Model6	0.333270	0.433740	7	292
Model8	0.193560	0.298716	4	256
Model9	0.043580	0.131135	20	476

functions. All models use minimum function for t-norm operator and maximum function for t-conorm operator. Although NEFPROX can use either center of gravity (COG) or mean of maximum (MOM) methods for defuzzification procedure, MOM was selected because the implementation of MOM procedure in NEFPROX is faster and produces almost the same results after learning (Nauck and Kruse, 1999). Same initialization parameters and learning restrictions were used for all models in order to get consistent results.

Obtained performance measures, time spent during training and generated rule counts are given in Table C.3. For the two-sample Kolmogorov-Simirnov test metric, KSTAT value gets lower as the probability that compared sets coming from the same population increases. Therefore, lower KSTAT values indicate better prediction performances. Similarly, as the root mean squared error value gets lower, prediction performance of network is better.

Table C.4: Performance metrics for neuro-fuzzy systems trained with Birecik data and tested with data from Bartın region.

Model	**Kolmogorov-Smirnov test (KSTAT)**	**RMSE**	**Prediction time (sec.)**
Model10	0.817580	0.440447	12
Model11	0.133570	0.279530	12
Model12	0.385850	0.356157	12
Model1	0.321000	0.341014	12
Model2	0.079289	0.289401	18
Model3	0.095203	0.259266	14
Model4	0.686750	0.444107	12
Model5	0.098323	0.303631	14
Model6	0.496310	0.372795	13
Model8	0.300880	0.303227	12
Model9	0.189580	0.297883	14

C.4.4 Testing Models with Different Geographical Region

Neuro-fuzzy models constructed from Birecik region were used for other geographical region, Bartın region, to test their prediction performance. Geographical regions are disjoint and have different characteristics (Figure C.2). The purpose of this test was to find the generic methods which give better prediction performances over different geographical regions. Neuro-fuzzy models trained with the data from Birecik region were tested with Bartın zone data. Results in Table C.4 show test results obtained by testing trained neuro-fuzzy models with unseen Bartın test data. Time given in Table C.4 is the time needed to accomplish the application of trained network to input data from geographically separated (disjoint) Bartın region.

For both KSTAT test metrics and RMSE values in Table C.4, Model3 is the best predictor for NEFPROX system. For ANFIS type neuro-fuzzy models metrics are not in agreement. According to KSTAT test metrics Model2, according to RMSE values Model11 produce better prediction performances. Since Model11 contains much less rules than Model2 and also requires less prediction time, Model11 was selected for ANFIS type system. In Table C.5, rules identified by Model3 and Model11 are given with the rules in FuzzyCell rule base (Rules C.1 and C.2).

Since Model11 rely on ANFIS architecture which is used to implement Sugeno-type fuzzy system in neural network structure, consequent parts of the fuzzy rules are functions of the input variables. Therefore, Model11 does not have output linguistic variable. Identified membership functions by models Model3 and Model11 are depicted in Figure C.3 and Figure C.4 respectively.

To compare interpretability of constructed rule bases, each membership function identified by the neuro-fuzzy models must be assigned with a name to make rule base more interpretable by considering functions and data ranges that function can take. For example identified membership functions by neuro-fuzzy models may be named as given in Table C.6.

Table C.5: Rules in the rule-bases of FuzzyCell and the best models for NEFPROX and ANFIS type neuro-fuzzy system. To shorten the rules following notation is used: Distance to road = r, Distance to town = t, Slope = s, Site Suitability = ss.

Model	**Rules**
Rules in FuzzyCell rule base	IF r is close and t is close and s is flat THEN ss is good
	IF r is close and t is close and s is gentle THEN ss is good
Identified rules by Model3	IF r is mf0 and t is mf1 and s is mf0 THEN ss is mf2
	IF r is mf1 and t is mf1 and s is mf0 THEN ss is mf1
	IF r is mf1 and t is mf2 and s is mf0 THEN ss is mf1
	IF r is mf1 and t is mf1 and s is mf1 THEN ss is mf1
	IF r is mf0 and t is mf1 and s is mf1 THEN ss is mf2
	IF r is mf0 and t is mf2 and s is mf0 THEN ss is mf1
	IF r is mf1 and t is mf2 and s is mf1 THEN ss is mf1
	IF r is mf0 and t is mf2 and s is mf1 THEN ss is mf1
	IF r is mf2 and t is mf2 and s is mf0 THEN ss is mf0
	IF r is mf1 and t is mf0 and s is mf0 THEN ss is mf1
	IF r is mf2 and t is mf2 and s is mf1 THEN ss is mf1
Identified rules by Model11	IF r is mf0 and t is mf1 and s is mf0 THEN -r*0.026401-t*0.075391-s*0.077778+0.435781
	IF r is mf0 and t is mf0 and s is mf0 THEN -r*0.266423+t*0.036360+s*0.022906+0.569266
	IF r is mf1 and t is mf1 and s is mf0 THEN -r*0.181756+t*0.034938+s*0.023866-0.749197
	IF r is mf1 and t is mf0 and s is mf0 THEN -r*0.026206+t*0.079974+s*0.147433-0.568073
	IF r is mf1 and t is mf1 and s is mf1 THEN -r*0.001481+t*0.000987-s*0.004933-0.883753
	IF r is mf0 and t is mf1 and s is mf1 THEN -r*0.018590-t*0.003683-s*0.001895+0.368105
	IF r is mf0 and t is mf0 and s is mf1 THEN -r*0.019436-t*0.011035+s*0.009854+0.507347
	IF r is mf1 and t is mf0 and s is mf1 THEN -r*0.003335+t*0.007968-s*0.011000-0.468688

Table C.6: Possible naming conventions for membership functions.

Model	**Linguistic Variables**			
	r	**t**	**s**	**ss**
Identified membership functions by Model3	mf0→ *Close*	mf0→ *Close*	mf0→ *Flat*	mf0→ *Bad*
	mf1→ *Average*	mf1→ *Average*	mf1→ *Gentle*	mf1→ *Average*
	mf2→ *Far*	mf2→ *Far*	mf2→ *Moderate*	mf2→ *Good*
	mf3→ *VeryFar*	mf3→ *VeryFar*	mf3→ *Steep*	
Identified membership functions by Model11	mf0→ *Close*	mf0→ *Close*	mf0→ *Gentle*	
	mf1→ *Far*	mf1→ *Far*	mf1→ *Moderate*	

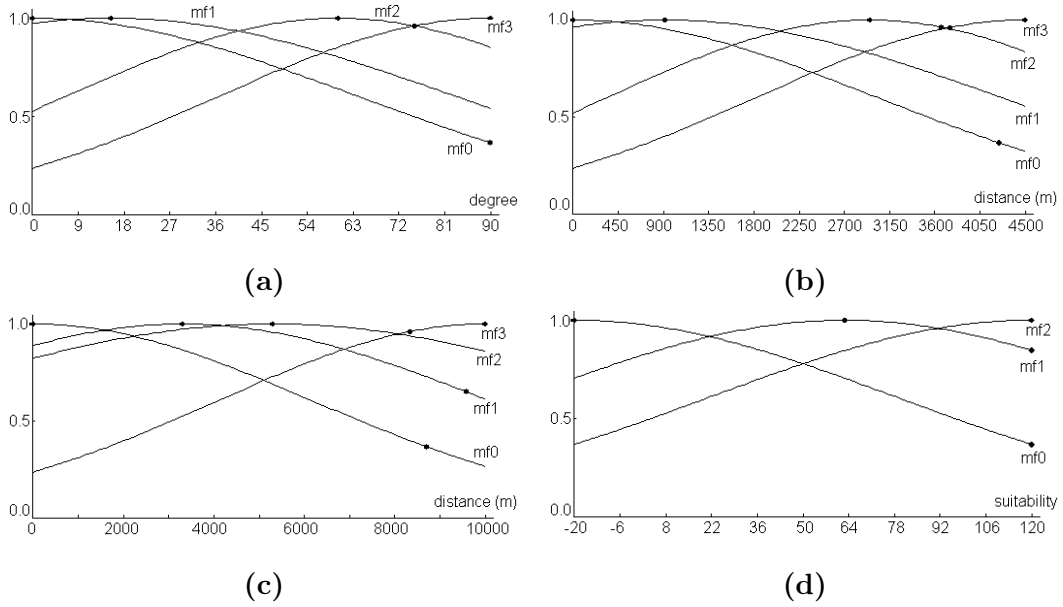


Figure C.3: Identified membership functions by Model3 (a) Slope, (b) Distance to road, (c) Distance to town, and (d) Suitability.

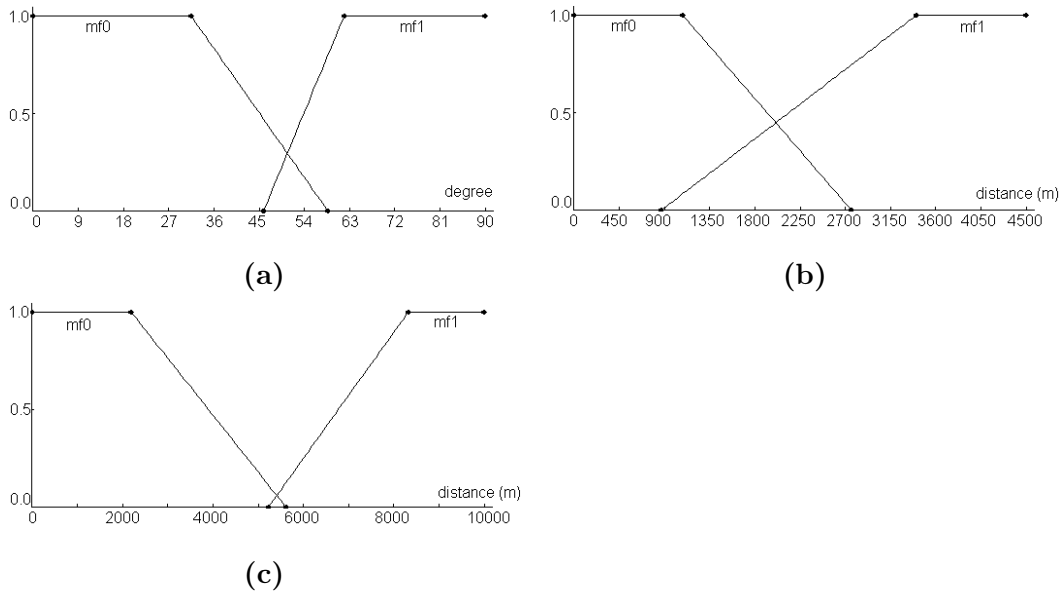


Figure C.4: Identified membership functions by Model11 (a) Slope, (b) Distance to road, and (c) Distance to town.

C.5 Discussion

Enhancing GIS operations with fuzzy set theory enables GIS user to design decision rules in the decision-making processes easier. Suitable fuzzy system for the decision problem can be built by using prior knowledge or experts' experiences. However, it is very difficult for human experts to build spatial analysis rules if the decision problem to be modeled is high dimensional. Even in some cases, it is quite difficult to adequately describe the solution steps, especially when the spatial nature of the phenomena is not entirely known. In such cases, based on observed input-output data for the phenomena decision models can be estimated.

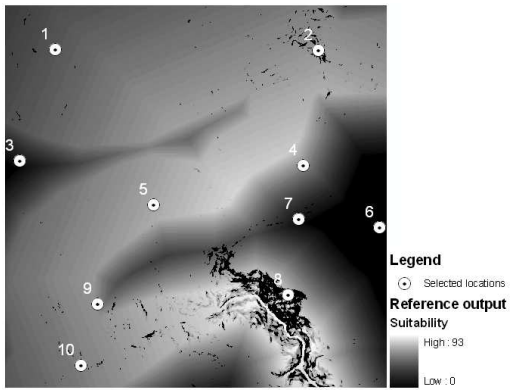
In this work, the combinations of neural networks and fuzzy systems, neuro-fuzzy systems, were examined since they can construct a set of fuzzy if-then rules with appropriate membership functions using input-output pairs. Neuro-fuzzy systems were trained with fuzzy measures calculated from GIS-based fuzzy inference system, FuzzyCell, against input data. Birecik region data were used for training. Then, prediction performances of constructed neuro-fuzzy models were tested with data from Bartın region. According to test metrics Model3 produced better predictions for NEFPROX system and Model11 produced better predictions for ANFIS system. Original output and outputs produced by best methods for NEFPROX and ANFIS systems are given in Figure C.5. To compare the values of reference output and outputs produced by best methods for NEFPROX and ANFIS systems, ten locations were randomly selected and associated values are given in Table C.7.

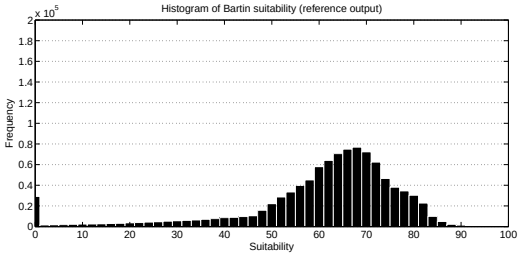
The best neuro-fuzzy model for the decision problem to be modeled could be found by trying many models and selecting the configuration which gives the smallest error value. However, in this work the actual fuzzy rule base was known previously. Therefore, selection of the neuro-fuzzy model properties was based on this prior knowledge.

In the training phase, all models based on ANFIS system produced better prediction performance metrics than NEFPROX based models. Although ANFIS models yield better approximation results for training data set, they did not produce as good results in the test data set as in the training data set. Moreover, best predictor for the test data set was based on NEFPROX system. This can be due to the generalization ability of the systems.

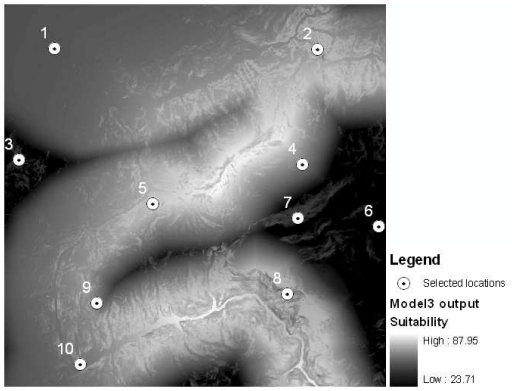
Since Sugeno-type systems trained by computationally demanding training algorithms based on gradient descent or least square technique, training time for ANFIS models were longer. On the other hand, prediction times for all models were almost similar. Moreover, prediction took much less time when compared to training phase.

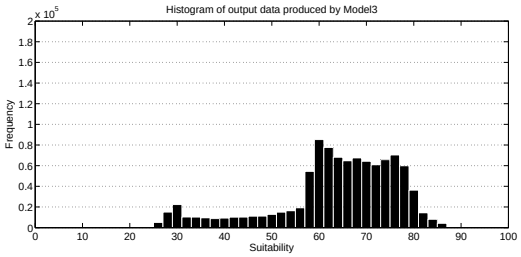
Produced outputs by neuro-fuzzy models, especially by NEFPROX, have some parts on the region which were overestimated. Especially, there are regions estimated as suitable by some degree where these regions are actually not suitable (i.e. suitability value is zero in the original image). However, there is a trade-off between interpretability and performance. Very good approximations may be achieved by other identification techniques but with less interpretable rule bases. Moreover, compared to ANFIS models, NEFPROX models gave more interpretable solutions. ANFIS models can represent Sugeno-type fuzzy models, which are not as easy to interpret as Mamdani models which NEFPROX can also represent (Nauck and Kruse, 1999). However, NEFPROX models did not always construct small and interpretable rule base. In such cases, human expert can further process the



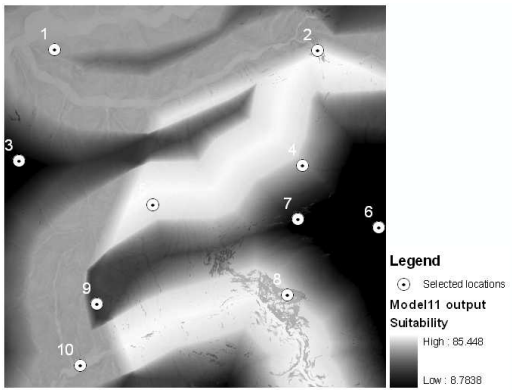


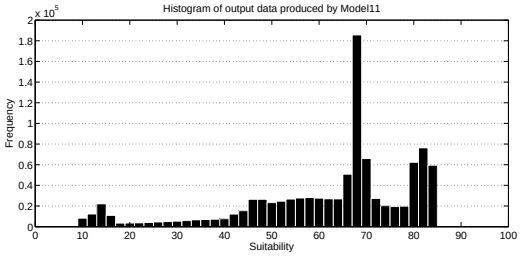
(a)





(b)





(c) **(d)**

Figure C.5: Graphs for (a) Bartın suitability (original output), (b) Suitability data produced by NEFPROX type model, Model3, (c) Suitability data produced by ANFIS type model, Model11, and (d) Histograms of suitability values.

Table C.7: Selected suitability values.

Location	Reference suitability	Suitability produced by Model3	Suitability produced by Model11
1	55	59.129	65.891
2	0	73.428	74.088
3	33	51.922	19.642
4	68	66.318	67.662
5	75	78.650	82.500
6	0	35.214	13.443
7	32	46.956	21.678
8	0	69.094	71.294
9	69	66.476	43.808
10	66	65.323	70.610

rules to produce more interpretable and more manageable (small number of rules) rule base. To produce more interpretable rule bases, learning algorithm should be constrained such that adjacent membership functions do not pass each other during training, may become asymmetric, or have a certain degree of overlapping (Nauck and Kruse, 1999). In Section C.4.4, the comparison of rule bases based on their interpretability would be more meaningful, if the constraint certain degree of overlapping has been implemented in the NEFPROX.

C.6 Conclusion

Fuzzy set theory is introduced into GIS to obtain more flexibility and more effective capability of handling and processing imprecise information about the real world. By enhancing GIS operations with fuzzy logic methodologies, the GIS user can approximate complex ill-defined problems in decision-making processes by capturing decision rules from experts' experiences in the form of fuzzy if-then rules. Fuzzy system properties, which consist of fuzzy if-then rules, input and output linguistic variables, membership function types and membership function parameters, can be selected depending on the problem (Robinson, 2003). Parameters, rules and all other choices forming a fuzzy system may be different for problems. Variety of results can be obtained by using different combinations of choices. Identifying a suitable fuzzy system for a given problem can be done by prior knowledge (i.e. experts' experiences), by learning from input-output data pairs, or by combination of both. Neuro-fuzzy methods can construct a set of fuzzy if-then rules with appropriate membership functions by means of learning methods obtained from neural networks.

This paper examined the use of neuro-fuzzy systems for decision-making problems of GIS by measuring their prediction accuracies and time required for learning and prediction. ANFIS and NEFPROX systems were used to construct rule base and membership function parameters for decision-making problems. These two systems were trained with input-output data pairs where output data were calculated by GIS-based fuzzy inference system. Then, constructed rule base and membership function parameters were compared with rule base and membership function parameters of GIS-based fuzzy inference system. While identifying a suitable fuzzy system, both prediction accuracy and interpretability of driven rule base are important. Since NEFPROX system implements Mamdani-

type fuzzy system, it produced more interpretable results. However, rules constructed by NEFPROX system still require human expert for further processing such as pruning, when used for GIS-based decision-making problems.

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APPENDIX D

FUZZY MODEL TUNING USING SIMULATED ANNEALING

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Submitted to Expert Systems with Applications

D.1 Abstract

This paper presents the use of simulated annealing metaheuristic for tuning Mamdani type fuzzy models. Structure of the Mamdani fuzzy model is learned from input-output data pairs using Wang and Mendel's method (Wang and Mendel, 1992) and fuzzy c-means clustering algorithm. Then, parameters of the fuzzy system are tuned through simulated annealing. In this paper, we perform experiments to examine effects of a) initial solution generated by Wang and Mendel's method and fuzzy c-means clustering method, b) membership function update procedure, c) probability parameter for the calculation of the initial temperature, d) temperature update coefficient used for cooling schedule, and e) randomness level in the disturbance mechanism used in simulated annealing algorithm on the tuning of Mamdani type fuzzy models. Experiments are performed with Mackey-Glass chaotic time series (Mackey and Glass, 1977). The results indicate that Wang and Mendel's method provides better starting configuration for simulated annealing compared to fuzzy c-means clustering method, and for the membership function update parameter, $MFChangeRate \in (0, 1]$, and the probability parameter for the calculation of the initial temperature, $P_0 \in (0, 1)$, values close to zero produced better results.

Keywords: Simulated annealing, Optimization, Fuzzy model tuning, Mamdani fuzzy model, Fuzzy model extraction

D.2 Introduction

Fuzzy systems based on fuzzy if-then rules are being used successfully for modeling of nonlinear, uncertain and complex systems. Fuzzy rules can be obtained from experts' knowledge. However, there is no standard method available for transforming experts' knowledge into the database of fuzzy systems (Jang, 1993; Yen and Langari, 1999; Yanar, 2003). In addition, expert rules are not sufficient to define complex partially unknown systems satisfactorily (Guillaume and Charnomordic, 2004).

Therefore, various methods have been applied to fuzzy systems for automatically generating and adjusting if-then rules (Jang, 1993; Guillaume and Charnomordic, 2004; Yen and Wang, 1998; Emami et al., 1998; Wang and Mendel, 1992; Shi and Mizumoto, 2000; Chen and Linkens, 2004; Jin, 2000; Nauck and Kruse, 1999; Guely et al., 1999).

Among the data driven, automatic fuzzy rule generation and tuning methods there are local optimization methods such as gradient descent algorithm and global optimization methods such as simulated annealing and genetic algorithms. Simulated annealing (SA) is an iterative search method inspired by the annealing of metals (Kirkpatrick et al., 1983; Cerny, 1985). It simulates the annealing of metal where annealing is a strategy to find optimum state by controlling the temperature. The technique starts with heating a metal to a temperature near its melting point and then the metal is cooled slowly by keeping at each stage temperature in sufficient duration. The method of controlling the temperature decrease leads to a stable crystallized solid state which corresponds to an obsolete minimum of energy. SA introduces a control parameter, temperature, in optimization and searches for global optimum by gradually decreasing the temperature similar to real annealing technique. Compared to gradient descent, simulated annealing has two advantages: simulated annealing is able to find the global minimum of the function to optimize under certain conditions (Aarts and Laarhoven, 1985; Hajek, 1988; Hajek and Sasaki, 1989; Kan and Timmer, 1987a,b) and it can handle any cost function. However its convergence speed is low unlike gradient descent. Moreover, since gradient descent based algorithms use derivatives they are mostly applied to Sugeno (Takagi and Sugeno, 1985) type fuzzy systems. These models are not as interpretable as Mamdani (Mamdani and Assilian, 1975) type fuzzy models since they use rules with linear models as consequents. For learning and tuning of fuzzy models global optimization methods such as simulated annealing (Mohamadi et al., 2008; Ghazanfari et al., 2007; Cordon et al., 2000; Liu and Yang, 2000; Cheng and Chen, 1997) and genetic algorithms (Antonelli et al., 2009; Marquez et al., 2007; Cordon and Herrera, 2001; Cordon et al., 2001; Roubos and Setnes, 2001; Setnes and Roubos, 2000) are also used. On the other hand, simulated annealing convergence has been demonstrated under more general assumptions than genetic algorithm (Aarts and Laarhoven, 1985) and genetic algorithm convergence depends on the way of coding parameters into genes.

This paper utilizes simulated annealing algorithm to fine-tune Mamdani type fuzzy models and reports experiments performed to determine the effects of simulated annealing parameters on the final prediction error. The proposed approach was tested with a chaotic time series given by Mackey-Glass differential equation. In the first experiment we generated two sets of rule bases. One set was created using fuzzy c-means clustering algorithm and the other set was generated by ad hoc data driven Wang and Mendel's method (Wang and Mendel, 1992). Then, the proposed approach was used to fine-tune the obtained rule bases. Tuned rule bases were evaluated using their prediction accuracies on test data and one rule base was selected for further testing the sensitivity of parameters involved in simulated annealing on final prediction accuracy. In our last experiment, we showed the random nature of the simulated annealing algorithm.

The paper is organized as follows. Section D.3 briefly describes generation of fuzzy-if then rules from input-output data, Section D.4 introduces simulated annealing method and describes the use

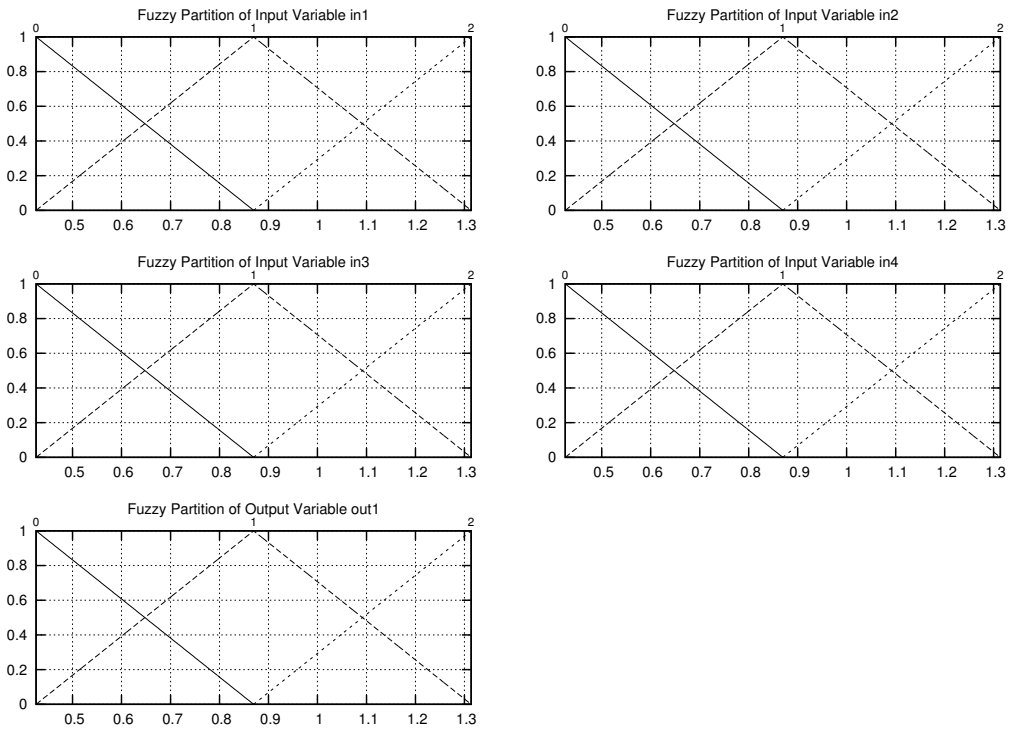

Figure D.1: Triangular fuzzy membership functions created by WM-method.

of simulated annealing for tuning parameters of a Mamdani fuzzy system whose structure is automatically generated from data, experiment results and discussions are reported in Section D.5 and conclusions are given in Section D.6.

D.3 Structure Learning

Fuzzy if-then rules and the number of fuzzy sets for each variable define the structure of a fuzzy system (Nauck, 2005). Structure of a fuzzy system can be given by experts or can be generated from data. For automatic rule generation from data there are three kinds of methods: the first kind uses a grid partitioning of the multidimensional space, the second kind uses clustering methods and the third kind uses a hybrid methods which utilize soft computing techniques (Guillaume, 2001).

In this study, two sets of rule bases were generated. This first set of rule bases were generated by Wang and Mendel's method (WM-method). Each variable of input and output space were divided into a number of (3, 5, 7, 10, 13, 16 and 20) symmetrical triangular membership fuzzy sets. Then fuzzy rules were generated using data as proposed by Wang and Mendel (1992). The second sets of rule bases were generated using fuzzy c-means (Dunn, 1973) (FCM) clustering algorithm. In FCM clustering space partitioning is derived from data partitioning and rule is associated to each cluster. To completely define rules, clustering was applied to input-output data where premise corresponds to input part and conclusion corresponds to the output part. The second set of rule bases also include rule bases with 3, 5, 7, 10, 13, 16 and 20 triangular membership fuzzy sets, like the first set.

Table D.1: Rules generated by WM-method

IF ((in1 is mf1) and (in2 is mf2) and (in3 is mf2) and (in4 is mf2)) THEN out1 is mf1
IF ((in1 is mf1) and (in2 is mf2) and (in3 is mf2) and (in4 is mf1)) THEN out1 is mf1
IF ((in1 is mf2) and (in2 is mf2) and (in3 is mf2) and (in4 is mf1)) THEN out1 is mf1
IF ((in1 is mf2) and (in2 is mf2) and (in3 is mf1) and (in4 is mf1)) THEN out1 is mf0
IF ((in1 is mf2) and (in2 is mf1) and (in3 is mf1) and (in4 is mf1)) THEN out1 is mf1
IF ((in1 is mf2) and (in2 is mf1) and (in3 is mf1) and (in4 is mf0)) THEN out1 is mf1
IF ((in1 is mf1) and (in2 is mf1) and (in3 is mf1) and (in4 is mf0)) THEN out1 is mf1
IF ((in1 is mf1) and (in2 is mf1) and (in3 is mf1) and (in4 is mf1)) THEN out1 is mf1
IF ((in1 is mf1) and (in2 is mf1) and (in3 is mf0) and (in4 is mf1)) THEN out1 is mf1
IF ((in1 is mf1) and (in2 is mf0) and (in3 is mf1) and (in4 is mf1)) THEN out1 is mf2
IF ((in1 is mf1) and (in2 is mf0) and (in3 is mf1) and (in4 is mf2)) THEN out1 is mf2
IF ((in1 is mf1) and (in2 is mf1) and (in3 is mf1) and (in4 is mf2)) THEN out1 is mf2
IF ((in1 is mf0) and (in2 is mf1) and (in3 is mf1) and (in4 is mf2)) THEN out1 is mf2
IF ((in1 is mf0) and (in2 is mf1) and (in3 is mf2) and (in4 is mf2)) THEN out1 is mf2
IF ((in1 is mf1) and (in2 is mf1) and (in3 is mf2) and (in4 is mf2)) THEN out1 is mf2
IF ((in1 is mf2) and (in2 is mf2) and (in3 is mf1) and (in4 is mf0)) THEN out1 is mf0
IF ((in1 is mf2) and (in2 is mf1) and (in3 is mf0) and (in4 is mf0)) THEN out1 is mf1
IF ((in1 is mf1) and (in2 is mf1) and (in3 is mf0) and (in4 is mf0)) THEN out1 is mf1
IF ((in1 is mf1) and (in2 is mf0) and (in3 is mf0) and (in4 is mf1)) THEN out1 is mf1
IF ((in1 is mf0) and (in2 is mf0) and (in3 is mf1) and (in4 is mf1)) THEN out1 is mf1
IF ((in1 is mf0) and (in2 is mf1) and (in3 is mf1) and (in4 is mf1)) THEN out1 is mf2
IF ((in1 is mf1) and (in2 is mf1) and (in3 is mf2) and (in4 is mf1)) THEN out1 is mf1
IF ((in1 is mf1) and (in2 is mf2) and (in3 is mf1) and (in4 is mf1)) THEN out1 is mf1
IF ((in1 is mf2) and (in2 is mf2) and (in3 is mf2) and (in4 is mf2)) THEN out1 is mf1

Table D.2: Rules generated by FCM-method

IF ((in1 is mf0) and (in2 is mf0) and (in3 is mf0) and (in4 is mf0)) THEN out1 is mf0
IF ((in1 is mf1) and (in2 is mf1) and (in3 is mf1) and (in4 is mf1)) THEN out1 is mf1
IF ((in1 is mf2) and (in2 is mf2) and (in3 is mf2) and (in4 is mf2)) THEN out1 is mf2

Membership functions created by both WM-method and FCM-method for three membership fuzzy set case are shown as example in Figure D.1 and Table D.2, respectively. Rules generated by the methods are given in Table D.1 and Table D.2.

D.4 Parameter Tuning Using SA

SA is considered as a metaheuristic. It does not guarantee finding an optimal solution. However, under certain constraints (Aarts and Laarhoven, 1985; Hajek, 1988; Hajek and Sasaki, 1989; Kan and Timmer, 1987a,b) SA probably converges towards a global optimum with a probability arbitrarily close to unity (Dreo et al., 2006). The SA algorithm is given in Figure D.3. SA starts with an initial solution which can be a randomly selected point within the search space of all the possible solutions. Current solution in search space is evaluated by an objective function. Objective function (evaluation function) measures the energy of the current solution. A new solution near the current solution is selected from the search space using disturbance mechanism. If energy of the newly selected solution is less than the current solution, then newly selected solution is accepted as the current solution. On

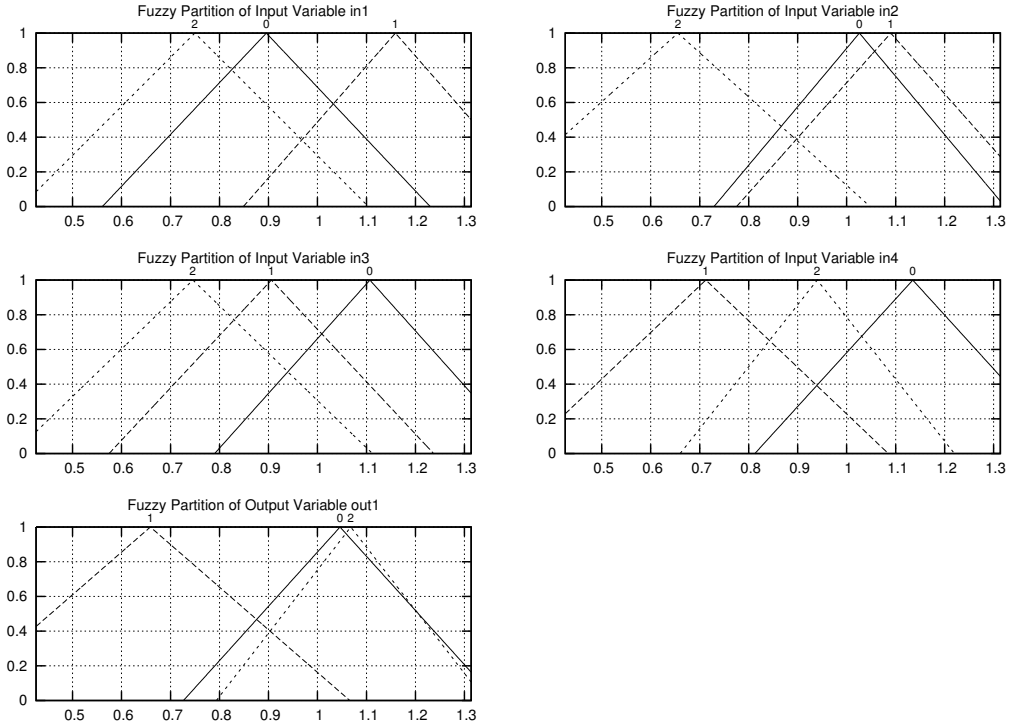

Figure D.2: Triangular fuzzy membership functions created by FCM-method.

```
Simulated_Annealing()
Begin
1. Choose an initial temperature, T.
2. Generate an initial solution, X.
3. Repeat
3.1. Repeat
3.1.1. Generate a new solution Y, near to X
3.1.2. If E(Y) < E(X) Then accept new solution
3.1.2.1. X = Y
3.1.3. Else use Metropolis acceptance rule
 for decision
3.1.4. If Metropolis_Acceptance(E(Y), E(X), T)
    returns true Then accept new solution
3.1.4.1. X = Y
3.2 Until temperature stage length is reached
3.3. Update T
4. Until T ≥ T_final
End
```

Figure D.3: Simulated annealing algorithm.

```
Metropolis_Acceptance(E_new, E_cur, T)
// E_new is the energy of the new solution.
// E_cur is the energy of the current solution.
// T is the current temperature.
Begin
1. Calculate change in energy, ΔE = E_new − E_cur
2. Calculate acceptance probability, p(T) = e^(−ΔE/T)
3. If Random(0, 1) < p(T) Then
3.1. Accept solution (return true)
4. Else
4.1. Reject solution (return false)
End
```

Figure D.4: Metropolis acceptance rule.

the contrary, if energy of the newly selected solution is higher than the energy of the current solution, SA does not automatically reject new candidate solution. Instead, it uses Metropolis Acceptance Criterion (Metropolis et al., 1953). Metropolis Acceptance Criterion will accept the new solution on a probabilistic basis. Bad moves in the search space are accepted with probability $p(T)$.

$$p(T) = e^{-\Delta E/T} \tag{D.1}$$

ΔE is the change in energy and T defines the temperature of the current configuration. Metropolis rule of acceptance is realized as in the following: a real number is drawn at random between 0 and 1. New solution causing ΔE change in the objective function is accepted if the random number drawn is lower than $p(T)$. At higher temperature probability of accepting bad configurations $p(T)$ is high, close to 1, therefore majority of the moves are accepted. At low temperature, $p(T)$ is low, close to 0, majority of the bad moves are rejected. Metropolis acceptance rule is given in Figure D.4.

SA starts with high temperature then initial temperature is reduced according to the selected cooling schedule. At each temperature SA performs selected number of iterations (i.e., temperature stage length) to allow the algorithm to settle into a balanced state.

Outline of the proposed approach for parameter tuning using SA is presented as follows:

Initial Solution: SA starts with an initial solution which was obtained from structure learning algorithm. Initial configuration which contains fuzzy if-then rules and initial membership function parameters for Mamdani fuzzy system was automatically generated from input-output data using WM-method and FCM-method. Both structure learning methods provide a good starting point for SA.

In the first experiment, we started with 7 different initial solutions obtained from both methods and reported final error values reached after optimizations.

Initial Temperature: Initial temperature was calculated using the method described by Wong and Liu (1986). According to the Metropolis rule of acceptance SA accepts an energy rise (worse solution), h, with probability $p(T)$ given in Equ. D.1 where T is the current temperature. The initial temperature, T_0, can be calculated from mean energy rises, h_{mean}, during the initialization. Before the start of the actual SA, the mean value of energy rises is estimated by a constant number of moves.

Then, initial temperature T_0 is calculated using the following formula. The formula is derived from the Metropolis function.

$$T_0 = \frac{-h_{mean}}{In(P_0)} \tag{D.2}$$

Selecting the initial probability, P_0, near to 1 allows SA to start with a high temperature and accepting worse solutions with high probability. If the initial probability, P_0, is adjusted near to 0 then SA starts with a low temperature which accepts worse solutions with low probability.

The initial solution was obtained from structure learning algorithms described above and we did not want to alter this initial knowledge too much therefore we wish to keep the initial probability, P_0, of accepting worse solutions low (Guely et al., 1999).

In the third experiment, the effect of initial probability, P_0, of accepting worse solution parameter on the final error was tested with all other parameters kept the same.

Objective Function: Output calculated from the tuned fuzzy system at current temperature can be evaluated using root mean square error (RMSE). Therefore, objective function to minimize was RMSE. Since, SA can use any cost function, any function measuring error between calculated output and target values can be used. However, evaluation function calculation must be direct and rapid to increase SA convergence speed and to decrease CPU consumption.

Disturbance Mechanism: SA can be used to solve many combinatorial optimization problems and some continuous variable problems (Bonomi and Lutton, 1984). Optimizing the parameters of fuzzy systems is a continuous variable problem. For selecting a new solution near the current solution in the search space, we introduce a change interval for each parameter which defines allowable minimum and maximum percentage of changes that can be made to each parameter. At each move, each parameter is changed proportional to the change rate randomly chosen in the interval $[-maxchangerate, +maxchangerate]$, where maxchangerate was calculated based on the current temperature. As the temperature decreases maxchangerate decreases. Therefore, at high temperatures each parameter has wider allowable change interval while at the lower temperatures allowable change interval is narrow.

In the second experiment, we tested optimization algorithm with different values of the change interval. Other parameters of the optimization algorithm were kept the same.

Decrease of the Temperature: The geometrical law of decrease $T_{k+1} = \alpha T_k$, where k defines temperature stage number and α is a constant between 0 and 1, was used to perform temperature decrease.

In the forth experiment, different values of cooling rate were used with all other parameters kept the same.

Temperature Stage Length: After performing a constant number of iterations at each temperature, temperature is decreased according to the cooling strategy.

Termination of SA algorithm: SA algorithm can be terminated when the temperature reaches the final temperature or after 3 successive temperature stages without any acceptance. Since our aim is to show the use of SA algorithm instead of finding a suitable model for test data, we terminated the SA algorithm after 100 iterations, which can be considered as a constant stopping criterion.

Table D.3: SA model parameters used in the experiments

SA Model Parameters	**Ranges of Parameters**
Initial solution	WM-method / FCM-method
Probability parameter for the calculation of the initial temperature, P_0	$0.03 \leq P_0 \leq 0.50$ (allowable range is $0 < P_0 < 1$)
Objective function	RMSE
Membership function update parameter, MFChangeRate, used for disturbance mechanism	$0.01 \leq MFChangeRate \leq 0.20$ (allowable range is $0 < MFChangeRate \leq 1$)
Temperature update parameter, α	$0.80 \leq \alpha \leq 0.99$ (allowable range is $0 < \alpha < 1$)
Temperature stage length	Rule base parameter count* $\times$ 2
Termination of SA algorithm	100 iterations

* Parameter counts for the rule bases are given in Table D.4 and Table D.5.

D.5 Experiments and Results

In the experiments, the proposed approach was tested with a chaotic time series given by Mackey-Glass differential equation. We performed five experiments. In the first four experiments, we examined the effects of initial solutions generated by the structure learning algorithms, membership function change interval, probability parameter for the calculation of the initial temperature and temperature update coefficient used in simulated annealing algorithm on the tuning of Mamdani type fuzzy models. Last experiment is divided into two parts. In the first part, we showed the random nature of the algorithm and in the second part we proposed an alternative disturbance mechanism to reduce randomness of the algorithm.

D.5.1 Test Data and Simulated Annealing Model Parameters

Proposed approach for constructing a Mamdani fuzzy system from data was tested with a chaotic time series given by Mackey-Glass differential equation (Mackey and Glass, 1977).

$$\dot{x}(t) = \frac{0.2x(t-\tau)}{1+x^{10}(t-\tau)} - 0.1x(t) \tag{D.3}$$

The problem consists of predicting future values of the series. In the experiments, the values $x(t-18)$, $x(t-12)$, $x(t-6)$ and $x(t)$ were used to predict $x(t+6)$. To obtain time series data Runge-Kutta method with 0.1 time step was used. Initial conditions for the time series were $x(0) = 1.2$ and $\tau = 17$. From Mackey-Glass time series 1000 input-output data pairs were generated between $t = 118$ and 1117. The first 500 data pair was used for training and the remaining 500 data pair was used for testing.

SA model parameters used in the experiments are summarized in Table D.3.

D.5.2 Experiment-1

In the first experiment, we examine the effect of initial solutions on the tuning of the Mamdani type fuzzy models. Initial solutions were generated by structure leaning methods namely WM-Method

Table D.4: Properties of rule bases generated by WM-method

Rule base name	Input fuzzy set count*	Output fuzzy set count*	Rule count	Parameter count
grid-3mf-Test1	3	3	24	45
grid-5mf-Test1	5	5	68	75
grid-7mf-Test1	7	7	116	105
grid-10mf-Test1	10	10	213	150
grid-13mf-Test1	13	13	304	195
grid-16mf-Test1	16	16	355	240
grid-20mf-Test1	20	20	413	300

* All linguistic variables have the same fuzzy set count.

Table D.5: Properties of rule bases generated by FCM-method

Rule base name	Input fuzzy set count*	Output fuzzy set count*	Rule count	Parameter count
fcm-3mf-Test1	3	3	3	45
fcm-5mf-Test1	5	5	5	75
fcm-7mf-Test1	7	7	7	105
fcm-10mf-Test1	10	10	10	150
fcm-13mf-Test1	13	13	13	195
fcm-16-mf-Test1	16	16	16	240
fcm-20mf-Test1	20	20	20	300

* All linguistic variables have the same fuzzy set count.

and FCM-Method. We generated 7 rule bases with WM-method. Each variable of input and output space were divided into symmetrical triangular membership fuzzy sets. Rule base properties generated by WM-method are given in Table D.4. The second sets of rule bases were generated using FCM-method. In order to define rules completely, clustering was applied to input-output data, where premise corresponds to input part and conclusion corresponds to the output part. Rule base properties generated by FCM-method are given in Table D.5. As an example for the generated rule bases, rule base created by WM-method "grid-3mf-Test1" and rule base "fcm-3mf-Test1" generated by FCM-method are shown in Figure D.1 and Figure D.2 respectively. Generated rules by the methods are given in Table D.1 and Table D.2. Generated fuzzy systems "grid-3mf-Test1" and "fcm-3mf-Test1" have 36 (i.e., $4 \times 3 \times 3$) premise parameters, 9 (i.e., $1 \times 3 \times 3$) consequent parameters and a total of 45 parameters.

Fuzzy systems learned from training data were used as initial solution for SA to optimize. Optimization starts with the calculation of the initial error and the initial temperature. To calculate initial temperature specified number of moves (i.e., temperature stage length) was made and the mean value of energy rises was estimated for each rule bases. Then, initial temperature T_0 was calculated with the selected initial probability as 25%. We chose initial probability near zero since we did not want to alter initial solution too much. Membership function change rate was selected as 2%, temperature update coefficient was chosen as 0.90 and we chose temperature stage lengths as twice of the parameter counts. Optimizations were ended after 100 iterations.

At each temperature stage SA performs selected number of iterations (i.e., temperature stage

Table D.6: Training and test data errors after optimization

Rule base name	Initial training error	Initial testing error	Final training error	Final testing error
grid-3mf-Test1	0.182128832717001	0.181332938414955	0.051293974826460	0.050551617372790
fcm-3mf-Test1	0.140500698321958	0.139089028431362	0.078924371420670	0.077601009623490
grid-5mf-Test1	0.067090942695495	0.065354930169926	0.037904107964340	0.037353257338010
fcm-5mf-Test1	0.113075237211503	0.110560368543713	0.064353429271540	0.063513924539640
grid-7mf-Test1	0.046433363724616	0.046199259813711	0.026913527065960	0.026855596131330
fcm-7mf-Test1	0.098854033131716	0.097474551961004	0.037469200208330	0.037606564592140
grid-10mf-Test1	0.032135461828215	0.030864573734693	0.020737285054710	0.022538351721490
fcm-10mf-Test1	0.078020749645363	0.075967057552711	0.021278026505080	0.021800062794140
grid-13mf-Test1	0.020227422404703	0.019976078411097	0.018415298211630	0.019595607238630
fcm-13mf-Test1	0.070818362261285	0.070954972110349	0.028628477201970	0.029525150198400
grid-16mf-Test1	0.017113632074282	0.017062889146294	0.020417443199310	0.022326597589060
fcm-16-mf-Test1	0.064910666069115	0.062670491780502	0.034262130245540	0.036598162900300
grid-20mf-Test1	0.015203573427025	0.014667227384729	0.019685296335970	0.021934103329990
fcm-20mf-Test1	0.057035467905985	0.056325876910200	0.022451010716630	0.024077184923930

length). At each move, to find a new solution near to the current solution, we changed each parameter of membership function belonging to each linguistic variable. We used 3 parameters (a, b, c) for triangular membership functions as given by Equ. D.4.

$$triangle(x : a, b, c) = \begin{cases} 0 & x < a \\ (x-a)/(b-a) & a \leq x \leq b \\ (c-x)/(c-b) & b \leq x \leq c \\ 0 & x > c \end{cases} \tag{D.4}$$

The parameters a and c locate the "feet" of the triangle and the parameter b locates the "peak". Each parameter of triangular membership functions were changed as follows: a random value is drawn between $[-0.5, +0.5]$. The effect of random value is reduced allowing only 1% change at a move (i.e., membership function change rate $\times$ a random value between $[-0.5, +0.5]$). Then, change rate is decreased by multiplying with the temperature decrease from the beginning of SA. Therefore, at the highest temperature maximum allowed change in each parameter was $\pm 1\%$ of the parameter value. As the temperature decreases, change in parameters decreases proportional to the temperature decrease. Training and test data errors after optimization are given in Table D.6 and final error values are presented graphically in Figure D.5. Generally structures learned using WM-method have less initial error values on both training and test data sets, only exception is the 3 membership fuzzy set case. Since rule bases learned using WM-method provide better starting configuration for SA algorithm, they have less final error values. On the other hand, error values of rule bases learned using FCM-method were changed more. Moreover, SA could not produce better solutions for rule bases "grid-16mf-Test1" and "grid-20mf-Test1".

Rule base "grid-13mf-Test1" has the best error value for test data, however SA algorithm could not tune rule base much. Therefore, we chose "fcm-10mf-Test1" rule base for the remaining tests since this rule base produces the second best error value for test data. Another factor for choosing "fcm-10mf-Test1" rule base was the execution time. Each linguistic variable in rule base "grid-13mf-Test1"

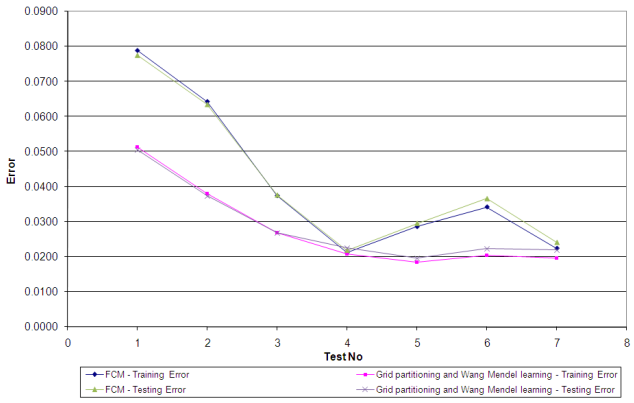

Figure D.5: Training and test data errors after optimization.

has 13 membership fuzzy sets and the rule base contains 304 rules, while each linguistic variable in rule base "fcm-10mf-Test1" has 10 membership fuzzy sets and the rule base contains only 10 rules. Therefore, optimization of rule base "grid-13mf-Test1" requires 37 times more execution time. Iterations took 1295.5736641 seconds for rule base "fcm-10mf -Test1", on the other hand time required for SA algorithm for "grid-13mf-Test1" rule base was 48394.4190356 seconds on Intel® Core™ 2 Quad Q6600 2.40GHz CPU machine with 2GB RAM (Windows®2003 Server SP2 platform).

D.5.3 Experiment-2

In the SA algorithm pseudo code shown in Figure D.3, Step 3.1.1 selects a new solution near to the current solution in the search space. To generate a new solution based on the current solution, an update for each parameter is calculated at each move. Update parameter is calculated using a random value which is drawn between $[-0.5, +0.5]$, membership function change rate which is given by the user as an optimization parameter and the current temperature as given in Equ. D.5.

$$\begin{aligned} \Delta Change &= Random(-0.5, +0.5) \\ &* MFChangeRate * \frac{T_{current}}{T_{initial}} \end{aligned} \tag{D.5}$$

At the initial temperature allowed change for each parameter is high. As the temperature decreases, change in parameters decreases proportional to the temperature decrease.

In the second experiment, our aim is to investigate the effect of the membership function change rate (MFChangeRate) on the proposed optimization. In this experiment, 20 different MFChangeRate parameters were used for optimization of rule base "fcm-10mf-Test1". Other parameters were selected as: 100 iterations for SA algorithm iteration count, 300 moves for temperature stage length, 0.90 for temperature update coefficient and 25% for initial probability of acceptance. Training and test data errors after optimization are given in Table D.7 and final error values are presented graphically in Figure D.6.

Although error values obtained after optimization show peaks and falls, there is an evidence for an increase in error values as the membership function change rate increases especially after membership

Table D.7: Membership function update parameter, MFChangeRate, values used in the SA algorithm and obtained error values after optimization

Test name	MFChange rate	Final training error	Final testing error
fcm-10mf-Test2-1	0.01	0.032580760211814	0.034482933503751
fcm-10mf-Test2-2	0.02	0.032591948510532	0.033392132982630
fcm-10mf-Test2-3	0.03	0.045522215875877	0.045283773571063
fcm-10mf-Test2-4	0.04	0.037250221958866	0.037111686343773
fcm-10mf-Test2-5	0.05	0.046859342753061	0.049512942168226
fcm-10mf-Test2-6	0.06	0.055710873762785	0.057387104672936
fcm-10mf-Test2-7	0.07	0.038593190277779	0.037691760335007
fcm-10mf-Test2-8	0.08	0.049405986659366	0.049606681226335
fcm-10mf-Test2-9	0.09	0.035560052878913	0.035040584929122
fcm-10mf-Test2-10	0.10	0.065161201280302	0.066034531924431
fcm-10mf-Test2-11	0.11	0.070715231866115	0.072737568138272
fcm-10mf-Test2-12	0.12	0.072491758454550	0.071444260694880
fcm-10mf-Test2-13	0.13	0.057367859895025	0.056450062456253
fcm-10mf-Test2-14	0.14	0.077969900413780	0.080257029618051
fcm-10mf-Test2-15	0.15	0.069258076957214	0.068363297497902
fcm-10mf-Test2-16	0.16	0.078020749645363	0.075967057552711
fcm-10mf-Test2-17	0.17	0.069279254319482	0.070267892090533
fcm-10mf-Test2-18	0.18	0.059555069215372	0.058699548712191
fcm-10mf-Test2-19	0.19	0.078020749645363	0.075967057552711
fcm-10mf-Test2-20	0.20	0.078020749645363	0.075967057552711

Figure D.6: Training and test data errors after optimization.

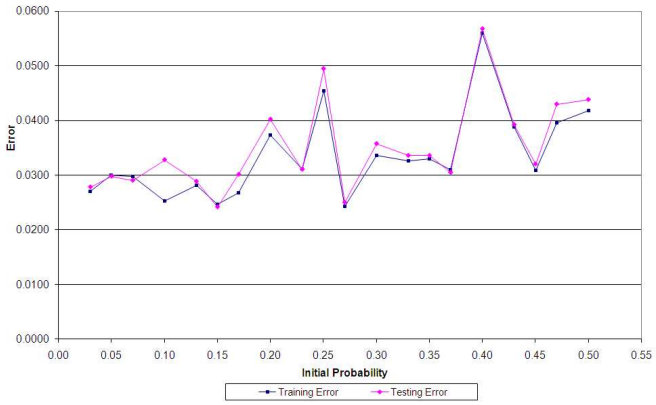

Figure D.7: Training and test data errors after optimization.

function change rate values above 0.09. Lowest error value on test data is obtained when membership function change rate is 0.02.

D.5.4 Experiment-3

Initial temperature can be given by the user or it can be calculated according to the probability, also chosen by the user. In this experiment, initial probability was given by the user to compute the initial temperature. Before starting the actual SA algorithm, a number of moves (i.e., temperature stage length) in the neighborhood of the initial rule base are made and new solutions are evaluated. During the initialization, mean value of energy rises, h_{mean}, is calculated using the formula given by Equ. D.6.

$$h_{mean} = \frac{1}{M_{bad}} \sum_{i=1}^{M_{bad}} \Delta Error_{bad} \tag{D.6}$$

where $\Delta Error_{bad}$ defines the energy rise of a bad move and M_{bad} is the number of bad moves made. Then, initial temperature T_0 is calculated using the formula given by Equ. D.2.

The user can start with a high temperature to accept worse solutions with high probability by tuning the probability, P_0, near to 1 or user can adjust P_0 near to 0 to start with a low temperature which accepts worse solutions with low probability. Starting with a low temperature is appropriate if user do not want to alter initial knowledge too much.

In the third experiment, the effect of initial probability, P_0, parameter was examined. In the experiment, 20 different probability parameters were used for optimization of rule base "fcm-10mf-Test1". Other parameters were selected as: 100 iterations for SA algorithm iteration count, 300 moves for temperature stage length, 0.90 for temperature update coefficient and 2% for membership function change rate. Training and test data errors after optimization are given in Table D.8 and final error values are presented graphically in Figure D.7.

Error values obtained after optimization show peaks and falls. Lowest error value on test data is obtained when probability is 0.15.

Table D.8: Probability parameter values, P_0, used for the calculation of the initial temperature and obtained error values after optimization

Test name	**Probability** P_0	**Final training error**	**Final testing error**
fcm-10mf-Test3-1	0.03	0.027049552287911	0.027869527137647
fcm-10mf-Test3-2	0.05	0.029956197338474	0.029829660111646
fcm-10mf-Test3-3	0.07	0.029706767182239	0.029079298999509
fcm-10mf-Test3-4	0.10	0.025233256318947	0.032839207577676
fcm-10mf-Test3-5	0.13	0.028108383024951	0.028903550365257
fcm-10mf-Test3-6	0.15	0.024723257924412	0.024207541432082
fcm-10mf-Test3-7	0.17	0.026744231653214	0.030178560416393
fcm-10mf-Test3-8	0.20	0.037303580573930	0.040250130879308
fcm-10mf-Test3-9	0.23	0.031059031170019	0.031098828253451
fcm-10mf-Test3-10	0.25	0.045389565363614	0.049498884978027
fcm-10mf-Test3-11	0.27	0.024294366227691	0.025061559123040
fcm-10mf-Test3-12	0.30	0.033570963106261	0.035780452130748
fcm-10mf-Test3-13	0.33	0.032578269279932	0.033617406936935
fcm-10mf-Test3-14	0.35	0.033021769309479	0.033618519921317
fcm-10mf-Test3-15	0.37	0.030999547372159	0.030512401946027
fcm-10mf-Test3-16	0.40	0.055932345066092	0.056781686915067
fcm-10mf-Test3-17	0.43	0.038780551326288	0.039264913365340
fcm-10mf-Test3-18	0.45	0.030843584680606	0.032059942003109
fcm-10mf-Test3-19	0.47	0.039539665936664	0.043011251124456
fcm-10mf-Test3-20	0.50	0.041774049038074	0.043849155959658

D.5.5 Experiment-4

In the SA algorithm pseudo code shown in Figure D.3, Step 3.3 updates temperature according to cooling strategy. In this work, geometrical law of decrease $T_{k+1} = \alpha T_k$, where k defines temperature stage number and α is the cooling rate parameter, $0 < \alpha < 1$, was used to perform temperature decrease. High cooling rate parameter leads to an excessive calculation time and low cooling rate parameter leads to the risk of evolving to a local minimum. In the experiment, α took values between $[0.80, 0.99]$.

In this experiment, the effect of α coefficient on the proposed optimization algorithm was examined. In the experiment, 20 different coefficients were used for optimization of rule base "fcm-10mf-Test1". Other parameters were selected as: 100 iterations for SA algorithm iteration count, 300 moves for temperature stage length, 2% for membership function change rate and 25% for initial probability of acceptance. Training and test data errors after optimization are given in Table D.9 and final error values are presented graphically in Figure D.8.

Although error values obtained after optimization show peaks and falls, there is an evidence for a decrease in error values as the coefficient value increases. On the other hand, there are some exceptional behaviors when coefficient values are 0.80, 0.85, 0.93 and 0.95. Lowest error value on test data is obtained when coefficient value is 0.97.

Table D.9: Temperature update parameter values, α, and obtained error values after optimization

Test name	α **coefficient**	**Final training error**	**Final testing error**
fcm-10mf-Test4-1	0.99	0.029026835077074	0.028326832465250
fcm-10mf-Test4-2	0.98	0.027777197636446	0.028659410138441
fcm-10mf-Test4-3	0.97	0.025672519214074	0.026026204822291
fcm-10mf-Test4-4	0.96	0.029759235867780	0.029996045236807
fcm-10mf-Test4-5	0.95	0.035546402545102	0.034864868319703
fcm-10mf-Test4-6	0.94	0.028193049851985	0.028270533502236
fcm-10mf-Test4-7	0.93	0.033324398812754	0.032960821576594
fcm-10mf-Test4-8	0.92	0.028136847672635	0.028029401015691
fcm-10mf-Test4-9	0.91	0.027984092493318	0.031211528735725
fcm-10mf-Test4-10	0.90	0.033322404863300	0.035016758634859
fcm-10mf-Test4-11	0.89	0.031917133745359	0.034114345905790
fcm-10mf-Test4-12	0.88	0.032445720605595	0.036761924729329
fcm-10mf-Test4-13	0.87	0.042040335158929	0.042430370726941
fcm-10mf-Test4-14	0.86	0.043826190250623	0.047584086162179
fcm-10mf-Test4-15	0.85	0.030392062758001	0.033358291518275
fcm-10mf-Test4-16	0.84	0.044645825142355	0.047110705252473
fcm-10mf-Test4-17	0.83	0.042474735507536	0.045331511498727
fcm-10mf-Test4-18	0.82	0.037630542191324	0.040724213443291
fcm-10mf-Test4-19	0.81	0.046103484209897	0.046745444622349
fcm-10mf-Test4-20	0.80	0.031979527957012	0.032640376540650

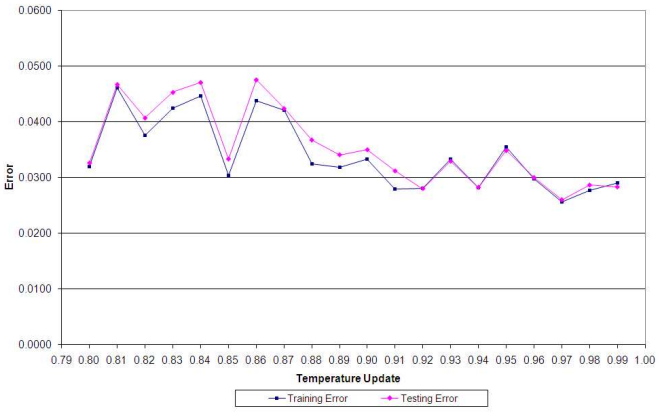

Figure D.8: Training and test data errors after optimization.

Table D.10: Training and test data errors after optimization

Test name	Final training error	Final testing error
fcm-10mf-Test5-1	0.031564486466301	0.031939684155499
fcm-10mf-Test5-2	0.022802840902982	0.023854559444832
fcm-10mf-Test5-3	0.030791731337729	0.031700077977207
fcm-10mf-Test5-4	0.020406376159823	0.020755203606649
fcm-10mf-Test5-5	0.023315952668870	0.024805128019452
fcm-10mf-Test5-6	0.025216722161838	0.026244743972233
fcm-10mf-Test5-7	0.024890721224761	0.025693350438340
fcm-10mf-Test5-8	0.024289979042150	0.026386516004149
fcm-10mf-Test5-9	0.031672059511228	0.031247557712458
fcm-10mf-Test5-10	0.024287407133265	0.024036721748655
fcm-10mf-Test5-11	0.025208654527442	0.026268854848332
fcm-10mf-Test5-12	0.020950259310876	0.021568865747721
fcm-10mf-Test5-13	0.028185466084554	0.028492139168233
fcm-10mf-Test5-14	0.024660307337206	0.025378469188651
fcm-10mf-Test5-15	0.018035446685474	0.017910462862281
fcm-10mf-Test5-16	0.021542658515521	0.021227765585768
fcm-10mf-Test5-17	0.016470763553281	0.016084958995410
fcm-10mf-Test5-18	0.026104224437659	0.026002423878585
fcm-10mf-Test5-19	0.024386712821907	0.025077005563244
fcm-10mf-Test5-20	0.020379414613201	0.020536928120313

D.5.6 Experiment-5

Since SA algorithm uses Metropolis Acceptance Criterion, it accepts worse solutions on a probabilistic basis. Therefore, results obtained from the algorithm may vary when the algorithm executed several times:

1. with different "seeds" for the generation of the random numbers,
2. with different initial configurations.

This experiment investigates the random nature of the algorithm. In the experiment, we used two different disturbance mechanisms to examine their effect on the final solutions. Therefore, we divided the experiment in two parts. In both parts of the experiment, the rule base "fcm-10mf-Test1" was used as initial solution and the algorithm was executed 20 times with the same initial solution and with the same parameters but with different seeds. Other parameters were selected as: 100 iterations for SA algorithm iteration count, 300 moves for temperature stage length, 2% for membership function change rate, 0.97 for temperature update coefficient and 15% for initial probability of acceptance.

Part1

In the first part, each parameter of a triangular membership function was changed during the generation of the new solution near to the current solution, as discussed in Section D.5.2. According to the disturbance mechanism all linguistic variables, all membership functions of each linguistic variable and all parameters of each membership function were changed. Training and test data errors after optimization are given in Table D.10 and final error values are presented graphically in Figure D.9.

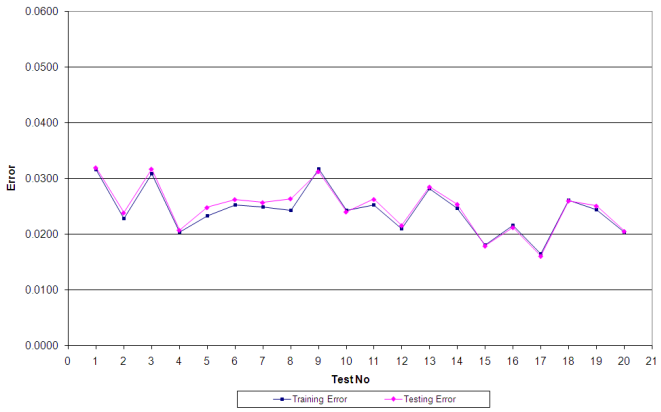

Figure D.9: Training and test data errors after optimization.

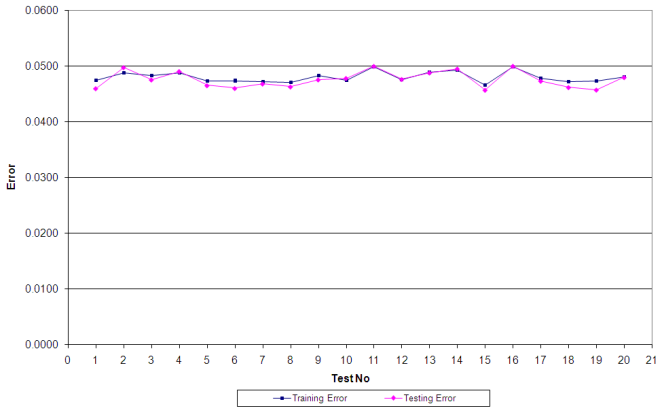

Figure D.10: Training and test data errors after optimization.

Although initial solution and all the parameters were the same, SA algorithm generated different tuned solutions with different seeds. Minimum and maximum error values for the test data are 0.016470763553281 and 0.031672059511228 respectively. Average error value for the test data is 0.024258109224803, where standard deviation is calculated as 0.004122075.

Part2

If we change disturbance mechanism in such a way that it alters less parameter, then results should not vary as the results obtained in the previous part. In the second part, only one membership function of one linguistic variable was changed. Linguistic variable and membership function was selected randomly. Each parameter of the membership function was changed as in the previous part. Training and test data errors after optimization are given in Table D.11 and final error values are presented graphically in Figure D.10.

In the second part, variation in the final solutions is decreased. As we decrease the number of changed parameters (i.e, as we decrease randomness of the algorithm), variation in the final solutions

Table D.11: Training and test data errors after optimization

Test name	Final training error	Final testing error
fcm-10mf-Test5-1	0.047528509468113	0.045970628326737
fcm-10mf-Test5-2	0.048747128906402	0.049712415319536
fcm-10mf-Test5-3	0.048369334423920	0.047528767895028
fcm-10mf-Test5-4	0.048768782612161	0.049011383074938
fcm-10mf-Test5-5	0.047394391155267	0.046507890548215
fcm-10mf-Test5-6	0.047424592345344	0.046009531275367
fcm-10mf-Test5-7	0.047288391081381	0.046802047863112
fcm-10mf-Test5-8	0.047155412732968	0.046281661714853
fcm-10mf-Test5-9	0.048314081192186	0.047533716220824
fcm-10mf-Test5-10	0.047494901529983	0.047789262605717
fcm-10mf-Test5-11	0.049856607977170	0.049943798781281
fcm-10mf-Test5-12	0.047638921685791	0.047612775582430
fcm-10mf-Test5-13	0.048855344137112	0.048768356490588
fcm-10mf-Test5-14	0.049238604504681	0.049470142262899
fcm-10mf-Test5-15	0.046652646803224	0.045696866606049
fcm-10mf-Test5-16	0.049866553542626	0.049953206071869
fcm-10mf-Test5-17	0.047817223953570	0.047301631752595
fcm-10mf-Test5-18	0.047249673199303	0.046175690001018
fcm-10mf-Test5-19	0.047344129831350	0.045733860336663
fcm-10mf-Test5-20	0.048131985347495	0.047948254104687

is also decreased. Minimum and maximum error values for the test data are 0.046652646803224 and 0.049866553542626 respectively. Average error value for the test data is 0.048056860821502. Standard deviation is calculated as 0.000914823 which is only 2/9 of the standard deviation of the previous part.

D.6 Conclusion

The aim of this paper was to introduce SA metaheuristic for tuning Mamdani type fuzzy models. Structures of the fuzzy models were learned from input-output data using two different methods namely WM-Method and FCM-Method. Then, parameters of the fuzzy rule bases were tuned using SA. SA technique is a general method, it is easy to understand and implement, can use any cost function, unlike gradient descent methods SA can use any type of membership functions, it does not depend on fuzzy logic operators, implication, defuzzification functions, etc.

SA can be used to solve many combinatorial optimization problems and some continuous variable problems. Optimizing the parameters of fuzzy rule bases is a continuous variable problem. Therefore, a specific method was needed for discretization of each parameter.

SA technique involves many parameters such as initial temperature, rate of decrease of the temperature, length of the temperature stages, termination criterion, etc. Although there are some methods to obtain them, generally they depend on the problem, therefore finding method requires empirical testing. In this paper we experiment with a) initial solution generated by WM-Method and FCM-Method, b) membership function update procedure, c) probability parameter for the calculation of the initial temperature, d) temperature update coefficient used for cooling schedule, and e) randomness

level in the disturbance mechanism used in the SA algorithm. Both WM-Method and FCM-Method provided good starting solutions to tune. Although WM-Method generated better initial solutions, they contained too many rules which are very difficult to interpret and required extensive calculation time to tune. For membership function update parameter, $MFChangeRate \in (0, 1]$, and probability parameter for the calculation of the initial temperature, $P_0 \in (0, 1)$, values close to zero generally produced better results. This may be due to the quality of the initial solutions. Taking update coefficient small for temperature leads to the risk of evolving to a local minimum, while taking update coefficient high leads to excessive calculation time. In our forth experiment, we used the same rule base, the same parameters except from the update coefficient and we stopped optimization after a constant number of iterations therefore we did not notice the difference between the calculation times required for different update coefficients. On the other hand, high values of the update coefficients gave better results. In the last experiment, as we decrease the number of changed parameters, variation in the final solutions was also decreased.

The computing time required by the SA technique is high; especially at low temperatures SA is greedy. Therefore, to reduce computation time, SA can be used in conjunction with an algorithm of local type such as gradient descent etc. SA can be terminated at a user specified error value and then local optimizer can further search the optimum locally. However, this approach adds another parameter that needs to be determined.

In this work, interpretability of fuzzy system is not considered while generation and tuning of the fuzzy rule bases. Addition of interpretation ability to data driven fuzzy rule base generation and tuning method presented in this work can be addressed as a future work.

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APPENDIX E

SIMPLIFIED FUZZY MODELS

The effectiveness of triangular membership functions for linguistic variables "longitude" and "latitude" are given in Figure E.1, Figure E.2, Figure E.3, Figure E.4, Figure E.5 and Figure E.6. The centers of the membership functions are drawn black and indicate membership degrees equal to unity. Shades of gray represent the membership degrees between zero and one where whiter regions represent membership degrees close to zero.

Initial and simplified fuzzy models for FCM_{1p}, GK_{1p} and GK_{2p} are given in Figure E.7, Figure E.8, Figure E.9, Figure E.10, Figure E.11 and Figure E.12, respectively. Initial fuzzy models were created by fuzzy clustering techniques and simplified fuzzy models were obtained by applying simplification algorithm to initially created fuzzy models.

Figure E.1: Membership function “east” for linguistic variable “longitude”.

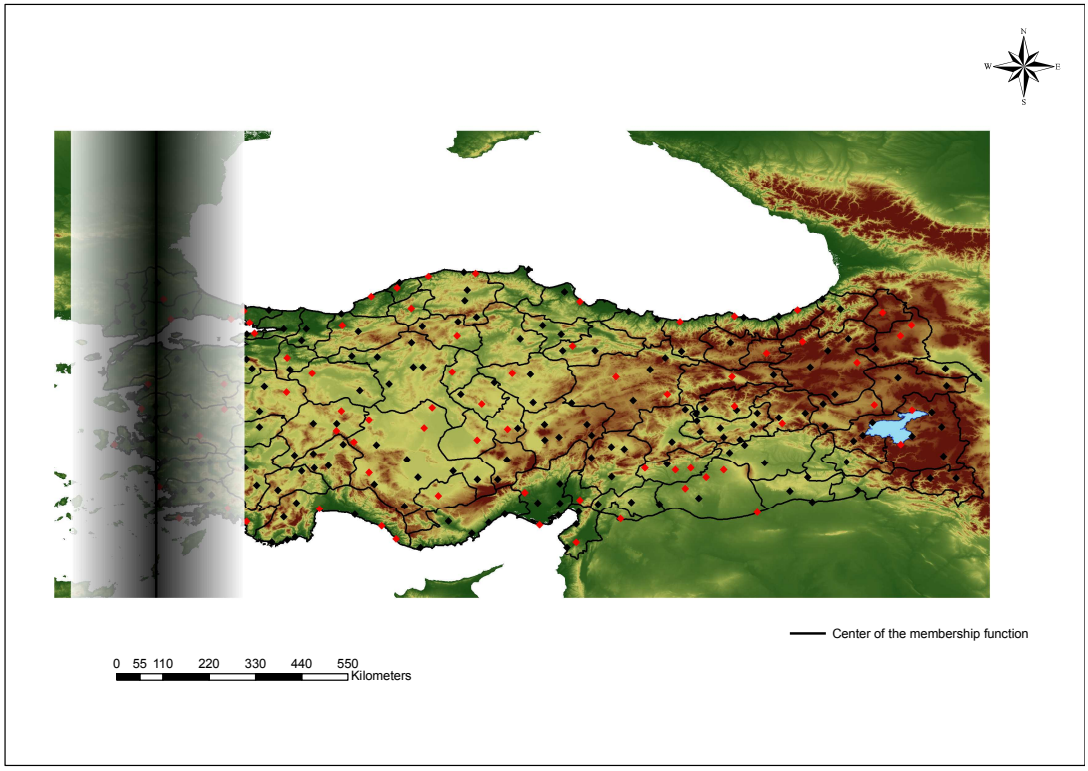

Figure E.2: Membership function “west” for linguistic variable “longitude”.

Figure E.3: Membership function “near-west” for linguistic variable “longitude”.

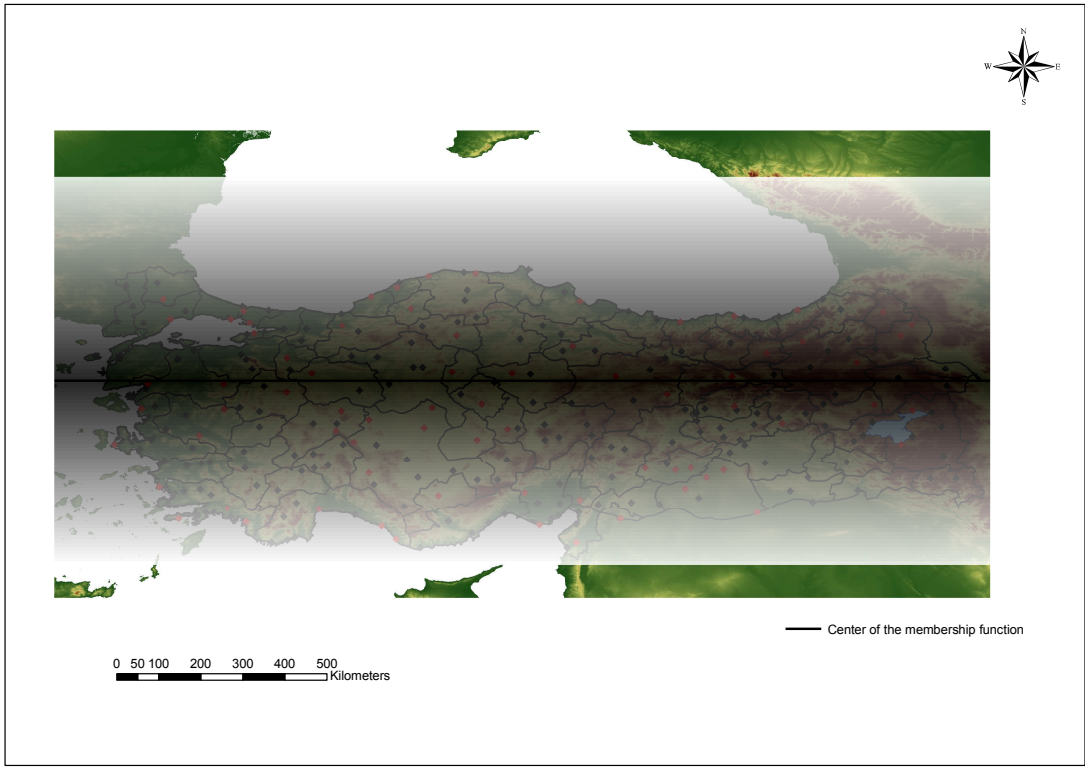

Figure E.4: Membership function “near-north” for linguistic variable “latitude”.

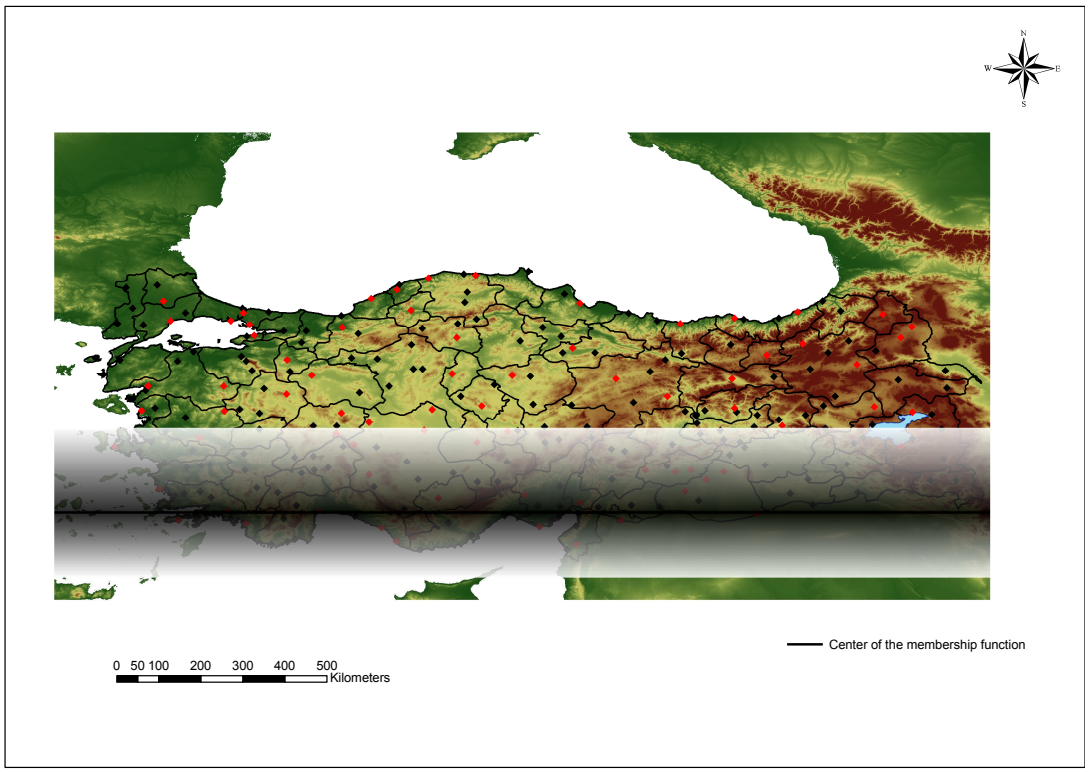

Figure E.5: Membership function “south” for linguistic variable “latitude”.

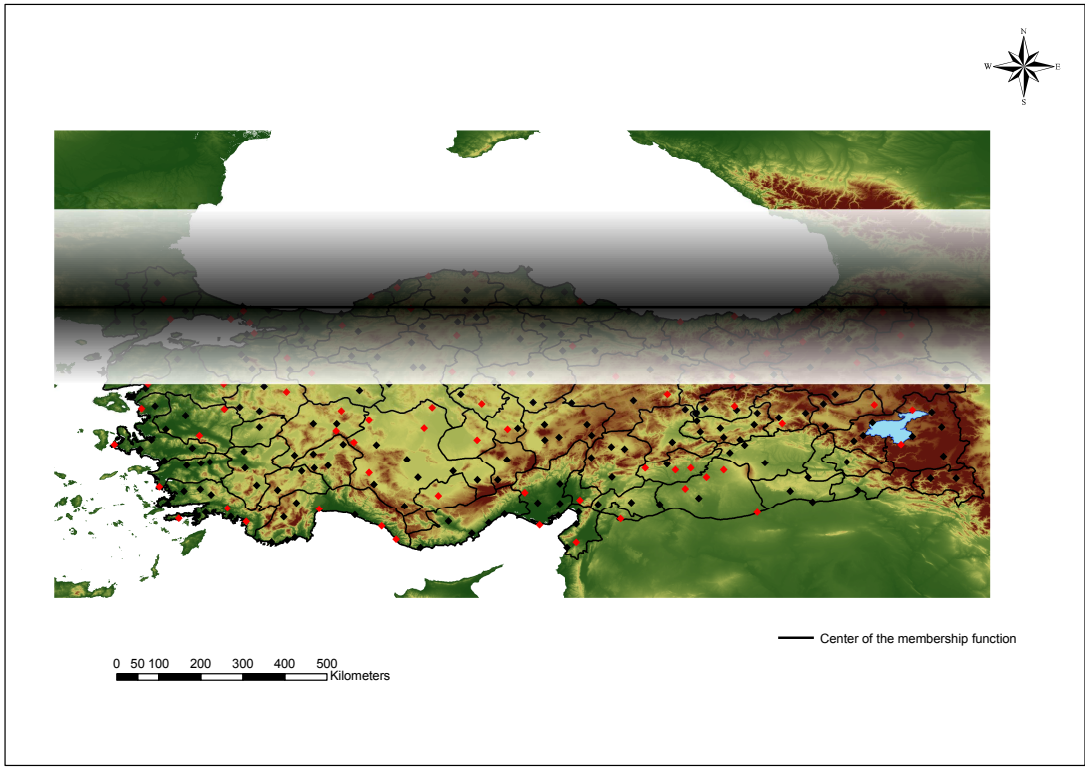

Figure E.6: Membership function “north” for linguistic variable “latitude”.

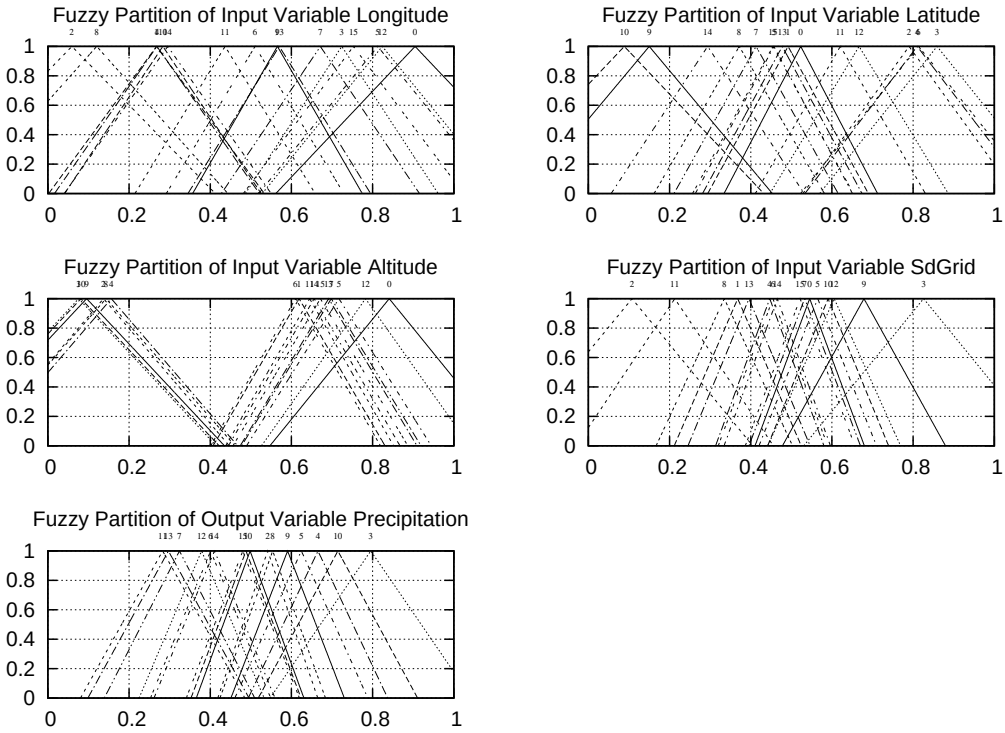

Figure E.7: Membership functions of initial fuzzy model FCM_{1p} before tuning. Initial fuzzy model rule base contains 16 rules.

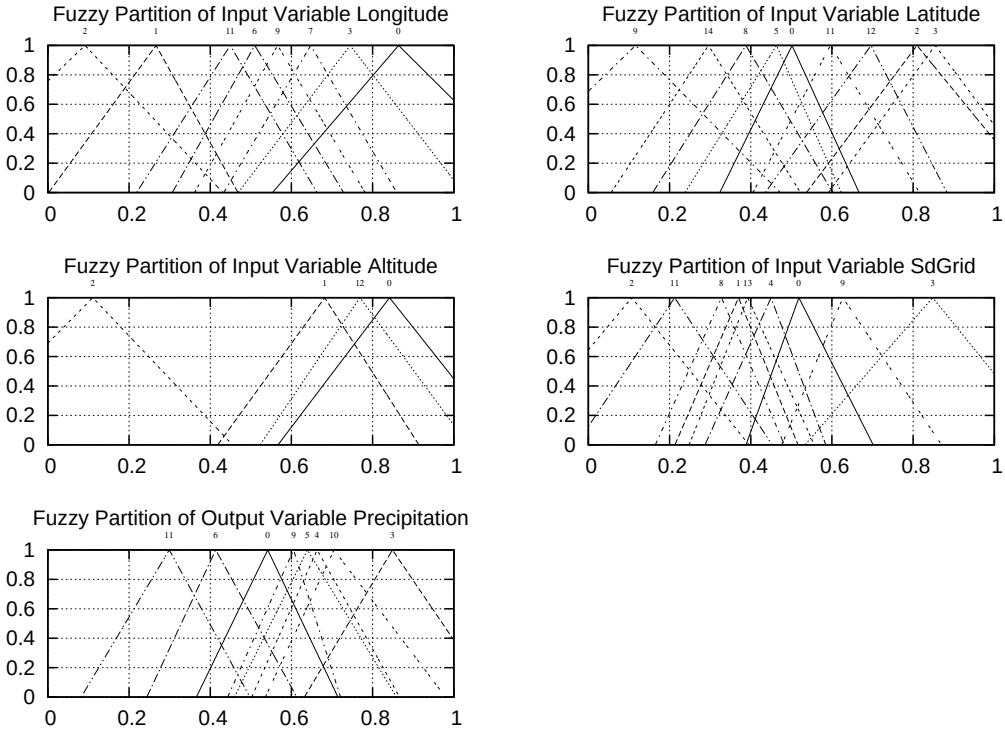

Figure E.8: Membership functions of simplified FCM_{1p} fuzzy model. Simplified fuzzy model rule base contains 15 rules.

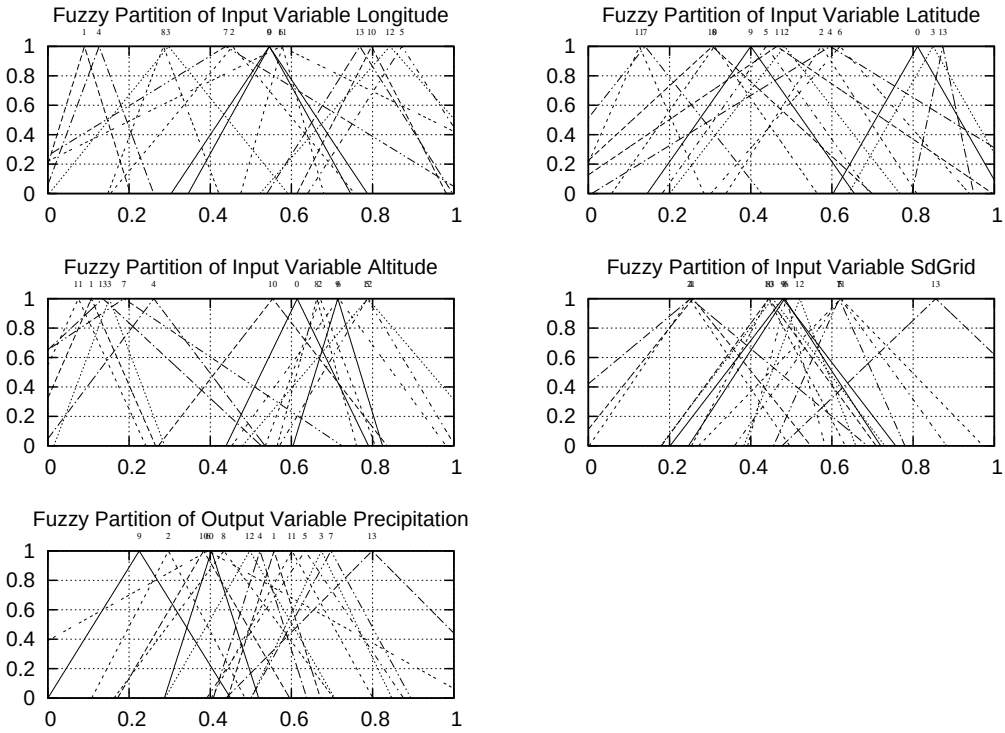

Figure E.9: Membership functions of initial fuzzy model GK_{1p} before tuning. Initial fuzzy model rule base contains 14 rules.

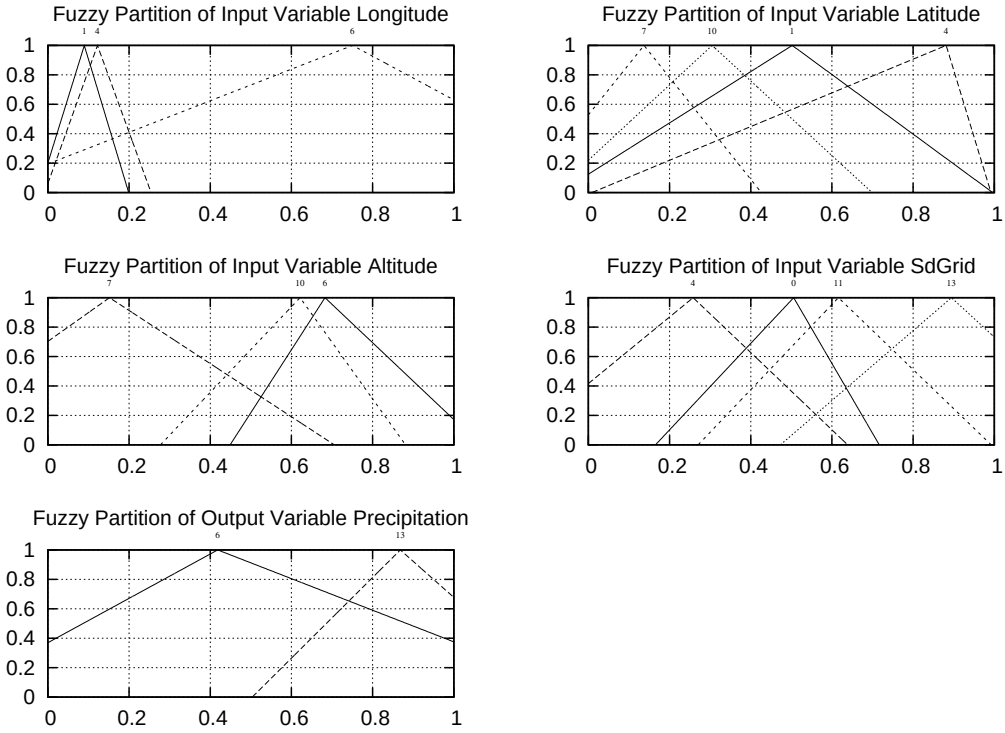

Figure E.10: Membership functions of simplified GK_{1p} fuzzy model. Simplified fuzzy model rule base contains 11 rules.

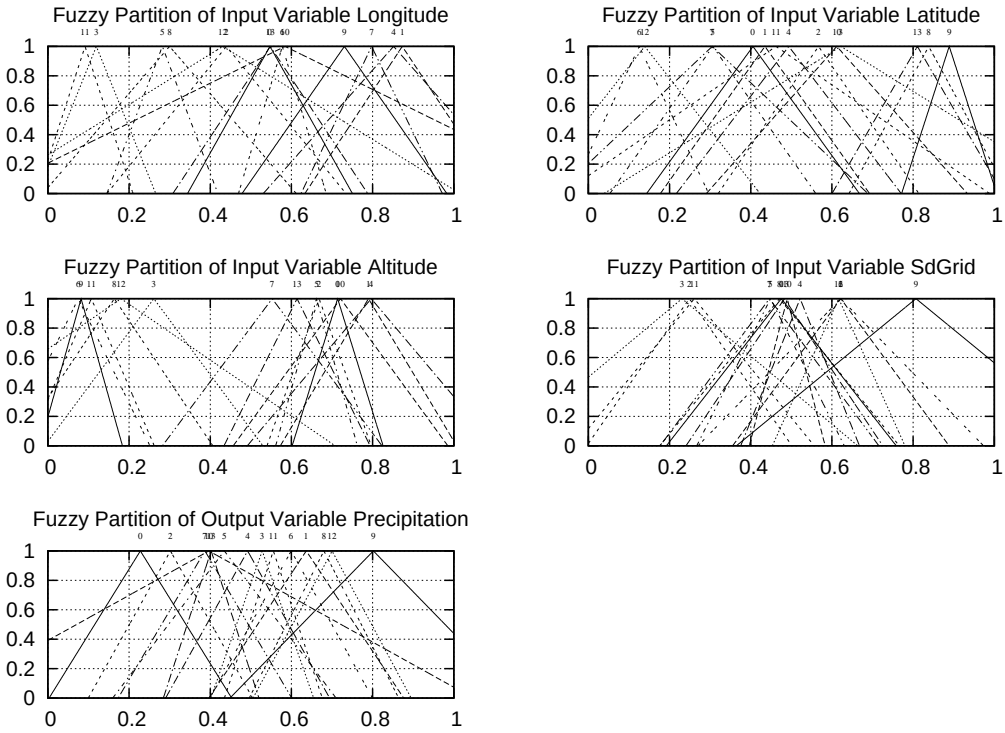

Figure E.11: Membership functions of initial fuzzy model GK_{2p} before tuning. Initial fuzzy model rule base contains 14 rules.

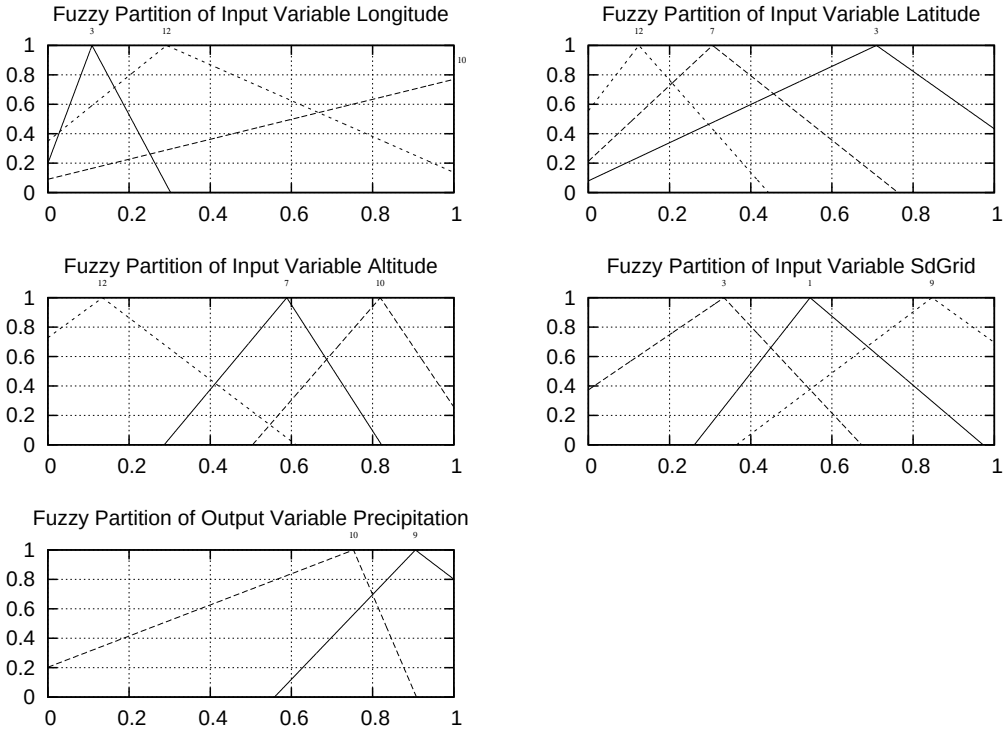

Figure E.12: Membership functions of simplified GK_{2p} fuzzy model. Simplified fuzzy model rule base contains 10 rules.

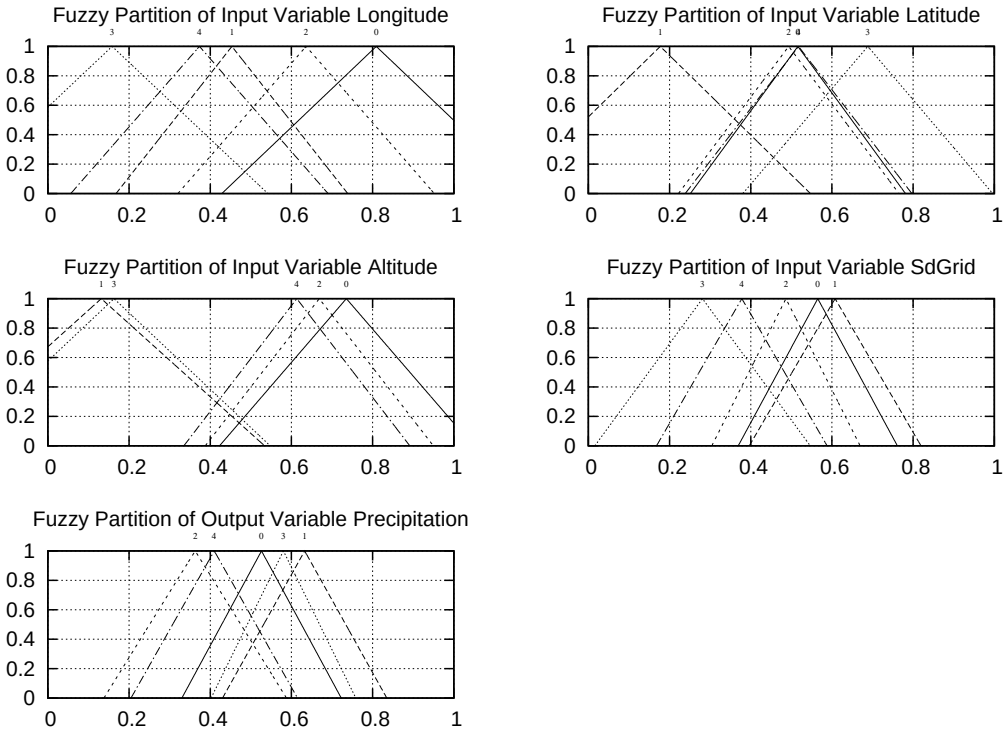

Figure E.13: Membership functions of initial fuzzy model FCM_{1p} before tuning. Initial fuzzy model is constructed with 5 clusters and it contains 5 rules.

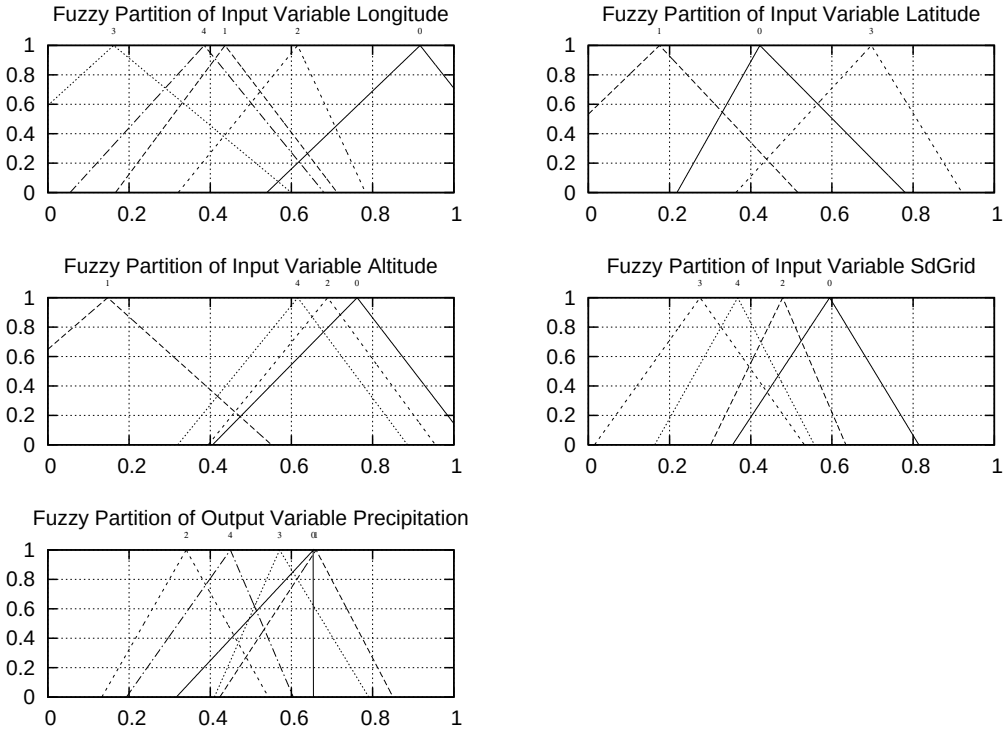

Figure E.14: Membership functions of simplified FCM_{1p} fuzzy model which are initially constructed with five clusters. Simplified fuzzy model rule base contains 5 rules.

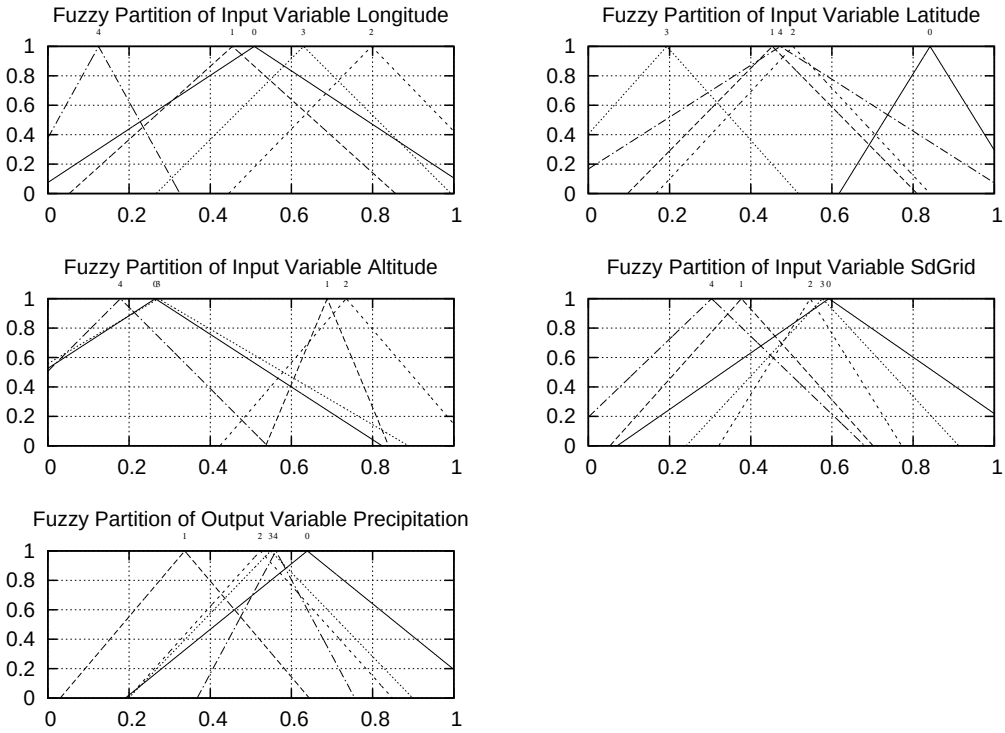

Figure E.15: Membership functions of initial fuzzy model GK_{1p} before tuning. Initial fuzzy model is constructed with 5 clusters and it contains 5 rules.

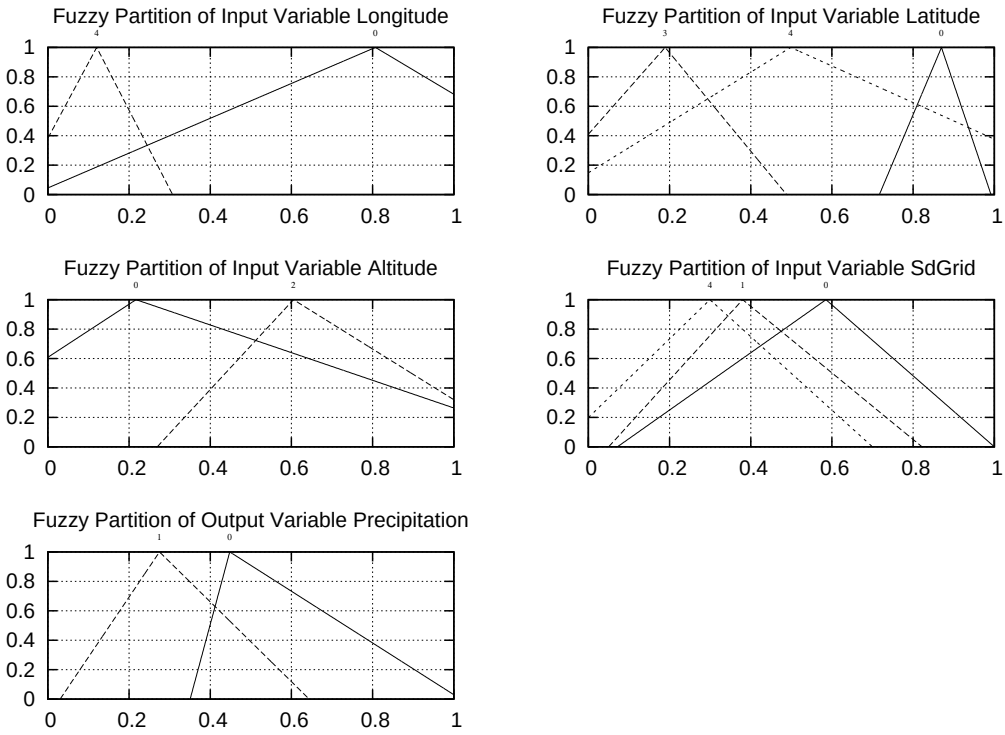

Figure E.16: Membership functions of simplified GK_{1p} fuzzy model which are initially constructed with five clusters. Simplified fuzzy model rule base contains 5 rules.

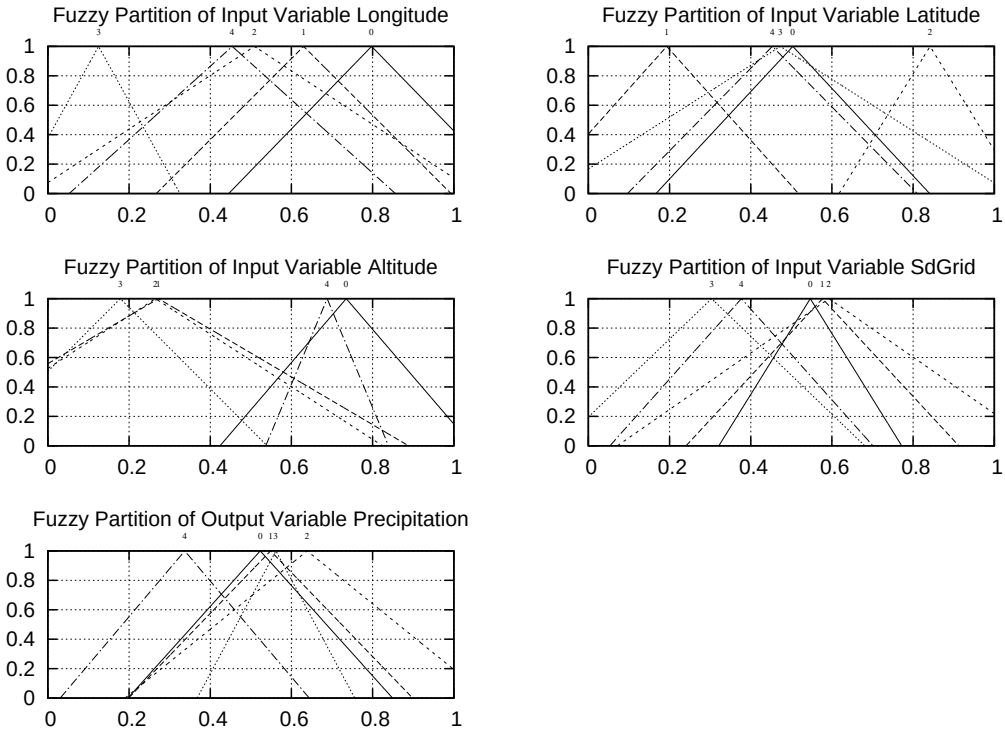

Figure E.17: Membership functions of initial fuzzy model GK_{2p} before tuning. Initial fuzzy model is constructed with 5 clusters and it contains 5 rules.

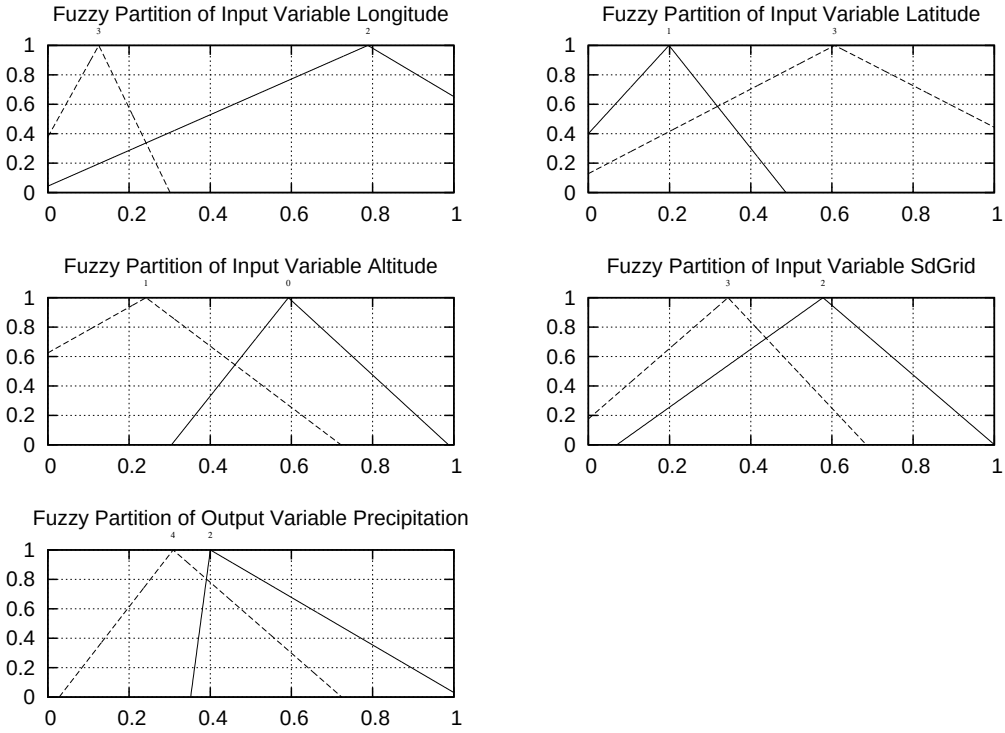

Figure E.18: Membership functions of simplified GK_{2p} fuzzy model which are initially constructed with five clusters. Simplified fuzzy model rule base contains 5 rules.

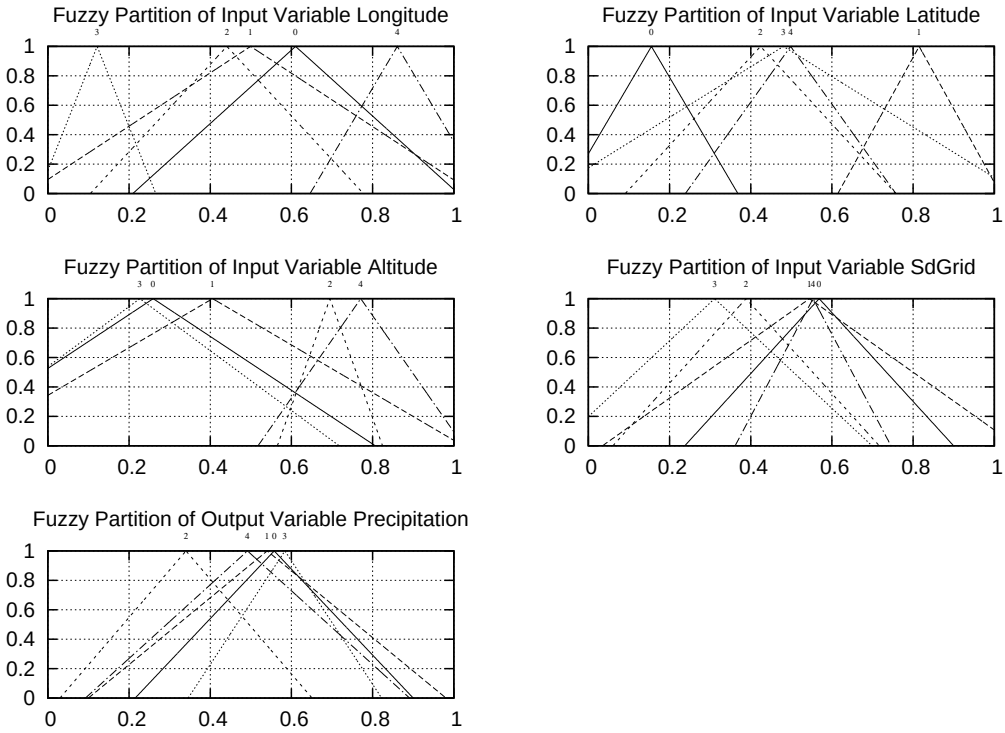

Figure E.19: Membership functions of initial fuzzy model GG_{3p} before tuning. Initial fuzzy model is constructed with 5 clusters and it contains 5 rules.

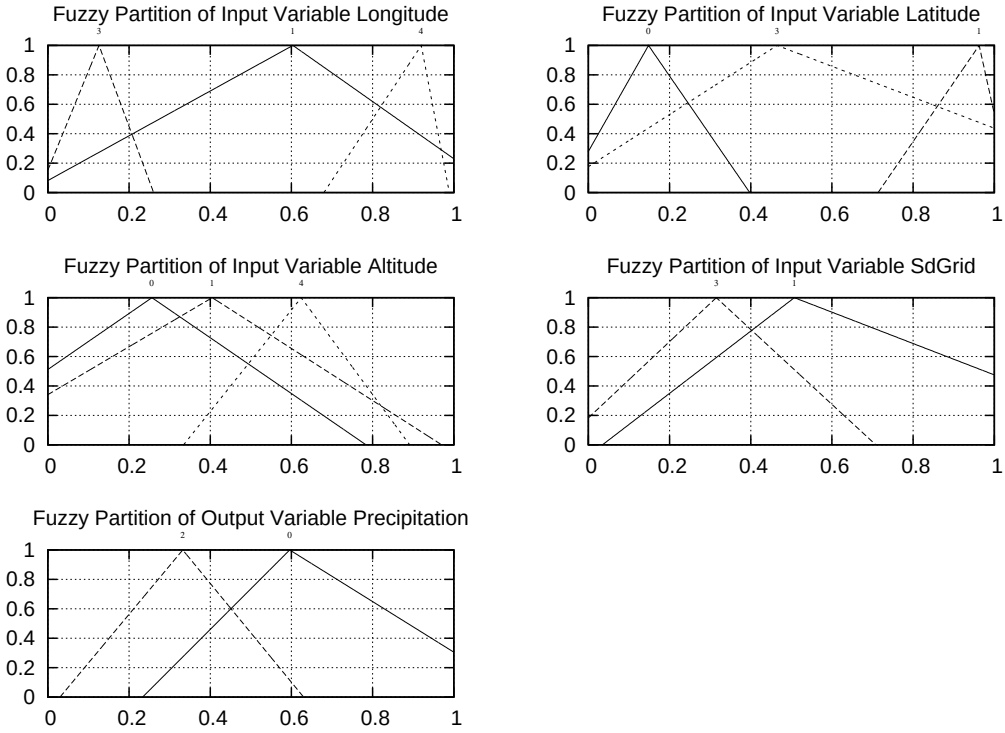

Figure E.20: Membership functions of simplified GG_{3p} fuzzy model which are initially constructed with five clusters. Simplified fuzzy model rule base contains 5 rules.

VITA

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