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Tikhonov Regularizationを用いた方程式の近似解法への再生核理論の応用

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Abstract

We shall show fundamental applications of the theory of reproducing kernels to the Tikhonov regularization that is powerful in best approximation problems in numerical analysis.

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1 Introduction

In the 2001 ISAAC Berlin Congress, the author [4] gave a plenary lecture in which the author showed that the theory of reproducing kernels is fundamental, beautiful and applicable widely in analysis. After then, the author found fundamental applications of the theory to the Tikhonov regularization that is powerful in best approximation problems in numerical analysis. In this survey article, we shall present their essences, simply.

At first, we recall a fundamental theorem for the best approximation by the functions in a reproducing kernel Hilbert space (RKHS) based on [1,3].

Let E be an arbitrary set, and let H_K be a RKHS admitting the reproducing kernel $K(p,q)$ on E. For any Hilbert space $\mathcal{H}$ we first consider a bounded linear operator L from H_K into $\mathcal{H}$. Then, we shall consider the best approximate problem

$$\inf_{f\in H_K} \|Lf - \mathbf{d}\|_{\mathcal{H}} \tag{1.1}$$

for a member $\mathbf{d}$ of $\mathcal{H}$. Then, we have

Proposition 1.1 *For a member* $\mathbf{d}$ *of* $\mathcal{H}$, *there exists a function* $\tilde{f}$ *in* H_K *such that*

$$\inf_{f\in H_K} \|Lf - \mathbf{d}\|_{\mathcal{H}} = \|L\tilde{f} - \mathbf{d}\|_{\mathcal{H}} \tag{1.2}$$

if and only if, for the RKHS H_k *defined by*

$$k(p,q) = (L^*LK(\cdot,q), L^*LK(\cdot,p))_{H_K}, \tag{1.3}$$

$$L^*\mathbf{d} \in H_k. \tag{1.4}$$

Furthermore, if the existence of the best approximation $\tilde{f}$ *satisfying (1.2) is ensured, then there exists a unique extremal function* f^* *with the minimum norm in* H_K, *and the function* f^* *is expressible in the form*

$$f_{\mathbf{d}}^*(p) = (L^*\mathbf{d}, L^*LK(\cdot,p))_{H_k} \quad on \quad E. \tag{1.5}$$

In Proposition 1.1, note that

$$(L^*\mathbf{d})(p) = (L^*\mathbf{d}, K(\cdot,p))_{H_K} = (\mathbf{d}, LK(\cdot,p))_{\mathcal{H}}; \tag{1.6}$$

that is, $L^*\mathbf{d}$ is expressible in terms of the known $\mathbf{d}, L, K(p,q)$ and $\mathcal{H}$. In Proposition 1.1, even when $L^*\mathbf{d}$ does not belong to H_k, the function

$$f_{\mathbf{d}}^{**}(p) = (\mathbf{d}, LL^*LK(\cdot,p))_{\mathcal{H}} \tag{1.7}$$

is still well defined and the function is the extremal function in the best approximate problem

$$\inf_{f\in H_K} \|L^*Lf - L^*\mathbf{d}\|_{H_K}, \tag{1.8}$$

as we see from Proposition 1.1, directly.

Let P be the projection map of $\mathcal{H}$ to $\overline{\mathcal{R}(L)}$ (closure). Then, there exists $\tilde{f}$ in H_K satisfying (1.2) if and only if $P\mathbf{d} \in \mathcal{R}(L)$. This condition is equivalent to

$$\mathbf{d} = P\mathbf{d} + (I-P)\mathbf{d} \in \mathcal{R}(L) + \mathcal{R}(L)^{\perp}.$$

Further, this condition is equivalent to

$$Lf - \mathbf{d} \in \mathcal{R}(L)^{\perp} = \mathcal{N}(L^*)$$

for some $f \in H_K$; that is, for some $f \in H_K$,

$$L^*Lf = L^*\mathbf{d}.$$

$f^*_{\mathbf{d}}$ in (1.5) is the Moore-Penrose generalized inverse of the equation

$$Lf = \mathbf{d}.$$

In particular, if the Moore-Penrose generalized inverse $f^*_{\mathbf{d}}$ exists, it coincides with $f^{**}_{\mathbf{d}}$ in (1.7).
Proposition 1.1 is rigid and is not practical in practical applications, because, practical data contain noises or errors and the criteria (1.4) is not suitable.
Meanwhile, the representation (1.7) is convenient in these senses. However, the function $f^{**}_{\mathbf{d}}(p)$ is, in general, not suitable for the problem (1.1). Indeed, we shall give an estimate of $\|Lf^{**}_{\mathbf{d}} - \mathbf{d}\|_{\mathcal{H}}$. We shall show good relationship between the Tikhonov regularization and the theory of reproducing kernels. For the Tikhonov regularization, see, for example, [2].

2 Tikhonov regularization

We shall introduce the Tikhonov regularization in the framework of the theory of reproducing kernels based on ([1],[3], pp. 50-53). However, from the viewpoint of Tikhonov regularization we shall give a further result constructing the associated reproducing kernels and a new viewpoint for the previous results.
Let L be a bounded linear operator from a reproducing kernel Hilbert space H_K admitting a reproducing kernel $K(p,q)$ on a set E into a Hilbert space $\mathcal{H}$. Then, by introducing the inner product, for any fixed positive $\lambda > 0$

$$(f,g)_{H_K(L;\lambda)} = \lambda(f,g)_{H_K} + (Lf, Lg)_{\mathcal{H}}, \tag{2.9}$$

we shall construct the Hilbert space $H_K(L;\lambda)$ comprising functions of H_K. This space, of course, admits a reproducing kernel and we shall denote it by $K_L(p,q;\lambda)$. Then, we first have the elementary properties:

LEMMA 2.1 *The reproducing kernel $K_L(p,q;\lambda)$ is determined as the unique solution $\tilde{K}(p,q;\lambda)$ of the equation:*

$$\tilde{K}(p,q;\lambda)+\frac{1}{\lambda}(L\tilde{K}_q,LK_p)_{\mathcal{H}}=\frac{1}{\lambda}K(p,q) \tag{2.10}$$

with

$$\tilde{K}_q=\tilde{K}(\cdot,q;\lambda)\in H_K \quad \textit{for} \quad q\in E. \tag{2.11}$$

Note here, in general, that the norm of the RKHS $H_{\lambda K}$ admitting the reproducing kernel $\lambda K(p,q)$ $(\lambda>0)$ is given by

$$\|f\|^2_{H_{\lambda K}}=\frac{1}{\lambda}\|f\|^2_{H_K} \tag{2.12}$$

and the members of functions of $H_{\lambda K}$ are the same of those of H_K.
We shall consider that the reproducing kernel $K(p,q)$ is known and we wish to construct the reproducing kernel $K_L(p,q;\lambda)$. For this construction we can obtain a very effective method by using the Neumann series. We define the bounded linear operator $\tilde{L}$ from H_K into H_K defined by

$$(\tilde{L}f)(p)=(Lf,LK_p)_{\mathcal{H}}=(L^*Lf)(p).$$

Then, from (2.10) we obtain directly

THEOREM 2.2 *If $\|L\|<\lambda$, then $K_L(p,q;\lambda)$ is expressible in terms of $K(p,q)$ by the Neumann series:*

$$K_L(p,q;\lambda)=\left(I+\frac{\tilde{L}}{\lambda}\right)^{-1}\frac{1}{\lambda}K(p,q)=\sum_{n=0}^{\infty}\left(-\frac{\tilde{L}}{\lambda}\right)^n\frac{1}{\lambda}K(p,q), \tag{2.13}$$

where $(I+\frac{\tilde{L}}{\lambda})^{-1}$ is a bounded linear operator from H_K into H_K satisfying

$$\left\|\frac{1}{I+\frac{\tilde{L}}{\lambda}}\right\|\leq\frac{1}{1-\|\frac{\tilde{L}}{\lambda}\|}.$$

Of course, if the operator $\tilde{L}$ is compact, then we can apply the spectral theory to the equation (2.10) without the restriction $\|L\|<\lambda$. In particular, $(I+\frac{\tilde{L}}{\lambda})^{-1}$ is a bounded linear operator and

$$K_L(p,q;\lambda)=\left(I+\frac{\tilde{L}}{\lambda}\right)^{-1}\frac{1}{\lambda}K(p,q).$$

Furthermore, we can obtain a further related result. See, for example, [2].

We shall consider the best approximation problem, for any given $f_0 \in H_K$ and $\mathbf{d} \in \mathcal{H}$:

$$\inf_{f \in H_K} \{\lambda \|f_0 - f\|^2_{H_K} + \|\mathbf{d} - Lf\|^2_{\mathcal{H}}\}, \tag{2.14}$$

in connection with the Tikhonov regularization for the equation $Lf = \mathbf{f}$. Then, we can obtain, from Proposition 1.1:

THEOREM 2.3 *In our situation, for any given $f_0 \in H_K$ and $\mathbf{d} \in \mathcal{H}$, the generalized solution f^* of the equations*

$$f_0 = f \quad \text{in} \quad H_K$$

and

$$\mathbf{d} = Lf \quad \text{in} \quad \mathcal{H}$$

in the sense

$$\inf_{f \in H_K} \{\lambda \|f_0 - f\|^2_{H_K} + \|\mathbf{d} - Lf\|^2_{\mathcal{H}}\}$$
$$= \lambda \|f_0 - f^*\|^2_{H_K} + \|\mathbf{d} - Lf^*\|^2_{\mathcal{H}} \tag{2.15}$$

exists uniquely and it is represented by

$$f^*(p)$$
$$= \lambda (f_0(\cdot), K_L(\cdot, p; \lambda))_{H_K} + (\mathbf{d}, LK_L(\cdot, p; \lambda))_{\mathcal{H}}. \tag{2.16}$$

In Theorem 2.3, in particular, we shall consider the best approximating function, for $f_0 = 0$

$$f^*_{\lambda,\mathbf{d}}(p) = (\mathbf{d}, LK_L(\cdot, p; \lambda))_{\mathcal{H}}, \tag{2.17}$$

which is the extremal function in the Tikhonov regularization (2.15) for $f_0 = 0$.

In general, in the Tikhonov regularization, the operator L is compact and the extremal functions are represented by using the singular values and singular functions of the selfadjoint operator L^*L. So, the representations are, in a sense, abstract. And the behaviour of the extremal functions as

λ tends to zero is an important problem, because the limit function may be expected as a solution of the equation $Lf = \mathbf{f}$ as in the Moore-Penrose generalized inverse.
From many examples in our situation ([5,6,7]), however we see that

$$\lim_{\lambda\to 0} K_L(p,q;\lambda) \tag{2.18}$$

and

$$\lim_{\lambda\to 0}(\mathbf{d}, LK_L(p,q;\lambda))_{\mathcal{H}} \tag{2.19}$$

do, in general, not exist.

3 Main Results

We now give our main results in this paper:

THEOREM 3.1 *For the two best approximate functions $f^*_{\lambda,\mathbf{d}}(p)$ in (2.17) and $f^{**}_{\mathbf{d}}(p)$ in (1.7) we have the estimate*

$$|f^*_{\lambda,\mathbf{d}}(p) - f^{**}_{\mathbf{d}}(p)| \le \left(\lambda\|L\| + \|LL^*LL^* - I\|\frac{1}{\sqrt{2\lambda}}\right)\sqrt{K(p,p)}\|\mathbf{d}\|_{\mathcal{H}}. \tag{3.20}$$

COROLLARY 3.2 *If LL^* is unitary, then we have for the two best approximate functions $f^*_{\lambda,\mathbf{d}}(p)$ in (2.17) and $f^{**}_{\mathbf{d}}(p)$ in (1.7) we have the estimate*

$$|f^*_{\lambda,\mathbf{d}}(p) - f^{**}_{\mathbf{d}}(p)| \le \lambda\|L\|\sqrt{K(p,p)}\|\mathbf{d}\|_{\mathcal{H}} \tag{3.21}$$

which shows that as λ tends to zero, $f^*_{\lambda,\mathbf{d}}(p)$ tends to $f^{**}_{\mathbf{d}}(p)$ with the order λ and the convergence is uniform on any subset of E satisfying $K(p,p) < \infty$.

For the best approximate function $f^{**}_{\mathbf{d}}(p)$ when there exists, we have

$$\begin{aligned} f^{**}_{\mathbf{d}}(p) &= (L^*\mathbf{d}, L^*LK(\cdot,p))_{H_K} \\ &= (L^*LL^*\mathbf{d})(p). \end{aligned} \tag{3.22}$$

For the image of $f^{**}_{\mathbf{d}}(p)$, we thus obtain the estimate

$$\|Lf^{**}_{\mathbf{d}} - \mathbf{d}\|_{\mathcal{H}} \le \|LL^*LL^* - I\|\|\mathbf{d}\|_{\mathcal{H}}. \tag{3.23}$$

The quantity $\|LL^*LL^* - I\|$ may be understood as a distance of the operator LL^* from being unitary..

THEOREM 3.3 *If L is a compact operator, then for the Moore-Penrose generalized inverse $f_{\mathbf{d}}^*$,*

$$\lim_{\lambda \to 0} f_{\lambda,\mathbf{d}}^*(p) = f_{\mathbf{d}}^*(p), \tag{3.24}$$

uniformly on any subset of E satisfying $K(p,p) < \infty$.

Proof: Since L is compact, we have, from (2.10)

$$K_L(p,q;\lambda) = \frac{1}{\lambda I + L^*L} K(p,q).$$

Then,

$$\begin{aligned} f_{\lambda,\mathbf{d}}^*(p) &= (\mathbf{d}, LK_L(\cdot,p;\lambda))_{\mathcal{H}} \\ &= (L^*\mathbf{d}, K_L(\cdot,p;\lambda))_{H_K} \\ &= \left(\frac{1}{\lambda I + L^*L} L^*\mathbf{d}, K(\cdot,p)\right)_{H_K}. \end{aligned}$$

As we see by using the singular value decomposition of L, for the Moore-Penrose generalized inverse $f_{\mathbf{d}}^*$, as $\lambda \to 0$,

$$\frac{1}{\lambda I + L^*L} L^*\mathbf{d} \to f_{\mathbf{d}}^*, \quad \text{in} \quad H_K$$

(see Section 5.1 in [2]). Hence, from the identity

$$\begin{aligned} &f_{\lambda,\mathbf{d}}^*(p) - f_{\mathbf{d}}^*(p) \\ &= \left(\frac{1}{\lambda I + L^*L} L^*\mathbf{d} - f_{\mathbf{d}}^*, K(\cdot,p)\right)_{H_K}, \end{aligned}$$

we have the desired result.

COROLLARY 3.4 *If $g \in \mathcal{N}(L)^{\perp}$, then*

$$\lim_{\lambda \to 0} f_{\lambda,Lg}^*(p) = f_{Lg}^*(p) = g(p) \tag{3.25}$$

uniformly on any subset of E satisfying $K(p,p) < \infty$.

Meanwhile,

COROLLARY 3.5 *If $\mathbf{d} \in \mathcal{H}$ belongs to $\mathcal{R}(H_K)$, then*

$$\lim_{\lambda \to 0} Lf_{\lambda,\mathbf{d}}^*(p) = \mathbf{d} \quad \textit{in} \quad \mathcal{H}. \tag{3.26}$$

For several concrete applications of our general theorems, see the forthcoming papers [5,6,7].

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