Bull. Nov. Comp. Center, Num. Anal., 7 (1996), 101–105

Optimization of energy functional for variational splines*

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The aim of this paper is to suggest optimization procedure for the refinement of energy functional in variational spline approximation problem. Our approach is based on a separation of measurement data between two sets. First is the set of basic measurements (nodes of spline), second is the set of control measurements (additional points). Additional data provides the reasonable choice of parameters in energy functional and may be the refinement of coefficients in mathematical model of the process we need to study.

The formulation of optimization problem in general form and example for D^m-splines with a tension are presented. Also the numerical algorithm of Newton's type is described.

1. General formulation

Let X, Y, Z_1, Z_2 be the Hilbert spaces with the corresponding scalar products $(\,,\,)_X$, $(\,,\,)_Y$, $(\,,\,)_{Z_1}$, $(\,,\,)_{Z_2}$, $A_1 : X \to Z_1$, $A_2 : X \to Z_2$ be two linear bounded operators, $z_1 \in Z_1$, $z_2 \in Z_2$ be two fixed elements.

Let us consider some open set $\mathcal{M} \subset R^n$ and mapping $\alpha \to T_\alpha$ from $\mathcal{M}$ to the space $L(X,Y)$ of linear bounded operators acting from X to Y, i.e., every point $\alpha \in \mathcal{M}$ corresponds to the operator $T_\alpha : X \to Y$. We formulate now the family of spline interpolation problems: for every fixed $\alpha \in \mathcal{M}$ find $\sigma_\alpha \in X$ as a solution of variational problem

$$\sigma_\alpha = \arg \min_{x \in A_1^{-1}(z_1)} \|T_\alpha x\|_Y^2, \tag{1}$$

where $A_1^{-1}(z_1) = \{x \in X : A_1 x = z_1\}$. We suppose problem (1) be uniquely solvable for every $\alpha \in \mathcal{M}$. This property is garanteed if [1]:

$$\begin{aligned} &1.\ A_1^{-1}(z_1) \neq \emptyset,\\ &2.\ N(A_1) + N(T_\alpha) \text{ is closed in } X\text{-norm},\\ &3.\ N(A_1) \cap N(T_\alpha) = \{\theta_X\}. \end{aligned} \tag{2}$$

Here $N(B)$ means null-space of operator B, θ_X is zero vector in the space X. In standard spline terminology Z_1 is the basic measurement operator,

*Supported by the Russian Foundation of Basic Research under Grant 95–01–000949.

T_α is energy operator which generates energy functional on (1) we need to minimize. In addition we introduce "control" operator $A_2 : X \to Z_2$ and define real valued aim function $\varphi(\alpha)$, $\alpha \in \mathcal{M}$ by the formula

$$\varphi(\alpha) = \left\| A_2\sigma_\alpha - z_2 \right\|^2_{Z_2}. \tag{3}$$

We call $\alpha_* \in \mathcal{M}$ optimal if

$$\alpha_* = \arg \min_{\alpha \in \mathcal{M}} \varphi(\alpha). \tag{4}$$

Let us suggest the mapping $\alpha \to T_\alpha$ be sufficiently smooth. Because $\mathcal{M}$ is an open set, then an optimal point α_* lies in interior of $\mathcal{M}$ and the equation

$$(\nabla\varphi)(\alpha_*) = 0 \tag{5}$$

takes place. It means

$$f_i(\alpha) = f_i(\alpha_1, \ldots, \alpha_n) = \left(A_2 \frac{\partial \sigma_\alpha}{\partial \alpha_i}, A_2\sigma_\alpha - z_2 \right)_{Z_2} = 0, \quad i = 1, 2, \ldots, n. \tag{6}$$

We obtain n nonlinear equations with respect to n variables $\alpha_1, \alpha_2, \ldots, \alpha_n$. We try to solve this system be Newton's method. Newton's iterations starting from the vector $\alpha^{(0)}$ have to be realized with the formula

$$\alpha^{(k+1)} = \alpha^{(k)} - J^{-1}(\alpha^{(k)}) \cdot F(\alpha^{(k)}), \tag{7}$$

where $F(\alpha^{(k)}) = \left(f_1(\alpha^{(k)}), f_2(\alpha^{(k)}), \ldots, f_n(\alpha^{(k)}) \right)^T$ is a column vector of residuals and $J(\alpha)$ is $n \times n$-Jacobi matrix of the elements

$$g_{ij}(\alpha) = \frac{\partial f_i}{\partial \alpha_j}(\alpha_1, \alpha_2, \ldots, \alpha_n), \quad i, j = \overline{1, n}. \tag{8}$$

Using the representation (6) we obtain

$$g_{ij}(\alpha) = \left(A_2 \frac{\partial \sigma_\alpha}{\partial \alpha_i \partial \alpha_j}, A_2\sigma_\alpha - z_2 \right)_{Z_2} + \left(A_2 \frac{\partial \sigma_\alpha}{\partial \alpha_i}, A_2 \frac{\partial \sigma_\alpha}{\partial \alpha_j} \right)_{Z_2}, \tag{9}$$

and the Jacobi matrix evidently is always symmetric.

It is well-known [1], the interpolating spline σ_α satisfies the system of operator equations

$$\begin{aligned} T_\alpha^* T_\alpha \sigma_\alpha + A_1^* \lambda_\alpha &= 0, \\ A_1 \sigma_\alpha &= z_1, \end{aligned} \tag{10}$$

where $\lambda_\alpha \in Z_1$ is an auxiliary vector of Lagrange's parameters. After the differentiation of (10) with respect to variable α_i we obtain

$$
\begin{aligned}
&T_\alpha^* T_\alpha \frac{\partial \sigma_\alpha}{\partial \alpha_i} + A_1^* \frac{\partial \lambda_\alpha}{\partial \alpha_i} = -\left[\frac{\partial}{\partial \alpha_i}(T_\alpha^* T_\alpha)\right]\sigma_\alpha; \\
&A_1 \frac{\partial \sigma_\alpha}{\partial \alpha_i} = 0,
\end{aligned}
\tag{11}
$$

i.e., to find $\partial\sigma_\alpha/\partial\alpha_i$ we need to solve the system of the same type as (10) but with the other right-hand part. Similarly, after the second differentiation of (11) with respect to α_j we have

$$
\begin{aligned}
T_\alpha^* T_\alpha \frac{\partial \sigma_\alpha}{\partial \alpha_i \partial \alpha_j} + A_1^* \frac{\partial \lambda_\alpha}{\partial \alpha_i \partial \alpha_j} &= -\left[\frac{\partial}{\partial \alpha_i \partial \alpha_j}(T_\alpha^* T_\alpha)\right]\sigma_\alpha - \\
&\left[\frac{\partial}{\partial \alpha_i}(T_\alpha^* T_\alpha)\right]\frac{\partial \sigma_\alpha}{\partial \alpha_j} - \left[\frac{\partial}{\partial \alpha_j}(T_\alpha^* T_\alpha)\right]\frac{\partial \sigma_\alpha}{\partial \alpha_i}, \\
A_1 \frac{\partial \sigma_\alpha}{\partial \alpha_i \partial \alpha_j} &= 0.
\end{aligned}
\tag{12}
$$

Finally, after the successive solving of systems (10), (11), (12) for $i, j = 1, 2, \ldots, n$ we obtain everything we need to realize one step of Newton's method.

It is useful to rewrite systems (10)–(12) in the weak form by the scalar multiplication of the first equations to the arbitrary element $v \in X$. In this case we obtain the following systems instead of the original ones:

$$
\begin{cases}
(T_\alpha \sigma_\alpha, T_\alpha v)_Y + (\lambda_\alpha, A_1 v)_{Z_1} = 0 \quad \forall v \in X, \\
A_1 \sigma_\alpha = z_1;
\end{cases}
\tag{10'}
$$

$$
\begin{cases}
\left(T_\alpha \frac{\partial \sigma_\alpha}{\partial \alpha_i}, T_\alpha v\right)_Y + \left(\frac{\partial \lambda_\alpha}{\partial \alpha_i}, A_1 v\right)_{Z_1} \\
\qquad = -\left(\frac{\partial T_\alpha}{\partial \alpha_i}\sigma_\alpha, T_\alpha v\right)_Y - \left(T_\alpha \sigma_\alpha, \frac{\partial T_\alpha}{\partial \alpha_i} v\right)_Y \quad \forall v \in X, \\
A_1 \frac{\partial \sigma_\alpha}{\partial \alpha_i} = 0;
\end{cases}
\tag{11'}
$$

$$
\begin{cases}
\left(T_\alpha \frac{\partial \sigma_\alpha}{\partial \alpha_i \partial \alpha_j}, T_\alpha v\right)_Y + \left(\frac{\partial \lambda_\alpha}{\partial \alpha_i \partial \alpha_j}, A_1 v\right)_{Z_1} \\
= -\left(\frac{\partial T_\alpha}{\partial \alpha_i} \cdot \frac{\partial \sigma_\alpha}{\partial \alpha_j}, T_\alpha v\right)_Y - \left(T_\alpha \frac{\partial \sigma_\alpha}{\partial \alpha_j}, \frac{\partial T_\alpha}{\partial \alpha_i} v\right)_Y - \left(\frac{\partial T_\alpha}{\partial \alpha_j} \cdot \frac{\partial \sigma_\alpha}{\partial \alpha_i}, T_\alpha v\right)_Y - \\
\quad \left(T_\alpha \frac{\partial \sigma_\alpha}{\partial \alpha_i}, \frac{\partial T_\alpha}{\partial \alpha_j} v\right)_Y - \left(\frac{\partial T_\alpha}{\partial \alpha_i \partial \alpha_j}\sigma_\alpha, T_\alpha v\right)_Y - \left(T_\alpha \sigma_\alpha, \frac{\partial T_\alpha}{\partial \alpha_i \partial \alpha_j} v\right)_Y - \\
\quad \left(\frac{\partial T_\alpha}{\partial \alpha_i}\sigma_\alpha, \frac{\partial T_\alpha}{\partial \alpha_j} v\right)_Y - \left(\frac{\partial T_\alpha}{\partial \alpha_j}\sigma_\alpha, \frac{\partial T_\alpha}{\partial \alpha_i} v\right)_Y \quad \forall v \in X, \\
A_1 \frac{\partial \sigma_\alpha}{\partial \alpha_i \partial \alpha_j} = 0.
\end{cases}
\tag{12'}
$$

2. Optimization of parameter for D^m-spline with tension

Let Ω be bounded domain in R^n, and $W_2^m(\Omega)$ be Sobolev space, $m > n/2$. Denote by $H(\Omega)$ some finite elēment subspace of $W_2^m(\Omega)$, and

$$H(\Omega) = \text{span}\,(\varphi_1, \varphi_2, \ldots, \varphi_N) \tag{13}$$

of the basic linear independent functions $\varphi_1, \varphi_2, \ldots, \varphi_N$. Let ω_h be the set of scattered points in Ω; and $\omega_h = \omega_h^{(1)} \cup \omega_h^{(2)}$, $\omega_h^{(1)} \neq \emptyset$, $\omega_h^{(2)} \neq \emptyset$, $\omega_h^{(1)} \cap \omega_h^{(2)} = \emptyset$. We denote

$$A_1 u = u\big|_{\omega_h^{(1)}}, \quad A_2 u = u\big|_{\omega_h^{(2)}} \tag{14}$$

the trace operators from $H(\Omega)$ to the sets $\omega_h^{(1)}$ and $\omega_h^{(2)}$ correspondingly, which act to Euclidian spaces of vectors of suitable dimensions. Let $\alpha \in R^1$. We formulate the problem for D^m-spline with tension by the following way:

$$\sigma_\alpha = \arg \min_{u \in A_1^{-1}(z_1)} \left(\|D^m u\|_{L_2}^2 + \alpha^2 \|u\|_{L_2}^2 \right), \tag{15}$$

where $A_1^{-1}(z_1) = \{u \in H(\Omega) : u\big|_{\omega_h^{(1)}} = z_1\}$, and $D^m u$ is the operator of generalized gradients of the order m, i.e., $D^m u$ is the vector function of components of the form $[m!/\beta!]^{1/2} D^\beta u$ under the condition for multi-index $|\beta| = \sum_{k=1}^{n} \beta_k = m$. In the other words, we have one-parametric family $T_\alpha : H(\Omega) \to Y(\Omega)$ of the energy composite operators which act to the Hilbert space $Y(\Omega) = L_2(\Omega) \times \prod_{|\beta|=m} L_2(\Omega)$ by the formula

$$T_\alpha u = [\alpha u, D^m u]. \tag{16}$$

It is clear, the 1-st and 2-nd derivatives of T_α with respect to scalar α are:

$$T'_\alpha = [E, \theta_2], \quad T''_\alpha = [\theta_1, \theta_2], \tag{17}$$

where E is the embedding operator from $W_2^m(\Omega)$ to $L_2(\Omega)$ and $\theta_{1,2}$ are zero operators. We suppose the problem (15) be uniqualy solvable. Because of

$$\sigma_\alpha = \sum_{k=1}^{N} C_k(\alpha) \varphi_k, \tag{18}$$

equations (10′), (11′), (12′) are equivalent to the following linear algebraic systems:

$$\sum_{k=1}^{N}(\alpha a_{ki}+b_{ki})C_k(\alpha)+\sum_{P\in\omega_h^{(1)}}\varphi_i(P)\lambda_P(\alpha)=0,\quad i=\overline{1,N},$$

$$\sum_{k=1}^{N}\varphi_k(P)C_k(\alpha)=z_1(P),\quad P\in\omega_h^{(1)}; \tag{10''}$$

$$\sum_{k=1}^{N}(\alpha a_{ki}+b_{ki})C_k'(\alpha)+\sum_{P\in\omega_h^{(1)}}\varphi_i(P)\lambda_P'(\alpha)=-\sum_{k=1}^{N}a_{ki}C_k(\alpha),\quad i=\overline{1,N},$$

$$\sum_{k=1}^{N}\varphi_k(P)C_k'(\alpha)=0,\quad P\in\omega_h^{(1)}; \tag{11''}$$

$$\sum_{k=1}^{N}(\alpha a_{ki}+b_{ki})C_k''(\alpha)+\sum_{P\in\omega_h^{(1)}}\varphi_i(P)\lambda_P''(\alpha)=-2\sum_{k=1}^{N}a_{ki}C_k'(\alpha),\quad i=\overline{1,N},$$

$$\sum_{k=1}^{N}\varphi_k(P)C_k''(\alpha)=0,\quad P\in\omega_h^{(1)}. \tag{12''}$$

Here $z_1(P)$ are given values at mesh $\omega_h^{(1)}$, and

$$a_{ki}=\int_\Omega \varphi_k\varphi_i\,d\Omega,\qquad b_{ki}=\sum_{|\beta|=m}\frac{m!}{\alpha!}\int_\Omega D^\beta\varphi_k D^\beta\varphi_i\,d\Omega.$$

Finally, after the solving of this system we can find σ_α, σ'_α, σ''_α. For the optimization problem

$$\alpha=\arg\min\sum_{P\in\omega_h^{(2)}}\left[\sigma_\alpha(P)-z_2(P)\right]^2 \tag{19}$$

we have Newton's iterative formula to improve the initial value $\alpha^{(0)}$:

$$\alpha^{(k+1)}=\alpha^{(k)}-\frac{\sum_{P\in\omega_h^{(2)}}\sigma'_{\alpha^{(k)}}(P)\cdot\left[\sigma_{\alpha^{(k)}}(P)-z_2(P)\right]}{\sum_{P\in\omega_h^{(2)}}\left[\sigma''_{\alpha^{(k)}}(P)\cdot\left[\sigma_{\alpha^{(k)}}(P)-z_2(P)\right]+\left[\sigma'_{\alpha^{(k)}}(P)\right]^2\right]}. \tag{20}$$

References

[1] A.Yu. Bezhaev, V.A. Vasilenko, *Variational Spline Theory*, NCC Bulletin, series Num. Anal., special issue 3(1993). XII+258p. NCC Publisher, Novosibirsk.