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LEAST SQUARES APPROXIMATION BY SPLINES WITH FREE KNOTS*

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Dedicated to Professor Dr.-Ing. habil. Dr. h.c. Helmut Heinrich on the occasion of his 90th birthday

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Abstract.

Suppose we are given noisy data which are considered to be perturbed values of a smooth, univariate function. In order to approximate these data in the least squares sense, a linear combination of B-splines is used where the tradeoff between smoothness and closeness of the fit is controlled by a smoothing term which regularizes the least squares problem and guarantees unique solvability independent of the position of knots. Moreover, a subset of the knot sequence which defines the B-splines, the so-called *free knots*, is included in the optimization process.

The resulting constrained least squares problem which is linear in the spline coefficients but nonlinear in the free knots is reduced to a problem that has only the free knots as variables. The reduced problem is solved by a generalized Gauss-Newton method. The method developed can be combined with a knot removal strategy in order to obtain an approximating spline with as few parameters as possible.

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1 Introduction.

Suppose we are given data $\{x_i, y_i\}$ where the $\{x_i\}$ are abscissae with

$$a \le x_1 < \ldots < x_i < x_{i+1} < \ldots < x_m \le b,$$

and the $\{y_i\}$ are noisy measurements of values of an unknown smooth function $f \in W_2^q[a, b]$, i.e.,

$$y_i = f(x_i) + \epsilon_i \qquad (i = 1, \ldots, m),$$

with ϵ_i being the error of the ith measurement.

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The function f is to be approximated by a function s from an appropriately chosen finite dimensional subspace S of $W_2^q[a,b]$ which

- can easily be computed,
- can be described by as few parameters as possible,
- represents the function within the noise level of the data.

Suppose that the errors $\{\epsilon_i\}$ are stochastically independent and identically normally distributed with

$$\boldsymbol{\epsilon} = (\epsilon_1, \ldots, \epsilon_m)^T = \mathcal{N}(\mathbf{0}, \sigma^2\mathbf{I}). \tag{1.1}$$

Under assumption (1.1), a natural measure of the goodness of the fit provided by s is given by

$$\varphi := \tfrac{1}{2}\sum_{i=1}^{m}[y_i - s(x_i)]^2. \tag{1.2}$$

Since splines provide a powerful tool for solving such problems, the function s will be taken from the n-dimensional spline space $\mathcal{S}_{k,\mathbf{t}}$ consisting of all polynomial splines s of order $k \geq 1$ with knot sequence $\mathbf{t} = \{t_j\}$ where

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

and $m \geq n$; in realistic problems there usually holds $m \gg n$.

For a given, fixed knot sequence $\mathbf{t}$ there exist several algorithms for the numerically stable computation of such splines, see [3]. However, if the knots are released and considered free, the approximation can significantly be improved, in general.

The aim of this paper is to develop a robust optimization algorithm that finds a good location of the free knots. Moreover, if the corresponding least squares error is smaller than the noise level of the data, the number of knots is reduced. This process is repeated until the data are approximated within their noise level using as few knots as possible.

Let us begin with some general remarks about free knot spline approximation and data reduction strategies.

Simple examples show that the problem of best approximation by splines with free knots has not always a solution in the set of splines with simple knots, whereas it can be proved that there always exists a solution in the set of splines with multiple knots.

In a first class, the algorithms start with only a few knots and iteratively add knots according to appropriate rules until the resulting spline satisfies some quality measuring criteria. To this class belongs de Boor's algorithm NEWKNOT [3] where the knots are chosen such that an indicator function depending on the kth derivative is equidistributed. In a recent paper, Hu [12] developed a similar algorithm where the same indicator is balanced over the knot intervals. However, the estimate of the kth derivative needed is computed in a preprocessing step using a spline of higher order with many knots.

In the second class of algorithms, initially a large number of starting knots is chosen from the set of data points $\{x_i\}$. Then certain knots which are less important for the approximation error are removed iteratively. A member of this class is the method of Lyche and Mørken [18].

Whereas the algorithms mentioned above do not seek an optimal knot placement with respect to the least squares error, the following methods try to minimize this error for a fixed, given number of knots.

De Boor and Rice [4] consider the case of L_2-approximation by cubic splines with variable knots. They do not allow the knots to coalesce, i.e., they require $t_{j+1} > t_j\,(j = k, \ldots, n)$, and they use a certain "coordinate relaxation" where each knot is varied cyclically so as to minimize the L_2-error as a function of this knot alone. Jupp [13] refers to the potentially high number of local extrema which may occur in approximation by splines with variable knots. With a logarithmic change of variables he transforms the constrained problem $(t_{j+1} \geq t_j)$ into an unconstrained one. He shows that this transformation in a certain sense mollifies the difficulties related with the original formulation. When solving the resulting unconstrained nonlinear least squares problem, he makes special use of the structure and separates the linear and nonlinear aspects. In his new book [7], Dierckx describes an algorithm originally developed in his Thesis [6]. There the linearly occuring parameters are eliminated, too. Unlike Jupp, the constraints for the knot position are treated via a certain barrier term in the objective function. The unconstrained problem obtained in this way is solved by the Fletcher/Reeves cg-method. Recently, Suchomski [24] proposed a new method of optimal variable-knot spline interpolation in the discrete L_2-norm. He explicitly enforces the Schoenberg-Whitney regularity condition, c.f. (2.8), to hold which leads to additional constraints for the knots. With a logarithmic change of variables similar to that of Jupp he transforms the constrained nonlinear least squares problem into an unconstrained one. Holt and Fletcher [11] developed a special algorithm for least squares problems with specially structured constraints and applied it to the problem of spline approximation with free knots. However, they did not separate the linear and nonlinear variables of the problem.

In all of the above approaches it is explicitly (sometimes even implicitly) assumed that any knot sequence encountered in the optimization process satisfies the Schoenberg-Whitney regularity condition – except in the paper [24] where some kind of simultaneous interpolation and approximation is used.

Unlike the algorithms mentioned, the method proposed in this paper

- does not suppose or enforce a Schoenberg-Whitney-like regularity condition but instead uses some type of regularization by a simple smoothing term which guarantees unique solvability independent on the position of knots.
- treats the linearly constrained nonlinear least squares problem directly, i.e., without any tranformation into an unconstrained problem as, e.g., the logarithmic transformation of Jupp. For the latter it is known that, when the knots become strongly nonuniformly spaced, the transformed variables approach zero. Therefore, the back transformation that requires the repeated evaluation of exponentials of very small numbers has to be performed in high precision, and loss of accuracy is likely.
- is able to find a good location of only a subset of the inner knots, in contrast

to the existing algorithms where all inner knots are included in the optimization process. This option is helpful when several data sets have to be fitted and one data set differs from the other only over a small region of the basic interval.

The paper is organized as follows: In Section 2, first the approximation and smoothing term are expressed as functions of the spline coefficients and the knot sequence. Then constraints on the free knots are posed which prevent the knots from coalescing, but allow groups of knots to become very closely spaced. This is sometimes essential, e.g., in approximating functions with peaks where there are regions of high curvature. On the other hand, the constraints keep the knots separated enough to avoid failure due to analytical and numerical instabilities as loss of differentiability, discontinuous tangent cones or others. In order to take into account the special structure, in Section 3 the full problem is reduced to a lower-dimensional one in the free knots only. In Section 4, a generalized Gauss-Newton method for solving the reduced problem is adapted from the literature. Special emphasize is given to the fast and numerically reliable solution of the linear least squares problems occuring as subproblems in each step of the optimization algorithm. Section 5 contains numerical examples with data taken from the literature. They show that the algorithm provides a robust and efficient tool for least squares approximation by splines with free knots.

2 Formulation of the Problem.

Let $\mathbf{t} = (t_1, \ldots, t_{n+k})^T$ with

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

be a knot sequence. The spline $s \in \mathcal{S}_{k,\mathbf{t}}$ is represented as

$$s = \sum_{j=1}^{n} B_{j,k}\alpha_j, \tag{2.1}$$

where $\{B_{j,k}\}$ denotes the sequence of normalized B-splines of order k with respect to the knot sequence $\mathbf{t}$. The B-splines $B_{j,k}$ are recursively defined by

$$B_{j,1}(t) := \begin{cases} 1 & \text{if} \quad t_j \leq t < t_{j+1} \\ 0 & \text{otherwise} \end{cases} \tag{2.2}$$

$$B_{j,k}(t) := \omega_{j,k}(t) \cdot B_{j,k-1}(t) + (1 - \omega_{j+1,k}(t)) \cdot B_{j+1,k-1}(t) \quad \text{for} \quad k > 1 \tag{2.3}$$

where

$$\omega_{j,k}(t) := \begin{cases} \frac{t - t_j}{t_{j+k-1} - t_j} & \text{if} \quad t_j < t_{j+k-1} \\ 0 & \text{otherwise.} \end{cases} \tag{2.4}$$

Because of $\operatorname{supp} B_{j,k} = [t_j, t_{j+k}]$, in case of $t_j = t_{j+k}$ it follows that $B_{j,k}(t) = 0$ for all $t \in [a, b]$. Therefore, it is natural to require that

$$t_{j+k} > t_j \qquad (j = 1, \ldots, n) \tag{2.5}$$

holds. Condition (2.5) implies the B-splines $B_{j,k}$ to be linearly independent, and then $\mathcal{S}_{k,\mathbf{t}}$ is the linear space $\tilde{\mathcal{S}}$ of all piecewise polynomials of order k or less with breakpoints t_j which are $k-1-\#t_j$ times continuously differentiable at t_j.

With the observation matrix $\mathbf{B} = (B_{j,k}(x_i))_{i=1,\dots,m,\, j=1,\dots,n} \in \mathbb{R}^{m,n}$, the vector of spline coefficients $\boldsymbol{\alpha} = (\alpha_j)_{j=1,\dots,n} \in \mathbb{R}^n$, and the right hand side $\mathbf{y} = (y_i)_{i=1,\dots,m} \in \mathbb{R}^m$, the approximation term introduced in (1.2) can be expressed as $\varphi = \varphi(\mathbf{t}, \boldsymbol{\alpha}) = \frac{1}{2}\left\|\mathbf{y} - \mathbf{B}(\mathbf{t})\boldsymbol{\alpha}\right\|^2$. Note that the elements of the observation matrix depend nonlinearly on the knots $\mathbf{t}$ and that $\mathbf{B}$ is a block banded matrix with bandwidth k.

For fixed knot sequence $\mathbf{t}$, the least squares problem

$$\min\left\{\varphi(\mathbf{t}, \boldsymbol{\alpha}) := \tfrac{1}{2}\left\|\mathbf{y} - \mathbf{B}(\mathbf{t})\boldsymbol{\alpha}\right\|^2 \;:\; \boldsymbol{\alpha} \in \mathbb{R}^n\right\} \tag{2.6}$$

has a unique solution if, and only if, $\mathbf{B}$ has full rank n. The following characterization of this full rank property is a consequence of the Schoenberg-Whitney Theorem, see [21].

THEOREM 2.1. *The observation matrix $\mathbf{B} \in \mathbb{R}^{m,n}$ has full rank if, and only if, there exists a subset $\{x_{i_j}\}$ of the data $\{x_i\}$ with*

$$B_{j,k}(x_{i_j}) \neq 0 \qquad (j = 1, \dots, n). \;\blacksquare \tag{2.7}$$

A neccessary (and in case of $t_{j+k} > t_j$ also sufficient) condition for (2.7) to hold is the *Schoenberg-Whitney-condition*

$$t_j < x_{i_j} < t_{j+k} \qquad (j = 1, \dots, n). \tag{2.8}$$

If this condition is not satisfied one can add an appropriately chosen regularization term $\mu\rho(\mathbf{t}, \boldsymbol{\alpha})$ to the approximation term (1.2). This leads to the problem

$$\min\left\{\varphi(\mathbf{t}, \boldsymbol{\alpha}) + \mu\rho(\mathbf{t}, \boldsymbol{\alpha}) \;:\; \boldsymbol{\alpha} \in \mathbb{R}^n\right\} \tag{2.9}$$

of *spline smoothing* where $\mu > 0$ is the *smoothing parameter*, and $\rho(\mathbf{t}, \boldsymbol{\alpha})$ is the *smoothing term* that characterizes the smoothness of the solutions which are denoted as *smoothing splines*. Such an approach is often used to control the tradeoff between closeness and smoothness of the fit, see e.g., [27].

A natural choice for the smoothing term is

$$\bar{\rho}(\mathbf{t}, \boldsymbol{\alpha}) := \tfrac{1}{2}\int_a^b \left[s^{(r)}(x)\right]^2 dx = \tfrac{1}{2}\left\|s^{(r)}\right\|_{L_2}^2 \tag{2.10}$$

with fixed $r \in \{0, \dots, k-1\}$; it corresponds to a semi-norm in W_2^q. An "optimal" smoothing parameter μ can be estimated, e.g., by generalized cross-validation, see again [27]. However, we will choose μ interactively.

Let us now come to the representation of $\bar{\rho}(\mathbf{t}, \boldsymbol{\alpha})$ in terms of the spline coefficients $\boldsymbol{\alpha}$ and the knots $\mathbf{t}$. It is well known that, if $t_{j+k-1} > t_j$ $(j = 2, \dots, n)$, then the derivative s' exists and is again a spline with

$$s' = \sum_{j=2}^{n} B_{j,k-1}\alpha'_j \quad \text{and} \quad \alpha'_j = \frac{\alpha_j - \alpha_{j-1}}{\frac{t_{j+k-1} - t_j}{k-1}} \qquad (j = 2, \dots, n).$$

Analogously, if

$$t_{j+k-r} > t_j \qquad (j = r+1, \ldots, n), \tag{2.11}$$

then there exists $s^{(r)}$ and can be expressed as

$$s^{(r)} = \sum_{j=r+1}^{n} B_{j,k-r}\alpha_j^{(r)} \tag{2.12}$$

where the coefficients $\boldsymbol{\alpha}^{(r)} := \left(\alpha_{r+1}^{(r)}, \ldots, \alpha_n^{(r)}\right)^T \in \mathbb{R}^{n-r}$ are related to the coefficients $\boldsymbol{\alpha}$ by

$$\boldsymbol{\alpha}^{(r)} = \mathbf{D}_r\boldsymbol{\alpha} \tag{2.13}$$

with $\mathbf{D}_0 := \mathbf{I} \in \mathbb{R}^{n,n}$, $\mathbf{D}_r := \mathbf{H}_r\mathbf{L}_r \ldots \mathbf{H}_1\mathbf{L}_1 \in \mathbb{R}^{n-r,n}$, and $\mathbf{H}_\nu$ and $\mathbf{L}_\nu$ are defined by

$$\mathbf{H}_\nu := (k-\nu)\mathrm{diag}\left(\frac{1}{t_{k+j-\nu} - t_j}\right)_{j=\nu+1,\ldots,n} \in \mathbb{R}^{n-\nu,n-\nu}$$

$$\mathbf{L}_\nu := \begin{bmatrix} -1 & 1 & & & & \\ & -1 & 1 & & & \\ & & \ddots & \ddots & & \\ & & & -1 & 1 & \\ & & & & -1 & 1 \end{bmatrix} \in \mathbb{R}^{n-\nu,n-\nu+1}$$

for $\nu = 1, \ldots, r$. The matrix $\mathbf{D}_r$ is upper triangular with bandwidth $r+1$. It is easy to show that it has full row rank $n-r$ if $t_{j+k-r} > t_j$ $(j = r+1, \ldots, n)$.

By inserting expression (2.13) into the smoothing term $\bar{\rho}$ and integrating over products of B-splines one obtains

$$\bar{\rho} = \tfrac{1}{2}\left\|\bar{\mathbf{S}}_r\boldsymbol{\alpha}\right\|^2$$

with an upper triangular and k-banded matrix $\bar{\mathbf{S}}_r = \bar{\mathbf{S}}_r(\mathbf{t}) \in \mathbb{R}^{n-r,n}$, see [23] for details.

Since the computation of $\bar{\rho}$ may be expensive we look for a cheaper approximation $\tilde{\rho}$. As in [23], we replace the L_2-semi-norm by its discrete analogue in $\mathcal{S}_{k-r,\mathbf{t}}$, i.e., by

$$\tilde{\rho}(\mathbf{t},\boldsymbol{\alpha}) := \tfrac{1}{2}\left\|s^{(r)}\right\|_{l_2}^2 := \tfrac{1}{2}\sum_{j=r+1}^{n}\left(\alpha_j^{(r)}\right)^2 \frac{t_{j+k-r} - t_j}{k-r}. \tag{2.14}$$

Note that both norms are equivalent in the following sense: There exist a constant d_{k-r} which does not depend on the knot sequence $\mathbf{t}$ so that there holds $d_{k-r}^{-1}\left\|s^{(r)}\right\|_{l_2} \le \left\|s^{(r)}\right\|_{L_2} \le \left\|s^{(r)}\right\|_{l_2}$ for all $s \in \mathcal{S}_{k,\mathbf{t}}$. By considering (2.14) and (2.13) we obtain

$$\tilde{\rho} = \tfrac{1}{2}\boldsymbol{\alpha}^T\mathbf{D}_r^T\tilde{\mathbf{F}}_r^T\tilde{\mathbf{F}}_r\mathbf{D}_r\boldsymbol{\alpha}$$

where $\tilde{\mathbf{F}}_r := \mathrm{diag}\left(\sqrt{\frac{t_{j+k-r}-t_j}{k-r}}\right)_{j=r+1,\ldots,n} \in \mathbb{R}^{n-r,n-r}$ and, finally,

$$\tilde{\rho} = \tfrac{1}{2}\left\|\tilde{\mathbf{S}}_r\boldsymbol{\alpha}\right\|^2.$$

The matrix $\tilde{\mathbf{S}}_r = \tilde{\mathbf{S}}_r(\mathbf{t}) := \tilde{\mathbf{F}}_r \mathbf{D}_r \in \mathbb{R}^{n-r,n}$ is again upper triangular but with bandwidth $r+1$ in contrast to k for the smoothing term $\bar{\rho}$. Because of the equivalence of the semi-norms, both matrices $\bar{\mathbf{S}}_r$ and $\tilde{\mathbf{S}}_r$ have full rank $n-r$ and the same kernel

$$\ker(\bar{\mathbf{S}}_r) = \ker(\tilde{\mathbf{S}}_r) = \left\{ \boldsymbol{\alpha} \in \mathbb{R}^n \,:\, \alpha_j^{(r)} = 0, j = r+1, \ldots, n \right\}$$

that corresponds to the linear space of all polynomials of order r in $\mathcal{S}_{k,\mathbf{t}}$.

By using either $\rho = \bar{\rho} = \frac{1}{2}\left\|\bar{\mathbf{S}}_r\right\|^2$, $\mathbf{S} = \bar{\mathbf{S}}_r$ or $\rho = \tilde{\rho} = \frac{1}{2}\left\|\tilde{\mathbf{S}}_r\right\|^2$, $\mathbf{S} = \tilde{\mathbf{S}}_r$ and its matrix representation, the functional to be minimized becomes

$$\begin{aligned}\psi(\mathbf{t}, \boldsymbol{\alpha}) := \varphi(\mathbf{t}, \boldsymbol{\alpha}) + \mu\rho(\mathbf{t}, \boldsymbol{\alpha}) &= \tfrac{1}{2}\left\|\mathbf{y} - \mathbf{B}(\mathbf{t})\boldsymbol{\alpha}\right\|^2 + \mu\tfrac{1}{2}\left\|\mathbf{S}(\mathbf{t})\boldsymbol{\alpha}\right\|^2 \\ &= \tfrac{1}{2}\left\| \begin{bmatrix} \mathbf{y} \\ \mathbf{0} \end{bmatrix} - \begin{bmatrix} \mathbf{B}(\mathbf{t}) \\ \sqrt{\mu}\mathbf{S}(\mathbf{t}) \end{bmatrix} \boldsymbol{\alpha} \right\|^2 .\end{aligned}$$

Suppose now and in the following that

$$m \geq r \tag{2.15}$$

holds. Then $\mathbf{B}\boldsymbol{\alpha} = \mathbf{0}$ and $\mathbf{S}\boldsymbol{\alpha} = \mathbf{0}$ imply $\boldsymbol{\alpha} = \mathbf{0}$. Therefore, for fixed knot sequence $\mathbf{t}$ and any $\mu > 0$, the problem

$$\min\left\{\varphi(\mathbf{t}, \boldsymbol{\alpha}) + \mu\rho(\mathbf{t}, \boldsymbol{\alpha}) \,:\, \boldsymbol{\alpha} \in \mathbb{R}^n\right\}$$

has a unique solution $\boldsymbol{\alpha} = \boldsymbol{\alpha}_\mu$ independent on whether the Schoenberg-Whitney condition (2.8) is fulfilled or not. The limit $\boldsymbol{\alpha}_0 = \lim_{\mu\to 0} \boldsymbol{\alpha}_\mu$ gives the unique best least squares fit with least semi-norm ρ, and $\boldsymbol{\alpha}_\infty = \lim_{\mu\to\infty} \boldsymbol{\alpha}_\mu$ is the unique best polynomial fit of order r, see [26].

In order to have greater flexibility, the optimization process will be restricted to a subset $\tilde{\mathbf{t}}$ of the whole knot sequence $\mathbf{t}$, the so-called *free knots*. This option is helpful when several data sets have to be fitted and one data set differs from the other only over a small region of the basic interval. In such a case, only the knots which lie in this small region should be considered free when changing from the current data set to the next one.

Let l denote the number and $\tilde{\mathbf{t}} = \left(t_{p(1)}, \ldots, t_{p(l)}\right)^T \in \mathbb{R}^l$ be the vector of free knots where $\mathbf{p} = (p(1), \ldots, p(l))^T$ contains the indices of the free knots which are supposed to satisfy

$$k < p(1) < \ldots < p(l) < n+1.$$

The last condition means that only inner knots $t_{k+1}, \ldots, t_n$ can be free knots which seems natural since the basic interval is usually prescribed by the user. It implies $l \leq n-k$.

Then the corresponding optimization problems are

$$\min\left\{\tfrac{1}{2}\left\|\mathbf{y} - \mathbf{B}(\tilde{\mathbf{t}})\boldsymbol{\alpha}\right\|^2 \,:\, \boldsymbol{\alpha} \in \mathbb{R}^n,\, \tilde{\mathbf{t}} \in \mathbb{R}^l\right\} \tag{2.16a}$$

or, with $\mu > 0$,

$$\min\left\{\tfrac{1}{2}\left\| \begin{bmatrix} \mathbf{y} \\ \mathbf{0} \end{bmatrix} - \begin{bmatrix} \mathbf{B}(\tilde{\mathbf{t}}) \\ \sqrt{\mu}\mathbf{S}(\tilde{\mathbf{t}}) \end{bmatrix} \boldsymbol{\alpha} \right\|^2 \,:\, \boldsymbol{\alpha} \in \mathbb{R}^n,\, \tilde{\mathbf{t}} \in \mathbb{R}^l\right\}, \tag{2.16b}$$

respectively.

Since the knot sequence $\mathbf{t}$ has to satisfy the order relation $t_{j+1}-t_j \geq 0$ $(j = 1, \ldots, n+k-1)$, the free knots occuring in (2.16) can not be chosen arbitrarily but have to fulfill the constraints

$$\begin{aligned} t_{p(j)} - t_{p(j)-1} &\geq 0 \\ t_{p(j)+1} - t_{p(j)} &\geq 0 \qquad (j = 1, \ldots, l). \end{aligned}$$

These constraints do not prevent the knots from coalescing and, hence, are not suitable for numerical purposes, cf. (2.5) and (2.11). Therefore, one could consider the modified constraints

$$t_{p(j)} - t_{p(j)-1} \geq \epsilon \tag{2.17a}$$

$$t_{p(j)+1} - t_{p(j)} \geq \epsilon \qquad (j = 1, \ldots, l) \tag{2.17b}$$

with a sufficiently small separation parameter $0 < \epsilon \ll 1$. The matrix formulation of (2.17) is given by $\mathbf{C}\tilde{\mathbf{t}} \geq \mathbf{h}$ with a certain matrix $\mathbf{C} \in \mathbb{R}^{ncstr,l}$ and a vector $\mathbf{h} \in \mathbb{R}^{ncstr}$ where $ncstr$ denotes the number of linear independent constraints. Here $ncstr$ as well as $\mathbf{C}$ and $\mathbf{h}$ depend on the relative position of the free knots and can easily be generated automatically.

In (2.17) the separation parameter ϵ represents a lower bound for the absolute distance between consecutive knots. However, if the spacing of the knots is very different from an equidistribution, instead the relative distance should be bounded from below according to, e.g.,

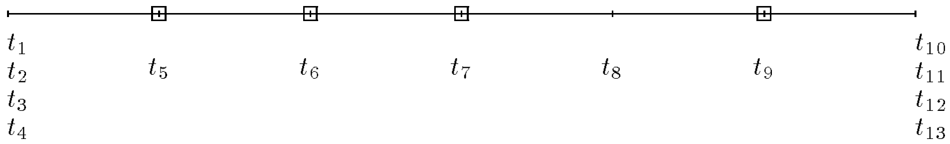
$$t_{p(j)} \geq t_{p(j)-1} + \epsilon \left(t_{p(j)+1} - t_{p(j)-1}\right) \tag{2.18a}$$

$$t_{p(j)} \leq t_{p(j)+1} - \epsilon \left(t_{p(j)+1} - t_{p(j)-1}\right) \qquad (j = 1, \ldots, l). \tag{2.18b}$$

These constraints have been introduced by de Boor and Rice [4] who used the value $\epsilon = 0.0625$.

Condition (2.18) leads to an analoguous matrix formulation $\mathbf{C}\tilde{\mathbf{t}} \geq \mathbf{h}$ with $\mathbf{C} \in \mathbb{R}^{2l,l}$, $\mathbf{h} \in \mathbb{R}^l$ where $\mathbf{C}$ contains at most three non-zero elements per row in contrast to two in (2.17). For illustration, let us give an example.

Example: $k = 4$, $n = 9$, $l = 4$, $p(1) = 5$, $p(2) = 6$, $p(3) = 7$, $p(4) = 9$



$$\begin{bmatrix} 1 & -\epsilon & & \\ -1 & 1-\epsilon & & \\ \epsilon-1 & 1 & -\epsilon & \\ \epsilon & -1 & 1-\epsilon & \\ & \epsilon-1 & 1 & \\ & \epsilon & -1 & \\ & & & 1 \\ & & & -1 \end{bmatrix} \begin{bmatrix} t_5 \\ t_6 \\ t_7 \\ t_9 \end{bmatrix} \geq \begin{bmatrix} (1-\epsilon)\,t_4 \\ -\epsilon\,t_4 \\ 0 \\ 0 \\ \epsilon\,t_8 \\ (\epsilon-1)\,t_8 \\ (1-\epsilon)\,t_8 + \epsilon\,t_{10} \\ -\epsilon\,t_8 + (\epsilon-1)\,t_{10} \end{bmatrix}$$

If the optimization algorithm is started with a knot sequence consisting of simple free knots then the free knots will remain simple throughout the optimization provided that the algorithm works with feasible points only (as our algorithm does). As a consequence, we have the highest degree of smoothness at the free knots. Of course, dependent on the order k of splines and the order r of derivative used in the smoothing term, also free knots of a given, fixed multiplicity could be allowed. For simplicity, in the following we restrict to the case of simple free knots.

Summarizing the results of this section, we achieve at the following problems referred to as *full approximation problem* or *full smoothing problem*, respectively:

$$\min\left\{\psi(\tilde{\mathbf{t}},\boldsymbol{\alpha}) := \tfrac{1}{2}\left\|\mathbf{y}-\mathbf{B}(\tilde{\mathbf{t}})\boldsymbol{\alpha}\right\|^2 \;:\; \mathbf{C}\tilde{\mathbf{t}} \geq \mathbf{h}\,,\, \tilde{\mathbf{t}}\in\mathbb{R}^l, \boldsymbol{\alpha}\in\mathbb{R}^n\right\} \tag{2.19a}$$

$$\min\left\{\psi(\tilde{\mathbf{t}},\boldsymbol{\alpha}) := \tfrac{1}{2}\left\|\begin{bmatrix}\mathbf{y}\\ \mathbf{0}\end{bmatrix} - \begin{bmatrix}\mathbf{B}(\tilde{\mathbf{t}})\\ \sqrt{\mu}\mathbf{S}(\tilde{\mathbf{t}})\end{bmatrix}\boldsymbol{\alpha}\right\|^2 \;:\; \mathbf{C}\tilde{\mathbf{t}} \geq \mathbf{h}\,,\, \tilde{\mathbf{t}}\in\mathbb{R}^l,\, \boldsymbol{\alpha}\in\mathbb{R}^n\right\}. \tag{2.19b}$$

Under condition (2.15), problem (2.19b) has, for arbitrary $\tilde{\mathbf{t}}$, always a unique and continuously differentiable solution $\boldsymbol{\alpha} = \boldsymbol{\alpha}(\tilde{\mathbf{t}})$ independent on whether $\mathbf{t}$ satisfies the Schoenberg-Whitney condition (2.8) or not since the extended system matrix has full rank, cf. Section 3 below. In problem (2.19a), however, the rank of the observation matrix $\mathbf{B}(\tilde{\mathbf{t}})$ depends on the position of the free knots with respect to the data $\{x_i\}$. Therefore, in order to guarantee unique and continuously differentiable solvability of problem (2.19a) for $\boldsymbol{\alpha}$ as function of $\tilde{\mathbf{t}}$, the Schoenberg-Whitney condition (2.8) has to be satisfied on open neighborhoods of all $\mathbf{t}$ encountered in the optimization algorithm. Let us note that in case of a rank deficient $\mathbf{B}(\tilde{\mathbf{t}})$ the solution $\boldsymbol{\alpha}$ can be made unique by choosing the minimum-norm solution $\mathbf{B}(\tilde{\mathbf{t}})^+\mathbf{y}$ as has been done in [13] but then the continuity is lost in a neighborhood of $\tilde{\mathbf{t}}$. Moreover, then the reduction of the problem described in the next section is not justified, cf. Theorem 3.1.

Therefore, the following assumption is supposed to be satisfied for the rest of this paper.

Assumption 1 (Regularity Conditions).

(i) For problem (2.19a), let the Schoenberg-Whitney condition (2.8) be fulfilled for all knot sequences $\mathbf{t}$ *which belong to free knots* $\tilde{\mathbf{t}}$ *from an open neighborhood of those* $\tilde{\mathbf{t}}^\nu$ *encountered as iterates in the optimization algorithm.*

(ii) For problem (2.19b), let the parameters r *and* μ *be chosen such that*

$$m \geq r \qquad \text{and} \qquad \mu > 0$$

holds. ∎

The efficient solution of both (2.19a) and (2.19b) is the aim of the rest of this paper.

3 Reduction of the Full Problem.

Problems (2.19a) and (2.19b) are nonlinear least squares problems where a subset of the variables occurs linearly. Such problems are called *linearly separable*. In the unconstrained case they were first analyzed in detail by Golub/Pereyra [9]. Later Ruhe/Wedin [20] generalized this class to problems in which the variables separate into two groups in such a way that the optimization with respect to one group of variables is easier than with respect to the other. In her Thesis, Parks [19] considered general constrained nonlinear approximation problems of this type.

In what follows let $\mathbf{y} \in \mathbb{R}^m$ be an arbitrary vector and

$$\mathbf{B}(.) : \tilde{\mathbf{t}} \in \mathbb{R}^l \to \mathbf{B}(\tilde{\mathbf{t}}) \in \mathbb{R}^{m,n}$$

an arbitrary, smooth matrix function which together define the unconstrained problem

$$\min\left\{\psi(\tilde{\mathbf{t}}, \boldsymbol{\alpha}) := \tfrac{1}{2}\left\|\mathbf{y} - \mathbf{B}(\tilde{\mathbf{t}})\boldsymbol{\alpha}\right\|^2 \,:\, \tilde{\mathbf{t}} \in \mathbb{R}^l, \boldsymbol{\alpha} \in \mathbb{R}^n\right\}. \tag{3.1}$$

For any fixed $\tilde{\mathbf{t}} \in \mathbb{R}^l$, the unique minimum-norm solution $\boldsymbol{\alpha}_{\text{opt}}$ of (3.1) with respect to $\boldsymbol{\alpha}$ is given by

$$\boldsymbol{\alpha} = \boldsymbol{\alpha}_{\text{opt}}(\tilde{\mathbf{t}}) = \mathbf{B}(\tilde{\mathbf{t}})^+\mathbf{y},$$

where $\mathbf{B}^+$ denotes the Moore-Penrose inverse of $\mathbf{B}$. By replacing the variable $\boldsymbol{\alpha}$ in (3.1) by its "optimal" value $\boldsymbol{\alpha}_{\text{opt}}(\tilde{\mathbf{t}})$ the *reduced problem*

$$\min\left\{\phi(\tilde{\mathbf{t}}) := \tfrac{1}{2}\Big\|\underbrace{\left[\mathbf{I} - \mathbf{B}(\tilde{\mathbf{t}})\mathbf{B}(\tilde{\mathbf{t}})^+\right]\mathbf{y}}_{=:\mathbf{G}(\tilde{\mathbf{t}})}\Big\|^2 = \tfrac{1}{2}\left\|\mathbf{G}(\tilde{\mathbf{t}})\right\|^2 \,:\, \tilde{\mathbf{t}} \in \mathbb{R}^l\right\} \tag{3.2}$$

is obtained. Recall that $\mathbf{P}_B^\perp := \mathbf{I} - \mathbf{B}(\tilde{\mathbf{t}})\mathbf{B}(\tilde{\mathbf{t}})^+$ is the orthogonal projector onto image $\mathbf{B}(\tilde{\mathbf{t}})^\perp$. Therefore $\phi(.)$ is called *variable projection functional*, and the described technique *variable projection method*, see [9]. The reduced problem (3.2) has only the l nonlinearly occuring parameters $\tilde{\mathbf{t}}$ as variables but is of higher complexity than the full problem (3.1).

Golub/Pereyra [9] showed that, under natural assumptions which guarantee the continuity of the Moore-Penrose inverse, the reduction described above is feasible in the following sense.

Theorem 3.1 (Golub/Pereyra [9]). *Let $\psi(\tilde{\mathbf{t}}, \boldsymbol{\alpha})$ and $\phi(\tilde{\mathbf{t}})$ be defined as above, and assume that $\mathbf{B}(\tilde{\mathbf{t}})$ has constant rank $r \leq \min(m, n)$ on the open set $\Omega \subset \mathbb{R}^l$.*

(i) If $\tilde{\mathbf{t}}^*$ is a critical point in Ω (or a global mimimizer on Ω) of $\phi(\tilde{\mathbf{t}})$, and

$$\boldsymbol{\alpha}^* = \mathbf{B}(\tilde{\mathbf{t}}^*)^+\mathbf{y}, \tag{3.3}$$

then $(\tilde{\mathbf{t}}^*, \boldsymbol{\alpha}^*)$ is a critical point (or a global mimimizer on $\{(\tilde{\mathbf{t}}, \boldsymbol{\alpha}) : \tilde{\mathbf{t}} \in \Omega, \boldsymbol{\alpha} \in \mathbb{R}^n\}$) of $\psi(\tilde{\mathbf{t}}, \boldsymbol{\alpha})$, and

$$\phi(\tilde{\mathbf{t}}^*) = \psi(\tilde{\mathbf{t}}^*, \boldsymbol{\alpha}^*).$$

(ii) If $(\tilde{\mathbf{t}}^*, \boldsymbol{\alpha}^*)$ is a global minimizer of $\psi(\tilde{\mathbf{t}}, \boldsymbol{\alpha})$ on $\{(\tilde{\mathbf{t}}, \boldsymbol{\alpha}) : \tilde{\mathbf{t}} \in \Omega, \boldsymbol{\alpha} \in \mathbb{R}^n\}$, then $\tilde{\mathbf{t}}^*$ is a global minimizer of $\phi(\tilde{\mathbf{t}})$ on Ω, and

$$\phi(\tilde{\mathbf{t}}^*) = \psi(\tilde{\mathbf{t}}^*, \boldsymbol{\alpha}^*).$$

Furthermore, if there is a unique $\boldsymbol{\alpha}^*$ among the minimizing pairs of $\psi(\tilde{\mathbf{t}}, \boldsymbol{\alpha})$, then $\boldsymbol{\alpha}^*$ must satisfy (3.3). ∎

Under the constant rank assumption of Theorem 3.1, the reduced function $\mathbf{G}(\tilde{\mathbf{t}})$ is differentiable. Moreover, if $\mathbf{B}$ has full rank on Ω which will be supposed in the following, then the Jacobian of $\mathbf{G}$ is given by

$$\mathbf{G}'(\tilde{\mathbf{t}})\mathbf{s} = \left\{\mathcal{A}(\tilde{\mathbf{t}})[\mathbf{s}] + \left(\mathcal{A}(\tilde{\mathbf{t}})[\mathbf{s}]\right)^T\right\}\mathbf{y} \quad \text{with} \tag{3.4a}$$

$$\mathcal{A}(\tilde{\mathbf{t}})[\mathbf{s}] := -\left[\mathbf{I} - \mathbf{B}(\tilde{\mathbf{t}})\mathbf{B}(\tilde{\mathbf{t}})^+\right]\left(\mathbf{B}'(\tilde{\mathbf{t}})[\mathbf{s}]\right)\mathbf{B}(\tilde{\mathbf{t}})^+ \quad \forall \mathbf{s} \in \mathbb{R}^l. \tag{3.4b}$$

Golub/Pereyra [9] solved the reduced problem (3.2) by applying the Gauss-Newton method to it. For doing so, the Gauss-Newton model

$$\mu_{GP}(\tilde{\mathbf{t}} + \mathbf{s}) := \tfrac{1}{2}\left\|\mathbf{G} + \mathbf{G}'\mathbf{s}\right\|^2 \approx \phi(\tilde{\mathbf{t}} + \mathbf{s}) \tag{3.5}$$

to $\mathbf{G}$ has to be built. In the following, this model will be called Golub-Pereyra model. Later Krogh [16] described a sophisticated realization of the linear algebra involved. However, the term $\mathcal{A}^T[.]\mathbf{y}$ complicates the index computations and the exploitation of the sparse structure which is typical in real applications (in our case we have band structure, see Section 4).

On the other hand, a closer look shows that

$$\left\|\mathbf{G} + \mathbf{G}'\mathbf{s}\right\|^2 = \left\|\mathbf{G} + \mathcal{A}[\mathbf{s}]\mathbf{y}\right\|^2 + \mathbf{s}^T\mathbf{T}_G\mathbf{s}$$

holds with

$$\begin{aligned}\mathbf{u}^T\mathbf{T}_G\mathbf{v} &:= \left\{\left(\mathcal{A}[\mathbf{u}]\right)^T\mathbf{y}\right\}^T\left\{\left(\mathcal{A}[\mathbf{v}]\right)^T\mathbf{y}\right\}\\ &= \mathbf{G}^T\left(\mathbf{B}'[\mathbf{u}]\right)\mathbf{B}^+\mathbf{B}^{+T}\left(\mathbf{B}'[\mathbf{v}]\right)^T\mathbf{G}.\end{aligned}$$

The term $\left(\mathcal{A}(\tilde{\mathbf{t}})[\mathbf{s}]\right)^T\mathbf{y}$ does not contribute to $\nabla\phi(\tilde{\mathbf{t}})$, and its contribution $\mathbf{T}_G$ to the Hessian of the Golub-Pereyra model is of order $\mathcal{O}\left(\|\mathbf{G}\|^2\right)$. Following the Gauss-Newton philosophy, this term can be omitted which leads to the simplified model

$$\mu_K(\tilde{\mathbf{t}} + \mathbf{s}) := \tfrac{1}{2}\left\|\mathbf{G} + \mathbf{K}\mathbf{s}\right\|^2 \quad \text{with} \tag{3.6a}$$

$$\mathbf{K}\mathbf{s} := \mathcal{A}(\tilde{\mathbf{t}})[\mathbf{s}]\mathbf{y} = -\left[\mathbf{I} - \mathbf{B}(\tilde{\mathbf{t}})\mathbf{B}(\tilde{\mathbf{t}})^+\right]\left(\mathbf{B}'(\tilde{\mathbf{t}})[\mathbf{s}]\right)\mathbf{B}^+\mathbf{y} \tag{3.6b}$$

named after Kaufman [14]. Note that omitting the term $\left(\mathcal{A}(\tilde{\mathbf{t}})[\mathbf{s}]\right)^T\mathbf{y}$ does not affect the gradient even when $\mathbf{B}^+$ is replaced by a "weaker" generalized inverse $\mathbf{B}^-$ that satisfies only the two Moore-Penrose conditions (P1) $\mathbf{B}\mathbf{B}^-\mathbf{B} = \mathbf{B}$ and (P3) $(\mathbf{B}\mathbf{B}^-)^T = \mathbf{B}\mathbf{B}^-$. Moreover, if additionally (P2) $\mathbf{B}^-\mathbf{B}\mathbf{B}^- = \mathbf{B}^-$ holds, then the corresponding $\mathbf{T}_G$ is again of order $\mathcal{O}\left(\|\mathbf{G}\|^2\right)$.

Numerical experiments reported in [14] and [20] show that, for unconstrained problems, methods based on the cheaper Kaufman model (3.6) perform not worse than those based on the Golub-Pereyra model.

Ruhe/Wedin examined the asymptotic R-convergence rates of the above algorithms. They proved that the algorithms are R-linearly convergent for small residual problems. However, if the Gauss-Newton method for the full (unreduced) problem converges superlinearly then the methods of Golub/Pereyra and Kaufman converge superlinearly, too.

Up to now the feasibility of the reduction has been shown only for the unconstrained case. Kaufman showed that the reduction is even feasible for separable least squares problems with linear inequality constraints for the nonlinearly occuring variables $\tilde{\mathbf{t}}$.

THEOREM 3.2 (KAUFMAN, CITED AFTER [19]). *A problem of the form*

$$\min\left\{\psi(\tilde{\mathbf{t}},\boldsymbol{\alpha}) := \tfrac{1}{2}\left\|\mathbf{y}-\mathbf{B}(\tilde{\mathbf{t}})\boldsymbol{\alpha}\right\|^2 \,:\, \mathbf{C}\tilde{\mathbf{t}} \geq \mathbf{h}\,,\, \tilde{\mathbf{t}} \in \mathbb{R}^l, \boldsymbol{\alpha} \in \mathbb{R}^n\right\}$$

is equivalent to

$$\min\left\{\phi(\tilde{\mathbf{t}}) := \tfrac{1}{2}\left\|\left[\mathbf{I}-\mathbf{B}(\tilde{\mathbf{t}})\mathbf{B}(\tilde{\mathbf{t}})^+\right]\mathbf{y}\right\|^2 = \tfrac{1}{2}\left\|\mathbf{P}_B^{\perp}(\tilde{\mathbf{t}})\mathbf{y}\right\|^2 \,:\, \mathbf{C}\tilde{\mathbf{t}} \geq \mathbf{h}\,,\, \tilde{\mathbf{t}} \in \mathbb{R}^l\right\}$$

followed by the back substitution

$$\boldsymbol{\alpha} = \mathbf{B}(\tilde{\mathbf{t}})^+\mathbf{y}. \ \blacksquare$$

Let us now come back to our original problems (2.19a) and (2.19b). The reduction technique described above can be applied to these problems. This leads to the *reduced approximation problem*

$$\text{(3.7a)}\quad \min\left\{\phi(\tilde{\mathbf{t}}) := \tfrac{1}{2}\Big\|\underbrace{\left[\mathbf{I}-\mathbf{B}(\tilde{\mathbf{t}})\mathbf{B}(\tilde{\mathbf{t}})^+\right]\mathbf{y}}_{=:\mathbf{G}(\tilde{\mathbf{t}})}\Big\|^2 = \tfrac{1}{2}\left\|\mathbf{G}(\tilde{\mathbf{t}})\right\|^2 \,:\, \mathbf{C}\tilde{\mathbf{t}} \geq \mathbf{h}\,,\, \tilde{\mathbf{t}} \in \mathbb{R}^l\right\},$$

in the following abbreviated as **RAP**, and the *reduced smoothing problem*

$$\text{(3.7b)}\quad \min\left\{\begin{aligned}\phi(\tilde{\mathbf{t}}) &:= \frac{1}{2}\left\|\left\{\begin{bmatrix}\mathbf{I}_m & \\ & \mathbf{I}_{n-r}\end{bmatrix} - \begin{bmatrix}\mathbf{B}(\tilde{\mathbf{t}}) \\ \sqrt{\mu}\mathbf{S}(\tilde{\mathbf{t}})\end{bmatrix}\begin{bmatrix}\mathbf{B}(\tilde{\mathbf{t}}) \\ \sqrt{\mu}\mathbf{S}(\tilde{\mathbf{t}})\end{bmatrix}^+\right\}\begin{bmatrix}\mathbf{y} \\ \mathbf{0}\end{bmatrix}\right\|^2 \\ &= \tfrac{1}{2}\left\|\mathbf{G}(\tilde{\mathbf{t}})\right\|^2 \,:\, \mathbf{C}\tilde{\mathbf{t}} \geq \mathbf{h}\,,\, \tilde{\mathbf{t}} \in \mathbb{R}^l\end{aligned}\right\}$$

denoted by **RSP**.

Unfortunately, for arbitrary data the matrix $\mathbf{B}(\tilde{\mathbf{t}})$ of the reduced problem **RAP** (3.7a) does not satisfy the constant rank condition of Theorem 3.1 for all feasible $\tilde{\mathbf{t}} \in \mathbb{R}^l$ whereas the matrix of the regularized problem **RSP** (3.7b) does.

THEOREM 3.3 (FEASIBILITY OF REDUCTION AND EXISTENCE OF SOLUTIONS).

(i) Suppose that $\mathbf{B}$ *has full rank at a feasible knot sequence* $\tilde{\mathbf{t}}^*$, *c.f. (2.8). Then the reduced function* $\mathbf{G}$ *of* **RAP** *is smooth on an open neighborhood* Ω^* *of* $\tilde{\mathbf{t}}^*$. *Moreover, if* $\tilde{\mathbf{t}}^*$ *is a local minimizer (or a stationary point) of the reduced problem* **RAP** *then* $(\tilde{\mathbf{t}}^*, \boldsymbol{\alpha}^*)$ *with*

$$\boldsymbol{\alpha}^* = \mathbf{B}(\tilde{\mathbf{t}}^*)^+\mathbf{y}$$

is also a local minimizer (or a stationary point) of the full problem (2.19a).

(*ii*) *Suppose that* $m \geq r$ *and* $\mu > 0$ *holds. Then the reduced function* $\mathbf{G}$ *of* **RSP** *is defined and smooth on the whole feasible set* $\{\tilde{\mathbf{t}} \in \mathbb{R}^l : \mathbf{C}\tilde{\mathbf{t}} \geq \mathbf{h}\}$*. Moreover, the reduced problem* **RSP** *is always solvable, and* $\tilde{\mathbf{t}}^*$ *is a global minimizer (or a local minimizer, or a stationary point) of* **RSP** *if and only if* $(\tilde{\mathbf{t}}^*, \boldsymbol{\alpha}^*)$ *with*

$$\boldsymbol{\alpha}^* = \begin{bmatrix} \mathbf{B}(\tilde{\mathbf{t}}^*) \\ \sqrt{\mu}\mathbf{S}(\tilde{\mathbf{t}}^*) \end{bmatrix}^+ \begin{bmatrix} \mathbf{y} \\ \mathbf{0} \end{bmatrix}$$

is a global minimizer (or a local minimizer, or a stationary point) of the full problem (2.19b). ■

Proof. Part (i): There exists a sufficiently small open neigborhood Ω^* of $\tilde{\mathbf{t}}^*$ so that $\mathbf{B}$ has full rank on Ω^*. Then the assertions follow from applying Theorems 2 and 3 to the intersection of Ω^* with the feasible set.
Part (ii): Under the assumption posed, the system matrix $\begin{bmatrix} \mathbf{B}(\tilde{\mathbf{t}}) \\ \sqrt{\mu}\mathbf{S}(\tilde{\mathbf{t}}) \end{bmatrix}$ of (3.7b) and its Moore-Penrose inverse are continuous functions of the knots. Therefore, the functional $\phi(\tilde{\mathbf{t}})$ is continuous on the closed – due to $\mathbf{C}\tilde{\mathbf{t}} \geq \mathbf{h}$ – and bounded – due to $a \leq t_{p(1)}, t_{p(l)} \leq b$ – feasible set $\{\tilde{\mathbf{t}} \in \mathbb{R}^l : \mathbf{C}\tilde{\mathbf{t}} \geq \mathbf{h}\}$. Hence, it attains its minimum. The equivalence of the reduced and full problems is again a consequence of Theorem 2 and 3 since the system matrix has full rank on the whole feasible set. □

Obviously, in case of the approximation problem **RAP**, the expressions for the Jacobian of the reduced function $\mathbf{G}$ defined with the "general" matrix $\mathbf{B}(\tilde{\mathbf{t}})$ of this section remain valid for the "special" $\mathbf{B}(\tilde{\mathbf{t}})$ given by the observation matrix introduced in Section 2. In order to get the Jacobian in case of the smoothing problem **RSP**, the pair $\{\mathbf{B}(\tilde{\mathbf{t}}), \mathbf{y}\}$ has to be replaced by the bordered quantities $\left\{\begin{bmatrix} \mathbf{B}(\tilde{\mathbf{t}}) \\ \sqrt{\mu}\mathbf{S}(\tilde{\mathbf{t}}) \end{bmatrix}, \begin{bmatrix} \mathbf{y} \\ \mathbf{0} \end{bmatrix}\right\}$.

4 Gauss-Newton-Like Methods for the Reduced Problem.

Whereas in almost all papers known to the authors the constrained reduced problem **RAP** is tranformed into an unconstrained one, cf. the Introduction, we directly treat both of the constrained problems **RAP** and **RSP** by some generalized Gauss-Newton-like methods. Applying these techniques to regularized problems as **RSP** seems to be new in the context of least squares spline approximation.

In the ν-th step of a generalized Gauss-Newton method, the Gauss-Newton model to $\mathbf{G}$ at the current iterate $\tilde{\mathbf{t}}^\nu$ has to be built. Remember that we have called this model Golub-Pereyra model. Then the quadratic subproblem

$$\min\left\{\mu_{GP}(\tilde{\mathbf{t}}^\nu + \mathbf{s}) = \tfrac{1}{2}\|\mathbf{G} + \mathbf{G}'\mathbf{s}\|^2 \,:\, \mathbf{C}\mathbf{s} \geq \mathbf{h} - \mathbf{C}\tilde{\mathbf{t}}^\nu \,,\, \mathbf{s} \in \mathbb{R}^l\right\} \tag{4.1}$$

with $\mathbf{G} := \mathbf{G}(\tilde{\mathbf{t}}^\nu)$, $\mathbf{G}' := \mathbf{G}'(\tilde{\mathbf{t}}^\nu)$ is to be solved for the generalized Gauss-Newton step $\mathbf{s}$. If the Jacobian $\mathbf{G}'$ has full rank then (4.1) has a unique solution $\mathbf{s}^\nu$ which defines the undamped generalized Gauss-Newton method

$$\tilde{\mathbf{t}}^{\nu+1} := \tilde{\mathbf{t}}^\nu + \mathbf{s}^\nu \qquad (\nu = 0, 1, 2, \ldots).$$

A convergence theory of generalized Gauss-Newton methods was developed by Bock [2], see also [15]. As in the unconstrained case, one can prove local Q-linear convergence for "small residual problems".

For evaluating $\mathbf{G}'$ or its Kaufman approximation $\mathbf{K}$, the derivative of $\mathbf{B}$ has to be computed. Expressions for the derivatives of a B-Spline with respect to its knots can be found, e.g., in [22]. In the smoothing case, additionally the derivative of the smoothing matrix $\mathbf{S}$ has to be provided using the defining formulas of Section 2. Of course, both derivatives can be computed by applying so-called *automatic differentiation* to the corresponding codes, see Griewank/Corliss [10] and the literature cited there for a description of this technique.

An alternative way consists of approximating the derivatives by appropriate finite differences. This will be done in the following.

When using the Golub-Pereyra model, the Jacobian $\mathbf{G}'(\tilde{\mathbf{t}}^{\nu})$ is approximated column-wise according to

$$\mathbf{G}'(\tilde{\mathbf{t}})\mathbf{e}^{\tau} \approx \frac{\mathbf{G}(\tilde{\mathbf{t}} + h_{\tau}\mathbf{e}^{\tau}) - \mathbf{G}(\tilde{\mathbf{t}})}{h_{\tau}} \qquad (\tau = 1, \ldots, l)$$

choosing, e.g., the stepsizes $h_{\tau} = \epsilon_1 \left(|t_{p(\tau)}| + \epsilon_2\right)$, $\epsilon_1 \approx \sqrt{\text{macheps}}$. Because here the discretization is done in the outermost part, we call this type of approximation *outer discretization*. The corresponding discretized Golub-Pereyra model to **RAP** or **RSP** is denoted by **RAP-GP-OD** or **RSP-GP-OD**, resp. Note that this approximation requires the additional factorization of $\mathbf{B}$ at the l auxiliary points $\tilde{\mathbf{t}}+h_{\tau}\mathbf{e}^{\tau}$ $(\tau = 1, \ldots, l)$.

When using the Kaufman model where $\mathbf{G}'$ is replaced by $\mathbf{K}$ defined in (3.6), the discretization is done in the inner part. In the approximation case **RAP**, the columns of $\mathbf{K} \in \mathbb{R}^{m,l}$ are defined by

$$\begin{aligned}
\mathbf{K}\mathbf{e}^{\tau} &= -\left[\mathbf{I} - \mathbf{B}(\tilde{\mathbf{t}})\mathbf{B}(\tilde{\mathbf{t}})^{+}\right]\left(\mathbf{B}'(\tilde{\mathbf{t}})[\mathbf{e}^{\tau}]\right)\mathbf{B}(\tilde{\mathbf{t}})^{+}\mathbf{y} \\
\left(\mathbf{B}'(\tilde{\mathbf{t}})\left[\mathbf{e}^{\tau}\right]\right)_{i,j} &= \frac{\partial B_j\left(x_i, \tilde{\mathbf{t}}\right)}{\partial t_{p(\tau)}} \qquad (i = 1, \ldots, m; j = 1, \ldots, n; \tau = 1, \ldots, l).
\end{aligned}$$

The derivatives of the B-splines with respect to the knots occuring above are approximated by finite differences

$$\left(\mathbf{B}'(\tilde{\mathbf{t}})\left[\mathbf{e}^{\tau}\right]\right)_{i,j} \approx \frac{B_j\left(x_i, \tilde{\mathbf{t}} + h_{\tau}\mathbf{e}^{\tau}\right) - B_j\left(x_i, \tilde{\mathbf{t}}\right)}{h_{\tau}}.$$

Here the discretization is done in the innermost part so that the fine structure of the Kaufman model is exploited. This type of discretization will be called *inner discretization*, and the corresponding discretized Kaufman model to **RAP** is abbreviated by **RAP-Ka-ID**. The matrix $\mathbf{K}$ can be evaluated efficiently because $\mathbf{B}$ and $\mathbf{B}'[\mathbf{e}^{\tau}]$ have bandwidth k, and the repeated evaluation of $\mathbf{B}^{+}\mathbf{u}$ for different $\mathbf{u}$ requires only one QR factorization of $\mathbf{B}$.

In the smoothing case **RSP**, the additional term $\sqrt{\mu}\mathbf{S}(\tilde{\mathbf{t}})$ and its derivative have to be considered. If the derivatives are approximated by inner discretization of $\mathbf{B}$ and $\mathbf{S}$ as described above, the corresponding Kaufman model is denoted by **RSP-Ka-ID**.

When comparing the discretized Golub-Pereyra and Kaufman model, one has to consider both the costs of realizing the linear algebra involved, and the approximation quality. The latter seems to be comparable, as numerical tests done by several authors show. The linear algebra costs depend strongly on the structure of $\mathbf{B}$ or its regularization. If $\mathbf{B}$ is dense, then using the Kaufman model is, in general, cheaper since the l additional least squares problems with different system matrices to be solved in the Golub-Pereyra model are replaced by l least squares problems with different right hand sides but the same system matrix. In our case, however, the matrix $\mathbf{B}$ is banded so that the costs for its factorization are comparable with the costs for handling a right hand side for the same matrix. On the other hand, the discretized Golub-Pereyra model is much easier to implement since it ignores the fine structure and requires only a code for computing the residual $\mathbf{G}(\tilde{\mathbf{t}})$.

For computing the residual $\mathbf{G}$ and the matrices $\mathbf{G}'$ or $\mathbf{K}$ of that quadratic model which is used in the optimization process, we need a fast and stable method to solve linear least squares problems

$$\min\left\{\tfrac{1}{2}\left\|\mathbf{y}-\mathbf{B}\boldsymbol{\alpha}\right\|^2 \,:\, \boldsymbol{\alpha}\in\mathbb{R}^n\right\}$$

in the approximation case, or

$$\min\left\{\tfrac{1}{2}\left\|\begin{bmatrix}\mathbf{y}\\ \mathbf{0}\end{bmatrix}-\begin{bmatrix}\mathbf{B}\\ \sqrt{\mu}\mathbf{S}\end{bmatrix}\boldsymbol{\alpha}\right\|^2 \,:\, \boldsymbol{\alpha}\in\mathbb{R}^n\right\}$$

in the smoothing case. We used numerically stable Givens rotations and reduced the matrices row by row to upper triangular form fully exploiting the band structure of the problem as done in [23]. For the repeated solution of these least squares problems with different right hand sides, the relevant information for reconstructing the Givens parameters is stored on the place of the band of $\mathbf{B}$.

In every step of the generalized Gauss-Newton methods we have to solve linear least squares problems with linear inequality constraints of the form

$$\min\left\{\tfrac{1}{2}\left\|\mathbf{G}+\mathbf{J}\mathbf{s}\right\|^2 \,:\, \mathbf{C}\mathbf{s}\geq\mathbf{h}-\mathbf{C}\tilde{\mathbf{t}}^{\nu}\,,\ \mathbf{s}\in\mathbb{R}^l\right\} \tag{4.2}$$

where $\mathbf{J}$ is either the outer difference approximation to $\mathbf{G}'$ (Golub-Pereyra model) or the inner approximation to $\mathbf{K}$ (Kaufman model). If $\mathbf{J}$ has full rank, then the problem is transformed by Householder reflections into a least distance problem as described in Lawson/Hanson [17]. The algorithms for solving the resulting least distance problem are taken from [17], too.

If $\mathbf{J}$ is nearly rank-deficient in the sense $\mathrm{cond}(\mathbf{R}) > 1/\sqrt{\mathrm{macheps}}$ where $\mathbf{R}$ is the upper triangular factor of the QR factorization of $\mathbf{J}$, then, following an idea of Dennis/Schnabel [5], the original problem (4.2) is replaced by the regularized problem

$$\min\left\{\tfrac{1}{2}\left\|\begin{bmatrix}\mathbf{G}\\ \mathbf{0}\end{bmatrix}+\begin{bmatrix}\mathbf{J}\\ \sqrt{\lambda}\mathbf{I}\end{bmatrix}\mathbf{s}\right\|^2 \,:\, \mathbf{C}\mathbf{s}\geq\mathbf{h}-\mathbf{C}\tilde{\mathbf{t}}^{\nu}\,,\ \mathbf{s}\in\mathbb{R}^l\right\} \tag{4.3}$$

with $\lambda=\sqrt{l\times\mathrm{macheps}}\,\left\|\mathbf{J}^T\mathbf{J}\right\|_1$.

The undamped generalized Gauss-Newton method considered up to now converges only locally and for small residual problems. In order to obtain global convergence as it is understood in nonlinear optimization, see [8] and [5], a damping technique is used. Since the constraints are linear, it is possible to work with feasible points only, and so the objective function $\phi(\tilde{\mathbf{t}}) = \frac{1}{2}\left\|\mathbf{G}(\tilde{\mathbf{t}})\right\|^2$ can be taken as merit function in the line search. We have implemented a safeguarded Armijo-Goldstein line search with mixed quadratic and cubic interpolation. The information available anyhow from the solution of the linear least squares problems allows to evaluate $\phi(\tilde{\mathbf{t}}^\nu + \gamma \mathbf{s}^\nu) = \frac{1}{2}\left\|\mathbf{G}(\tilde{\mathbf{t}}^\nu + \gamma \mathbf{s}^\nu)\right\|^2$ without computing the residual vector $\mathbf{G}(\tilde{\mathbf{t}}^\nu + \gamma \mathbf{s}^\nu)$ explicitly. In the numerical examples of Section 5, the number of rejected trial points was comparatively small when using the line search described. Let us note that the popular line search of Al-Baali/Fletcher [1], which models each individual component of the residual by a quadratic polynomial, requires the explicit knowledge of the residual vector.

Summarizing the preceeding discussion, the final algorithm will be formulated.

ALGORITHM 4.1 (DAMPED GENERALIZED GAUSS-NEWTON METHOD).

S1: Choose a feasible initial knot sequence $\tilde{\mathbf{t}}^0 \in \mathbb{R}^l$
$\delta \in (0, \frac{1}{4})$
$\nu := 0$

S2: Iteration
Repeat

S2.1: $\mathbf{G} := \mathbf{G}(\tilde{\mathbf{t}}^\nu) = \left[\mathbf{I} - \mathbf{B}(\tilde{\mathbf{t}}^\nu)\mathbf{B}(\tilde{\mathbf{t}}^\nu)^+\right] \mathbf{y}$
{ Compute residual function }
$\mathbf{J} :\approx \mathbf{G}'(\tilde{\mathbf{t}}^\nu)$
{ Compute an approximation to the Jacobian (Golub-Pereyra or Kaufman model) }

S2.2: Compute a descent direction s^ν from

$$\min \left\{ \tfrac{1}{2}\left\|\mathbf{G} + \mathbf{J}\mathrm{s}\right\|^2 \,:\, \mathbf{C}\mathrm{s} \geq \mathbf{h} - \mathbf{C}\tilde{\mathbf{t}}^\nu ,\, \mathrm{s} \in \mathbb{R}^l \right\}$$

If the problem is ill-conditioned, compute s^ν from the regularized problem

$$\min \left\{ \tfrac{1}{2}\left\| \begin{bmatrix} \mathbf{G} \\ \mathbf{0} \end{bmatrix} + \begin{bmatrix} \mathbf{J} \\ \sqrt{\lambda}\mathbf{I} \end{bmatrix} \mathrm{s} \right\|^2 \,:\, \mathbf{C}\mathrm{s} \geq \mathbf{h} - \mathbf{C}\tilde{\mathbf{t}}^\nu ,\, \mathrm{s} \in \mathbb{R}^l \right\}$$

with $\lambda = \sqrt{l \times \text{macheps}}\,\left\|\mathbf{J}^T\mathbf{J}\right\|_1$

S2.3: Safeguarded line search
$\gamma := 1.0$
while $\phi(\tilde{\mathbf{t}}^\nu) - \phi(\tilde{\mathbf{t}}^\nu + \gamma \mathrm{s}^\nu) < -\gamma\delta\nabla\phi(\tilde{\mathbf{t}}^\nu)^T \mathrm{s}^\nu$ do
$\gamma := \gamma * \alpha$
{ Here α is chosen so that $\gamma * \alpha$ is the minimizer of a quadratic or cubic polynomial that models $\phi(\tilde{\mathbf{t}} + \gamma \mathrm{s}^\nu)$ provided that α is not to close to the boundary points 0 or 1 }

S2.4: $\tilde{\mathbf{t}}^{\nu+1} := \tilde{\mathbf{t}}^\nu + \gamma \mathrm{s}^\nu$
$\nu := \nu + 1$

until $\nu > \nu max$ or *convergence*

The algorithm exits if at least one of the following conditions is fulfilled

1	$\|\mathbf{G}\| \leq \varepsilon_0$
2	$\|\mathbf{J}^T\mathbf{G}\| \leq \varepsilon_3$
3	$\|\mathbf{G}^T\mathbf{J}\mathbf{s}\| \leq \varepsilon_4$
4	$\|\tilde{\mathbf{t}}^{\nu+1} - \tilde{\mathbf{t}}^{\nu}\| \leq \varepsilon_1(\|\tilde{\mathbf{t}}^{\nu}\| + \varepsilon_2)$
5	$\nu > \nu max$
6	failed otherwise

5 Numerical Examples.

In this section the capabilities of the new method will be demonstrated. It will be shown that the method is a robust tool in locating a good knot sequence, and that the algorithm can be used in combination with data reduction strategies. An experimental code has been implemented in PASCAL and run on a 486DX50 PC using IEEE double precision arithmetic. Since the block sparse structure of the matrices is exploited, the requirements concerning memory and floating point performance are moderate. To compare our algorithm with standard algorithms in nonlinear optimization, all tests have been run also with MATLAB's CONSTR routine. The relative knot separation parameter was chosen to be $\epsilon = 0.0625$ as first used by de Boor/Rice.

One of the best investigated examples in approximation by splines with free knots is the titanium heat data set, see [4], [13] and [3]. The $m = 49$ data values lie on a curve that is relatively flat except the peak in the region $x = 900$. In order to allow a direct comparison with the results of [4] and [13], we approximate these data by $n = 9$ B-splines of order $k = 4$ and do not use smoothing. Moreover, all $l = 5$ inner knots are considered free.

The optimization is started with the three knot sequences provided by Jupp:

$\tilde{\mathbf{t}}_1$	initial point near the interior optimum,
$\tilde{\mathbf{t}}_2$	initial point used by de Boor/Rice [4],
$\tilde{\mathbf{t}}_3$	equidistant knots.

	$\tilde{\mathbf{t}}_1$	MATLAB CONSTR	RAP-Ka-ID	RAP-GP-OD
t_5	838.2	835.481	835.457	835.457
t_6	876.6	876.470	876.506	876.506
t_7	895.8	898.228	898.166	898.166
t_8	915.0	916.225	916.280	916.280
t_9	979.0	974.084	974.017	974.017
$\|\mathbf{G}\|$	$1.011427E-01$	$8.748072E-02$	$8.748003E-02$	$8.748003E-02$
steps		500 funct. calls	10	10
time		252 sec.	0.142 sec.	0.148 sec.
$\|\mathbf{G}^T\mathbf{J}\mathbf{s}\|$			$9.414131E-11$	$9.410049E-11$
$\|\mathbf{J}^T\mathbf{G}\|$			$1.041312E-07$	$1.041355E-07$
Ret. Code		terminated	3	3

	$\tilde{\mathbf{t}}_2$	MATLAB CONSTR	RAP-Ka-ID	RAP-GP-OD
t_5	725	835.453	835.457	835.457
t_6	850	876.506	876.506	876.506
t_7	910	898.170	898.167	898.166
t_8	975	916.275	916.280	916.280
t_9	1040	974.017	974.017	974.017
$\|\mathbf{G}\|$	$1.008965E+00$	$8.748005E-02$	$8.748003E-02$	$8.748003E-02$
steps		500 funct. calls	16	13
time		243 sec.	0.220 sec.	0.209 sec.
$\|\mathbf{G}^T\mathbf{J}\mathbf{s}\|$			$3.059450E-11$	$5.660746E-11$
$\|\mathbf{J}^T\mathbf{G}\|$			$6.562935E-08$	$8.750237E-07$
Ret. Code		terminated	3	3

	$\tilde{\mathbf{t}}_3$	MATLAB CONSTR	RAP-Ka-ID	RAP-GP-OD
t_5	675	689.386	803.307	610.104
t_6	755	839.781	864.915	836.671
t_7	835	877.214	869.022	877.901
t_8	915	897.038	897.214	897.006
t_9	995	908.161	908.327	908.131
$\|\mathbf{G}\|$	$1.235202E+00$	$2.515804E-01$	$2.450117E-01$	$2.525756E-01$
steps		359 funct. calls	11	12
time		179 sec.	0.175 sec.	0.197 sec.
$\|\mathbf{G}^T\mathbf{J}\mathbf{s}\|$			$2.006475E-11$	$1.571279E-10$
$\|\mathbf{J}^T\mathbf{G}\|$			$1.060480E-04$	$9.329193E-05$
Ret. Code		successfully	3	4

Jupp [13] mentioned that there are four stationary points for this problem (probably found there in lower accuracy arithmetic):

	$\tilde{\mathbf{t}}^*$ interior optimum	$\tilde{\mathbf{t}}^1$ local minimum	$\tilde{\mathbf{t}}^2$ saddle point	$\tilde{\mathbf{t}}^3$ local minimum
t_5	835.9670	803.5453	796.9648	836.2518
t_6	876.4016	866.2870	852.4528	878.7197
t_7	898.1462	866.3510	885.2259	890.6851
t_8	916.3146	901.2944	885.9946	905.0262
t_9	973.9075	905.5165	910.5168	905.0902
$\|\mathbf{G}\|$	$8.752539E-02$	$2.440692E-01$	$2.493385E-01$	$2.510164E-01$

Fig. 5.1 and 5.2 show the splines belonging to the initial knot sequence $\tilde{\mathbf{t}}_2$ and to the interior optimum $\tilde{\mathbf{t}}^*$. In all figures, a small circle or a cross mark a data point or a knot, resp.

In the second example, the new method is combined with a knot removal strategy in order to achieve a maximal data reduction. For a given estimate Δ to the noise level

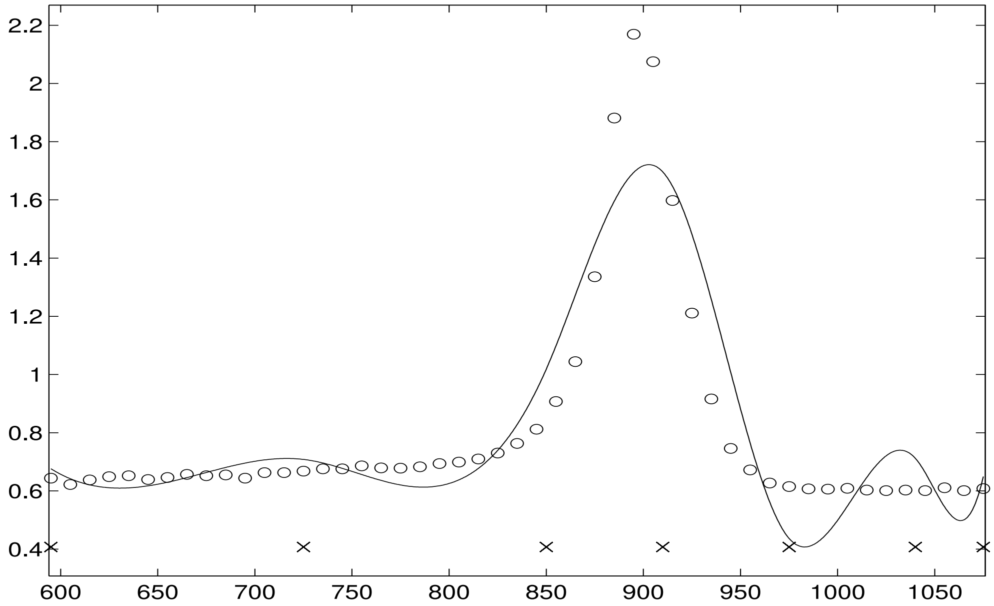


Figure 5.1: Titanium heat data, $n = 9$, initial knot sequence $\tilde{\mathbf{t}}_2$

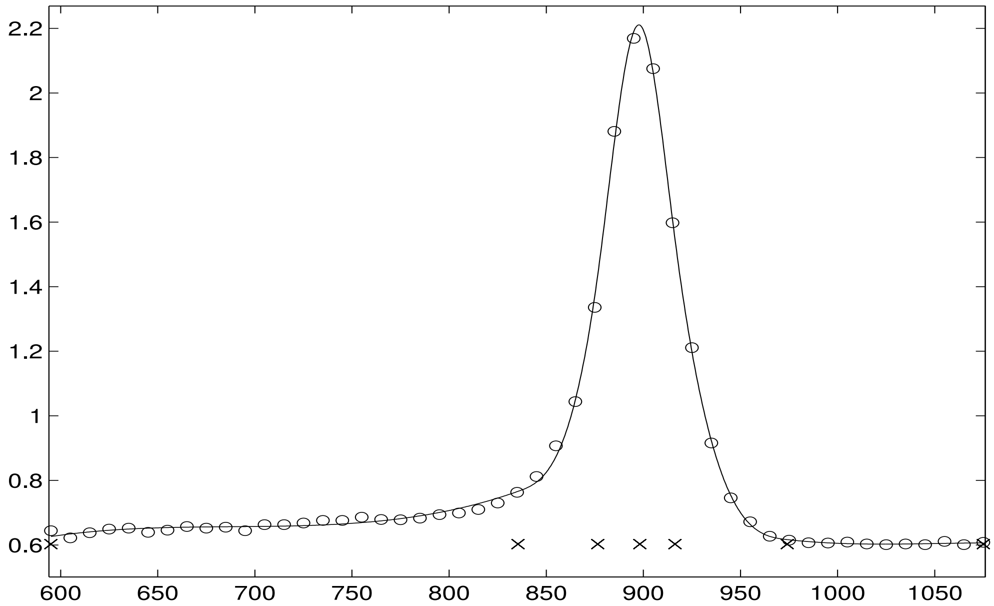


Figure 5.2: Titanium heat data, $n = 9$, interior optimum $\tilde{\mathbf{t}}^*$

measured by the least squares error $||\mathbf{G}||$, we want to approximate the data within this level with as few B-splines as possible. In the following, let us call a knot sequence $\tilde{\mathbf{t}}$ *acceptable* if the least squares error of the corresponding spline is not greater than the prescribed estimate Δ, i.e., if $||\mathbf{G}(\tilde{\mathbf{t}})|| \leq \Delta$.

Our strategy is similar to that of Lyche/Mørken [18]. We start the process with an acceptable knot sequence consisting of a larger number of knots whereas, in contrast to Lyche/Mørken, these knots need not be placed at data points. In one step of the iterative process, at first the current knot sequence is optimized using our algorithm. Then the interior knots are ranked according to their importance for the approximation which is measured by the jump in the first discontinuous derivative. If removing the less important knot leads to a knot sequence which is not acceptable, then the iteration is terminated, and the old (last acceptable) knot sequence is taken as final knot sequence. Otherwise, the iteration is repeated with the new, shortened knot sequence where the less important knot is dropped.

The difference to other known knot removal strategies is that we try to locate an "optimal" knot sequence in every step whereas in other strategies no relocating is done at all. However, because relocating the knots in *every* step is expensive, a compromise between these extremes is sought for, and the knot removal process is split into two stages: In the first stage, we start with a fixed, acceptable knot sequence. Then we remove knots as described above but without optimizing the new knot sequence. This cheap process is repeated as long as the knot sequence remains acceptable. When the acceptibility gets lost, we start the second stage and try to remove further knots by applying our first strategy, i.e., by relocating the knots in every step.

Let us illustrate this two-stage strategy on hand of the following example: We sample the function $f(x) = \frac{10x}{1+100x^2}$ at $m = 90$ equidistant points x_i in $[-2, 2]$. Adding some random noise $\{\epsilon_i\}$ chosen as pseudo random numbers with $-0.05 \leq \epsilon_i \leq 0.05$, we generate the perturbed data $y_i = f(x_i) + \epsilon_i$, $i = 1, \ldots, m$. We want to approximate these data by a smoothing spline of order $k = 5$ with a smoothing term of order $r = 2$ using the estimate $\Delta = 0.3$ for the least squares error $||\mathbf{G}||$. As value of the smoothing parameter μ we take $\mu = 1.0E - 10$. The approximation is started with $l = 15$ equidistant inner knots which, however, are not acceptable. Therefore, one preprocessing knot optimization step is performed which leads to the acceptable knot sequence of Fig. 5.3. This sequence is taken as input for stage I. The knot removing process of this stage (without relocation) ends up with an acceptable knot sequence consisting of $l = 12$ inner knots. Switching to stage II gives a further reduction to $l = 5$ inner knots; the final knot sequence and the corresponding spline are shown in Fig. 5.4.

The results of the whole procedure including the preprocessing step are summarized in Table 5.1. The model used in the knot optimization process was **RSP-GP-OD**.

We performed the same procedure using the discretized Kaufman model **RSP-Ka-ID**. Here the preprocessing step leads to an optimized knot sequence the least square error of which is slightly greater, namely $||\mathbf{G}|| = 2.2486127E - 01$. Nevertheless, the number of inner knots is reduced to $l = 9$ in stage I; the error is $||\mathbf{G}|| = 2.7768012E-01$. In the final stage II, however, the same least squares error as with **RSR-GP-OD** is achieved with the same number $l = 5$ of free inner knots.

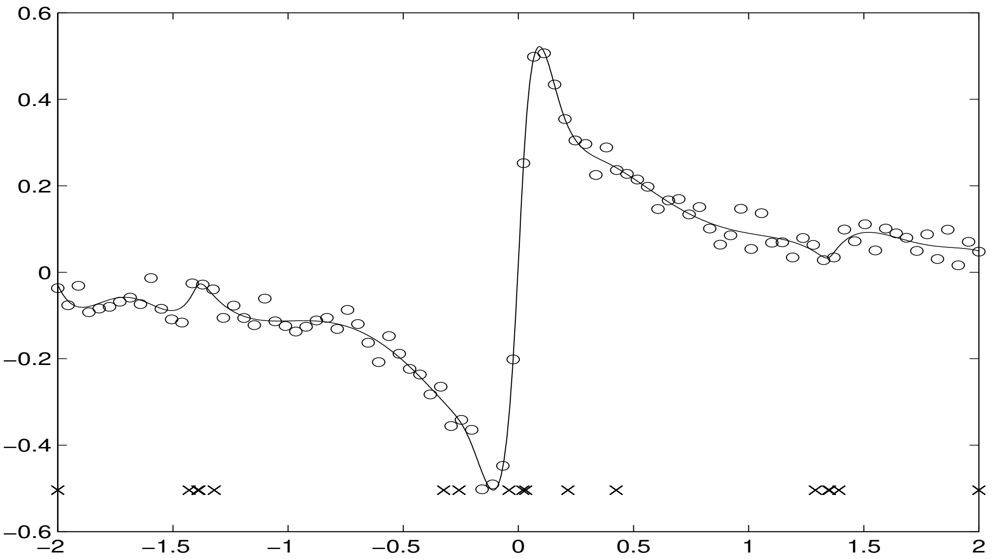


Figure 5.3: Preprocessing step: optimized location of knots starting from an equidistant distribution (no removal), $n = 20$, $l = 15$

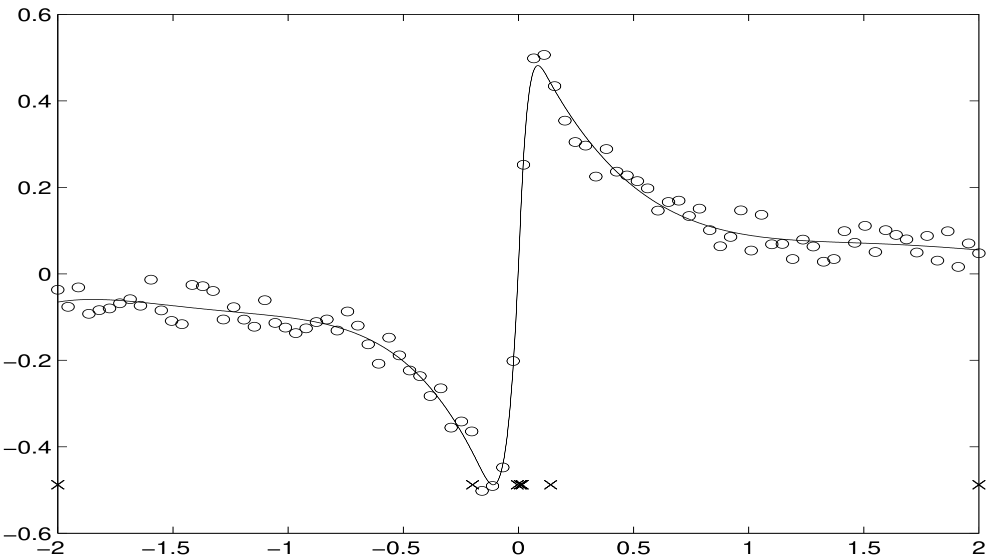


Figure 5.4: Knot removal and relocation algorithm: final result of stage II, $n = 10$, $l = 5$

Table 5.1: Knot removal algorithm

equidistant inner knots	$n = 20$	$\|\|\mathbf{G}\|\|$	$= 5.3641288E-01$
	$l = 15$	$\|\|\mathbf{y}-\mathbf{B}\boldsymbol{\alpha}\|\|$	$= 5.3641269E-01$
optimized knot sequence	$n = 20$	$\|\|\mathbf{G}\|\|$	$= 2.2395534E-01$
(Fig. 5.3)	$l = 15$	$\|\|\mathbf{y}-\mathbf{B}\boldsymbol{\alpha}\|\|$	$= 2.2395367E-01$
knot removal algorithm, stage I	$n = 17$	$\|\|\mathbf{G}\|\|$	$= 2.6486237E-01$
	$l = 12$	$\|\|\mathbf{y}-\mathbf{B}\boldsymbol{\alpha}\|\|$	$= 2.6486161E-01$
knot removal algorithm, stage II	$n = 10$	$\|\|\mathbf{G}\|\|$	$= 2.7195137E-01$
(Fig. 5.4)	$l = 5$	$\|\|\mathbf{y}-\mathbf{B}\boldsymbol{\alpha}\|\|$	$= 2.7194998E-01$

The last example shows an essential further advantage of the combined knot removal and relocation algorithm for the approximation of noisy data. The final spline does not only reproduce the data within the noise level with only $l = 5$ instead of $l = 15$ inner knots. In addition, it is visually more pleasant in that it avoids the "overfitting" caused by too many parameters, cf. Fig. 5.3. The reduced number of degrees of freedom in the final approximation implies some kind of "regularization by reduction of dimension", see [25] and [27] for a discussion (and exploitation) of this effect.

The examples listed above and further one‘s performed by the authors show that the new knot optimizing algorithm combined with a reasonable knot removing strategy provides an efficient tool for fitting noisy data by splines with free knots. Especially when used with a smoothing term, it is rather robust since it does not depend on the location of the free knots.

REFERENCES

1. M. Al-Baali and R. Fletcher, *An efficient line search for nonlinear least squares*, J. Optim. Theory Appl., 48 (1986), pp. 359–377.
2. H. G. Bock, *Randwertproblemmethoden zur Parameteridentifizierung in Systemen nichtlinearer Differentialgleichungen (Habilitationschrift)*, Bonner Mathematische Schriften Nr.183, Universität Bonn, 1987.
3. C. de Boor, *A practical guide to splines*, Springer-Verlag, New York, Heidelberg, Berlin, 1978.
4. C. de Boor and J. R. Rice, *Least squares cubic spline approximation II – variable knots*, Technical Report CSD TR 21, Computer Science Department, Purdue University, 1968.
5. J. E. Dennis and R. B. Schnabel, *Numerical Methods for Unconstrained Optimization and Nonlinear Equations*, Prentice Hall, Inc., 1983.
6. P. Dierckx, *Het aanpassen van krommen en oppervlakken aan meetpunten met behulp van spline funkties*, PhD thesis, Katholieke Universiteit Leuven, 1979.
7. ———, *Curve and surface fitting with splines*, Oxford University Press, 1993.
8. R. Fletcher, *Practical Methods of Optimization*, John Wiley & Sons, 1987.
9. G. H. Golub and V. Pereyra, *The differentiation of pseudoinverses and nonlinear least squares problems whose variables separate*, SIAM J. Numer. Anal., 10 (1973), pp. 413–432.

10. A. Griewank and G. Corliss, eds., *Automatic Differentiation of Algorithms: Theory, Implementation, and Application*, Philadelphia, 1991, SIAM Publications.
11. J. N. Holt and R. Fletcher, *An algorithm for constrained nonlinear least squares*, J. Inst. Math. Appl., 23 (1979), pp. 449–463.
12. Y. Hu, *An algorithm for data reduction using splines with free knots*, IMA J. Numer. Anal., 13 (1993), pp. 365–381.
13. D. L. B. Jupp, *Approximation to data by splines with free knots*, SIAM J. Numer. Anal., 15 (1978), pp. 328–343.
14. L. Kaufman, *A variable projection method for solving separable nonlinear least squares problems*, BIT, 15 (1975), pp. 49–57.
15. O. Knoth, *A globalization scheme for the generalized Gauss-Newton method*, Numer. Math., 56 (1989), pp. 591–607.
16. F. T. Krogh, *Efficient implementation of a variable projection algorithm for nonlinear least squares problems*, Comm. ACM, 17 (1974), pp. 167–169.
17. C. L. Lawson and R. J. Hanson, *Solving Least Squares Problems*, Prentice Hall, Inc., Englewood Cliffs, N. J., 1974.
18. T. Lyche and K. Mørken, *A data reduction strategy for splines with applications to the approximation of functions and data*, IMA J. Numer. Anal., 8 (1988), pp. 185–208.
19. T. A. Parks, *Reducible Nonlinear Programming Problems*, PhD thesis, Houston Univ., Dept. of Mathematics, Houston, 1985.
20. A. Ruhe and P. Å. Wedin, *Algorithms for separable nonlinear least squares problems*, SIAM Rev., 22 (1980), pp. 318–337.
21. I. J. Schoenberg and A. Whitney, *On Pólya frequency functions III: The positivity of translation determinants with an application to the interpolation problem by spline curves*, Trans. Amer. Math. Soc., 74 (1953), pp. 246–259.
22. L. L. Schumaker, *Spline Functions: Basic Theory*, John Wiley and Sons, New York, 1981.
23. H. Schwetlick and V. Kunert, *Spline smoothing under constraints on derivatives*, BIT, 33 (1993), pp. 512–528.
24. P. Suchomski, *Method of optimal variable-knot spline interpolation in the L_2 discrete norm*, Internat. J. Systems Sci., 22 (1991), pp. 2263–2274.
25. J. M. Varah, *A spline least squares method for numerical parameter estimation in differential equations*, SIAM J. Sci. Statist. Comput., 3 (1982), pp. 28–46.
26. M. von Golitschek and L. L. Schumaker, *Data fitting by penalized least squares*, in Algorithms for Approximation II, J. C. Mason and M. G. Cox, eds., London-New York, 1988, Chapman and Hall, pp. 210–227.
27. G. Wahba, *Spline Models for Observational Data*, SIAM Publications, Philadelphia, 1990.