Comm. Korean Math. Soc. **12** (1997), No. 1, pp. 165–176

ON THE REGULARIZATION WITH NONLINEAR SPLINES*

S. K. CHUNG AND S. M. JOE

ABSTRACT. In order to overcome computational ill-posedness which arises when we solve the least square problems, nonlinear smoothing splines are used. The existence and the convergence on nonlinear smoothing spline are shown with numerical experiments.

1. Introduction

The problem of least squares arises in a broad class of scientific areas such as signal processing, automatic control, statistics, economics, biology, etc. It is a problem to find a curve $f(x) \in X$ which is the solution of

$$\min_{f \in X} \sum_{i=1}^{n} \{y_i - f(x_i)\}^2, \tag{1.1}$$

where the data $(x_i, y_i), a = x_1 < x_2 < \cdots < x_n = b$, are given and X is an appropriate set of functions.

Of course, (1.1) is minimized if we take $f(x)$ as an interpolating function of (x_i, y_i). But in many practical problems the obtained data y_i consist of errors;

$$y_i = f(x_i) + \epsilon_i, \quad 1 \le i \le n, \tag{1.2}$$

where ϵ_i are white noisy, that is, ϵ_i are uncorelated with zero means.

Received August 16, 1996. Revised December 5, 1996.
1991 AMS Subject Classification: 65D10.
Key words and phrases: least square problems, regularization, nonlinear splines.
*This work is supported by KOSEF under grant No. KOSEF 941–0100–030–2.

Because of errors in data, it is not meaningful to seek an interpolating functional. Hence we would better not to try to obtain an interpolating functional when we solve the problem of least squares. But the problem of least squares turns out to be computationally ill-posed in many cases. In order to avoid this ill-posedness Tikhonov[13] first introduced a regularization method which is to find the solution of

$$\min_{f\in X}[\sum_{i=1}^{n}\{y_i - f(x_i)\}^2 + \lambda\Omega(f)], \tag{1.3}$$

where $\Omega(\cdot)$ is a nonnegative smoothing functional and λ is a regularization parameter instead of solving (1.1) directly.

Among various ways to choose $\Omega(f)$, one of the most popular smoothing functionals is

$$\Omega(f) = \int \{f''(x)\}^2 dx. \tag{1.4}$$

The solution of minimization problem (1.4) is well known as the cubic spline. The problem (1.3) with (1.4) has been studied by Schoenberg[11]. In [11], the author showed that the solution of (1.3) converges to the linear solution of least squares problem of (1.1) as $\lambda \to \infty$ and to the cubic spline interpolating $(x_i, f(x_i))$ as $\lambda \to 0$. The existence of solution for (1.3) and (1.4) has been studied by Lukas[7]. The method of finding optimal regularization parameter by cross validations is discussed by Wahba[15]. For more theoretical background on (1.3), see Locker and Prenter[6], Lukas[7], Morozov[9], Neubauer[10], and Tikhonov and Arsenin[14].

Since the interpolating cubic spline is not invariant under the rigid motion, we may take a functional $\Omega(f)$ as

$$\Omega(f) = \int \{\kappa(f; s)\}^2 ds, \tag{1.5}$$

where $\kappa(f; s)$ is the curvature of $f(x)$. The functional $\Omega(f)$ in (1.5) is known to be invariant under the rigid motion. The solution of minimizing (1.5) interpolating $(x_i, f(x_i))$ is called a nonlinear spline. Note that

(1.4) is a linearization of (1.5). The existence and convergence of nonlinear spline interpolation has been considered by Jerome[3]–[4]. Numerical solutions of nonlinear cubic splines can be seen in Lee and Forsythe[5], Malcolm[8] and Horn[1]. And the methods of finding invariant solutions for (1.1) under the rigid motion can be found in Van Huffel and Vandewalle [2].

In this paper we will consider the nonlinear spline smoothing problem

$$\text{(1.6)} \qquad \min J(f) := \min_{f\in X}[\sum_{i=1}^{n}\{y_i - f(x_i)\}^2 + \lambda \int \{\kappa(f;s)\}^2 ds].$$

The problem (1.6) may be rewritten as

$$\text{(1.7)} \quad \min J(f) := \min_{f\in X}[\sum_{i=1}^{n}\{y_i - f(x_i)\}^2 + \lambda \int_a^b \frac{(f''(x))^2}{\{1+(f'(x))^2\}^{\frac{5}{2}}} dx].$$

In section 2, the existence and convergence of a nonlinear smoothing spline will be shown. In section 3, numerical solutions of (1.7) will be considered by using finite difference methods.

2. Existence and uniqueness

In this section, we consider the existence of (1.7) in an appropriate function space X. For the existence of nonlinear interpolating splines, we need to take X as

$$X = \{f \in H^2[a,b] : |f'(x)| \le M \text{ for all } x \in [a,b] \text{ and } |f(x_0)| \le C \text{ for } x_0 \in [a,b]\}.$$

Then it is clear that X is convex and closed since derivative evaluations are continuous linear functionals on $H^2[a,b]$.

For the simple notations we introduce a linear operator $A : X \subset H^2 \to \mathbb{R}^n$ defined by

$$\text{(2.1)} \qquad Af = (f(x_1), f(x_2), \ldots, f(x_n)), \quad \forall f \in X.$$

For $y = (y_1, y_2, \ldots, y_n)$ let

$$\|Af - y\|^2 = \sum_{i=1}^{n} \{y_i - f(x_i)\}^2 \tag{2.2}$$

and a differential operator $T : X \subset H^2 \to L_2$ be

$$Tf = \frac{f''}{[1 + (f')^2]^{5/4}}. \tag{2.3}$$

Then the smoothing functional in (1.5) is $\Omega(f) = \|Tf\|^2$. Jerome[3] has shown the following Theorem 2.1 which tells that a nonlinear spline interpolating (x_i, y_i) exists in X.

THEOREM 2.1. *Let U_o be any closed convex subset of $H^2[a,b]$ with the property that for some $x_o \in [a,b], |f(x)| \le C$ for $f \in U_o$ and a constant $C > 0$. Define*

$$U = U_o \cup \{f \in H^2[a,b] : |f''(x)| \le M \text{ for all } x \in [a,b]\}.$$

The minimization problem

$$\min_{f \in U} \|Tf - g\| \tag{2.4}$$

has a solution for each $g \in L_2[a,b]$.

Along the ideas of the proof in [3], we may prove the following lemma.

LEMMA 2.1. *Let the operator A and the functional Ω be defined as in (2.1) and (1.5), respectively. Then the following hold.*

1. *The set $\{f \in X : \Omega(f) < \infty\}$ is nonempty.*
2. *For any sequence $\{f_k\}$ in X converging weakly to f in X with $\{Af_k\}$ bounded in $\mathbb{R}^n$, $\{Af_k\}$ converges weakly to Af.*
3. *For any constant $\alpha > 0$ and any sequence $\{f_k\}$ in H^2 satisfying $\Omega(f) \le \alpha$, there is a subsequence $\{f_{k_r}\}$ which converges weakly to f in X and $\Omega(f) \le \alpha$. Further, $\{Tf_k\}$ converges weakly to Tf.*

PROOF. (1) Since the set X is clearly a closed convex subset of H^2 satisfying (2.5) and $\Omega(f) \leq \int |f''(x)|^2 dx$, $\Omega(f) < \infty$ for each $f \in X$ and the problem (2.4) has a solution f in X by Theorem 2.1. Hence $\{f \in X : \Omega(f) < \infty\}$ is clearly nonempty.

(2) Since $f_k(x) = f_k(x_0) + f_k'(\xi)(x - x_0)$ for some ξ between x and x_0, $|f_k(x)| \leq C + M(b-a)$. Hence any sequence $\{f_k\}$ in X is bounded and actually uniformly bounded on $[a, b]$. We may choose a subsequence $\{f_{k_r}\}$ of $\{f_k\}$ which converges weakly to f in X.

Since the operator A is continuous and $\{f_{k_r}\}$ is bounded, $\{Af_{k_r}\}$ is bounded. Thus $\{Af_{k_r}\}$ converges weakly to Af by the Closed Graph Theorem.

(3) Let $\{f_k\}$ be a sequence from H^2 with $\Omega(f_k) \leq \alpha$ for a positve constant α. Then we may choose a subsequence $\{f_{k_r}\}$ which converges weakly to $f \in H^2$. Since for any $\varphi \in H^2$

$$(f_k, \varphi) + (f_k', \varphi') + (f_k'', \varphi'') \to (f, \varphi) + (f', \varphi') + (f'', \varphi'')$$

and by the Sobolev imbedding theorem $\{f_k\}$ and $\{f_k'\}$ converge uniformly to f and f', respectively,

$$(f_k'', \varphi'') \to (f'', \varphi'').$$

That is, $\{f_k''\}$ converges weakly to $f'' \in L_2$. This implies that $\{Tf_k\}$ converges weakly to Tf and the proof is completed. □

LEMMA 2.2. *Let A and Ω be defined as (2.1) and (1.5), respectively. Then there exists a solution f^* of*

$$\min_{f \in X} \|Af - y\|, \tag{2.5}$$

where f^* is the weak limit of a minimizing sequence $\{f_k\}$ of (2.5) and $y = (g(x_1), g(x_2), \ldots g(x_n))$ for $g \in L_2$.

PROOF. Let $Y_\beta = \{f \in X : \Omega(f) \leq \beta\}$. Then since $Tf \in L_2$ for $f \in X$, Y_β is nonempty.

Let $\{f_k\}$ be a minimizing sequence of (2.5) on Y_β. Then $\{Af_k\}$ is clearly bounded. It follows from Lemma 2.1 that there exists a subsequence $\{f_{k_r}\}$ of $\{f_k\}$ which converges weakly to $f^* \in X$ with $\Omega(f^*) \leq \beta$. This implies that $f^* \in Y_\beta$.

Hence by Lemma 2.1 $\{Af_k\}$ converges weakly to Af^* and

$$\|Af^* - y\|^2 \le \liminf \|Af_k - y\|^2 = \inf_{f \in Y_\beta} \|Af - y\|^2.$$

Therefore, the minimum of (2.5) is attained at $f^* \in Y_\beta$. □

We are now ready to show that the solution of (1.7) exists with the aid of [9].

THEOREM 2.2. *The minimization problem (1.7) has a solution f in X.*

PROOF. Let $\{f_k\}$ be a minimizing sequence of (1.7) in Y_β. Then both $\{Af_k\}$ and $\{\Omega(f_k)\}$ are bounded. Hence we can choose a subsequence $\{f_{k_r}\}$ of $\{f_k\}$ which converges weakly to f and $\{Af_{k_r}\}$ and $\{\Omega(f_{k_r})\}$ converge weakly to Af and $\Omega(f)$, respectively. It follows from Lemma 2.1 and Lemma 2.2 that the minimum of $\{\|Af_k - y\|\}$ and $\{\Omega(f_k)\}$ are obtained at f simultaneously. This completes the proof. □

Let $s(x)$ be the cubic spline interpolating the given data (x_i, y_i) and $q_1(x)$ the least square polynomial of degree one. Schoenberg[11] has shown that the solution $s(x,\lambda)$ of (1.3) with (1.4) has the property

$$\lim_{\lambda \to 0} s(x,\lambda) = s(x), \qquad \lim_{\lambda \to \infty} s(x,\lambda) = q_1(x).$$

As in [11], we can easily show that the following behaviour of nonlinear smoothing solution along the smoothing parameter λ.

THEOREM 2.3. *Let f_λ be the solution of (1.7), $q_1(x)$ the least square polynomial of degree one and $s(x)$ the nonlinear cubic spline interpolating (x_i, y_i). Then*

$$\lim_{\lambda \to 0} f_\lambda(x) = s(x), \qquad \lim_{\lambda \to \infty} f_\lambda(x) = q_1(x).$$

3. Discrete solutions

In this section we consider numerical solutions of (1.7) using finite difference schemes. Let $u_i = f(x_i)$ and take $h = x_{i+1} - x_i$ for the simplicity of calculation. For the discretization of (1.7), the central difference schemes

$$\nabla u_i = \frac{u_{i+1} - u_{i-1}}{2h}, \quad \Delta u_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2},$$

for the approximations of $f'(x_i)$ and $f''(x_i)$, respectively. Then the functional $J(u)$ in (1.7) becomes

$$J_h(u) = \sum_{i=1}^{n}(u_i - y_i)^2 + \lambda h \sum_{i=1}^{n} \frac{(\Delta u_i)^2}{\{1 + (\nabla u_i)^2\}^{5/2}}, \tag{3.1}$$

where $u = (u_1, u_2, \ldots, u_n)$. In order to find the minimum of (3.1) we have to solve a system of nonlinear equations

$$\frac{\partial J_h(u)}{\partial u_i} = 0, \quad i = 1, 2, \ldots, n. \tag{3.2}$$

In order to solve (3.2), we will use the generalized Newton's method;

$$u_i^{(k+1)} = u_i^{(k)} - \omega \frac{\partial J_h(u_1^{(k+1)}, \ldots, u_{i-1}^{(k+1)}, u_i^{(k)}, \ldots, u_n^{(k)})/\partial u_i}{\partial^2 J_h(u_1^{(k+1)}, \ldots, u_{i-1}^{(k+1)}, u_i^{(k)}, \ldots, u_n^{(k)})/\partial^2 u_i}, \tag{3.3}$$

where the components of the gradient $\partial J_h(u)/\partial u$ of $J_h(u)$ are

$$\begin{aligned}\frac{\partial J_h(u)}{\partial u_i} = &- 2(u_i - y_i) + \xi_{i-1}(u_i - 2u_{i-1} + u_{i-2}) \\ &+ \xi_{i+1}(u_{i+2} - 2u_{i+1} + u_i) \\ &+ \eta_{i-1}(u_i - u_{i-2}) - \eta_{i+1}(u_{i+2} - u_i),\end{aligned}$$

and the components of the Hessian $\partial^2 J_h(u)/\partial^2 u$ of $J_h(u)$ are

$$\begin{aligned}\frac{\partial^2 J_h(u)}{\partial^2 u_i} =& 2 + \xi_{i-1} - \frac{5}{2h^2}\xi_{i-1}(u_i - u_{i-2}) + \frac{35}{32h^4}\tau_{i-1} \\ &- \frac{5}{8h^2}\zeta_{i-1}(u_i - 2u_{i-1} + u_{i-2}) + 4\xi_i + \xi_{i+1} \\ &+ \frac{5}{2h^2}\zeta_{i+1}(u_{i+2} - u_i) + \frac{35}{32h^4}\tau_{i+1} \\ &+ \frac{5}{8h^2}\zeta_{i+1}(u_{i+2} - 2u_{i+1} + u_i).\end{aligned}$$

Here

$$\xi_i = \{1 + (u_{i+1} - u_{i-1})^2/(4h^2)\}^{-7/2},$$

$$\eta_i = \frac{5}{8h^2}(u_{i+1} - 2u_i + u_{i-1})^2\{1 + (u_{i+1} - u_{i-1})^2/(4h^2)\}^{-7/2},$$

$$\zeta_i = (u_{i+1} - 2u_i + u_{i-1})\{1 + (u_{i+1} - u_{i-1})^2/(4h^2)\}^{-7/2},$$

and

$$\tau_i = (u_{i+1} - 2u_i + u_{i-1})(u_{i+1} - u_{i-1})^2\{1 + (u_{i+1} - u_{i-1})^2/(4h^2)\}^{-9/2}.$$

NUMERICAL EXAMPLES. We consider the linear smoothing cubic spline

$$\min[\sum_{i=1}^{n}\{u_i - y_i\}^2 + \lambda\int_a^b (u''(x))^2 dx] \tag{3.3}$$

and the nonlinear smoothing cubic spline

$$\min[\sum_{i=1}^{n}\{u_i - y_i\}^2 + \lambda\int_a^b \frac{(u''(x))^2}{\{1 + (u'(x))^2\}^{5/2}} dx], \tag{3.4}$$

interpolating $(x_i, y_i), i = 1, 2, \ldots, n$.

$$y_i = u(x_i) = x_i^2 e^{-5x_i} - 0.5x_i\cos(\pi x_i) + \epsilon_i, \tag{3.5}$$

with

$$\epsilon_i \sim N(0, 0.04), \quad h = \frac{3}{100}, \quad x_i = ih.$$

Figure 1 and Figure 2 show the numerical results for linear and nonlinear cubic spline regularization problems, respectively. In the figures, the dotted line is the graph of $u(x) = x^2e^{-5x} - 0.5xcos(\pi x)$ and the solid lines are graphs of numerical solutions for the regularization problem with regularization parameter $\lambda = 1.0$. In order to solve systems of nonlinear equations we used generalized Newton's method with relaxation parameter $\omega = 0.5$.

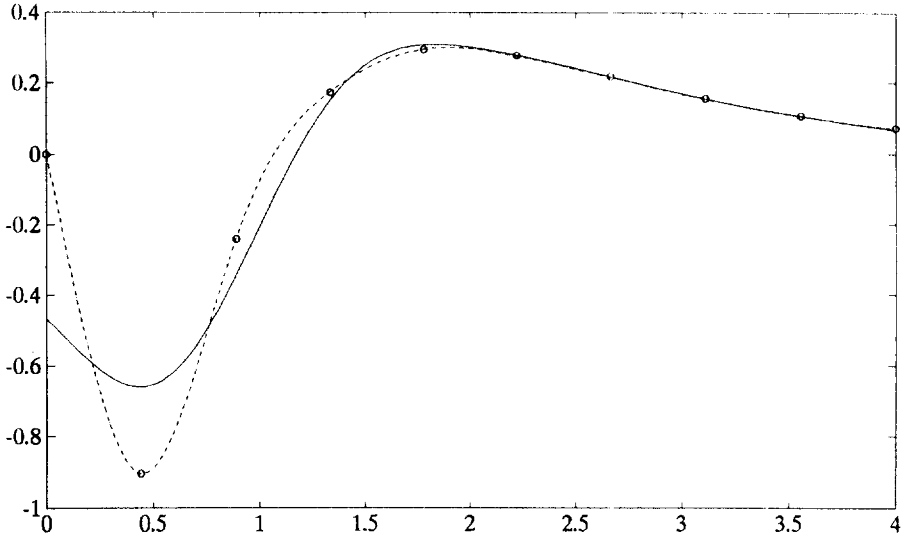

Figure 1 : Linear spline with $\lambda = 1.0$ for (3.5)

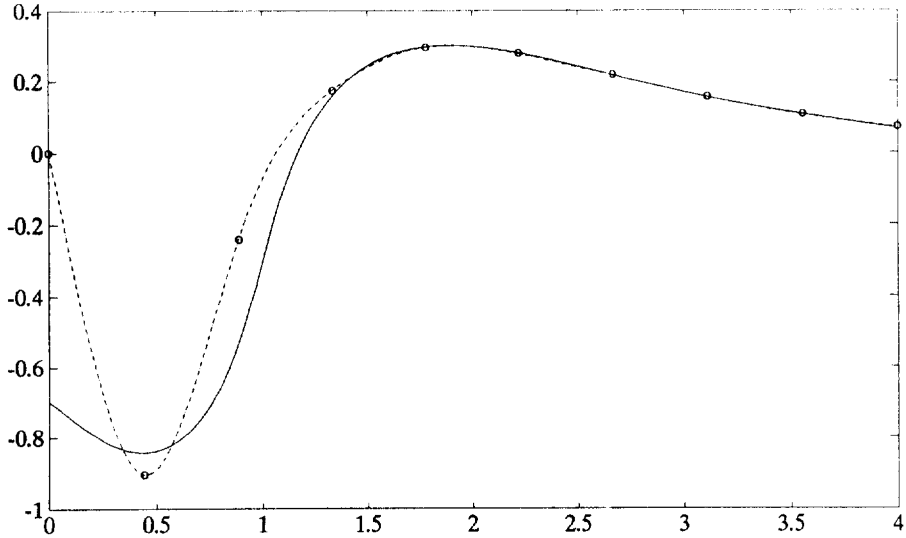

Figure 2 : Nonlinear spline with $\lambda = 1.0$ for (3.5)

$$y_i = u(x_i) = x_i^2 e^{-5x_i} - 0.5 x_i \sin(\pi x_i) + \epsilon_i, \tag{3.6}$$

with

$$\epsilon_i \sim N(0, 0.04), \quad h = \frac{3}{100}, \quad x_i = ih.$$

Figure 3 and Figure 4 show the numerical results for nonlinear cubic spline regularization problems for $u(x) = x^2 e^{-5x} - 0.5x sin(\pi x)$ with $\lambda = 0.06$ and $\lambda = 10.0$, respectively. We may see that nonlinear cubic splines with larger λ is close to a straight line which is a solution of least square problem.

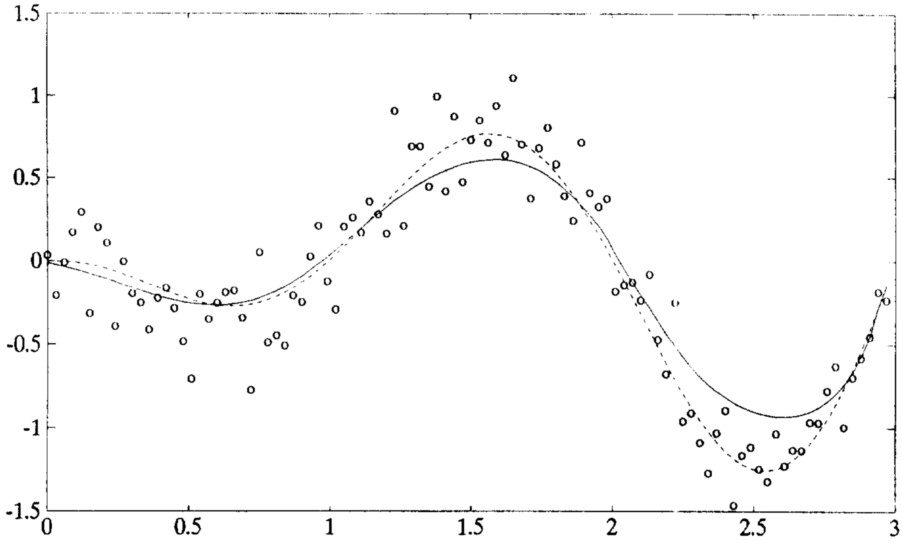

Figure 3 : Nonlinear spline with $\lambda = 0.06$ for (3.6)

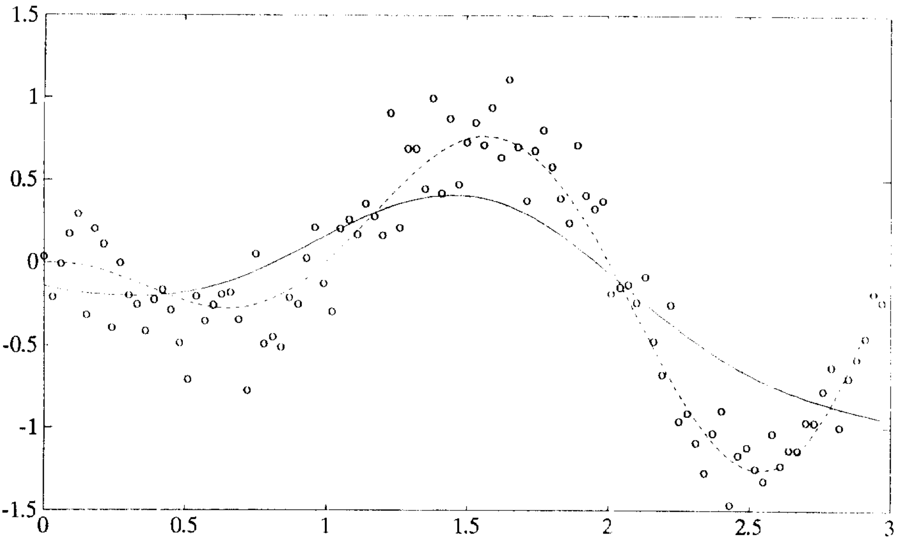

Figure 4 : Nonlinear spline with $\lambda = 10.0$ for (3.6)

References

1. B. K. P. Horn, *The curve of least energy*, ACM Trans. Math. Soft. **9** (1983), 441–460.
2. S. Van Huffel and J. Vandewalle, *The total least squares problem*, SIAM, Philadelphia, 1991.
3. J. W. Jerome, *Minimization problems and linear and nonlinear spline functions, I: Existence*, SIAM J. Numer. Anal. **10** (1973), 808–819.
4. ———, *Minimization problems and linear and nonlinear spline functions, II: Convergence*, SIAM J. Numer. Anal. **10** (1973), 820–830.
5. E. H. Lee and G. E. Forsythe, *Variational study of nonlinear spline curves*, SIAM Review **15** (1973), 120–133.
6. J. Locker and P. M. Prenter, *Regularization with differential operators I. General Theory*, J. of Math. Anal. and Appl. **74** (1980), 504–529.
7. M. A. Lukas, *Regularization*, The application and numerical solution of integral equations, ed. by R. S. Anderssen, F. R. de Hoog and M. A. Lukas, Sijthoff and Noordhoff, Alphen aan den Rijin, 1980.
8. M. A. Malcolm, *On the computation of nonlinear spline functions*, SIAM J. Numer. Anal. **14** (1977), 254–282.
9. V. A. Morozov, *Methods for solving incorrectly posed problems*, translated by Z. Nashed, Springer-Verlag, New York, 1984.
10. A. Neubauer, *Tikonov regularization of nonlinear ill-posed problems in Hilbert scales*, Applicable Analysis **46** (1992), 59–72.

11. I. J. Schoenberg, *Spline functions and the problem of graduation*, Proc. Nat. Acad. Sci. **52** (1964), 451–454.
12. T. I. Seidman and C. R. Vogel, *Well-posedness and convergence of some regularization methods for nonlinear ill-posed problems*, CMA-R48-86, CMA, Australian National University, Canberra, Australia.
13. A. N. Tikhonov, *Solution of incorrectly formulated problems and the regularzation method*, Soviet Math. Dolk. **4** (1963), 1035–1037.
14. A. N. Tikhonov and A. Y. Arsenin, *Solutions of ill-posed problems*, translated by F. John, V. H. Winston & Sons, Washington, D.C., 1977.
15. G. Wahba, *Spline models for observational data*, CBMS-NSF Regional Conference Series in Applied Mathematics 59, SIAM, 1990.

S. K. Chung
Department of Mathematics Education
Seoul National University
Seoul 151-742, Korea

S. M. Joe
Department of Computer Science
Shingu Technical College
Seongnam 462-743, Korea