Bull. Nov. Comp. Center, Num. Anal., 7 (1996), 79–86

On optimal choice of spline-smoothing parameter

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In this paper we consider an abstract spline smoothing problem in Hilbert space and express Newton's iteration formula for an optimal choice of the smoothing parameter α in terms of the residual operator $R_\alpha z = z - A\sigma_\alpha$.

We also obtain expansions of $A\sigma_\alpha$ and $z - A\sigma_{1/\beta}$ by series based on the operators R_α and $Q_\beta = I - R_{1/\beta}$ respectively, and derive the estimates $\|\sigma_\alpha - \sigma_0\| = O(\alpha)$ and $\|\sigma_\alpha - \sigma_\infty\| = O(\alpha^{-1})$ as an easy consequences of these expansions.

1. Introduction

We use the following notations. Throughout the paper X, Y, Z are some Hilbert spaces. The norm and the scalar product in X will be denoted by $\|\cdot\|_X$ and $(\cdot,\cdot)_X$ respectively, with omitting the subscript in the case where no ambiguity arises. The null element of the space X will be denoted by the symbol 0. $L(X,Y)$ will stand for the Banach space of linear bounded operators acting from X into Y. The notations $N(A)$ and $R(A)$ will denote the kernel and the image of an operator $A \in L(X,Y)$.

Let operators $T \in L(X,Y)$ and $A \in L(X,Z)$ form a *spline-pair*, i.e.,

(a) $R(T)$ and $R(A)$ are closed in Y and Z respectively;

(b) $N(T) + N(A)$ is closed in X;

(c) $N(T) \cap N(A) = \{0\}$.

It is well-known [1–3] that the spline-pair (T, A) defines an equivalent norm

$$\|x\|_* = \left(\|Tx\|^2 + \|Ax\|^2\right)^{1/2} \tag{1}$$

in X, and a unique solvability of a spline smoothing problem

$$\sigma_\alpha = \arg\min_{x \in X} \alpha\|Tx\|^2 + \|Ax - z\|^2 \tag{2}$$

takes place at any $z \in Z$, $\alpha > 0$.

A *residual criterion*

$$\varphi(\alpha) \overset{df}{=} \|A\sigma_\alpha - z\| = \varepsilon \tag{3}$$

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

is usually used to choose the smoothing parameter α. Here $\varepsilon > 0$ is a residual level required.

The function $\varphi(\alpha)$ monotonically increases [2] from $\varepsilon_{\min} = \varphi(0) = \min_{x\in X} \|Ax - z\|$ up to $\varepsilon_{\max} = \varphi(\infty) \min_{x\in N(T)} \|Ax - z\|$.

We will assume that $\varepsilon_{\min} \neq \varepsilon_{\max}$. In this case the function $\varphi(\alpha)$ is strictly monotone, and problem (3) has a unique solution for any $\varepsilon \in [\varepsilon_{\min}, \varepsilon_{\max}]$. Usually, the equivalent problem

$$\psi(\beta) \stackrel{df}{=} \varphi^{-1}(1/\beta) = \varepsilon^{-1} \tag{4}$$

is proposed instead of (3), and the Newton method

$$\beta_{k+1} = \beta_k - \frac{\psi(\beta_k) - \varepsilon^{-1}}{\psi'(\beta_k)} \tag{5}$$

is applied for the optimal choice of the smoothing parameter. ($\psi(\beta)$ is strictly monotonically increasing upper convex function [2].)

2. Step of Newton's iteration

Let us denote $\alpha = 1/\beta$. Then

$$\psi'(\beta) = [\varphi^{-1}(1/\beta)]' = \frac{\varphi'(1/\beta)}{\beta^2\varphi^2(1/\beta)} = \frac{\alpha^2\varphi'(\alpha)}{\varphi^2(\alpha)}. \tag{6}$$

Using the notation $r_\alpha = z - A\sigma_\alpha$, we obtain

$$\varphi'(\alpha) = [(r_\alpha, r_\alpha)^{1/2}]' = \varphi^{-1}(\alpha) \cdot (r_\alpha, r'_\alpha).$$

Introduce the *residual operator* $R_\alpha : Z \to Z$ by the rule $R_\alpha z = z - A\sigma_\alpha$. Then

$$\varphi'(\alpha) = \varphi^{-1}(\alpha) \cdot (R_\alpha z, R'_\alpha z). \tag{7}$$

To obtain R'_α, we use the representation of the spline σ_α via the operator's equation [4]

$$(\alpha T^*T + A^*A)\sigma_\alpha = A^*z. \tag{8}$$

We have

$$R_\alpha = I - A(\alpha T^*T + A^*A)^{-1}A^* \tag{9}$$

and

$$A\sigma_\alpha = (I - R_\alpha)z. \tag{10}$$

To find $r'_\alpha = -A\sigma'_\alpha$, let us diffirentiate (8) by α:

$$(\alpha T^*T + A^*A)\sigma'_\alpha = -T^*T\sigma_\alpha = -\frac{1}{\alpha}(\alpha T^*T + A^*A - A^*A)\sigma_\alpha$$
$$= -\frac{1}{\alpha}(A^*z - A^*A\sigma_\alpha) = -\frac{1}{\alpha}A^*r_\alpha.$$

Therefore,

$$\sigma'_\alpha = -\frac{1}{\alpha}(\alpha T^*T + A^*A)^{-1}A^*r_\alpha.$$

Multiplying this equality to A and using (9), we obtain

$$A\sigma'_\alpha = -\frac{1}{\alpha}A(\alpha T^*T + A^*A)^{-1}A^*r_\alpha = \frac{1}{\alpha}(I - R_\alpha)r_\alpha.$$

Hence,

$$R'_\alpha = \frac{1}{\alpha}(I - R_\alpha)R_\alpha. \tag{11}$$

Substituting this formula to (7), we derive

$$\varphi'(\alpha) = \frac{\varphi(\alpha)}{\alpha}\cdot\frac{(R_\alpha z, (I - R_\alpha)R_\alpha z)}{\varphi^2(\alpha)}$$
$$= \frac{\varphi(\alpha)}{\alpha}\cdot\frac{(R_\alpha z, R_\alpha z) - (R_\alpha z, R_\alpha^2 z)}{(R_\alpha z, R_\alpha z)}$$
$$= \frac{\varphi(\alpha)}{\alpha}(1 - \omega(\alpha)), \tag{12}$$

where

$$\omega(\alpha) = \frac{(R_\alpha z, R_\alpha^2 z)}{(R_\alpha z, R_\alpha z)}. \tag{13}$$

Applying (12) into (6), we have

$$\psi'(\beta) = \frac{\alpha^2\varphi'(\alpha)}{\varphi^2(\alpha)} = \frac{\alpha}{\varphi(\alpha)}(1 - \omega(\alpha)). \tag{14}$$

Finally, Newton's iteration formula (5) looks as follows:

$$\alpha_{k+1} = \alpha_k\frac{1 - \omega(\alpha_k)}{\varphi(\alpha_k)/\varepsilon - \omega(\alpha_k)}. \tag{15}$$

Remark 1. Since σ_α is a solution to problem (2), it is easy to obtain that $\|R_\alpha\| \le 1$.

Remark 2. Applying the conditions $\psi'(\beta) > 0$ and $\psi''(\beta) \le 0$, one can find the following inequalities

$$\varphi(\alpha)/\varepsilon_{\max} \le \omega(\alpha) < 1. \tag{16}$$

Remark 3. Let us denote $\bar{r}_\alpha = r_\alpha/\|r_\alpha\|$. Then $\omega(\alpha) = (\bar{r}_\alpha, R_\alpha\bar{r}_\alpha)$.

3. How to start iterations?

The Newton iterations (5) converge if the inequality $\psi(\beta_0) \leq \varepsilon^{-1}$ is valid. It is the best choice to start iterations from $\beta_0 = 0$, but a calculation of $\psi'(0)$ is not easy, because it requires the solving of a special linear system [2]. At the same time the calculation of $\psi(0)$ is a simple least squares problem

$$\varepsilon_{\max}^2 = \psi^{-2}(0) = \min_{x \in N(T)} \|Ax - z\|^2.$$

To avoid difficulties arising when $\psi'(0)$ is computed, we suggest the following method:

0. Let us start iterations from an arbitrary $\beta_0 = \alpha_0^{-1} > 0$.
1. If $\varphi(\alpha_k) \geq \varepsilon$, the Newton iteration (15) is applied. In this case all consequent iterations will be also Newton's, and the sequence α_k will be monotonically decreasing.
2. If $\varphi(\alpha_k) < \varepsilon$, we construct a ratio function $\eta(\beta) = (a + b\beta)/(1 + c\beta)$ to satisfy the following conditions

$$\eta(0) = \psi(0) = \varepsilon_{\max}^{-1}, \quad \eta(\beta_k) = \psi(\beta_k), \quad \eta'(\beta_k) = \psi'(\beta_k),$$

and give β_{k+1} as a solution to the equation $\eta(\beta) = \varepsilon^{-1}$. (It is easy to prove that the solution is unique.)

The iteration formula for the ratio's approximation is the following:

$$\alpha_{k+1} = \alpha_k \frac{(1 - \varphi(\alpha_k)/\varepsilon_{\max}) - (1 - \varphi(\alpha_k)/\varepsilon) \cdot \delta(\alpha_k)}{\varphi(\alpha_k)/\varepsilon - \varphi(\alpha_k)/\varepsilon_{\max}}, \tag{17}$$

where

$$\delta(\alpha) = \frac{\varphi(\alpha)/\varepsilon_{\max} - \omega(\alpha)}{1 - \omega(\alpha)}.$$

4. Taylor expansions of $A\sigma_\alpha$ and $z - A\sigma_{1/\beta}$

It is easy to obtain from (11) the following differential rule

$$D^k R_\alpha = (-1)^{k+1} \frac{k!}{\alpha^k} R_\alpha^k (I - R_\alpha), \quad k \geq 1.$$

Using this formula, we derive a formal Taylor expansion of the operator R_α at the neighbourhood of a point $\alpha_0 > 0$:

$$R_\alpha = R_{\alpha_0} + \sum_{k=1}^{\infty} \frac{(\alpha - \alpha_0)^k}{k!} D^k R_{\alpha_0} = R_{\alpha_0} - \sum_{k=1}^{\infty} (-1)^k \frac{(\alpha - \alpha_0)^k}{\alpha_0^k} R_{\alpha_0}^k (I - R_{\alpha_0}),$$

and applying (10), we obtain the formal identity

$$A\sigma_\alpha = (I - R_\alpha)z = \Big(I - R_{\alpha_0} + \sum_{k=1}^{\infty}(-1)^k \frac{(\alpha-\alpha_0)^k}{\alpha_0^k} R_{\alpha_0}^k (I - R_{\alpha_0})\Big) z$$
$$= \Big[\sum_{k=0}^{\infty} \frac{(\alpha_0-\alpha)^k}{\alpha_0^k} R_{\alpha_0}^k\Big] \cdot (I - R_{\alpha_0})z = \Big[\sum_{k=0}^{\infty} \frac{(\alpha_0-\alpha)^k}{\alpha_0^k} R_{\alpha_0}^k\Big] A\sigma_{\alpha_0}. \quad (18)$$

Since $\|R_\alpha\| \leq 1$, the series

$$\sum_{k=0}^{\infty} \frac{(\alpha_0-\alpha)^k}{\alpha_0^k} R_{\alpha_0}^k$$

is absolutely convergent when $|\alpha - \alpha_0| < \alpha_0$. An interval of it's convergence could be enlarged due to the fact, that this series acts at the vector $A\sigma_\alpha$ belonging to $R(A)$.

Denote the restriction of the operator R_α at the subspace $R(A)$ by $\tilde{R}_\alpha$.

Theorem 1. $\|\tilde{R}_\alpha\| = \rho_\alpha < 1$ *for any* $\alpha \in (0, \infty)$, *and* $\rho_\alpha = O(\alpha)$ *as* $\alpha \to 0$.

As it was remarked in Section 1, the scalar product

$$(x_1, x_2)_* \stackrel{df}{=} (Tx_1, Tx_2)_Y + (Ax_1, Ax_2)_Z$$

induces an equivalent norm in X. Therefore, we can regard below the operators A^* and T^* be adjoined to A and T with respect to the scalar product $(\cdot,\cdot)_*$. Note that the operators A^*A and T^*T become commutative (due to the identity $A^*A + T^*T = I$).

Proof. Since $R(A)$ is closed, the operator A^* has a closed image $R(A^*)$ coinciding with $N(A)_*^\perp$ (the orthogonal complement to $N(A)$ with respect to $(\cdot,\cdot)_*$). Denote by $\tilde{B}_\alpha$ the restriction of the operator $\alpha T^*T + A^*A$ at $N(A)_*^\perp$. To prove the theorem we will use the following facts: the operator $\tilde{B}_\alpha$ carries out one-to-one correspondence of $N(A)_*^\perp$ onto itself; the operators $\tilde{B}_\alpha$ and A^*A are commutative.

Since the operator $\tilde{R}_\alpha$ is self-adjoined, its norm coincides with the spectral radius $\rho(\tilde{R}_\alpha) = \sup \lambda(\tilde{R}_\alpha)$. We will estimate it with the help of a scalar product $(A^*z_1, A^*z_2)_*$, which induces an equivalent norm in $R(A)$. We have

$$\inf \lambda(I - \tilde{R}_\alpha) = \inf_{z\in R(A)} \frac{(A^*(I - R_\alpha)z, A^*z)_*}{(A^*z, A^*z)_*} = \inf_{z\in R(A)} \frac{(A^*A\tilde{B}_\alpha^{-1}A^*z, A^*z)_*}{(A^*z, A^*z)_*}$$
$$= \inf_{x\in N(A)_*^\perp} \frac{(A^*A\tilde{B}_\alpha^{-1}x, x)_*}{(x,x)_*} = \inf_{x\in N(A)_*^\perp} \frac{(A^*A\tilde{B}_\alpha^{-1/2}x, \tilde{B}_\alpha^{-1/2}x)_*}{(x,x)_*}$$
$$= \inf_{x\in N(A)_*^\perp} \frac{(A^*Ax, x)_*}{(\tilde{B}_\alpha x, x)_*} = \inf_{x\in N(A)_*^\perp} \frac{\|Ax\|^2}{\alpha\|Tx\|^2 + \|Ax\|^2}. \quad (19)$$

Taking into account an equivalence of norms $(\alpha\|Tx\|^2+\|Ax\|^2)^{1/2}$ and $\|Ax\|$ on $N(A)_*^\perp$, we conclude that a real number $c_\alpha < \infty$ exists, such that

$$\alpha\|Tx\|^2 + \|Ax\|^2 \le c_\alpha\|Ax\|^2 \qquad \forall x \in N(A)_*^\perp.$$

Let this estimate be exact. Then, substituting it into (19), we obtain

$$\inf \lambda(I - \tilde{R}_\alpha) = c_\alpha^{-1} > 0.$$

Hence

$$\|\tilde{R}_\alpha\| = \sup \lambda(\tilde{R}_\alpha) = 1 - \inf \lambda(I - \tilde{R}_\alpha) = 1 - c_\alpha^{-1} \stackrel{df}{=} \rho_\alpha < 1. \tag{20}$$

Finally, to prove the estimate $\rho_\alpha = O(\alpha)$, let us substitute (19) into (20):

$$\|\tilde{R}_\alpha\| = \sup_{x\in N(A)_*^\perp} \frac{\alpha\|Tx\|^2}{\alpha\|Tx\|^2 + \|Ax\|^2} \le \alpha \cdot \sup_{x\in N(A)_*^\perp} \frac{\|Tx\|^2}{\|Ax\|^2}.$$

The expression $\|Tx\|^2/\|Ax\|^2$ is bounded on $N(A)_*^\perp$ due to the boundedness of the operator T and an equivalence of the norm $\|Ax\|$ to the original one on the subspace $N(A)_*^\perp$. □

Corollary 1. *Let $\alpha_0 > 0$. Then*

$$A\sigma_\alpha = \Big[\sum_{k=0}^{\infty}\Big(\frac{\alpha_0 - \alpha}{\alpha_0}\Big)^k R_{\alpha_0}^k\Big] A\sigma_{\alpha_0} \tag{21}$$

for any $\alpha \in [0, 2\alpha_0]$, and the series in (21) is absolutely convergent.

Corollary 2. *The smoothing spline σ_α converges to the pseudo-interpolating spline σ_0 (the limiting smoothing spline at $\alpha = 0$) with a linear rate, i.e., $\|\sigma_\alpha - \sigma_0\|_X = O(\alpha)$.*

Consider now a behaviour of the spline σ_α near $\alpha = \infty$. Denote

$$\Sigma_\beta = \sigma_{1/\beta}, \qquad Q_\beta = I - R_{1/\beta}.$$

It is easy to verify that

$$D^k Q_\beta = (-1)^{k+1}\frac{k!}{\beta^k} Q_\beta^k (I - Q_\beta), \quad k \ge 1.$$

Hence

$$\begin{aligned} z - A\Sigma_\beta &= z - Q_\beta z = z - Q_{\beta_0} z - \sum_{k=1}^{\infty} \frac{(\beta-\beta_0)^k}{k!} D^k Q_{\beta_0} z \\ &= (I - Q_{\beta_0})z + \sum_{k=1}^{\infty} (-1)^k \frac{(\beta-\beta_0)^k}{\beta_0^k} Q_{\beta_0}^k (I - Q_{\beta_0}) z \\ &= \left[\sum_{k=0}^{\infty} \left(\frac{\beta_0 - \beta}{\beta_0}\right)^k Q_{\beta_0}^k\right] (z - A\Sigma_{\beta_0}). \end{aligned} \tag{22}$$

It is clear that the series in (22) is absolutely convergent when $|\beta - \beta_0| < \beta_0$. The convergence interval could be enlarged if we will take into account the special structure of the vector $z - A\Sigma_{\beta_0}$.

Let us express the vector z in the form $z_* + z_{**}$, where $z_* \in R(A)$, $z_{**} \in R(A)^\perp$. It is known [2] that the pseudo-interpolating spline $\sigma_0 \equiv \Sigma_\infty$ satisfies an interpolating condition $A\Sigma_\infty = z_*$. Therefore,

$$z - A\Sigma_{\beta_0} = z_{**} + A(\Sigma_\infty - \Sigma_{\beta_0}),$$

and only the component $A(\Sigma_\infty - \Sigma_{\beta_0})$ influence on the convergence of the series in (22) (z_{**} is annihilated by the operator Q_{β_0}). One can obtain from (8) that the vector $\Sigma_\infty - \Sigma_{\beta_0}$ is orthogonal to the subspace $\mathcal{N} \overset{df}{=} N(T) + N(A)$ with respect to $(\cdot,\cdot)_*$, i.e., it belongs to $\mathcal{N}_*^\perp$.

Denote the restriction of the operator Q_β at the subspace $A\mathcal{N}_*^\perp$ by $\tilde{Q}_\beta$, and introduce an operator $\tilde{C}_\beta$ as the restriction of the operator $T^*T + \beta A^*A$ at $\mathcal{N}_*^\perp$. We have

$$\tilde{Q}_\beta = A(\beta^{-1}T^*T + A^*A)^{-1}A^* = \beta A\tilde{C}_\beta^{-1}A^*.$$

It is clear that the operator $\tilde{C}_\beta$ carries out one-to-one correspondence of $\mathcal{N}_*^\perp$ onto itself, and $A^*A\mathcal{N}_*^\perp = \mathcal{N}_*^\perp$. Using these facts and applying the scalar product $(A^*z_1, A^*z_2)_*$, we obtain

$$\begin{aligned} \|\tilde{Q}_\beta\| &= \sup_{z \in A\mathcal{N}_*^\perp} \beta \frac{(A^*A\tilde{C}_\beta^{-1}A^*z, A^*z)_*}{(A^*z, A^*z)_*} = \sup_{x \in \mathcal{N}_*^\perp} \beta \frac{(A^*A\tilde{C}_\beta^{-1}x, x)_*}{(x,x)_*} \\ &= \sup_{x \in \mathcal{N}_*^\perp} \frac{\beta\|Ax\|_Z^2}{\|Tx\|_Y^2 + \beta\|Ax\|_Z^2} = 1 - \inf_{x \in \mathcal{N}_*^\perp} \frac{\|Tx\|_Y^2}{\|Tx\|_Y^2 + \beta\|Ax\|_Z^2}. \end{aligned} \tag{23}$$

Taking into account an equivalence of norms $\|Tx\|$ and $\|Ax\|$ on the subspace $\mathcal{N}_*^\perp$, we obtain from (23) the following

Theorem 2. $\|\tilde{Q}_\beta\| = q_\beta < 1$ *for any* $\beta \in (0, \infty)$, *and* $q_\beta = O(\beta)$ *as* $\beta \to 0$.

Corollary 1. *Let $\beta_0 > 0$. Then*

$$z - A\Sigma_\beta = \left[\sum_{k=0}^{\infty}\left(\frac{\beta_0 - \beta}{\beta_0}\right)^k Q_{\beta_0}^k\right](z - A\Sigma_{\beta_0}) \tag{24}$$

for any $\beta \in [0, 2\beta_0]$, and the series in (24) is absolutely convergent.

Corollary 2. *The smoothing spline σ_α converges to σ_∞ with a rate $1/\alpha$, i.e., $\|\sigma_\alpha - \sigma_\infty\|_X = O(\alpha^{-1})$.*

Using expansions (21) and (24) we can construct an algorithm of the optimal choice of a smoothing parameter α_{opt} based on "freezing" ideas: give any α_0 and calculate $\varphi(\alpha_0)$; if $\varphi(\alpha_0) > \varepsilon$, then α_{opt} may be found from the equation (21) with required precision; otherwise α_{opt}^{-1} may be found from (24).

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