Comparing Methods for Knowledge-Driven and Data-Driven Fuzzy Modeling: A Case Study in Textile Industry

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Abstract: The aim of this study is to compare different approaches to fuzzy systems design from different perspectives: knowledge-driven versus data-driven and rule-based (flat) versus tree-based (hierarchical). More specifically, our comparison is focused on two of the arguably most important criteria in fuzzy systems design, namely accuracy and interpretability. We compare two approaches to data-driven fuzzy modeling, namely fuzzy rule-based inference using the well-established Takagi-Sugeno approach, and so-called fuzzy pattern trees, an alternative approach that has been proposed only recently. In contrast to the flat structure of fuzzy rule systems, pattern trees are hierarchical models. These methods are compared in the context of a concrete case study, namely the modeling of color yield in polyester high temperature dyeing as a function of disperse dyes concentration, temperature and time. As a baseline, we include Mamdani models designed in a knowledge-driven way. Our results show that, at least in this particular application, Takagi-Sugeno systems offer the best predictive accuracy, whereas Mamdani models are preferable in terms of interpretability. Fuzzy pattern trees seems to offer a good trade-off between both criteria.

1 Introduction

While aspects of knowledge representation and reasoning have dominated research in fuzzy logic for a long time, problems of automated learning and knowledge acquisition have more and more come to the fore during the recent years. This is not very surprising in view of the fact that the "knowledge acquisition bottleneck" seems to remain one of the key issues in the design of intelligent and knowledge-based systems. Indeed, experience has shown that a purely knowledge-driven approach, which aims at formalizing problem-relevant human expert knowledge, is difficult, intricate, and tedious most of the time. Consequently, a kind of data-driven construction of fuzzy systems is often worthwhile [1]. In fact, such a "tuning" even suggests itself in many applications where data is readily available. In some applications, such as learning on data streams, where models need to be learned and updated continuously in an online manner, data-driven adaptation is even essential [2, 3].

The transparency and interpretability of fuzzy systems is often emphasized as one of their key advantages, especially in comparison to so-called "black-box" approximation methods such as neural networks. Indeed, a primary motivation for the development of fuzzy sets was to provide an interface between a numerical scale and a symbolic scale usually composed of linguistic terms. Thus, fuzzy sets have the capability to interface quantitative patterns with qualitative knowledge structures expressed in terms of natural language. This makes the application of fuzzy technology very appealing from a knowledge representational point of view.

However, if models are extracted from data in an automatic way instead of being designed by a human expert, interpretability becomes a critical issue. For example, a lin-

guistic representation may become difficult if the fuzzy sets have been induced by the learning algorithm in a data-driven way, since the existence of appropriate linguistic interpretations cannot be guaranteed in that case. Another problem that may hamper interpretability concerns the complexity of models consisting of a potentially large number of interacting pieces, for example rules in a rule-based system. Since accurate models typically require a certain level of complexity, accuracy and understandability are to some extent conflicting goals [4, 5].

Due to these reasons, the interpretability of fuzzy models is clearly not self-evident and does not come for free, especially when these models are constructed in a data-driven way. Research in this field is still hampered by the lack of accepted criteria for measuring interpretability in a more or less objective way, although some advances have recently been made [6, 7]. In this paper, we therefore opt for another approach: Instead of looking for generic evaluation measures, we compare different methods in the context of a concrete case study, namely the modeling of color yield in polyester high temperature dyeing.

More specifically, we compare fuzzy rule-based inference and so-called fuzzy pattern trees (FPT), an alternative approach to fuzzy systems design that has been proposed only recently. Whereas rule-based systems have a "flat" structure, fuzzy pattern trees are hierarchical models. As argued in [8], they are thus able to represent models in more compact way. Regarding fuzzy inference systems (FIS), we compare a knowledge-driven and a data-driven approach, namely Mamdani [9] and Takagi-Sugeno systems [10]. In fact, wile the former are quite convenient from a modeling perspective, more efficient learning algorithms exist for the latter.

The remainder of the paper is organized as follows. In

the next section, we briefly recall the basic conception of the fuzzy models included in our study. Our application, the modeling of color yield in polyester high temperature dyeing, is outlined in Section 3. The results of our case study are then presented and discussed in Section 4. The paper ends with some concluding remarks in Section 5.

2 METHODS

Due to space restrictions, we mainly restrict to a description of the architectures of the fuzzy models used in our study, without explaining algorithms for learning them from data. For technical details of that kind, we refer to the related literature. We also refrain from explaining Mamdani models, which we assume to be widely known.

2.1 Takagi-Sugeno Systems

Takagi-Sugeno (TS) fuzzy systems allow for modeling $\mathbb{R}^p \to \mathbb{R}$ mappings in a convenient and flexible way [10]. A single rule in a (single output) TS fuzzy system is of the form

$$\begin{array}{ll} \text{IF} & (x_1 \text{ IS } \mu_{i1}) \text{ AND ... AND } (x_p \text{ IS } \mu_{ip}) \\ \text{THEN} & l_i = w_{i0} + w_{i1}x_1 + w_{i2}x_2 + \ldots + w_{ip}x_p \end{array}$$

where $\boldsymbol{x}=(x_1,\ldots,x_p)$ is the p-dimensional input vector and μ_{ij} the fuzzy set describing the j-th antecedent of the rule. Typically, these fuzzy sets are associated with a linguistic label. The AND connective is modeled in terms of a t-norm, i.e., a generalized logical conjunction [11]. The output $l_i=l_i(\boldsymbol{x})$ is the so-called consequent function of the rule.

The output of a TS system consisting of C rules is a linear combination of the outputs produced by the individual rules, where the contribution of each rule is given by its normalized degree of activation:

$$\hat{f}(\boldsymbol{x}) = \hat{y} = \sum_{i=1}^{C} \Psi_i(\boldsymbol{x}) \cdot l_i(\boldsymbol{x})$$
 (1)

with

$$\Psi_i(\boldsymbol{x}) = \frac{\mu_i(\boldsymbol{x})}{\sum_{j=1}^C \mu_j(\boldsymbol{x})} , \qquad (2)$$

where $\mu_i(x)$ denotes the activation degree of the *i*-th rule. The latter is defined by the conjunctive (t-norm) combination of the rule antecedents, i.e., the degrees of membership of the feature values x_i in the fuzzy sets μ_{ij} :

$$\mu_i(\boldsymbol{x}) = \bigotimes_{j=1}^p \mu_{ij}(x_j) \tag{3}$$

As can be seen, a TS fuzzy model is a parameterized mapping which is defined by the choice of the input space (via feature selection) including its dimensionality p, the number of rules, C, and the parameters of each single rule, i.e., the fuzzy sets μ_{ij} $(j=1,\ldots,p)$ and the weight vector $w_i=(w_{i0},w_{i1},\ldots w_{ip})$. For learning TS models from data, i.e., from a given set if examples (x_i,y_i) , we make use of the method proposed in [12].

2.2 Fuzzy Pattern Trees

Pattern tree induction was recently introduced as a novel machine learning method for classification in [13] and further developed for regression in [8]. Roughly speaking, a

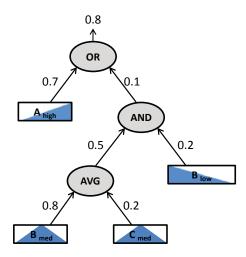


Fig. 1: Example of a fuzzy pattern tree: The output is large if attribute A is high or if the truth degree of a second criterion is high, namely that B is low and that the average between the conditions that B and C are medium is high. The tree also shows the concrete propagation of values from the bottom to the top; in this case, the output is high to the degree 0.7.

fuzzy pattern tree is a hierarchical, tree-like structure, whose inner nodes are marked with generalized (fuzzy) logical and arithmetic operators (namely t-norms, t-conorms, average and ordered weighted average operators), and whose leaf nodes are associated with fuzzy predicates on input attributes (fuzzy subsets of the attribute's domain, possibly associated with a linguistic term); see Fig. 1 for an illustration. A pattern tree propagates information from the bottom to the top: A node takes the values of its descendants as input, combines them using the respective operator, and submits the output to its predecessor.

Just like TF models, a pattern tree can implement a mapping $\mathbb{R}^p \to \mathbb{R}$. Note that the direct output of a pattern tree is in [0,1]. One can think of this value as the degree of membership of a fuzzy subset G of an underlying domain $\mathcal{Y} \subseteq \mathbb{R}$. For example, if \mathcal{Y} is an interval [a,b], i.e., if the original output variable is lower-bounded by a and upper-bounded by b, then the membership function could be given by a simple linear scaling

$$G: y \mapsto \frac{y-a}{b-a}$$
.

Thus, the corresponding fuzzy set could be interpreted as a model of the linguistic term "large". Likewise, if the original output is unbounded, a possible re-scaling is

$$G: y \mapsto \frac{1}{1 + \exp(-\alpha y)}$$
.

Considering the fuzzy set G as a fuzzy predicate or, say, property of the output variable (e.g., being large), a fuzzy pattern tree can be seen as a model that specifies criteria on the input attributes which imply this property to hold. From a modeling point of view, the pattern tree approach is based on three important conceptions:

- fuzzification of input attributes;
- hierarchical structuring of a functional dependency through recursive partitioning of criteria into sub-criteria;
- flexible aggregation of sub-criteria by means of parameterized fuzzy operators.

Pattern trees are interesting for several reasons. From a learning point of view, they offer a flexible model class that is able to fit non-linear functions in a quite accurate way, possesses desirable monotonicity properties and can easily handle missing or imprecise input values [14]. Moreover, pattern trees are interesting from an interpretation point of view. A tree can be considered as a kind of generalized logical description of properties that guarantee a "large" output. The description itself is compact and modular due to its hierarchical structure.

Different algorithms have been proposed for learning a pattern tree classifier from a given set of data, namely methods that construct trees in a bottom-up [13] and in a top-down manner [14]. A variant of pattern tree induction suitable for learning regression functions was proposed in [8].

3 POLYESTER DYEING

The most important man made fiber is Polyethylene terphethalate (PET) commonly known as polyester. This polymer contains ester groups (-CO-O-) in its main molecular chain and is produced by melt spinning process. Ester groups are a result of the reaction between bi-functional carboxylic acids and bi-functional alcohols. The absence of reactive groups, capable of undergoing reaction with anionic and cationic dyes as well as being a hydrophob, has limited dyeing and printing of unmodified polyethylene terphethalate fibers to only disperse dyes. Moreover, under normal dyeing conditions, the compact structure of polyethylene terphethalate fibers makes the penetration of disperse dyes inside them very difficult. Dyeing of polyethylene terephthalate fibers therefore requires special conditions such as high temperature $(\sim 130^{\circ}\text{C})$, dry heat $(190\text{-}220^{\circ}\text{C})$, or using carrier in the dye bath [15, 16, 17, 18].

The chemical structure of disperse dyes contains polar groups such as -NHR, -OH and NH₂ but there are no ionic groups present which leads to their very low solubility in water [15, 19, 20]. Azo, anthraquinone, and nitro diphenylamine constitue the three main chemical structure of disperse dyes. However, as far as the application is concerned, these dyes are divided into four groups namely A, B, C, and D [15, 20]. Temperature, time, and disperse dye concentration are the primary factors affecting the color yield in dyeing polyethylene terephthalate. The overall picture of the relative importance of these factors can be seen in models representing the color yield as a function of them. These models may also have applications in processing and cost minimization [15].

Our objective is to present a model for the color yield of polyethylene terephthalate dyed with specific disperse dyes by high temperature method. The model will represent color yield as a function of time, temperature and dye concentration for each dye. K/S has a direct relationship with the color yield. K/S shows the ratio of absorbed light by an opaque substrate relative to the scattered light from it. This ratio is calculated by Kubelka-Munk theory as follows:

$$(K/S)_{\lambda} = \frac{(1 - R_{\lambda})^2}{2R_{\lambda}} ,$$

where R_{λ} is the reflectance of sample of infinite thichness to light of given wavelength, expressed in fractional form [15, 21].

Dye Concentr. (% owf)	Temperature (°C)	Time (min)
0.75	100	12
1,50	110	24
3,00	115	36
4.50	120	48
6,00	125	
	130	

TABLE I: DYEING CONDITIONS.

Index Name	Chromophore
C.I. Disperse Blue 266	Mono Azo
C.I. Disperse Brown 1	
C.I. Disperse Blue 56	Anthraquinone
C.I. Disperse Red 60	
C.I. Disperse Yellow 7	Diazo
C.I. Disperse Yellow 23	
Mixture	Not Known

TABLE II: THE DISPERSE DYES EMPLOYED FOR SAMPLES DYEING.

4 Modeling of Polyester Dyeing

As mentioned before, the present study aims to model variations of color yield of polyester samples dyed with different disperse dyes versus time, temperature, and disperse dye concentration in the high temperature (HT) polyester dyeing process. To this end, Mamdani and Takagi-Sugeno systems as well as fuzzy pattern trees are used.

Dyeing of the samples (5 g) was carried out by Polymat laboratory dyeing machine (AHIBA 1000) with the following recipe:

Disperse dye	х%
pН	5.5
L:R	50:1

and according to a set of values for dye concentration, dyeing temperature and dyeing time in the form of a matrix shown in Table i [22]. After dyeing, reduction clearing for the samples was carried out for 10 minutes in a bath (65 °C) containing sodium hydroxide 38 °Be, sodium dithionite and a nonionic detergent [15, 22]. The disperse dyes employed are listed in Table ii [15, 22].

From the values for concentration, temperature and time, 120 combinations were constructed, for which the output K/S was determined experimentally. Thus, for a single disperse dye, a data set with 120 observations was obtained (hence 7 such data sets in total), where each observations consists of three values of the input attributes (concentration, temperature, time) and one value for the output (K/S).

4.1 Fuzzy Models

The Mamdani inference system, representing the color yield of C.I. Disperse Blue 266 as a function of time, temperature, and disperse dye concentration in the high temperature (HT) polyester dyeing, was developed in a knowledge-driven way, formalizing expert knowledge in a proper way [23]: First, membership functions for input and output variables regarding HT dyeing of polyester for C.I. Disperse Blue 266, one of mono Azo Disperse Dyes, have been determined.

	Concentration		Time		Temperature	
Fuzzy Set	Mean	Std	Mean	Std	Mean	Std
Low	0.30	1.00	13.1	14.2	100	7.8
Medium	3.38	0.89	_	—	117	3.0
High	5.86	1.33	44.4	11.7	129	4.0

TABLE III: PARAMETERS OF GAUSSIAN FUZZY SETS FOR INPUT VARIABLES.

Fuzzy Set	Mean	Std
Very Low	0.00	3.30
Low	4.11	1.42
Medium	12.8	1.69
High	19.3	1.86
Very High	29.80	3.50

TABLE IV: PARAMETERS OF GAUSSIAN FUZZY SETS FOR OUTPUT VARIABLE.

Gaussian membership functions were used for all input and output variables. The values for mean and standard deviation of membership functions for each variable are given in Tables iii and iv.

In the second stage, the eight rules blow were defined according to the physical and chemical structure of polyester fiber, HT dyeing of polyester, and the behavior of 120 samples dyed in C.I. Disperse Blue 266 [23]:

- 1. If (temperature is low) and (time is low) and (concentration is low), then (K/S is very low).
- 2. If (temperature is medium) and (concentration is high), then (K/S is high).
- 3. If (temperature is high) and (concentration is low), then (K/S is medium).
- 4. If (temperature is low) and (time is high) and (concentration is low), then (K/S is very low).
- 5. If (temperature is high) and (concentration is high), then (K/S is very high).
- 6. If (temperature is medium) and (time is low) and (concentration is high), then (K/S is medium).
- 7. If (temperature is medium) and (time is high) and (concentration is high), then (K/S is high).
- 8. If (Temperature is low) and (time is low) and (concentration is high), then K/S is low.

In a manner similar to the one described above, the proposed method was applied to C.I. Disperse Brown 1, which has a chemical structure similar to C.I. Disperse Blue 266, with no changes in the FIS designed for the previous dye. The obtained FIS has been applied for Anthraquinone dyes.

Regarding to different chemical structure of other dyes, the behavior of each of them has been studied and the parameters of temperature according to change of color yield in each of them during change of temperature have been defined as shown in Table v.

As mentioned before, the TS fuzzy systems and the fuzzy pattern trees have been determined in a purely data-driven manner, using the learning algorithms proposed in [12] and [8], respectively.

	Mixture		Diaz	ZO
Fuzzy Set	Mean	Std	Mean	Std
Low	106.70	9.68	100.00	5.00
Medium	123.10	2.43	115.00	5.00
High	131.70	4.00	130.00	5.00

TABLE V: PARAMETERS OF FUZZY SETS FOR VARIABLE 'TEMPERATURE' FOR MIXTURE AND ANTHRAOUNONE DYES.

Dyes	Mamdani	TS	FPT
Blue 266	3.3663	1.28 ± 0.13	2.23 ± 0.16
Brown 1	4.3129	2.25 ± 0.14	2.68 ± 0.13
Blue 56	3.7985	1.46 ± 0.07	2.74 ± 0.28
Red 60	4.6461	2.09 ± 0.07	3.03 ± 0.14
Yellow 7	4.9089	1.11 ± 0.08	2.29 ± 0.08
Yellow 23	4.1213	1.31 ± 0.11	$2.84{\pm}0.16$
Mixture	3.9760	1.39 ± 0.07	1.92 ± 0.04

Table VI: Accuracy in terms of RMSE \pm standard deviation.

4.2 Accuracy

The accuracy of the three models has been determined by means of a 5-fold cross validation, repeated 10 times. The average results in terms of root mean squared error (RMSE) are shown in Table vi for all 7 data sets. These results convey a relatively clear picture: TS models provide the most accurate solutions, followed by fuzzy pattern trees. The knowledge-driven Mamdani models cannot compete with the two data-driven approaches and produce a significantly higher error.

4.3 Interpretability

From an interpretability point of view, the situation is quite different. Obviously, Mamdani models are well interpretable, since these models have been designed by hand.

The models produced by the Takagi-Sugeno approach are much less interpretable, for several reasons. First of all, rules of the TS type are arguably more difficult to understand than Mamdani rules. Besides, a TS model as a whole is sometimes difficult to grasp, especially if the number of rules is large. In our study, despite the low dimensionality of the input space, the number of rules can become as large as 13; see Table vii for an overview of the model size.

Second, the models learned in a data-driven way do not reflect the chemical structures and behavior of each dye in a proper way. For example, the fuzzy partitions induced for the input variables are often non-intuitive. As an illustration, Table viii shows the parameters of the Gaussian fuzzy sets induced for the attribute 'temperature' for C.I. Disperse Blue

		# fuzzy sets		
Dyes	# rules	Te	Co	Ti
C.I. Disperse Blue 266	13	3	4	4
C.I. Disperse Brown 1	8	2	2	3
C.I. Disperse Blue 56	10	3	2	4
C.I. Disperse Red 60	9	3	2	2
C.I. Disperse Yellow 7	9	2	3	2
C.I. Disperse Yellow 23	13	5	4	3
Mixture	12	4	4	3

TABLE VII: SIZE OF TAKAGI-SUGENO MODELS.

	Blue 266		Brown 1		Yellow 7	
Fuzzy Set	Mean	Std	Mean	Std	Mean	Std
Low	104.3	6.97	105.8	8.42	110.1	13.11
Medium	121.4	8.42	_	_	_	_
High	130.0	0.30	121.1	8.23	123.2	4.81

Table VIII: Parameters of fuzzy sets for variable 'temperature' in different data sets.

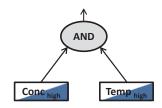


Fig. 2: Fuzzy pattern tree for dyes mixture.

266, C.I. Disperse Brown 1 and C.I. Disperse Yellow 7, respectively. Consider the fuzzy sets for temperature in the case of C.I. Disperse Blue 266 and C.I. Disperse Brown 1. These fuzzy sets are not at all in agreement with our expectation. C.I. Disperse Blue 266 needs higher temperature than C.I. Disperse Brown 1 to have a high color yield, and if we select a lower standard deviation for "low" in Table 3 or shift the mean of temperature variable to lower variables, we can obtain better results and lower RMSE for C.I. Disperse Brown 1. As can be seen in Table viii, mean and standard deviation of "low" for C.I. Disperse Brown 1 are higher than for C.I. Disperse Blue 266.

Another point concerns the influence of individual input variables on the model output. As an example, the effect of the variable 'time' for the above-mentioned dyes can be considered. Although time has not an important effect in comparison with temperature and concentration, and these dyes are not sensible toward time, in comparison with temperature and concentration, variable 'time' has more fuzzy sets for these dyes; see Table vii. We can consider the fuzzy sets for temperature in the case of C.I. Disperse Yellow 7 as another example. The K/S values of the samples dyed with C.I. Disperse Yellow 7 rise steadily with time and reach a peak at 110°c, but beyond this value, an increase of temperature does not have a significant effect on K/S. Therefore, the mean value 110.10 °c, regarding Table viii, is not acceptable as a mean of the fuzzy set for 'low' for this dye. In general, Takagi-Sugeno models learned in a data-driven way are not monotone, despite the fact that the output (K/S) is a monotone increasing function of all input variables (time, temperature, concentration), and this monotonicity also holds for the data sets.

In comparison, fuzzy pattern trees are easier to interpret; see Fig. 2 for an example of a very simple model and Fig. 3 for a more complex (but still manageable) one. The first model can simply be interpreted as follows: The output (K/S) is high if the concentration is high and the temperature is high.

The selection of relevant variables, as realized by pattern trees, appears to be quite reasonable. As an example, we can consider the above result for C.I. Disperse Yellow 7, but also for C.I. Disperse Red 60. The variable 'time' does not have an important effect on dyeing regarding chemical structure of these dyes. This is indeed reflected by the corresponding fuzzy pattern trees, in which this variable does either not occur

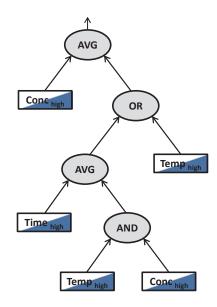


Fig. 3: Fuzzy pattern tree for dyes C.I. Disperse Yellow 7.

at all, or at least does not play an important role. In contrast, time plays a significant roll for mixture dye in high temperature conditions, and in these cases, it indeed occurs repeatedly in the fuzzy pattern trees. In the same way, results of fuzzy pattern trees for Diazo dyes, C.I. Disperse Yellow 7 and C.I. Disperse Yellow 23 show the importance of concentration, as it was expected.

As another nice feature of pattern trees, let us mention that they can easily guarantee a monotone influence of an input variable on the output. This is simply accomplished by restricting the choice of fuzzy sets in the leaf nodes to the single fuzzy set 'high'.

5 CONCLUSIONS

There are at least two important conclusions that can be drawn from our case study. First, regarding the comparison of fuzzy rule-based inference systems, we can confirm previous experience with Mamdani and Takagi-Sugeno models: The former are quite amenable to a knowledge-driven design, whereas a specification of TS models by hand is much more difficult. On the other hand, TS models can be learned quite efficiently in a data-driven way. In fact, the models thus produced are more accurate than Mamdani models. The price to pay, however, is a loss in terms of interpretability.

Second, fuzzy pattern trees can be considered as a viable alternative for fuzzy systems design, as they seem to offer a reasonable compromise between accuracy and interpretability. Due to their hierarchical structure, pattern trees are often more compact than a flat rule base, and thus offer models of smaller size. This model class is clearly worth further investigation.

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