J. Inv. Ill-Posed Problems, Vol. 10, No. 4, pp. 1–26 (2002)

Regularized data-driven construction of fuzzy controllers

M. BURGER*, J. HASLINGER† U. BODENHOFER†, and H.W. ENGL‡

Received March 24, 2002

Abstract — This paper is devoted to the mathematical analysis and the numerical solution of data-driven construction of fuzzy controllers. We show that for a special class of controllers (so-called *Sugeno controllers*), the design problem is equivalent to a nonlinear least squares problem, which turns out to be *ill-posed*. Therefore we investigate the use of regularization in order to obtain stable approximations of the solution. We analyze a smoothing method, which is common in spline approximation, as well as Tikhonov regularization with respect to stability and convergence.
In addition, we develop an iterative method for the regularized problems, which uses the special structure of the problem and test it in some typical numerical examples. We also compare the behavior of the iterations for the original and the regularized least squares problems. It turns out that the regularized problem is not only more robust but also favors solutions that are interpretable easily, which is an important criterion for fuzzy systems.

1. INTRODUCTION

Fundamentally, the idea of fuzzy sets and systems, dated back to Zadeh [34, 35], is to provide a mathematical model that can present and process vague, imprecise and uncertain knowledge. It has been modeled on human thinking and the ability of humans to perform approximate reasoning, so that precise and yet significant statements can be made on the behavior of a complex system.

*Numerical and Symbolic Scientific Computing and Industrial Mathematics Institute, Johannes Kepler Universität, Linz, Altenbergerstr., 69, A-4040 Linz, Austria.

†Software Competence Center Hagenberg, Hauptstrasse 99, A-4232 Hagenberg. E-mail: josef.haslinger@scch.at

‡Industrial Mathematics Institute, Johannes Kepler Universität, Linz, Altenbergerstr., 69, A-4040 Linz, Austria.

The work of M. Burger is supported by the Austrian National Science Foundation FWF (grant SFB F013/08). J. Haslinger and U. Bodenhofer are working in the framework of the Kplus Competence Center Program which is funded by the Austrian Government, the Province of Upper Austria, and the Chamber of Commerce of Upper Austria.

Successful applications of fuzzy logic control include automatic train operation systems, elevator control, temperature control, power plant control, fuzzy refrigerators, washing machines, etc. The main advantage of fuzzy controllers in comparison with other adaptive systems like neural networks is the linguistic interpretability of the controller.

1.1. Fuzzy Control

Basically, a fuzzy logic controller consists of three components [1, 7, 17]:

1. The rules, i.e. a verbal description of the relationships usually of a form as the following (n is the number of rules):
$$\text{if } x \text{ is } A_i \text{ then } u \text{ is } B_i \ (i = 1, \dots, n)$$
2. The fuzzy sets (membership functions), i.e. the semantics of the vague expressions A_i, B_i used in the rules. More precisely (cf. [2]): Given a universe of discourse X a fuzzy subset A of X is characterized by its membership function
$$\mu_A : X \to [0, 1]$$
where for $x \in X$ the number $\mu_A(x)$ is interpreted as the degree of membership of x in the fuzzy set A.
3. An inference machine, i.e. a mathematical methodology for processing a given input through the rule base. The general inference process proceeds in three (or four) steps: first the *fuzzification*, then the *inference* itself, the *composition* and finally the (optional) *defuzzification*.

In the following we assume that a reasonable inference scheme—a Sugeno controller [30], where the output membership functions are crisp values—is given. For a complete definition of a Sugeno controller, see Section 2.

There are still two components left which have to be specified in order to design a fuzzy controller—the rules and the fuzzy sets. Recent effort has been concentrated on developing new techniques which may be able to design the membership functions and rule base automatically from measured data. Genetic algorithms have played a special role in fuzzy control design as well as methods treating fuzzy systems as artificial neural networks to adjust membership functions using back propagation. For references see the article of Tan and Hu [31]. Also classical optimization algorithms, such as the method of steepest descent have been applied in tuning small and medium sized controllers.

Under the quite natural assumptions that product is used as fuzzy inference rule, summation as the composition scheme, and center of gravity as the defuzzification method, the tuning of a Sugeno controller reduces to fitting a set of data $\{(x_i, y_i)\}_{i=1,\dots,m}$ by a linear combination of membership functions in the least squares sense, i.e. seeking a solution of the minimization problem

$$\sum_{i=1}^{m} \Big(y_i - \sum_{j=1}^{n} \alpha_j b_j(x_i; \boldsymbol{t}) \Big)^2 = \min_{(\boldsymbol{\alpha}, \boldsymbol{t})}, \tag{1.1}$$

where b_j represents the membership functions and $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_n)^\top$ the coefficients. The concrete shape of the membership functions depends on the knot sequence $\boldsymbol{t}$, which is also included in the optimization procedure. Therefore, the minimization problem (1.1) is nonlinear.

Among the wide range of possible membership functions for Sugeno controllers, we will concentrate on two different kinds: trapezoidal and B-spline membership functions, firstly for the one-dimensional case (see Section 2). The more general class of B-spline membership functions for Sugeno controllers, including the often used triangular membership functions, were proposed in Zhang and Knoll [36]. We mention that in a more abstract setting such approximations have been introduced as abstract splines by Sard [20] and generalized by Groetsch [12].

1.2. Ill-posedness and regularization

Assuming for the moment that the knot sequence $\boldsymbol{t}$ is fixed, we end up with a linear least squares problem

$$\|\boldsymbol{y} - B(\boldsymbol{t})\alpha\|^2/2 = \min_{\boldsymbol{\alpha}}, \tag{1.2}$$

where $B(\boldsymbol{t}) := (b_j(x_i, \boldsymbol{t}))_{i=1,\ldots,m;\, j=1\ldots,n}$ is the so-called observation matrix. (1.2) has a unique solution, if and only if the observation matrix B has full rank which is equivalent to the—in approximation theory well-known—Schoenberg-Whitney condition [6]. In our case, we also have to take into account data errors. Usually, the data $\boldsymbol{y}$ is the result of measurements contaminated by noise. Often, the exact position x_i of the measurement is only known approximately, i.e. we get a set of noisy data $(\boldsymbol{x}^\gamma, \boldsymbol{y}^\delta)$ with error bounds γ and δ. Then, (1.2) belongs to the class of *ill-posed problems* and we have to use regularization techniques to obtain a stable solution to our problem.

In the case of linear ill-posed problems, the regularization theory is very well developed [8]. It is shown by a simple example in Section 2, that the full nonlinear minimization problem (1.1) is indeed ill-posed in the sense that solutions do not necessarily depend on the data in a continuous way. Generally, the theory for nonlinear ill-posed problems (cf. [8], Chapter 10) involves more technical problems as the linear case. The case of an ill-posed nonlinear least squares problem, where no "attainability assumption" is fulfilled, is even more complicated and by far not so well developed [3]. As a characteristic of our problem is that it is linear in one set of variables (the coefficients α) and nonlinear in the set of free knots $\boldsymbol{t}$, we cite [24], where the problem of regularizing an operator consisting of a linear and nonlinear part is considered in a more abstract framework.

We note that an analogous ill-posed problem arises in the problem of function approximation with neural networks. In this case the problem is also given by (1.2), the basis functions are usually of the form

$$b_j(x; \boldsymbol{a}, \boldsymbol{b}) = \sigma(a_j^\top x + b_j), \tag{1.3}$$

with $a_j \in \mathbb{R}^N$ and $b_j \in \mathbb{R}$. The so-called activation function σ is usually chosen to be a *sigmoidal function*, i.e., a monotone and piecewise continuous function on $\mathbb{R}$, which satisfies

$$\lim_{t\to-\infty} \sigma(t) = 0 \qquad \lim_{t\to\infty} \sigma(t) = 1.$$

Similar to our problem in fuzzy control, the minimization is performed with respect to the weights and also with respect to the parameters a_j and b_j on which the output depends in a nonlinear way. The main difference is that in the approximation with neural networks one is not interested in the behavior of the parameters a_j and b_j, since they do not have a particular meaning, but one rather wants to achieve convergence of the approximating output $f_n := \sum_{j=1}^{n} \alpha_j b_j(x; \boldsymbol{a}, \boldsymbol{b})$ to the function from which the samples y_i are taken. For this reason the results obtained in the sequel cannot be transferred directly to neural networks, but there are several techniques that could be carried over to that field in future work. For further details we refer the reader to the monograph by Bishop [4] and also to [5, 10, 28].

In the following (Section 3) we investigate smoothing—a stabilization approach commonly used in the area of spline approximation—which is only a regularization method under the severe restriction of additional constraints on the free knots. Then, we investigate classical Tikhonov regularization. We develop existence, stability, and convergence results without any restrictions as in the case of smoothing. Finally, in Section 5 numerical experiments verify theoretical results obtained in Section 4. It turns out, that Tikhonov regularization gives the best results with respect to stability and interpretability of fuzzy controllers.

1.3. Approximation properties of Sugeno controllers

It has been shown by several authors [16, 32, 15], that fuzzy controllers are universal approximators in the sense that it is possible to construct such rule bases that approximate uniformly any continuous function defined on a compact subset of $\mathbb{R}^m$ with arbitrary accuracy. Proofs are based upon the Stone—Weierstrass Theorem and purely existential in nature. From a practical—fuzzy control oriented—point of view, these theorems suffer from the fact that the number of rules in the base is not bounded, in addition to that even the supports of the terms in the rules are not bounded (e.g. Gaussian membership functions).

As already mentioned, the tuning of a Sugeno controller reduces to a data fitting problem by a linear combination of membership functions. From a purely mathematical point of view, we now let both the number of membership functions and data points tend to infinity and examine the approximation power. We consider the case of B-spline membership functions, where a wide range of convergence results exists [6, 27].

We can approximate a large class of functions arbitrarily well by splines of a fixed order if we are willing to use many knots. The order of approximation attainable will increase with the smoothness of the class of functions being approximated. Additionally, substantial gains in the rate of convergence can be achieved when using the knots as free parameters that can be adjusted to the particular function being approximated (cf. [27], Chapters 6-7).

2. OPTIMIZATION OF SUGENO CONTROLLERS

2.1. Basic definitions of Sugeno controller and membership functions

If we look at a Sugeno controller from the point of view of mappings which assign to each crisp observation a crisp value (vector) in the output space, i.e., there is a function $F_s : X \to \mathbb{R}^{d_o}$ associating to each input x its corresponding output y, it is possible to construct an explicit formula substituting the fuzzy control system completely.

Definition 2.1. Let X be an input space, let $A_1, A_2, \dots, A_n$ be normalized fuzzy subsets of X with $\sum \mu_{A_i}(x) > 0$ for all $x \in X$, and $f_1, f_2, \dots, f_n$ be functions from X to $\mathbb{R}^{d_o}$, and consider the rulebase $(i = 1, 2, \dots, n)$

$$\text{if } x \text{ is } A_i \text{ then } u = f_i(x).$$

Then the Sugeno controller defines the following input-output function F_s : $X \to \mathbb{R}^{d_o}$

$$F_s(x) = \sum \mu_{A_i}(x)\, f_i(x) \Big/ \sum \mu_{A_i}(x). \tag{2.1}$$

In the following we consider the special case, that for $i = 1, 2, \dots, n$ the functions f_i are constant, that is $f_i(x) \equiv \alpha_i$. In a first step, we restrict ourselves to the one-dimensional case, i.e., a single input-single output controller. However, for the output variable this is no restriction. If the number of output variables is higher than one, it can easily be shown [15] that in every case it is possible to decompose the controller into as many independent controllers as many output variables we have.

Among the class of membership functions, we consider first the classical trapezoidal ones. Let the knot sequence $\boldsymbol{t} = \{t_i\}$, where

$$a = t_1 \leq t_2 \leq ... \leq t_{2n-1} \leq t_{2n} = b \tag{2.2}$$

be a partition of the universe of an input variable defined over $[a, b]$, corresponding to n linguistic terms. Then the mathematical formulation of the trapezoidal membership functions b_j ($j \in \{2, \dots, n-1\}$) is as follows:

$$b_j(x, \boldsymbol{t}) := \begin{cases} (x - t_{2j-2})/(t_{2j-1} - t_{2j-2}) & \text{if } x \in (t_{2j-2}, t_{2j-1}) \\ 1 & \text{if } x \in [t_{2j-1}, t_{2j}] \\ (-x + t_{2j+1})/(t_{2j+1} - t_{2j}) & \text{if } x \in (t_{2j}, t_{2j+1}) \\ 0 & \text{otherwise} \end{cases}$$

with appropriate definitions for $j = 1$ and $j = n$ (Figure 1).

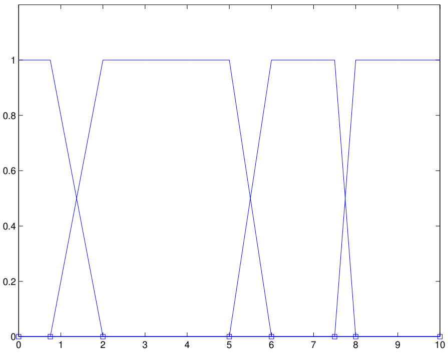

Figure 1. Trapezoidal membership functions

Now we turn to the more general class of B-spline membership functions for Sugeno controllers. Assume that x is an input variable of a Sugeno controller that is defined on the interval $[a,b]$. Given a sequence of ordered knots $\boldsymbol{t} = \{t_i\}$, where

$$t_1 = \ldots = t_k = a < t_{k+1} \le \ldots \le t_n < b = t_{n+1} = \ldots = t_{n+k} \tag{2.3}$$

let $b_{j,k}$ denote the *j-th* normalized B-spline basis function of order k for the knot sequence $\boldsymbol{t}$. For an exact definition see e.g. [6]. The complete knots consist of two parts, the interior knots that lie within the universe of discourse, and extended knots that are generated at both ends of the universe for a unified definition of B-splines (leading to the so-called marginal linguistic terms in [36]).

From the point of view of fuzzy control, B-splines have some properties such as positivity, local support, and partition of unity $\sum_{j=1}^{n} b_{j,k}(x,\boldsymbol{t}) = 1$ which qualify them well as membership functions.

2.2. Tuning of Sugeno controllers as an ill-posed least squares problem

Assume $(\boldsymbol{x},\boldsymbol{y})$ is a set of so-called training data, where $\boldsymbol{x} = (x_1, x_2, \ldots, x_m)^\top$ is the training data vector, and $\boldsymbol{y} = (y_1, y_2, \ldots, y_m)^\top$ the desired output for $\boldsymbol{x}$. It follows immediately from (2.1), and the partition of unity (2.1), that designing a Sugeno controller from training data, is then equivalent to the least squares problem

$$\sum_{i=1}^{m} \Big(y_i - \sum_{j=1}^{n} \alpha_j b_j(x_i;\boldsymbol{t}) \Big)^2 = \min_{((\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\ldots,\boldsymbol{\alpha}_n),\boldsymbol{t}) \in \mathbb{R}^n \times [a,b]^\ell}, \tag{2.4}$$

where $(b_j)_{j=1,\ldots,n}$ is one of the membership functions introduced above. The concrete shape of the membership functions is determined by the ℓ-dimensional knot vector $\boldsymbol{t}$. ℓ represents the number of free knots.

As already mentioned, we have to consider data errors in $\boldsymbol{y}$ and $\boldsymbol{x}$, i.e., instead

$$\|\boldsymbol{x} - \boldsymbol{x}^\gamma\|_{\ell^2} \leq \gamma \tag{2.5}$$

$$\|\boldsymbol{y} - \boldsymbol{y}^\delta\|_{\ell^2} \leq \delta, \tag{2.6}$$

where $\|\boldsymbol{x}\|_{\ell^2} := \sqrt{\sum_{i=1}^m x_i^2}$ denotes the usual ℓ_2 norm.

The following example shows that the problem of finding a minimum to (2.4) is ill-posed, even if we have complete information about the function f, from which the samples y are taken.

Example 2.1. Let $n = 2$, $k \in \mathbb{N}$, $k \geq 2$, $a = t_1^k = 0$, $t_2^k = k^{-3}$ and $t_3^k = 2k^{-3}$, $t_4^k = b = 1$, and choose $\alpha_1^k = k$, $\alpha_2^k = 0$. The fuzzy membership functions b_1 and b_2 are defined by

$$b_1(x;\boldsymbol{t}) = \begin{cases} 1 & \text{if } x \leq t_2 \\ (t_3 - x)(t_3 - t_2) & \text{if } t_2 < x < t_3 \\ 0 & \text{if } t_3 \leq x \end{cases} \tag{2.7}$$

$$b_2(x;\boldsymbol{t}) = 1 - b_1(x;\boldsymbol{t}). \tag{2.8}$$

Then $f^k = \alpha_1^k b_1(x;\boldsymbol{t}^k) + \alpha_2^k b_2(x;\boldsymbol{t}^k)$ converges to zero in $L_2([0,1])$, but α^k has no bounded subsequence. Hence, the optimization problem is unstable with respect to perturbations in the data.

In the remainder of the paper we will assume that the functions b_j satisfy the Lipschitz-estimate

$$|b_j(x,\boldsymbol{t}) - b_j(\tilde{x},\boldsymbol{t})| \leq L|x - \tilde{x}|, \qquad \forall\, x, \tilde{x}, \quad \forall \boldsymbol{t} \in [a,b]^\ell$$

with some nonnegative real constant L.

3. SMOOTHING

In the following we investigate a common stabilization approach for spline approximation (cf e.g. [23]), which consists of replacing (2.4) by

$$\sum_{i=1}^m \Big(y_i - \sum_{j=1}^n \alpha_j b_j(x_i;\boldsymbol{t})\Big)^2 + \beta \Big|\sum_{j=1}^n \alpha_j b_j(\,\cdot\,;\boldsymbol{t})\Big|^2_{H^k(\Omega)} = \min_{(\boldsymbol{\alpha},\boldsymbol{t})}, \tag{3.1}$$

where $|\cdot|_{H^k(\Omega)}$ denotes the norm or seminorm in the Sobolev space $H^k(\Omega)$. Especially in classical approximation theory, this spline smoothing problem is often considered, where the smoothing term characterizes the smoothness of the spline (cf. [6] for fixed knots). It should be mentioned that in practical applications, the smoothness of the controller output is one of the most important design requirements.

However, one can easily show by an adaptation of Example 2.1 that the minimization problem (3.1) is ill-posed itself and thus, this minimization is not a regularization method. So, in addition we impose the constraints

$$t_{j+1} - t_j \geq \epsilon, \qquad j = 1, \ldots, \ell - 1, \tag{3.2}$$

which are necessary to remove the possible instabilities caused by two equal or almost equal knots.

For notational simplicity, we do not bother with multiple knots at the end of the intervals (cf. the definition of the knot sequences (2.2), (2.3)). We will show that (3.1) subject to (3.2) is a well-posed problem and its solution will converge to a minimizer of the original problem with the additional constraint (3.2) for fixed ϵ and appropriately chosen $\beta \to 0$ as $\gamma, \delta \to 0$. However, we cannot show convergence as $\epsilon \to 0$, which is a serious disadvantage.

Now we turn our attention to the stabilized problem (3.1) supplemented by (3.2). For the sake of simplicity we restrict our analysis to the case of $\Omega = (0,1)$, trapezoidal functions b_j and the H^1-norm defined by

$$\|u\|^2_{H^1(\Omega)} = \int_\Omega \left(|u|^2 + |\nabla u|^2\right)\, dx$$

as the stabilizer. Obviously, the number of inner grid points must be even in this case to ensure that the output equals one in the intervals $(0, t_1)$ and $(t_\ell, 1)$. The number of basis functions is then given by $n = \frac{\ell}{2} + 1$. We note that a similar but technically much more complicated reasoning is possible for other spline basis functions, but the technical details would shadow the basic concepts. Therefore, they are omitted here.

The stabilizing term can be transformed to a bilinear expression in terms of the variable $\boldsymbol{\alpha}$ via

$$\Big\| \sum_{j=1}^{n} \alpha_j b_j(.;\boldsymbol{t}) \Big\|^2_{H^1(\Omega)} = \boldsymbol{\alpha}^\top A(\boldsymbol{t})\boldsymbol{\alpha} + \boldsymbol{\alpha}^\top B(\boldsymbol{t})\boldsymbol{\alpha}, \tag{3.3}$$

where the symmetric, positive definite matrices $A(\boldsymbol{t})$ and $B(\boldsymbol{t})$ are defined by

$$A(\boldsymbol{t}) = \Big(\int_0^1 b_i(x;\boldsymbol{t}) b_j(x;\boldsymbol{t})\, dx \Big)_{i,j=1,\ldots,n} \tag{3.4}$$

$$B(\boldsymbol{t}) = \Big(\int_0^1 b_i'(x;\boldsymbol{t}) b_j'(x;\boldsymbol{t})\, dx \Big)_{i,j=1,\ldots,n}. \tag{3.5}$$

Now we define a new grid s_j, which does not include the intervals (t_{2j}, t_{2j+1}), on which $b_i' = 0$ for all i, more precisely,

$$s_1 = t_1, \quad s_{j+1} = s_j + t_{2j} - t_{2j-1}, j = 1, \ldots, \ell/2. \tag{3.6}$$

This allows us to find an equivalent definition for the matrix $B(\boldsymbol{t})$:

Lemma 3.1. *Let $\{\phi_j\}_{j=1,\dots,\ell/2}$ denote the usual piecewise affinely linear finite elements on the grid $\{s_j\}_{j=1,\dots,\ell/2}$, i.e.,*

$$\phi_j|_{(s_i,s_{i+1})} \text{ is affinely linear }, \quad \phi_j(s_i) = \delta_{ij}, \forall\, i,j,$$

where δ_{ij} denotes the Kronecker delta symbol. Then the matrix $\tilde{B}(\boldsymbol{t})$ defined by

$$\tilde{B}(\boldsymbol{t}) = \Big(\int \phi_i'(s)\phi_j'(s)\,ds \Big)_{i,j=1,\dots,\ell/2}$$

equals $B(\boldsymbol{t})$ defined by (3.5). Furthermore, the matrix $A(\boldsymbol{t})$ can be represented in the form

$$A(\boldsymbol{t}) = \Big(\int \phi_i(s)\phi_j(s)\,ds \Big)_{i,j=1,\dots,\ell/2} + A_0(\boldsymbol{t}), \tag{3.7}$$

where $A_0(\boldsymbol{t})$ is a positive semidefinite matrix.

Proof. Since $b_j' = 0$ on (t_{2i}, t_{2i+1}) for all i, j and $b_j'(x;\boldsymbol{t}) = \phi_j'(S_i(x))$ on (t_{2i-1}, t_{2i}), where S_i is the unique transformation of the form $S_i(x) = x + \sigma_i$ that maps (t_{2i-1}, t_{2i}) onto (s_i, s_{i+1}) we obtain

$$\int_0^1 b_i'(x;\boldsymbol{t})b_j'(x;\boldsymbol{t})\,dx = \int \phi_i'(s)\phi_j'(s)\,ds$$

and consequently $\tilde{B}(\boldsymbol{t}) = B(\boldsymbol{t})$.

An analogous argument yields the decomposition

$$A(\boldsymbol{t}) = \Big(\int \phi_i(s)\phi_j(s)\,ds \Big)_{i,j=1,\dots,n} + \Big(\int_{(0,1)-S} b_i(s)b_j(s)\,ds \Big)_{i,j=1,\dots,n},$$

where $S = \cup(t_{2i-1}, t_{2i})$. We now define $A_0(\boldsymbol{t})$ as the second term in the previous identity and since

$$b_i(s)b_j(s) = \begin{cases} 1 & \text{if } i=j,\ s \in (t_{2i-2}, t_{2i-1}) \\ 0 & \text{else for } s \in (0,1) - S \end{cases},$$

A_0 is a diagonal matrix with nonnegative entries and therefore positive semidefinite. $\square$

To carry out the stability analysis we will use the following result adapted from stability estimates in finite element theory:

Lemma 3.2. *For each $c_0 > 0$ there exists a positive real number c_1 such that for all $\boldsymbol{t}$ satisfying $\inf_{j\in\{1,\dots,\ell-1\}}\{t_{j+1} - t_j\} \geq c_0/\ell$, the estimate*

$$\sum_{j=1}^{n} \alpha_j^2 \leq c_1 \ell \Big\| \sum_{j=1}^{n} \alpha_j b_j(x;\boldsymbol{t}) \Big\|_{H^1(\Omega)}^2 \tag{3.8}$$

holds.

Proof. Lemma 3.1 and (3.3) yield the identity

$$\Big\| \sum_{j=1}^{n} \alpha_j b_j(x;\boldsymbol{t}) \Big\|_{H^1(\Omega)}^2 = \alpha^\top \Phi \alpha + \alpha^\top A_0(\boldsymbol{t})\alpha \geq \alpha^\top \Phi \alpha,$$

where

$$\Phi = \Big(\int \left[\phi_i(s)\phi_j(s) + \phi_i'(s)\phi_j'(s)\right]\, ds \Big)_{i,j=1,\ldots,n}.$$

A standard argument from finite-element theory (cf. [29]) implies that the minimal eigenvalue of the symmetric matrix Φ is bounded below by $c_1\ell$, where c_1 depends only on $c_0/2$, which is a lower bound for the length of the interval (s_1, s_n). $\square$

Now we are able to show that the stabilized problem 3.1 is well-posed, i.e., a minimizer exists and the dependence of the minimizers on the data is stable (in a set-valued way), which is expressed in the following propositions:

Proposition 3.1 [Existence of a minimizer]. *For all* $\boldsymbol{y} \in \mathbb{R}^m$ *and* $\boldsymbol{x} \in [0,1]^m$ *there exists a minimizer of* (3.1), *if* $\epsilon > 0$ *and* $\beta > 0$.

Proof. Since a minimizer must yield an output less or equal than the one from $\boldsymbol{\alpha} = 0$, we may add the additional constraint (using Lemma 3.2, $\epsilon = c_0/\ell$ and the notation $C = c_1/c_0$)

$$\sum_{j=1}^{n} \alpha_j^2 \leq \frac{C}{\beta\epsilon} \sum_{i=1}^{m} y_i^2.$$

The resulting set of admissible points is compact in $\mathbb{R}^n \times \mathbb{R}^\ell$ and since the objective functional is continuous, the existence of a minimizer follows from a standard principle in optimization. $\square$

Proposition 3.2 [Stability]. *Let* $\beta > 0$, $\epsilon > 0$, $\boldsymbol{y}^k \to \boldsymbol{y}$ *and* $\boldsymbol{x}^k \to \boldsymbol{x}$. *Then the according sequence of minimizers of* (3.1) *has a convergent subsequence and the limit of every convergent subsequence is a minimizer of* (3.1).

Proof. As in the proof of Proposition 3.1 we obtain the estimate

$$\sum_{j=1}^{n} |\alpha_j^k|^2 \leq \frac{C}{\beta\epsilon} \sum_{i=1}^{m} |y_i^k|^2.$$

Consequently, the sequence $(\boldsymbol{\alpha}^k, \boldsymbol{t}^k)$ is bounded, which implies the existence of a convergent subsequence. Let $(\boldsymbol{\alpha}^{k_\ell}, \boldsymbol{t}^{k_\ell})$ be a convergent subsequence with limit $(\boldsymbol{\alpha}, \boldsymbol{t})$, then the continuity of the objective functional together with the definition of $(\boldsymbol{\alpha}^k, \boldsymbol{t}^k)$ implies that $(\boldsymbol{\alpha}, \boldsymbol{t})$ is a minimizer of (3.1). $\square$

Finally, we want to investigate the question of convergence of minimizers of the regularized problem as the noise level (γ, δ) and the regularization parameter β tend to zero. Of course, it would be of interest to let ϵ tend to zero, too, but in this case one cannot guarantee that the minimizers are uniformly bounded.

Theorem 3.1 [Convergence under constraints].. *Let $\epsilon > 0$ be fixed, let (γ^k, δ^k) be a monotone sequence convergent to $(0,0)$ and let $(x^{\gamma^k}, y^{\delta^k})$ be a corresponding data sequence satisfying* (2.5), (2.6) *with* $(\gamma, \delta) = (\gamma^k, \delta^k)$. *Moreover, let the regularization parameter β^k be chosen such that*

$$\beta^k \to 0, \qquad \max\{\gamma^k, \delta^k\}/\beta^k \to 0.$$

If a minimizer of (2.4) *with exact data exists, then each sequence of minimizers* $(\boldsymbol{\alpha}^k, \boldsymbol{t}^k)$ *of* (3.1), (3.2) *with noisy data* $(x^{\gamma^k}, y^{\delta^k})$ *and* $\beta = \beta^k$ *has a convergent subsequence and the limit of each convergent subsequence is a minimizer of the least squares problem* (2.4) *subject to* (3.2).

Proof. Let $(\hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{t}})$ be a minimizer of the problem with exact data, then the definition of $(\boldsymbol{\alpha}^k, \boldsymbol{t}^k)$ implies

$$\begin{aligned}
&\sum_{i=1}^m \Big(y_i^{\delta^k} - \sum_{j=1}^n \alpha_j^k b_j(x_i^{\gamma^k}, \boldsymbol{t}^k)\Big)^2 + \beta^k \frac{\epsilon}{C} \sum_{j=1}^n (\alpha_j^k)^2 \\
&\quad \leq \sum_{i=1}^m \Big(y_i^{\delta^k} - \sum_{j=1}^n \alpha_j^k b_j(x_i^{\gamma^k}, \boldsymbol{t}^k)\Big)^2 + \beta^k (\boldsymbol{\alpha}^k)^\top [A(\boldsymbol{t}^k) + B(\boldsymbol{t}^k)]\boldsymbol{\alpha}^k \\
&\quad \leq \sum_{i=1}^m \Big(y_i^{\delta^k} - \sum_{j=1}^n \hat{\alpha}_j b_j(x_i^{\gamma^k}, \hat{\boldsymbol{t}})\Big)^2 + \beta^k \hat{\boldsymbol{\alpha}}^\top [A(\hat{\boldsymbol{t}}) + B(\hat{\boldsymbol{t}})]\hat{\boldsymbol{\alpha}} \\
&\quad \leq \sum_{i=1}^m \Big(y_i - \sum_{j=1}^n \hat{\alpha}_j b_j(x_i, \hat{\boldsymbol{t}})\Big)^2 + c_1(\delta^k + L\|\hat{\boldsymbol{\alpha}}\|_{\ell^1}\gamma^k) + c_2\beta^k \sum_{j=1}^n \hat{\alpha}_j^2
\end{aligned}$$

for some constants c_1, c_2. The noisy residual can be estimated by

$$\begin{aligned}
&\sum_{i=1}^m \Big(y_i^{\delta^k} - \sum_{j=1}^n \alpha_j^k b_j(x_i^{\gamma^k}, \boldsymbol{t}^k)\Big)^2 \\
&\qquad \geq \sum_{i=1}^m \Big(y_i - \sum_{j=1}^n \hat{\alpha}_j b_j(x_i, \hat{\boldsymbol{t}})\Big)^2 - c_1(\delta^k + L\|\boldsymbol{\alpha}^k\|_{\ell^1}\gamma^k),
\end{aligned}$$

and hence,

$$\sum (\alpha_j^k)^2 \leq \frac{c_1 C}{\epsilon \beta_k}(2\delta^k + L[\|\hat{\boldsymbol{\alpha}}\|_{\ell^1} + \|\boldsymbol{\alpha}^k\|_{\ell^1}]\gamma^k) + \frac{c_2 C}{\epsilon} \sum \hat{\alpha}_j^2.$$

Finally, with the standard estimate $\|\boldsymbol{\alpha}^k\|_{\ell^1} \leq \sqrt{n}\|\boldsymbol{\alpha}^k\|_{\ell^2}$ we conclude that

$$\sum (\alpha_j^k)^2 \leq \frac{c_1 C}{\epsilon}\Big(4\frac{\delta^k}{\beta_k} + 2L\|\hat{\boldsymbol{\alpha}}\|_{\ell^1}\frac{\gamma^k}{\beta^k}\Big) + L^2\frac{c_1^2 C^2}{\epsilon^2}\Big(\frac{\gamma^k}{\beta^k}\Big)^2 + 2\frac{c_2 C}{\epsilon}\sum \hat{\alpha}_j^2,$$

which implies

$$\limsup \sum (\alpha_j^k)^2 \le 2\frac{c_2 C}{\epsilon} \sum \hat{\alpha}_j^2.$$

Thus, the sequence $(\boldsymbol{\alpha}_j^k, \boldsymbol{t}^k)$ is bounded and therefore there exists a convergent subsequence. The fact that the limit of a convergent subsequence is a minimizer of (2.4) follows from

$$\limsup \sum_{i=1}^{m} \Big(y_i^{\delta^k} - \sum_{j=1}^{n} \alpha_j^k b_j(x_i^{\gamma^k}, \boldsymbol{t}^k) \Big)^2 \le \sum_{i=1}^{m} \Big(y_i - \sum_{j=1}^{n} \hat{\alpha}_j b_j(x_i, \hat{\boldsymbol{t}}) \Big)^2.$$

□

4. TIKHONOV REGULARIZATION

In this section we investigate a different approach to the regularization of the least squares problem (2.4), namely the classical Tikhonov regularization in the parameter space $\mathbb{R}^n \times \mathbb{R}^\ell$, it consists of minimizing the functional

$$\sum_{i=1}^{m} \Big(y_i^\delta - \sum_{j=1}^{n} \alpha_j b_j(x_i^\gamma; \boldsymbol{t}) \Big)^2 + \beta_1 \sum_{j=1}^{n} \alpha_j^2 + \beta_2 \sum_{j=1}^{\ell} (t_j - t_j^*)^2 = \min_{(\boldsymbol{\alpha}, \boldsymbol{t})} \tag{4.1}$$

for appropriately chosen β_1 and β_2 (in dependence of δ and $\boldsymbol{y}^\delta$), where $\boldsymbol{t}^*$ is a prior for $\boldsymbol{t}$, e.g. the uniform grid points. In this case we can show convergence for appropriate choice of $\beta_1 \to 0$ as the noise level tends to zero even for $\beta_2 = 0$, which is due to the compactness of the set of admissible $\{t_i\}$.

We restrict our attention again to the case $\Omega = (0, 1)$, but we note that the method and all proofs can be carried out in the same way (but with vectors t_j). In the general theory (cf. e.g. [3, 8, 9]), the existence of a minimizer of problem (4.1) can be shown if $\beta_1 > 0$ and $\beta_2 > 0$. In our special case, the positivity of the second regularization parameter β_2 is not necessary to guarantee the existence, since we have the additional information that the parameters t_i are contained in the compact set Ω:

Proposition 4.1 [Existence of a minimizer]. *For all* $\boldsymbol{y} \in \mathbb{R}^m$ *and* $\boldsymbol{x} \in [0, 1]^m$ *there exists a minimizer of* (4.1), *if* $\beta_1 > 0$.

Proof. As in the proof of Proposition 3.1 it suffices to show that the set of admissible $\boldsymbol{\alpha}$ can be restricted to a compact set by an a-priori estimate. Again from a comparison with the output functional at the point $\boldsymbol{\alpha} = 0$, we may conclude that a minimizer $(\boldsymbol{\alpha}, \boldsymbol{t})$ of (4.1) must satisfy

$$\sum_{j=1}^{n} \alpha_j^2 \le \frac{1}{\beta_1} \sum_{i=1}^{m} |y_i^\delta|^2.$$

□

We note that the stability and convergence analysis of Tikhonov regularization with respect to the perturbation in the output $\boldsymbol{y}$ can be carried over directly from [9, 25]. Since we are also interested in perturbations in the positions $\boldsymbol{x}$, we need some modifications, which we will prove in the following:

Proposition 4.2 [Stability]. *Let $\beta_1 > 0$, $\boldsymbol{y}^k \to \boldsymbol{y}$ and $\boldsymbol{x}^k \to \boldsymbol{x}$. Then the according sequence of minimizers $(\boldsymbol{\alpha}^k, \boldsymbol{t}^k)$ of* (4.1) *has a convergent subsequence and the limit of every convergent subsequence is a minimizer of* (4.1).

Proof. Again we compare the value of the objective functional achieved at $(\boldsymbol{\alpha}^k, \boldsymbol{t}^k)$ for the data $\mathbf{x}^k$ and $\boldsymbol{y}^k$ with the one achieved with $(\mathbf{0}, \boldsymbol{t}^k)$ and obtain the a-priori estimate

$$\sum_{j=1}^{n} \alpha_j^2 \leq \frac{1}{\beta_1} \sum_{i=1}^{m} |y_i^k|^2.$$

Since $\boldsymbol{y}^k \to \boldsymbol{y}$, the right-hand side is uniformly bounded as $k \to \infty$ and therefore the set of minimizers is bounded, which implies the existence of a weakly convergent subsequence.

By standard techniques (as in [25]) one can show that a convergent subsequence (without restriction of generality $(\boldsymbol{\alpha}^k, \boldsymbol{t}^k)$ itself and limit $(\bar{\boldsymbol{\alpha}}, \bar{\boldsymbol{t}})$) satisfies

$$\begin{aligned} &\sum_{i=1}^{m} \Big(y_i - \sum_{j=1}^{n} \bar{\alpha}_j b_j(x_i; \bar{\boldsymbol{t}}) \Big)^2 + \beta_1 \sum_{j=1}^{n} \bar{\alpha}_j^2 + \beta_2 \sum_{j=1}^{\ell} (\bar{t}_j - t_j^*)^2 \\ &\quad \leq \sum_{i=1}^{m} \Big(y_i - \sum_{j=1}^{n} \alpha_j b_j(x_i; \boldsymbol{t}) \Big)^2 + \beta_1 \sum_{j=1}^{n} |\alpha_j|^2 + \beta_2 \sum_{j=1}^{\ell} (t_j - t_j^*)^2 \end{aligned}$$

for all admissible $(\boldsymbol{\alpha}, \boldsymbol{t})$ and thus, the limit is again a minimizer of (4.1). □

The convergence result in this case holds for the full problem (2.4), not only for a constrained version:

Theorem 4.1 [Convergence]. *Assume that a minimizer of problem* (4.1) *exists. Moreover, let (γ^k, δ^k) be a sequence converging to $(0,0)$ and denote by $(\boldsymbol{\alpha}^k, \boldsymbol{t}^k)$ the according sequence of minimizers of* (4.1) *with data $(\boldsymbol{x}^\gamma, \boldsymbol{y}^\delta)$, satisfying* (2.5), (2.6). *Then $(\boldsymbol{\alpha}^k, \boldsymbol{t}^k)$ has a convergent subsequence and the limit of every convergent subsequence is a minimizer of* (4.1) *with exact data $(\boldsymbol{x}, \boldsymbol{y})$ if the regularization parameters satisfy*

$$\beta_1^k \to 0, \quad \beta_2^k \to 0, \quad \max\{\gamma^k, \delta^k\}/\beta_1^k \to 0, \qquad \exists \epsilon > 0 : \ \beta_1^k/\beta_2^k \geq \epsilon. \quad (4.2)$$

Proof. By similar reasoning to the proof of Theorem 3.1 we can deduce that

$$\limsup \sum (\alpha_j^k)^2 \leq \sum \hat{\alpha}_j^2 + \limsup \frac{\beta_2^k}{\beta_1^k} \sum (\hat{t}_j - t_j^*)^2$$

for a minimizer $(\hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{t}})$ of (2.4). The remaining steps of the proof are the same as for Theorem 3.1. □

Finally, we want to investigate the rate of convergence of the regularized solutions as $\delta \to 0$. For this sake we need additional smoothness of the *parameter-to-output map*, which we will define and analyze in the following Lemma:

Lemma 4.1. *Let $b_j \in C([0,1]^{\ell+1})$ for all $j \in \{1,\dots,n\}$, then the nonlinear parameter-to-output operator F defined by*

$$\begin{aligned} F : \mathbb{R}^n \times [0,1]^\ell \to \quad & \mathbb{R}^m \\ (\boldsymbol{\alpha}, \boldsymbol{t}) \quad \mapsto & \Big(\textstyle\sum_{j=1}^n \alpha_j b_j(x_i; \boldsymbol{t}) \Big)_{i=1,\dots,m} \end{aligned} \tag{4.3}$$

is continuous. Moreover, if the partial derivatives $\partial b_j / \partial t_k$ exist and are continuous functions for all $j \in \{1,\dots,n\}$, $k \in \{1,\dots,\ell\}$, then F is continuously Frèchet-differentiable with partial derivatives

$$\frac{\partial}{\partial \alpha_k} F(\boldsymbol{\alpha}, \boldsymbol{t}) = (b_k(x_i; \boldsymbol{t}))_{i=1,\dots,m} \tag{4.4}$$

$$\frac{\partial}{\partial t_k} F(\boldsymbol{\alpha}, \boldsymbol{t}) = \Big(\sum_{j=1}^n \alpha_j \frac{\partial b_j}{\partial t_k}(x_i; \boldsymbol{t}) \Big)_{i=1,\dots,m}. \tag{4.5}$$

If the partial derivatives above are all Lipschitz-continuous, then F' is Lipschitz-continuous, too.

For convergence rates, we restrict our attention to the case of $\gamma = 0$, which corresponds to an implicit assumption that errors in the input variables can be transformed to errors in the output variables. Of course, this may be a severe restriction, but so far it is the only one enabling the application of the standard theory of Tikhonov regularization. As usual for ill-posed problems, the convergence can be arbitrarily slow in general (cf. e.g. [21]), rates can only be achieved under additional conditions on the solution. A standard condition of this kind is the *source condition*

$$\exists\ \boldsymbol{w} \in \mathbb{R}^m \ :\ (\bar{\boldsymbol{\alpha}}, \bar{\boldsymbol{t}} - \boldsymbol{t}^*) = F'(\bar{\boldsymbol{\alpha}}, \bar{\boldsymbol{t}})^* \boldsymbol{w}, \tag{4.6}$$

which is an abstract smoothness condition. The adjoint of the operator F' defined in (4.3) is given by

$$F'(\alpha, \boldsymbol{t})^*(u, v) = \begin{pmatrix} \sum_{i=1}^n b_k(x_i; \boldsymbol{t}) u_i \\ \sum_{i=1}^n \sum_{j=1}^m \alpha_j \dfrac{\partial b_j}{\partial t_k}(x_i; \boldsymbol{t}) v_i \end{pmatrix} \tag{4.7}$$

Theorem 4.2 [Rate of convergence]. *Let $\boldsymbol{y}^\delta \in \mathbb{R}^m$ satisfy (2.6) and let $\boldsymbol{\alpha}_0, \boldsymbol{t}_0$ be a solution of minimal distance (in the product space $\ell^2 \times \ell^2$) to the prior $(0, \boldsymbol{t}^*)$. Furthermore, let the metric projection of the exact data y onto $\mathcal{R}(F)$ be unique and equal the projection of $\mathcal{R}(F) \cap B_\epsilon(F(\boldsymbol{\alpha}_0, \boldsymbol{t}_0))$. Finally, let $b_j \in C^{1,1}([0,1])$ and denote by L_F the resulting Lipschitz-constant of F' in $B_r(\boldsymbol{\alpha}_0, \boldsymbol{t}_0)$ due to Lemma 4.1. If (4.6) holds with*

$$L_F \|w\|_{\ell^2} < 1, \tag{4.8}$$

then the choice $\beta_1 = \beta_2 \sim \sqrt{\delta}$ *yields*

$$\|(\boldsymbol{\alpha}^\delta - \boldsymbol{\alpha}_0, \boldsymbol{t}^\delta - \boldsymbol{t}_0)\|_{\ell^2 \times \ell^2} = \mathcal{O}(\sqrt{\delta}), \tag{4.9}$$

where $(\boldsymbol{\alpha}^\delta, \boldsymbol{t}^\delta)$ *denotes the solution of* (4.1) *with noisy data* $\boldsymbol{y}^\delta$.

The assertion follows by an application of Theorem 3.7 in [3].

Remark 4.1. It is clear that the source condition is a severe restriction if $m < n + \ell$, since the set of parameters that can fulfill the source condition is a lower-dimensional manifold. However, the case of $m \gg n + \ell$ usually arises in practical applications and thus, the source condition is mainly an assumption on the regularity of the distribution of the parameters t_k with respect to the grid points. To illustrate this, we consider the case of cubic B-splines on the unit interval, where the free knots are given by $t_2, ..., \ldots, t_{n-1}$ and we have $t_1 = 0$ and $t_n = 1$. Suppose that the following condition is fulfilled:

$$\forall\ k \in \{1, \ldots, n-1\} \quad \exists\ i_1(k), i_2(k) \quad x_{i_1(k)}, x_{i_2(k)} \in (t_k, t_{k+1}),$$

then we can set $w_i = 0$ for all $i \notin \{i_1(k), i_2(k)\}_{k \in \{1,\ldots,n-1\}}$ and write the source condition as a system for $(w_{i_1(1)}, w_{i_2(1)}, \ldots, w_{i_1(n-1)}, w_{i_2(n-1)})$, which is an upper-diagonal system of size $2n - 2 \times 2n - 2$. Since the diagonal entries are all nonzero (note that $x_{i_1(k)}$ and $x_{i_2(k)}$ are in the interior of the interval (t_k, t_{k+1}), there exists a unique solution. Hence, the source condition (4.6) is satisfied and (4.8) holds if in addition $\|\alpha\|$ and $\|\boldsymbol{t} - \mathbf{t}^*\|$ are sufficiently small.

5. NUMERICAL SOLUTION OF THE REGULARIZED PROBLEM

In this section we want to verify theoretical results obtained above by numerical experiments. The description of the optimization algorithm—a generalized Gauss—Newton like method—follows Schütze [22, 23].

5.1. Description of the optimization algorithm

The common characteristic of both the primal nonlinear least squares problem (2.4) as well as the regularized problems (3.1), (3.2) and (4.1) is that they are linear in one set of variables (the coefficients $\boldsymbol{\alpha}$) but nonlinear in the set of free knots $\boldsymbol{t}$. In the unconstrained case such semi-linear separable problems were first analyzed in detail by Golub/Pereyra [11]. Later Parks [19] treated general constrained nonlinear problems of this type.

Consider the following semi-linear least squares problem with linear inequality constraints:

$$\min_{\boldsymbol{\alpha}, \boldsymbol{t}} \{\|G(\boldsymbol{t})\boldsymbol{\alpha} - y(\boldsymbol{t})\|^2 \mid C\boldsymbol{t} \geq \boldsymbol{h},\ \boldsymbol{t} \in [0,1]^\ell,\ \boldsymbol{\alpha} \in \mathbb{R}^n\} \tag{5.1}$$

representing (3.1), (3.2) with appropriately chosen regularized observation matrix $G \in \mathbb{R}^{m+p,n}$, ($p = n - k$ in case of (3.1), $p = n + \ell$ for (4.1)) vector of coefficients $\boldsymbol{\alpha} \in \mathbb{R}^n$ and data vector $\boldsymbol{y} \in \mathbb{R}^m$. The constraints (3.2) on the knot positions are expressed equivalently in matrix formulation. In the case of (4.1) we do not include the inequality constraints.

The linear subproblem

$$\min_{\boldsymbol{\alpha}}\{\|G(\boldsymbol{t})\boldsymbol{\alpha} - \boldsymbol{y}(\boldsymbol{t})\|^2 \mid \boldsymbol{\alpha} \in \mathbb{R}^n\} \tag{5.2}$$

can be solved easily for fixed $\boldsymbol{t}$, e.g. by reducing G to upper triangular form by a series of Givens rotations, leading to the minimum norm solution

$$\boldsymbol{\alpha}(\boldsymbol{t}) = G^\dagger(\boldsymbol{t})\boldsymbol{y}(\boldsymbol{t}). \tag{5.3}$$

where $G^\dagger(\boldsymbol{t})$ is the pseudoinverse of $G(\boldsymbol{t})$. It follows that the original separable problem can be written

$$\min_{\boldsymbol{t}}\{\|G(\boldsymbol{t})\, G^\dagger(\boldsymbol{t})\, \boldsymbol{y}(\boldsymbol{t}) - \boldsymbol{y}(\boldsymbol{t})\|^2 \mid \boldsymbol{t} \in [0,1]^\ell\} \tag{5.4}$$

which is now a nonlinear least squares problem in the free knots $\boldsymbol{t}$ only.

Golub and Pereyra [11] showed that under natural assumptions which guarantee the continuity of the pseudoinverse, the reduction is feasible in the sense that the change from minimizing the full problem to minimizing the reduced problem does not add any critical points and does not exclude the solution of the original problem. Such a natural assumption is that the rank of the matrix $G(\boldsymbol{t})$ is constant on an open neighborhood which contains the solution. The constant rank assumption, even the full rank assumption on $G(\boldsymbol{t})$ is satisfied in the case of the regularized problem (4.1) and (3.1) together with (3.2).

Since $G(\boldsymbol{t})\, G^\dagger(\boldsymbol{t})$ is the orthogonal projector on the range of $G(\boldsymbol{t})$, algorithms based on (5.4) are often called variable projection algorithms. A variable projection algorithm using a Gauss—Newton method applied to the reduced problem (5.4) was used to solve the original least squares problem. The Gauss—Newton method is based on a sequence of linear approximations of the residuum. If $\boldsymbol{t}^\nu$ denotes the current approximation, then a correction $\boldsymbol{p}^\nu$ is computed as a solution to the quadratic problem

$$\min_{\boldsymbol{p}}\{\|[I - G(\boldsymbol{t}^\nu)\, G^\dagger(\boldsymbol{t}^\nu)]\, \boldsymbol{y}(\boldsymbol{t}^\nu) + J(\boldsymbol{t}^\nu)\boldsymbol{p}\|^2 \mid \boldsymbol{p} \in \mathbb{R}^\ell\}. \tag{5.5}$$

with J the Jacobi matrix of $R(\boldsymbol{t}) := [I - G(\boldsymbol{t})\, G^\dagger(\boldsymbol{t})]\, \boldsymbol{y}(\boldsymbol{t})$ evaluated at $\boldsymbol{t}^\nu$. If the Jacobian has full rank then (5.5) has a unique solution $\boldsymbol{p}^\nu$ which defines the new approximate

$$\boldsymbol{t}^{\nu+1} = \boldsymbol{t}^\nu + \boldsymbol{p}^\nu. \tag{5.6}$$

The Gauss—Newton method can be generalized to constrained problems. A search direction $\boldsymbol{p}^\nu$ is then computed as a solution to

$$\min_{\boldsymbol{p}}\{\|R(\boldsymbol{t}^\nu) + J(\boldsymbol{t}^\nu)\boldsymbol{p}\|^2 \mid C(\boldsymbol{t} + \boldsymbol{p}) \geq \boldsymbol{h},\ \boldsymbol{p} \in \mathbb{R}^\ell\} \tag{5.7}$$

by first transforming (5.7) by Householder reflections into a least distance problem and finally using an active set strategy for solving the resulting nonnegative least squares problem [18].

For evaluating J, the derivative of R has to be computed. Expressions for the derivatives of B-splines with respect to its knots can be found, e.g. in [22], the formulas for the Frèchet derivative of an orthogonal projector in [11]. Alternatively the derivatives can be approximated by finite differences. Then l additional least squares problems have to be solved in each computation of the derivative. However, in our case, the (regularized) observation matrix G is banded, so that the costs of realizing the linear algebra involved are relatively cheap.

The undamped generalized Gauss-Newton method converges only locally and for small residual problems. In order to globalize the method, a Armijo—Goldstein line search has been implemented. To be robust the algorithm must employ stabilizing techniques for the Gauss—Newton steps when the Jacobian J is nearly rank deficient. This is done by applying a Levenberg—Marquardt method.

Jupp [14] referred to the potentially high number of local extrema for free knot least squares problems. Not surprisingly, the local minimum to which the optimization algorithm converges heavily depends on the starting knot sequence $\boldsymbol{t}^0$. Hence, the generalized Gauss—Newton method is rerun several times with equally distributed random starting values.

5.2. Results for fixed error levels

In the following we compare the results of reconstructing an a-priori given function from noisy measurements taking into account spline approximation, smoothing and Tikhonov regularization. The exact data values are perturbed with uniformly distributed random noise. In these examples we show that regularization both leads to stable function approximations as well as stable fuzzy sets and consequent values. In the last example we take a more careful look onto constructing an interpretable fuzzy controller.

In the figures, the starting knot sequences for the reduced free knot optimization problem are marked with $*$ whereas the locations of the resulting (local) optimal knots are labeled with $\square$. The noisy data are represented by dots, the solid line represents the 'optimal' spline approximation.

In the tables, we compare the residuals $r_{0,0}$ and $r_{\gamma,\delta}$ for exact and noisy data, i.e.

$$r_{\gamma,\delta} := \Big[\sum_{i=1}^{m} \Big(y_i^\delta - \sum_{j=1}^{n} \alpha_j^{\gamma,\delta}\; b_j(x_i^\gamma; \boldsymbol{t}^{\gamma,\delta}) \Big)^2 \Big]^{1/2} \tag{5.8}$$

where $\boldsymbol{\alpha}^{\gamma,\delta}$ and $\boldsymbol{t}^{\gamma,\delta}$ denote the solutions to the (regularized) optimization problems with noisy data.

Example 5.1. The first example deals with the reconstruction of the function

$$f_1(x) := 10x/(1 + 100x^2) \qquad x \in [-2, 2] \tag{5.9}$$

(see Figure 2), a function already considered in [13] and [22] in the context of spline approximation and smoothing.

Table 1. Example 1: Results for different solution strategies

	Approximation	Smoothing	Tikhonov reg.
$r_{0,0}$	4.99659	0.55853	0.52923
$r_{\gamma,\delta}$	0.16833	0.59593	0.59760
$\|\boldsymbol{\alpha}\|_{\ell^2}$	8.19528	0.56305	0.60057
$\|\boldsymbol{t}-\boldsymbol{t}^*\|_{\ell^2}$	1.11397	0.83290	0.41486

Table 2. Example 1: Starting and optimized knot sequences

$\boldsymbol{t}^0=\boldsymbol{t}^*$	-1.566	-1.111	-0.667	-0.222	0.222	0.667	1.111	1.556
Appr.	-1.803	-1.012	-0.192	-0.032	-0.030	0.069	1.405	1.705
Smoothing	-1.872	-0.788	-0.226	-0.224	0.186	0.190	1.037	1.802
Tikhonov	-1.563	-1.120	-0.711	-0.237	0.062	0.288	1.126	1.558

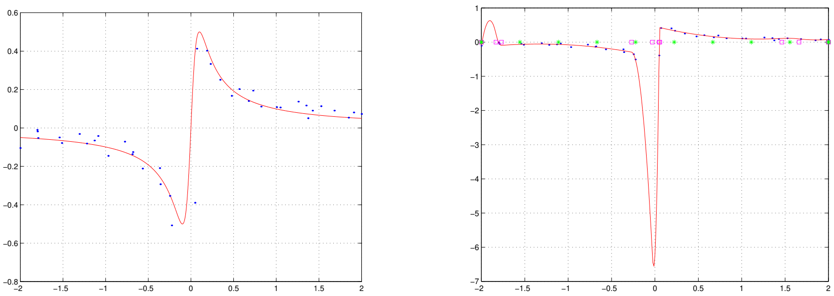

Figure 2. Example 1: The function $10x/(1+100x^2)$ and noisy data (left) and raw approximation with 11 quadratic B-splines (right; $\varepsilon = 0.001$)

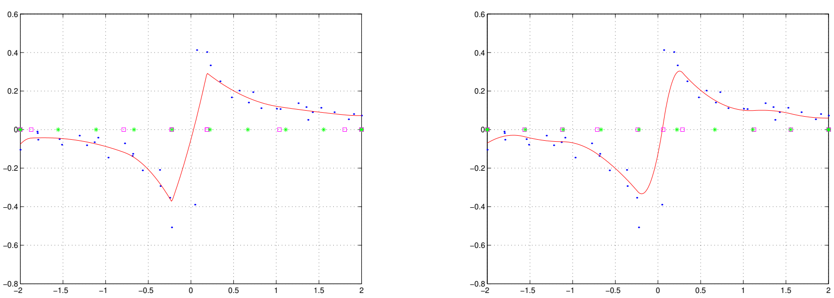

Figure 3. Example 1: Reconstruction with 11 quadratic B-splines with smoothing (left; $k = 1$, $\beta = 0.06$, $\varepsilon = 0.001$) and Tikhonov regularization(right; $\beta_1 = 0.4$, $\beta_2 = 0.4$)

Both the abscissa as well as the data values are perturbed with uniformly distributed random noise. The perturbations of the 40 data samples are within a level of 5% and 12%, respectively leading to noise levels $\gamma = 0.364$ and $\delta = 0.199$. For the reconstruction 11 B-splines of order 3 (quadratic splines) are used. The optimization algorithm for the 8 free knots is started with an equidistant knot sequence.

When approximating f_1 without including any smoothing terms, the resulting function is rather arbitrary (cf. Figure 2, right); in most cases the optimization procedure breaks down. The Schoenberg—Whitney condition is not satisfied for the knot sequences in the iterative optimization process, the system matrix becomes singular. In smoothing some positions of the optimized knot sequence nearly coincide. However, the minimal distance requirement between knots stabilizes the calculations. In Tikhonov regularization knots are quite separated due to the choice of $\boldsymbol{t}^*$.

When comparing residuals for exact data, Tikhonov regularization gives better results than smoothing, and of course, much better results than approximation without applying any regularization technique. But Tikhonov regularization also gives better results with regard to the linguistic interpretability of the resulting fuzzy controller, as we will see in the next example.

Example 5.2. Similar to the paper of Setnes et.al. [26] we want to construct a transparent rule-based model from noisy data measurements considering the spectral data function

$$f_2(x) := 12\,\mathrm{e}^{-(x-4.8)(x-5.8)/0.7} - 12\mathrm{e}^{-(x+3.5)^2} + 0.8x, \quad x \in [-10, 10] \tag{5.10}$$

(cf. Figure 4, left). By using inputs x uniformly distributed in $[-10, 10]$ 50 samples of $f_2(x)$ were obtained and then disturbed with uniformly distributed noise within a noise level of 10% (δ =9.5804, maximal error =2.0398).

When constructing a Sugeno controller from measurements, the question on the optimal number of rules or equivalently knots arises. In the context of spline approximation and smoothing, Schütze [22] proposes a knot removal strategy leading to a nearly optimal number of knots. However, we just fix the number of rules to be equal to eight. Accordingly, the universe of discourse is split into eight fuzzy sets interpretable linguistically as negative big, negative medium, negative small, negative very small, positive very small, positive small, positive medium and positive big. To be interpretable easily, the shape of the membership functions is chosen to be triangular.

Figure 4 and Figure 5 show the results for approximation, smoothing and Tikhonov regularization of the noisy data problem. Although the residuum is smaller for approximation than for smoothing and Tikhonov regularization (Table 3), only the later succeeds in constructing an interpretable fuzzy controller since knots are separated appropriately. In approximation and smoothing knots of the optimized sequence nearly coincide (Table 4) leading to questionable and not linguistically interpretable membership functions (Figure 4, right and Figure 5, lower parts). For Tikhonov regularization $\boldsymbol{t}^*$ is chosen to be equidistant

Table 3. Example 2: Results for different solution strategies

	Approx	Smoothing	Tikhonov
$r_{0,0}$	12.0859	14.6041	14.5291
$r_{\gamma,\delta}$	12.3130	14.7508	16.9215
$\|\boldsymbol{\alpha}\|_{\ell^2}$	32.6938	25.8770	22.7836
$\|\boldsymbol{t}-\boldsymbol{t}^*\|_{\ell^2}$	4.1379	4.4046	1.8854

Table 4. Example 2: Starting and optimized knot sequences

$\boldsymbol{t}^0 = \boldsymbol{t}^*$	-7.143	-4.286	-1.429	1.429	4.286	7.143
Appr.	-5.585	-2.661	-2.608	3.999	5.658	5.668
Smoothing	-5.372	-3.119	-2.399	4.215	4.346	4.655
Tikhonov	-7.124	-3.718	-0.989	2.790	5.354	7.354

Table 5. Sugeno controller identified from noisy data

Rule: Antecedent		Consequent singleton	Consequent label
R1 : If x is *Negative Big*	then	$y=-7.605$	*Negative Medium*
R2 : If x is *Negative Medium*	then	$y=-5.025$	*Negative Medium*
R3 : If x is *Negative Small*	then	$y=-11.063$	*Negative Big*
R4 : If x is *Negative very Small*	then	$y=-0.460$	*Negative very Small*
R5 : If x is *Positive very Small*	then	$y=1.367$	*Positive very Small*
R6 : If x is *Positive Small*	then	$y=15.095$	*Positive Big*
R7 : If x is *Positive Medium*	then	$y=4.968$	*Positive Medium*
R8 : If x is *Positive Big*	then	$y=7.682$	*Positive Medium*

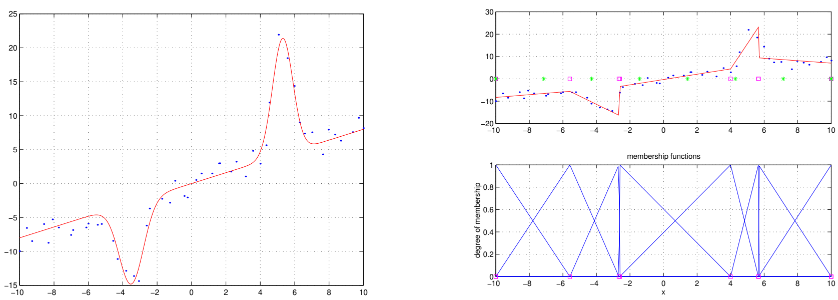

Figure 4. Spectral data function f_2 and noisy measurements (left) and raw approximation with 8 triangular membership functions (right; $k=1$, $\varepsilon=0.01$)

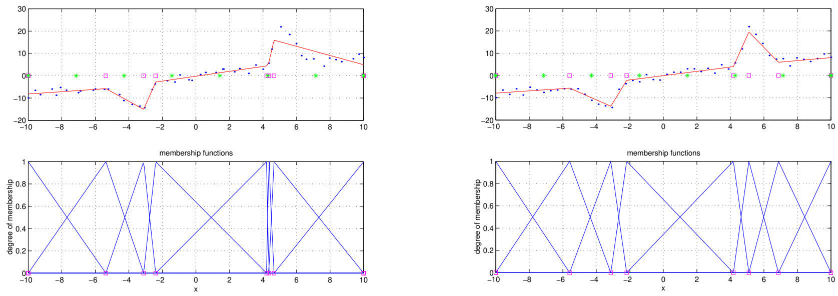

Figure 5. Approximation with 8 triangular membership functions with smoothing (left; $k = 1$, $\beta = 0.01$, $\varepsilon = 0.01$) and Tikhonov regularization (right; $\beta_1 = \beta_2 = 0.5$)

Table 6. Consequent values for two different noisy data sets

Appr.	-8.190	-4.879	-11.067	5.506	-0.842	19.804	5.124	7.751
	-8.362	-3.800	-15.577	-1.186	1.505	18.874	2.065	15.428
Tikhonov	-8.648	-4.307	-13.382	-1.380	-0.110	19.405	5.758	7.280
	-8.268	-3.984	-14.710	-0.716	-0.291	21.700	4.100	7.595

within the underlying interval. The linguistic fuzzy model constructed from Tikhonov regularization is given in Table 5.

Furthermore, we demonstrate that Tikhonov regularization leads not only to stable output functions but also to stable and well-interpretable fuzzy sets and consequent values as opposed to raw approximation. The calculations were done with 50 data samples perturbed with random noise within a 2 % level for measurement locations and an 8 % level for output values. Two such noisy data sets were generated. Figure 6 and Table 6 show that Tikhonov regularization leads to consequent values and fuzzy membership functions, which coincide quite well for the two differently perturbed data sets, which is not the case without regularization and demonstrates that Tikhonov regularization is a powerful tool in the numerical optimization of fuzzy controllers.

5.3. Results for error level tending to zero

Again, we consider the reconstruction of the function f_1 (cf. (5.9), Figure 2) and try to validate the convergence properties stated in Theorem 4.2. We take 90 data samples equidistant in $[-2, 2]$ and perturb the y-values with uniformly distributed random noise up to a noise level of 20 % (maximal error = 0.0986, maximal $\delta = 0.5226$). 15 B-splines of order 5 act as membership functions in Tikhonov regularization. It is easily shown that the assumptions of Theorem 4.2 are satisfied.

The residuum for the least squares approximation of the exact data is equal to 0.004322. The resulting knot sequence

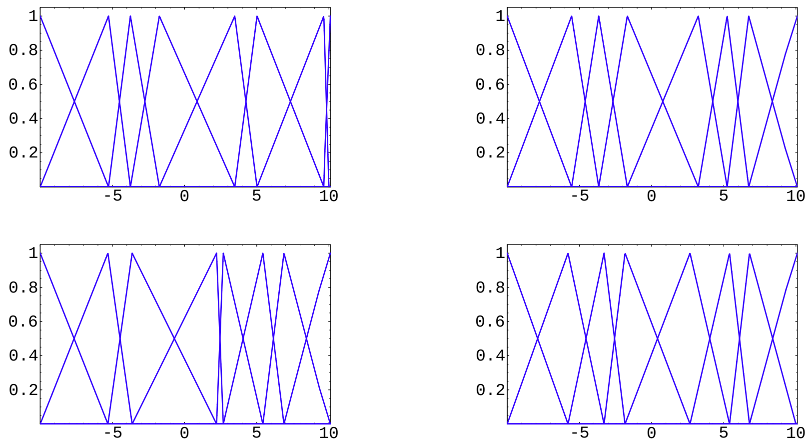

Figure 6. Optimized fuzzy membership functions for two different noisy data sets with raw approximation (left) and Tikhonov regularization(right; $\beta_1 = 0.5$, $\beta_2 = 20$)

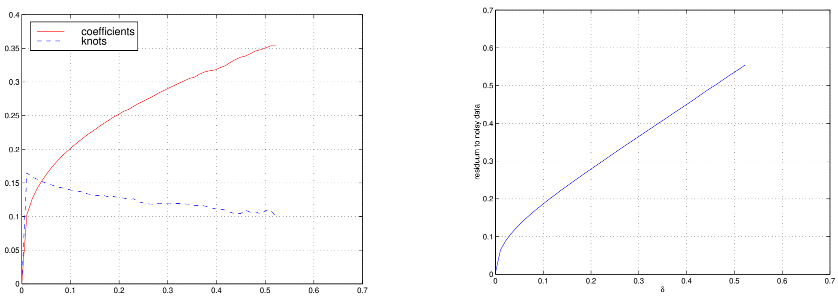

Figure 7. $\|\boldsymbol{\alpha}^\delta - \boldsymbol{\alpha}\|_{\ell_2}$ and $\|\boldsymbol{t}^\delta - t^*\|_{\ell_2}$ vs. δ (left) and residuum $\|F(\boldsymbol{\alpha}^\delta, \boldsymbol{t}^\delta) - \boldsymbol{y}^\delta\|_{\ell_2}$ of Tikhonov regularized approximation to noisy data vs. noise level (right)

$$\begin{aligned}\overline{\boldsymbol{t}} = \{&-1.2665, -0.7356, -0.1896, -0.0351, -0.0350,\\ &0.0349, 0.0350, 0.1896, 0.7355, 1.2656\}\end{aligned}$$

is taken as the prior $\boldsymbol{t}^*$. The regularization parameters are chosen according to the theory ($\beta_1 = \beta_2 = \mathcal{O}(\sqrt{\delta})$), where one has to take into account appropriate equilibration of the two parameters. Figure 7 (left) shows the ℓ_2 difference of the coefficients and knots obtained from exact data vs. noisy data. It is noticeable that the difference between the knot sequences is nearly constant or even declines with increasing δ, which could be explained by the increased weighting of the β_2 term in the objective functional. The ℓ_2 difference of the coefficients is quite well in agreement with the theory. Finally, in Figure 7 (right) the residuum of the Tikhonov regularized approximation to noisy data is plotted against the error level δ.

6. EXTENSIONS AND OPEN PROBLEMS

We have seen in the preceding sections that regularization leads to stable approximations of the minimizers and, in addition, improves the interpretability of the arising fuzzy systems, because grid points are separated. So far, we have restricted our analysis to a one-dimensional situations, but multi-dimensional problems arise in many applications. Under the assumptions of the previous sections, the input-output function F_s of a Sugeno controller with d-dimensional input variable is given by

$$F_s(x_1, x_2, \dots, x_d) \\ = \alpha_{j_1, j_2, \dots, j_d} \sum_{j_1=1}^{n_1} \sum_{j_2=1}^{n_2} \dots \sum_{j_d=1}^{n_d} b_{j_1}(x_1, \boldsymbol{t}_1) \cdot b_{j_2}(x_2, \boldsymbol{t}_2) \cdot \ldots \cdot b_{j_d}(x_d, \boldsymbol{t}_d).$$

F_s represents a d-dimensional tensor product spline. However, the results on Tikhonov regularization can be carried over to a multi-dimensional situation without many modifications (except with respect to notation). In the case of smoothing the change to higher dimensions is more difficult, since it is not obvious how the singular values of the system matrix can be estimated for arbitrary parameters $\boldsymbol{t}$.

Since our analysis seems to be a novel approach to the optimization of fuzzy systems, there are still open problems connected to it, which might be of importance for application. In particular we want to mention the so-called *generalization error* (cf. [33]), which means the error of the approximator at points $x \notin \{x_i\}_{i=1,\dots,m}$. A desirable property of the approximators would be convergence to the function from which the samples are taken, as the number of grid points m tends to infinity. However, such a convergence result can be obtained only if also $n \to \infty$, which is often not desirable for fuzzy systems. Nevertheless a meaningful approximation should yield boundedness (and smallness) of the error as $m \to \infty$.

If the grid is regular enough one could consider the case $h \to 0$, where h is a real number such that $|x_i - x_{i-1}| < h$ for all i, which allows a rather standard deterministic analysis. For more irregular distributions of sampling points, one should use different concepts such as stochastic models for the locations. This will be one of our main items for future research.

REFERENCES

1. R. Babuška, *Fuzzy Modeling for Control.* Kluwer Academic Publishers, Boston, 1998.

2. P. Bauer, E. P. Klement, B. Moser, and A. Leikermoser, Modeling of control functions by fuzzy controllers. In: *Theoretical Aspects of Fuzzy Control.* H. T. Nguyen, M. Sugeno, R. M. Tong, and R. R. Yager (Eds). John Wiley & Sons, New York, 1995, Ch. 5, 91–116.

3. A. Binder, H. W. Engl, C. W. Groetsch, A. Neubauer, and O. Scherzer, Weakly closed nonlinear operators and parameter identification in parabolic equations by Tikhonov regularization. *Appl. Anal.* (1994) **55**, 215–234.

4. C. M. Bishop, *Neural Networks for Pattern Recognition.* Clarendon Press, Oxford, 1995.

5. M. Burger and H. W. Engl, Training neural networks with noisy data as an ill-posed problem. *Adv. Comp. Math.* (2000) **13**, 335–354.

6. C. de Boor, *A Practical Guide to Splines.* Springer-Verlag, New York—Heidelberg—Berlin, 1978.

7. D. Driankov, H. Hellendoorn, and M. Reinfrank, *An Introduction to Fuzzy Control.* Springer, Heidelberg, 1993.

8. H. W. Engl, M. Hanke, and A. Neubauer, *Regularization of Inverse Problems.* Kluwer, Dordrecht, 1996.

9. H. W. Engl, K. Kunisch, and A. Neubauer, Convergence rates for Tikhonov regularization of nonlinear ill-posed problems. *Inverse Problems* (1989) **5**, 523–540.

10. F. Girosi, M. Jones, and T. Poggio, Regularization theory and neural networks architectures. *Neural Computation* (1995) **7**, 219–269.

11. G. H. Golub and V. Pereyra, The differentiation of pseudoinverses and nonlinear least squares problems whose variables separate. *SIAM J. Numer. Anal.* (1973) **10**, 413–432.

12. C. W. Groetsch, Generalized inverses and generalized splines. *Numer. Funct. Anal. Optimiz.* (1980) **2**, 93–97.

13. Y. Hu, An algorithm for data reduction using splines with free knots. *IMA J. Numer. Anal.* (1993) **13**, No. 3, 65–381.

14. D. L. B. Jupp, Approximation to data by splines with free knots. *SIAM J. Numer. Anal* (1978) **15**, No. 2, 328–343.

15. E. P. Klement, L. T. Koczy, and B. Moser, Are fuzzy systems universal approximators? *Int. J. General Systems* (1999) **28**, No. 2, 3, 259–282.

16. B. Kosko, Fuzzy systems as universal approximators. In: *IEEE Int. Conf. on Fuzzy Systems.* San Diego, 1992, 1153–1162.

17. R. Kruse, J. Gebhardt, and F. Klawonn, *Foundations of Fuzzy Systems.* John Wiley & Sons, New York, 1994.

18. C. L. Lawson and R. J. Hanson, *Solving Least Squares Problems.* SIAM Publications, Philadelphia, 1995.

19. T. A. Parks, *Reducible Nonlinear Programming Problems.* PhD thesis, Houston Univ., Department of Mathematics, 1985.

20. A. Sard, Approximations based on nonscalar observations. *J. Approx. Theory* (1973) **8**, 315–334.

21. E. Schock, Approximate solution of ill-posed equations: arbitrarily slow convergence vs. superconvergence. In: *Constructive Methods for the Practical Treatment of Integral Equations.* G. Hämmerlin and K. H. Hoffmann (Eds). Birkhäuser, Basel, 1985, 234–243.

22. T. Schütze, *Diskrete Quadratmittelapproximation durch Splines mit freien Knoten.* PhD Thesis. Technical University Dresden, Department of Mathematics, 1997.

23. H. Schwetlick and T. Schütze, Least squares approximation by splines with free knots. *BIT* (1995) **35**, No. 3, 361–384.

24. A. Seidel and H. W. Engl, Recovering discrete and continuous parts of the solution of linear ill-posed problems by Tikhonov regularization. *J. Inv. Ill-Posed Problems* (1999) **7**, 165–183.

25. T. I. Seidman and C. R. Vogel, Well-posedness and convergence of some regularization methods for nonlinear ill-posed problems. *Inverse Problems* (1989) **5**, 227–238.

26. M. Setnes, R. Babuška, and H. B. Verbruggen, Rule-based modeling: Precision and transparency. *IEEE Trans. Syst. Man Cybern. Part C* (1998) **28**, No. 1, 165–169.

27. L. L. Shumaker, *Spline Functions: Basic Theory.* John Wiley and Sons, New York, 1981.

28. J. Sjöberg and L. Ljung, Overtraining, regularization and searching for a minimum, with application to neural networks. *Int. J. Control* (1995) **62**, 1391–1407.

29. G. Strang and G. J. Fix, *An Analysis of the Finite Element Method.* Prentice-Hall, Englewood Cliffs, 1973.

30. T. Takagi and M. Sugeno, Fuzzy identification of systems and its applications to modeling and control. *IEEE Trans. Syst. Man Cybern.* (1985) **15**, No. 1, 116–132.

31. G. V. Tan and X. Hu, On designing fuzzy controllers using genetic algorithms. In: *Proc. FUZZ-IEEE'96.* 1996. **II**, 905–911.

32. L. X. Wang, Fuzzy systems are universal approximators. In: *IEEE Int. Conf. on Fuzzy Systems.* San Diego, 1992, 1163–1169.

33. D. H. Wolpert (Ed), The mathematics of generalization. In: *SFI Studies in the Sciences of Complexity.* Santa Fe Institute, Sante Fe, 1995. Addison-Wesley, 1996, **20**; In: *Proc. of the SFI/CNLS workshop on formal approaches to supervised learning.* Summer, 1992.

34. L. A. Zadeh, Fuzzy sets. *Inform. Control* (1965) **8**, 338–353.

35. L. A. Zadeh, Outline of a new approach to the analysis of complex systems and decision processes. *IEEE Trans. Syst. Man Cybern.* (1973) **3**, No. 1, 28–44.

36. J. Zhang and A. Knoll, Constructing fuzzy controllers with B-spline models. In: *Proc. FUZZ-IEEE'96* 1996, **I**, 416–421.