

On the Asymptotic Distribution of the Eigenvalues of Discretizations of a Compact Operator

G.N. Newsam

Abstract

It is well known that bounds on the asymptotic decay rate of the eigenvalues of the symmetric integral operator with kernel $k(s,t)$ may be obtained from the smoothness of $k(s,t)$ [1,4,7,9,11]. Some recent numerical results suggested that these bounds also applied to the eigenvalues of matrices with entries $K_{mn} = k(s_m, t_n)$ that occur in various discretizations of the continuous operator. This note shows that, in certain common situations, this is indeed the case.

1. Introduction

The canonical ill-posed problem is the solution of the equation $\mathcal{K}f = g$, where \mathcal{K} is a compact linear operator. In the presence of data or model errors, the full solution f can be obtained from the equation as it stands (for a review of this see [2,8]). The maximum amount of obtainable information can be quantified in terms of the noise levels and the singular values of the matrix [8,13], but to do so requires some *a priori* knowledge of the distribution of the singular values.

Such knowledge is often available for the exact operator. If \mathcal{K} is an integral operator, i.e.

$$(\mathcal{K}f)(s) \equiv \int_{\Omega} k(s,t) f(t) dt \quad s \in \Omega$$

then the asymptotic distribution of the singular values of \mathcal{K} is related to the smoothness of the kernel k [9]. If \mathcal{K} is also symmetric and positive definite, the results in [9] can be improved; e.g., if Ω is a finite interval on the real line and k is p times differentiable in either variable then the eigenvalues $\lambda_n(\mathcal{K})$ decay as $o(n^{-(p+1)})$ [4,11]. In the special case when \mathcal{K} is also a convolution operator, i.e. when $k(s,t) = k(s-t)$, then the

distribution of its eigenvalues is governed by the asymptotic decay of the Fourier transform $K(\omega)$ of the kernel $k(t)$ [1,7].

In many cases, however, the practical problem centres on an operator K that is a discretization of \mathcal{K} , rather than on \mathcal{K} itself, and what is required is *a priori* knowledge of the distribution of the singular values of K . For example, in geostatistics the smooth interpolation via kriging of N scattered data values at the points $\{s_n\}_{n=1}^N$ in the region Ω requires the inversion of matrices of the form:

$$K_{mn} = k(s_m, s_n) \quad (1)$$

(see [3,12] for details). Alternatively, if the data function $g(s)$ in the model problem is only available in the form of point values g_n sampled at the points $\{s_n\}_{n=1}^N$, then the operator of real interest is $K : L^2(\Omega) \rightarrow \mathbb{R}^N$, where

$$[Kf]_n \equiv \int_{\Omega} k(s_n, t) f(t) dt . \quad (2)$$

In either case, if the points s_n are reasonably distributed then at least the larger singular values of the discrete operator K should approximate those of the continuous operator \mathcal{K} . This note proposes the following much stronger result: if \mathcal{K} is symmetric and L^∞ norms of the eigenfunctions of the continuous operator are uniformly bounded, the singular values of the discrete operator are essentially bounded above by those of the exact operator.

Results of this nature are immediate for discretizations based on Galerkin's method. In such cases the discrete operators are essentially representations of the operator $\mathcal{P}_U \mathcal{K} \mathcal{P}_V$, where U and V are finite dimensional subspaces of test functions and \mathcal{P}_U and \mathcal{P}_V are the associated orthogonal projection operators. The minimax characterization of singular values now establishes that

$$\sigma_p(\mathcal{P}_U \mathcal{K} \mathcal{P}_V) \leq \sigma_p(\mathcal{K}) .$$

Thus the singular values of the discrete operator must consistently underestimate those of

the continuous operator. This sort of behaviour is evident in Figure 1. The graph shows the eigenvalues of a discretization of the symmetric convolution operator with kernel

$$k(s,t) \equiv \frac{1}{\pi[1 + (s-t)^2]} \quad \text{s.t. } \in [-c,c]$$

for the particular case $c = 2$. This operator is associated with problems in analytic continuation. Theory [1,7] predicts that the eigenvalues of the exact operator are asymptotically distributed as:

$$\lambda_p(\ell) \sim e^{-2\pi(p/4c)}.$$

This exponential decay is mirrored in the distribution of the larger eigenvalues of the discrete operator. However, beyond $p \sim 40$ the discretization is no longer an accurate approximation of the true operator, so the eigenvalues begin to fall away more rapidly.

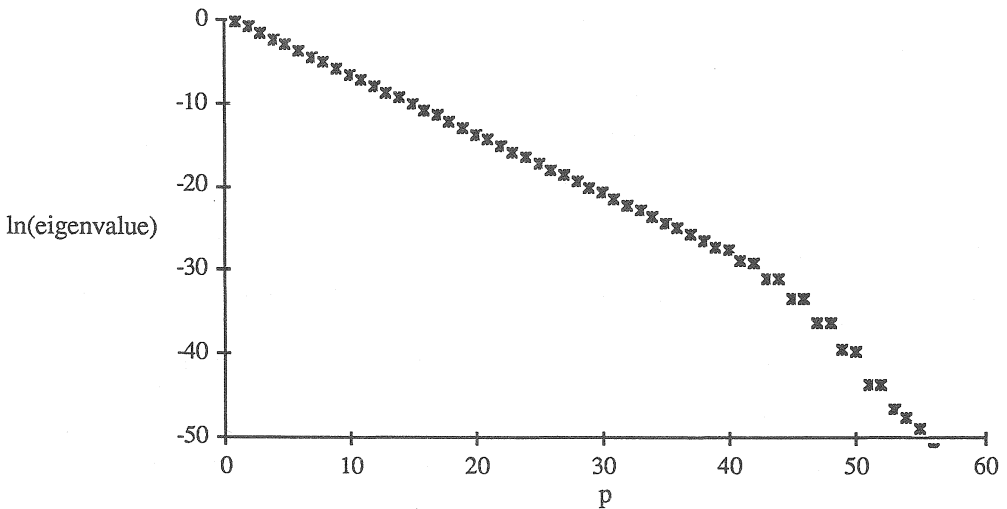


Figure 1: Plot of $\ln(\lambda_p)$ against p for a 56 point Gaussian discretization of the analytic continuation kernel with $c = 2$.

This accelerated decay is in contrast to the behaviour in Figure 2, which shows the eigenvalues for the case $c = 1$. Here, at $p \sim 35$, the eigenvalues reach the level of

machine precision, and the impact of random errors arising in numerical calculations now levels them off.

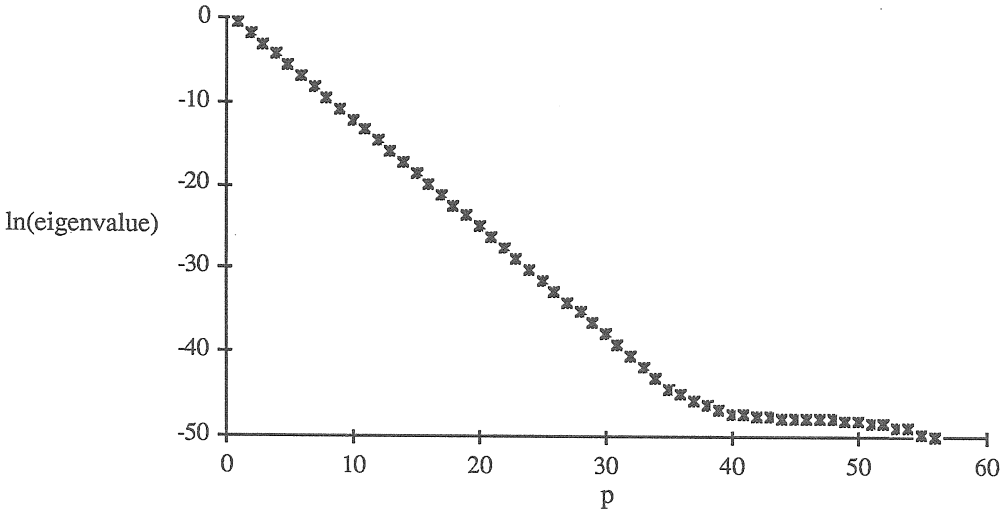


Figure 2: Plot of $\ln(\lambda_p)$ against p for a 56 point Gaussian discretization of the analytic continuation kernel with $c = 1$.

While the eigenvalues of a Galerkin approximation will show an accelerated fall-off once the accuracy of the approximation has been reached, one might expect that the eigenvalues of a discrete approximation, such as (1), would actually level off at these accuracy limits, corresponding to the levelling off that occurs at the level of machine precision. In practice, however, the singular values of discrete approximations show much the same accelerated fall-off as those of Galerkin approximations. The eigenvalues in Figure 1 are actually those of a discretization based on Gaussian quadrature. Moreover, Figure 3 shows the eigenvalues of several different realizations of (1) for the above kernel with $c = 2$ and with various choices of mesh $\{s_n\}$. In each case the asymptotic decay of the eigenvalues is faster than that predicted for the eigenvalues of the continuous operator.

The aim of the paper is to explain this accelerated decay by establishing the upper bound result described above. The explanation centres on construction of an imbedding of the domain and range of the continuous operator within larger Hilbert spaces that include

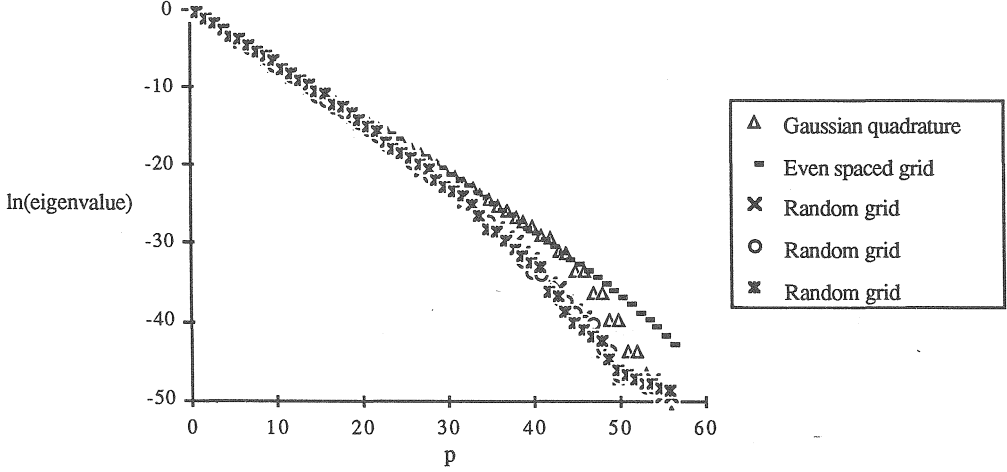


Figure 3: Plot of $\ln(\lambda_p)$ against p for five 56 point Gaussian discretization of the analytic continuation kernel with $c = 2$.

delta functions. The discrete operator can now be viewed as analogous to a Galerkin approximation to the continuous operator formed by projecting into subspaces spanned by the appropriate delta functions, and its eigenvalues estimated accordingly. This explanation is not, however, the complete story; the construction rests on an assumption that, while it holds in many cases of interest, it is not valid for all operators. Nevertheless, the explanation gives a good insight into the observed behaviour.

The structure of the paper is as follows. The next section establishes the necessary concepts and notation for the imbedding, and sets up a subspace of delta functions together with an associated operator \mathcal{S} that plays much the same role as the Galerkin projection \mathcal{P}_U . Section 3 then uses such an imbedding to show that, for a symmetric positive definite operator \mathcal{K} , the discrete operator K of (1) may be expressed as the product $\mathcal{S}^* \tilde{\mathcal{K}} \mathcal{S}$, where the operator $\tilde{\mathcal{K}}$ is a slight modification of \mathcal{K} . This product is then used in Section 4 to derive bounds both on the individual eigenvalues of K and on its determinant, through the inequality

$$\lambda_p(K) \leq \min \lambda_{p+1-q}(\tilde{\mathcal{K}}) \lambda_q(\mathcal{S}^* \mathcal{S}).$$

Finally the results of Section 4 are used in Section 5 to establish similar bounds for the singular values of the discrete operator K of (2).

2. Subspaces of Delta Functions

Let $\mathcal{K} : L^2(\Omega) \rightarrow L^2(\Omega)$ be a symmetric, positive definite, compact linear integral operator with continuous kernel $k(s,t)$. Then \mathcal{K} has an associated eigendecomposition with eigenvalues $\{\lambda_p\}_{p=1}^{\infty}$ and eigenfunctions $\{\psi_p(t)\}_{p=1}^{\infty}$, and by Mercer's Theorem [6]

$$k(s,t) = \sum_{p=1}^{\infty} \lambda_p \psi_p(s) \psi_p(t).$$

As the functions ψ_p form an orthonormal basis for $L^2(\Omega)$, they may be used to identify $L^2(\Omega)$ with the space ℓ^2 of square summable sequences through the usual isomorphism

$$\{\alpha_p\}_{p=1}^{\infty} \in \ell^2 \mapsto f(t) = \sum_{p=1}^{\infty} \alpha_p \psi_p(t) \in L^2(\Omega).$$

ℓ^2 itself can be considered as the member h^0 of the one-parameter family of sequence spaces $h^{-\varepsilon}$ where

$$h^{-\varepsilon} \equiv \left\{ \{\alpha_p\}_{p=1}^{\infty} : \sum_{p=1}^{\infty} \frac{|\alpha_p|^2}{p^{2\varepsilon}} < \infty \right\}.$$

The space $h^{-\varepsilon}$ may in turn be identified with the following formal function space

$$H^{-\varepsilon} \equiv \left\{ f(t) : f(t) = \sum_{p=1}^{\infty} f_p \psi_p(t) \quad \text{where} \quad \{f_p\}_{p=1}^{\infty} \in h^{-\varepsilon} \right\}.$$

$H^{-\varepsilon}$ is a Hilbert space under the inner product

$$(f,g)_{H^{-\varepsilon}} \equiv \sum_{p=1}^{\infty} \frac{f_p g_p}{p^{2\varepsilon}}$$

and has an orthonormal basis in the functions

$$\left\{ \tilde{\psi}_p(t) : \tilde{\psi}_p(t) \equiv \frac{\psi_p(t)}{p^{\varepsilon}} \right\}_{p=1}^{\infty}. \quad (3)$$

The delta function $\delta_s(t) \equiv \delta(t-s)$ may now be placed within this framework by identifying it with the sequence $\{\psi_p(s)\}_{p=1}^{\infty}$. However placing δ_s in one of the spaces $H^{-\epsilon}$ requires some further assumptions about the function ψ_p . In particular, the following assumption is now made and will be used throughout the rest of the paper.

Assumption. The functions ψ_p are uniformly bounded. That is, there exists some constant d such that $|\psi_p(s)| < d$ for all p and s . //

The assumption is by no means greatly restrictive; it is satisfied by many standard basis functions, such as the trigonometric functions on the Rademacher functions. It is not satisfied by all standard bases, however; for example, if P_n denotes the n -th Legendre polynomial normalized so that $\|P_n\|_2 = 1$, then $\|P_n\|_{\infty} \sim \sqrt{n}$ as $n \uparrow \infty$. The author has so far not been able to find any simple conditions on the kernel under which the assumption would be true. However, it seems likely that there are kernels for which this assumption does not hold, and consequently for which the asymptotic bounds here are not valid.

In any case, the next lemma follows immediately from the assumption.

Lemma. $\delta_s \in H^{-\epsilon} \quad \forall \epsilon > \frac{1}{2}$, and $\|\delta_s\|_{H^{-\epsilon}}^2 \leq d^2 \zeta(2\epsilon)$. //

Here $\zeta(2\epsilon)$ is the Riemann zeta function, i.e.

$$\zeta(2\epsilon) = \sum_{p=1}^{\infty} \frac{1}{p^{2\epsilon}}.$$

Now let $\{s_n\}_{n=1}^N$ be any collection of N points in Ω , and let $\delta_n(t) \equiv \delta(t-s_n)$ be the delta function centred on s_n . Then it follows from the lemma that the subspace

$$U_N \equiv \text{span}\{\delta_n\}_{n=1}^N$$

is contained in $H^{-\epsilon}$. Moreover, if E^N denotes Euclidean N -space (i.e. \mathbb{R}^N with the

standard inner product norm), then there is a natural map $\mathcal{S} : E^N \rightarrow H^{-\varepsilon}$ relating U_N and E^N :

$$\mathcal{S}(a) \equiv \sum_{n=1}^{\infty} a_n \delta_n(t).$$

Clearly \mathcal{S} is a compact linear operator. And if $S : E^N \rightarrow E^N$ is defined by $S = \mathcal{S}^* \mathcal{S}$, then S is a symmetric non-negative definite matrix with eigenvalues $\{\rho_n\}_{n=1}^N$. Since

$$\begin{aligned} S_{mn} &= (e_m, \mathcal{S}^* \mathcal{S} e_n)_{E^N} = (\mathcal{S} e_m, \mathcal{S} e_n)_{H^{-\varepsilon}} \\ &= (\delta_m, \delta_n)_{H^{-\varepsilon}} \\ &= \sum_{p=1}^{\infty} \frac{\Psi_p(s_m) \Psi_p(s_n)}{p^{2\varepsilon}} \leq d^2 \zeta(2\varepsilon) \\ \Rightarrow \text{tr}(S) &= \sum_{n=1}^N \rho_n = \sum_{n=1}^N s_{nn} \leq N d^2 \zeta(2\varepsilon) \gamma(\varepsilon). \end{aligned} \quad (4)$$

It follows immediately from this bound on the trace that

$$\det(S) = \prod_{n=1}^N \rho_n \leq [d^2 \zeta(2\varepsilon)]^N. \quad (5)$$

3. Reformulation of the Discrete Operator

The machinery set up in Section 2 can now be used to recast the matrix K of (1) as a product of operators. Consider the operator $\tilde{\mathcal{K}} : H^{-\varepsilon} \rightarrow H^{-\varepsilon}$ defined by

$$(\tilde{\mathcal{K}}f)(s) \equiv \sum_{p=1}^{\infty} p^{2\varepsilon} \lambda_p \tilde{\Psi}_p(s) (f, \tilde{\Psi}_p)_{H^{-\varepsilon}}$$

where the $\tilde{\Psi}_p$ are defined as in (3). As long as $p^{2\varepsilon} \lambda_p \downarrow 0$ as $p \uparrow \infty$, then $\tilde{\mathcal{K}}$ is also symmetric, positive definite and compact. If the $N \times N$ matrix K is defined by

$$K \equiv \frac{|\Omega|}{N} \mathcal{S}^* \tilde{\mathcal{K}} \mathcal{S} \quad (6)$$

then

$$K_{mn} = (e_m, K e_n)_{E^N} = \frac{|\Omega|}{N} (e_m, \mathcal{S}^* \tilde{\mathcal{K}} \mathcal{S} e_n)_{H^{-\varepsilon}}$$

$$\begin{aligned}
&= \frac{|\Omega|}{N} (\mathcal{S}e_m, \tilde{\mathcal{K}}\mathcal{S}e_n)_{H^{-\epsilon}} \\
&= \frac{|\Omega|}{N} (\delta_i, \tilde{\mathcal{K}}\delta_j)_{H^{-\epsilon}}.
\end{aligned}$$

But

$$\begin{aligned}
(\tilde{\mathcal{K}}\delta_j)(s) &= \sum_{p=1}^{\infty} p^{2\epsilon} \lambda_p \tilde{\psi}_p(s) (\delta_n, \tilde{\psi}_p)_{H^{-\epsilon}} \\
&= \sum_{p=1}^{\infty} p^{2\epsilon} \lambda_p \tilde{\psi}_p(s) \frac{\psi(s_n)}{p^\epsilon} \\
\Rightarrow (\delta_i, \tilde{\mathcal{K}}\delta_j)_{H^{-\epsilon}} &= \left[\sum_{p=1}^{\infty} \psi_p(s_m) \psi_p(s), \sum_{q=1}^{\infty} q^\epsilon \lambda_q \psi_q(s_n) \tilde{\psi}_q(s) \right]_{H^{-\epsilon}} \\
&= \sum_{p=1}^{\infty} p^\epsilon \lambda_p \psi_p(s_n) \psi_p(s_n) (\psi_p, \tilde{\psi}_p)_{H^{-\epsilon}} \\
&= \sum_{p=1}^{\infty} \lambda_p \psi_p(s_m) \psi_p(s_n) = k(s_m, s_n). \\
\Rightarrow K_{mn} &= \frac{|\Omega|}{N} k(s_m, s_n).
\end{aligned}$$

Note the introduction of a normalizing factor $|\Omega|/N$; this simply rescales the discrete operator so that its norm is approximately the same as that of the continuous operator. Failure to rescale simply introduces a factor of N in all the bounds; this can be interpreted as being the improvement one would expect in the discrete operator simply due to sampling at a large number of points (see Section 5 for a further discussion of this point).

4. Asymptotic Bounds on $\lambda_p(K)$

The eigenvalues $r_p \equiv \lambda_p(K)$ can now be bounded in terms of the original eigenvalues $\lambda_p \equiv \lambda_p(\mathcal{K})$ and the eigenvalues ρ_p of S through (6). The bound is constructed as follows. First note that, as $\tilde{\mathcal{K}}$ is symmetric and positive definite, it has a square root $\tilde{\mathcal{K}}^{1/2}$ and

$$K = \frac{|\Omega|}{N} (\tilde{\mathcal{K}}^{1/2} \mathcal{S})^* (\tilde{\mathcal{K}}^{1/2} \mathcal{S}).$$

Therefore $\lambda_p = \sigma_p^2(\tilde{\kappa}^{1/2} \mathcal{S})$, where $\sigma_p(\cdot)$ denotes the p^{th} singular values of a compact operator. Squaring both sides of the following inequality from [5]

$$\sigma_p(\tilde{\kappa}^{1/2} \mathcal{S}) \leq \min_{1 \leq q \leq p} \sigma_{p+1-q}(\tilde{\kappa}^{1/2}) \sigma_q(\mathcal{S})$$

gives

$$r_p \leq \frac{|\Omega|}{N} \min_{1 \leq q \leq p} \tilde{\lambda}_{p+1-q} \rho_q \quad (7)$$

where $\tilde{\lambda}_p = p^{2\epsilon} \lambda_p$.

It remains to show that (7) is a sufficiently tight bound to enforce that $r_p \leq \lambda_p$, where the bound is interpreted in some asymptotic sense yet to be made precise. (Note that $p \leq N$ as r_p is not defined for $p > N$.) Allowing the ρ_q to be arbitrary, save for the constraints that $\rho_q \geq 0$ and that $\text{tr}(\mathcal{S})$ be bounded as in (4), gives that r_p is bounded above by the solution of the following optimization problem

$$r_p \leq \frac{|\Omega|}{N} \max_{\rho} \min_{1 \leq q \leq p} \tilde{\lambda}_{p+1-q} \rho_q$$

subject to

- i) $\rho_q \geq 0 \quad 1 \leq q \leq p$
- ii) $\sum_{q=1}^{\infty} \rho_q \leq N d^2 \zeta(2\epsilon)$.

This problem can be recast as a simple linear program where optimum can easily be found to be achieved at

$$\rho_q = \frac{1}{\tilde{\lambda}_{p+1-q}} \frac{N d^2 \zeta(2\epsilon)}{\sum_{q=1}^p 1/\tilde{\lambda}_{p+1-q}}$$

giving the bound

$$r_p \leq \frac{\gamma(\epsilon)}{\sum_{q=1}^p 1/\tilde{\lambda}_q} \quad (8)$$

where $\gamma(\epsilon) \equiv |\Omega|/d^2 \zeta(2\epsilon)$. (8) gives the immediate

$$r_p \leq \gamma(\varepsilon) \tilde{\lambda}_p \leq \gamma(\varepsilon) p^{2\varepsilon} \lambda_p .$$

Since 2ε can be made arbitrarily close to 1, r_p decays more slowly than λ_p by at most a factor that grows essentially linearly in p . It is easy to see, however, that the worst case can only be achieved when λ_p , and therefore r_p , is in fact decaying very rapidly. For suppose that λ_p decays asymptotically as $p^{-\alpha}$, i.e. $\lambda_p \sim p^{-\alpha}$. Then $\tilde{\lambda}_p \sim p^{2\varepsilon-\alpha}$ and

$$\begin{aligned} \sum_{q=1}^p \frac{1}{\tilde{\lambda}_q} &\sim \sum_{q=1}^p q^{\alpha-2\varepsilon} \sim \frac{1}{\alpha+1-2\varepsilon} p^{\alpha+1-2\varepsilon} \\ \Rightarrow r_p &\leq \gamma(\varepsilon) (\alpha+1-2\varepsilon) p^{\alpha+1-2\varepsilon} \\ &\sim \gamma(\varepsilon) (\alpha+1) \lambda_p \end{aligned}$$

since $2\varepsilon-1$ can be made arbitrarily small. Then r_p decays asymptotically at least as fast as λ_p .

The bounds on r_p are reinforced by the following bounds on the determinant of K . It is straightforward to show that

$$\det(K) \leq \left[\frac{|\Omega|}{N} \right]^N \prod_{n=1}^N \tilde{\lambda}_n \det(S)$$

and so by (5) that

$$\begin{aligned} \det(K) &\leq [\gamma(\varepsilon)]^N \cdot \prod_{n=1}^N \lambda_n \prod_{n=1}^N p^{2\varepsilon} N^{-N} \\ &\sim [\gamma(\varepsilon)]^N \prod_{n=1}^N \lambda_n \left[\frac{N}{e} \right]^{2\varepsilon N} N^{-N} \\ &= \left[\frac{\gamma(\varepsilon)}{e^{2\varepsilon}} \right]^N [N^N]^{2\varepsilon-1} \prod_{k=1}^N \lambda_k . \end{aligned}$$

Thus the asymptotic decay rates of $\prod r_n$ and $\prod \lambda_n$ can be made arbitrarily close.

5. Extensions and Conclusions

The results of the previous section show that, for symmetric operators satisfying the

assumption, no significant improvement can be expected in the conditioning of any discrete operator. Indeed the reverse is most likely. As expected, these results extend to the unsymmetric case.

Let $\mathcal{K} : L^2(\Omega) \rightarrow L^2(\Lambda)$ now be an arbitrary compact integral operator with kernel $k(s,t)$, let $\{s_n\}_{n=1}^N$ be an arbitrary set of points in Λ and let $K : L^2(\Omega) \rightarrow E^N$ be the operator defined by (2), i.e.

$$[Kf]_n = \int_{\Omega} k(s_n, t) f(t) dt .$$

The problem is to now bound the singular values $\sigma_p(K)$ of K by the singular values of $\sigma_p(\mathcal{K})$ of \mathcal{K} . To do so, first note that $\sigma_p^2(\mathcal{K}) = \lambda_p(\mathcal{K}\mathcal{K}^*)$, and that $\mathcal{K}\mathcal{K}^*$ is a symmetric, positive definite, integral operator with kernel

$$k_2(s,u) \equiv \int_{\Omega} k(s,t) k(u,t) dt .$$

Likewise $\sigma_p^2(K) = \lambda_p(KK^*)$, and as

$$(K^* a)(t) = \sum_{n=1}^N a_n k(s_n, t)$$

KK^* is a matrix with entries

$$[KK^*]_{mn} = \int_{\Omega} k(s_m, t) k(s_n, t) dt = k_2(s_m, s_n) .$$

The results of Section 4 now give that (modulo a constant)

$$\begin{aligned} \lambda_n(KK^*) &\leq N \lambda_n(\mathcal{K}\mathcal{K}^*) & n = 1, \dots, N \\ \Rightarrow \sigma_n(K) &\leq \sqrt{N} \sigma_n(\mathcal{K}) . \end{aligned} \tag{9}$$

(9) has important implications for data gathering. It essentially says that clever placement of data points will not result in a discrete problem with substantially better conditioning than that of the underlying continuous problem. The best that can be hoped for by increasing the number of points is the usual $O(\sqrt{N})$ improvement in accuracy that

would be expected anyway on statistical grounds.

This is not to say, however, that point placement is not important. Poor placement may substantially worsen the conditioning of the discrete problem. And in some cases, e.g. when \mathcal{K} is a totally positive operator, theory suggests that an optimal set of data locations $\{s_n\}_{n=1}^N$ may exist for which $\sigma_N(\mathbf{K}) \sim \sqrt{N} \sigma_N(\mathcal{K})$, i.e. the points achieve the upper bound on $\sigma_N(\mathbf{K})$ (see [10] for details).

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Centre for Mathematical Analysis
The Australian National University
Box 4, G.P.O.
Canberra A.C.T. 2601 Australia