On the Influence of Multiplication Operators on the Ill-Posedness of Inverse Problems

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Numerical Analysis Seminar, University of Bath

8th October 2004

Inverse problems and well-posedness

The operator equation

$$F(x) = y, \quad x \in D \subset X, \quad y \in Y$$

is said to be **well-posed** according to Hadamard, if the following three conditions hold:

- For every $y \in Y$ there exists at least one $x \in D$ satisfying $F(x) = y$ (existence).
- The element x satisfying $F(x) = y$ is uniquely determined in D (uniqueness).
- The solution x depends continuously on the right hand side y (stability).

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Chemical reaction I

Ordinary differential equation

$$u'(t) = x(t)u(t), \quad u(0) = u_0$$

Direct problem: determination of $u(t)$ for $0 \leq t \leq T$, with given u_0 and $x(t)$

$$[F(x)](s) = u_0 \exp\left(\int_0^s x(t)dt\right), \quad (0 \leq s \leq T)$$

or

$$F = N \circ J, \quad [J(x)](s) := \int_0^s x(t)dt, \quad (0 \leq s \leq T).$$

Chemical reaction II

- Inverse problem: identification of $x(t)$ in $[0, T]$ with given concentration $u(t)$.
- Fréchet derivative $F'(x_0)$:

$$[F'(x_0)(h)](t) = [F(x_0)](t)[J(h)](t), \; h \in X = L^2(0, T)$$

or $F'(x_0) = M \circ J$ with the **multiplication operator**:

$$m(t) := [F(x_0)](t), \quad 0 < c \leq |m(t)| \leq C < \infty.$$

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Heat conduction I

$$\frac{\partial u(z,t)}{\partial t} = x(t)\frac{\partial^2 u(z,t)}{\partial z^2}, \quad (0 < z < 1,\ 0 < t < T),$$

- $x(t)$, $(0 \leq t \leq T)$ is the coefficient of thermal conductivity
- $u(z,t)$, $(0 \leq z \leq 1,\ 0 \leq t \leq T)$: temperature field
- initial condition

$$u(z,0) = \sin(\pi z), \quad (0 \leq z \leq 1).$$

homogenous boundary conditions given by

$$u(0,t) = u(1,t) = 0 \quad (0 \leq t \leq T).$$

- temperature in the middle of the rod, i.e. at $z = \frac{1}{2}$ is known:

$$y(t) := u\left(\frac{1}{2}, t\right)$$

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Heat conduction II

- Direct problem: nonlinear mapping $x(t) \to y(t)$.
- Solution y to the above problem:

$$y(t) = \exp\left(-\pi^2 \int_0^t x(\tau) d\tau\right).$$

- Inverse problem: identification of the thermal conductivity $x(t)$ in $[0, T]$, i.e. finding the solution to the nonlinear problem

$$[F(x)](t) = \exp\left(-\pi^2 \int_0^t x(\tau) d\tau\right), \quad (0 \le t \le T),$$

which may also be written as a composition $F = N \circ J$.
- as before: $F'(x_0) = M \circ J$ with the **multiplication operator**: $m(t) := -\pi^2 [F(x_0)](t)$

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Option pricing I

Fair option prices $u(t)$ on arbitrage-free markets are explicitely given by the Black-Scholes-type formula

$$u(t) = u_{BS}(X, K, r, t, S(t)), \quad (0 \leq t \leq T),$$

where $S(t)$ is given by

$$S(t) := \int_0^t x(\tau) d\tau.$$

- Inverse problem: finding the volatility function $x(t)$
- Nemytskii operator:

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- Fréchet derivative $F'(x_0) = M \circ J$

$$[F'(x_0)(h)](t) = m(t)[J(h)](t),\ h \in X = L^2(0, T)$$

where

$$m(t) = \frac{\partial k(t, [J(x_0)](t))}{\partial s}, \quad (0 \leq t \leq 1).$$

- We may estimate (see Hofmann/Hein (2003))

$$m(t) \sim \exp\left(-\frac{1}{t^{\alpha}}\right).$$

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SVD of compact operators

Linear operator equations

$$Ax = y, \quad x \in D \subset X, \quad y \in Y \quad A \in \mathcal{L}(X, Y)$$

For each compact operator A there exists a singular system

$$\{\sigma_j, u_j, v_j\}, \quad j = 1, \dots, \infty$$

where

$$\{\sigma_j\}_{j \in J} \quad \text{is non-increasing and} \quad \lim_{j \to \infty} \sigma_j = 0$$

$$Au_j = \sigma_j v_j \, (j \in J) \quad \text{and} \quad A^* v_j = \sigma_j u_j \, (j \in J).$$

For all $x \in X$ there exists an element $x_0 \in N(A)$ with

$$x = x_0 + \sum_{j \in J} \langle x, u_j \rangle_X u_j \quad \text{and} \quad Ax = \sum_{j \in J} \sigma_j \langle x, u_j \rangle_X v_j.$$

The degree of ill-posedness I

- We have
$$A^*Au_j = \sigma_j^2 u_j \quad \text{and} \quad AA^*v_j = \sigma_j^2 v_j.$$
- With the help of singular value decomposition we may define a minimum norm solution:
$$x_{mn} = A^\dagger y = \sum_{j\in J} \frac{\langle y, v_j\rangle_Y}{\sigma_j} u_j, \quad y \in R(A) \oplus R(A)^\perp.$$
- *Picard condition*
$$\sum_{j=1}^{\infty} \frac{\langle y, v_j\rangle_Y^2}{\sigma_j^2} < \infty$$
has to be satisfied

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The degree of ill-posedness II

- Let $Ax = y$ be given and the Pseudo-Inverse $A^\dagger$ be applied to a perturbed right hand side $y_\delta = y + \delta$ for a small δ
- error in the solution is given by

$$\begin{aligned} \|x_{mn}^\delta - x_{mn}\|_X &= \|A^\dagger y_\delta - A^\dagger y\|_X \\ &\leq \|A^\dagger\|_{\mathcal{L}(Y,X)} \cdot \delta. \end{aligned}$$

- Let $A \in \mathcal{L}(X, Y)$ and separable Hilbert spaces X, Y. Then $Ax = y$ has got a **degree of ill-posedness** of $\nu > 0$ if there exist constants $0 \leq \underline{C} \leq \overline{C} < \infty$, such that

$$\underline{C} n^\nu \leq \frac{1}{\sigma_n} \leq \overline{C} n^\nu, \quad n = 1, 2, \ldots$$

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A Volterra integral operator

$$[Jx](s) = \int_0^s x(t)dt, \quad (0 \leq s \leq 1).$$

Eigenvalue equation:

$$[J^* Ju](\tau) = \sigma^2 u(\tau) = \int_\tau^1 \int_0^s u(t)dtds, \quad (0 \leq \tau \leq 1),$$

which leads to the boundary value problem

$$-u(t) = \sigma^2 u''(t) \quad \text{with} \quad u(1) = u'(0) = 0,$$

with singular values

$$\sigma_n = \frac{2}{(2n-1)\pi}, \quad n = 1, 2, \dots,$$

i.e. $\nu = 1$.

An integral operator with infinite degree of ill-posedness

- Heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad (x,t) \in [0,\pi] \times [0,1], \quad u(0,t) = u(\pi,t) = 0.$$

- given $u(x,1) = f(x)$
- task: determine the initial temperature $u(x,0) = g(x)$
- solution to the heat equation:

$$u(x,t) = \sum_{n=1}^{\infty} a_n e^{-n^2 t} \sin(nx), \quad a_n = \frac{2}{\pi} \int_0^{\pi} u(x,0) \sin(ny) dy.$$

$$u(x,1) = f(x) = \frac{2}{\pi} \sum_{n=1}^{\infty} e^{-n^2} \sin(nx) \int_0^{\pi} g(x) \sin(ny) dy := [Ag](x).$$

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Multiplication operators

- Problem: Finding the singular value asymptotics of the composite operator $B : L^2(0,1) \to L^2(0,1)$:

$$[Bx](s) := m(s) \left(\int_0^s x(t)dt \right), \quad (0 \leq s \leq 1)$$

for special multiplier functions $m(s)$.

- $B = M \circ J$ is a compact operator, if J is compact and $m \in L^\infty(0,1)$
- If m has got a positive essential infimum, then J and B are spectrally equivalent
- Consider special multiplier functions

$$m(s) = s^\alpha \quad \text{or} \quad m(s) = \exp\left(-\frac{1}{s^\alpha}\right), \quad \alpha > 0.$$

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Some analytical results I

- Vu Kim Tuan/Gorenflo (1994):

$$[s^{-\alpha} J_r x](s) := s^{-\alpha} \int_0^s \frac{(s-t)^{r-1}}{\Gamma(r)} x(t)dt, \quad (0 \le s \le 1)$$

yields $\sigma_n(J_r) \sim n^{-r}$, for all $r > 0$ as $n \to \infty$ if $r > 2\alpha \ge 0$.

- Write $B = M \circ J$ as Fredholm integral equation

$$[Bx](s) = \int_0^1 k(s,t)x(t)dt, \quad (0 \le s \le 1)$$

with

$$k(s,t) = \begin{cases} m(s), & (0 \le t \le s \le 1) \\ 0, & (0 \le s \le t \le 1). \end{cases}$$

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$$k(s,t) = \begin{cases} m(s), & (0 \le t \le s \le 1) \\ 0, & (0 \le s \le t \le 1). \end{cases}$$

Some analytical results II

- Chang (1952): $k \in L^2((0,1)^2) \Rightarrow \sigma_n(B) = o(n^{-\frac{1}{2}})$
- Minimax principle:

$$\sigma_n(B) = \min_{x \in \text{span}(u_1,\dots,u_n)\setminus\{0\}} \frac{\|Bx\|_Y}{\|x\|_X}$$

and

$$\|Bx\|_{L^2(0,1)} = \|M(Jx)\|_{L^2(0,1)} \leq \|m\|_{L^\infty(0,1)}\|Jx\|_{L^2(0,1)}$$

i.e.

$$\sigma_n(B) = \sigma_n(M \circ J) \leq \|m\|_{L^\infty(0,1)}\sigma_n(J) \leq Cn^{-1}$$

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Some analytical results III

- Eigenvalues of B^*B:

$$[B^*Bx](\tau) = \int_0^1 \left(\int_0^1 k(s,\tau)k(s,t)ds \right) x(t)dt$$

Reade (1984): The eigenvalues of operators B^*B Lipschitz continuous self-adjoint positive definite kernels satisfy

$$\lambda_n(B^*B) = \mathcal{O}(n^{-2})$$

Formulation as a Sturm-Liouville problem

Formulate

$$[Bx](s) = \int_0^s m(s)x(t)dt, \quad (0 \leq s \leq 1),$$

as a boundary value problem, using the eigenvalue equation $B^*Bu = \sigma^2 u$:

$$\sigma^2 \left(\frac{u'(\tau)}{m^2(\tau)} \right)' = -u(\tau), \quad m(\tau) \neq 0, u \in C^2[0,1]$$

or

$$-(a(\tau)u'(\tau))' = \lambda u(\tau), \quad u(1) = \lim_{\tau \to 0} a(\tau)u'(\tau) = 0,$$

where $\lambda = \frac{1}{\sigma^2}$ and $a(\tau) = \frac{1}{m^2(\tau)}$.

Finite difference methods for the SL-problem

- Boundary value problem:

$$-(a(\tau)u'(\tau))' = \lambda u(\tau)$$

$$u(1) = 0 \quad \text{and} \quad \lim_{\tau \to 0} a(\tau)u'(\tau) = 0.$$

- apply classical finite difference method:

$$\left(\frac{a_{i+1} - a_{i-1}}{4h^2} - \frac{a_i}{h^2}\right) u_{i-1} + \frac{2a_i}{h^2} u_i + \left(\frac{a_{i-1} - a_{i+1}}{4h^2} - \frac{a_i}{h^2}\right) u_{i+1} = \lambda u_i$$

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Results for $m(s) = s^{\alpha}$

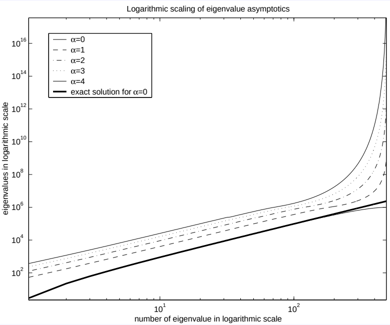

Figure: Computed eigenvalues of Sturm-Liouville problem $-(au')' = \lambda u$ for $n = 500$ in logarithmic scales

$$\lambda_n^{\text{approx}}(A) = (\alpha + 1)^2 \pi^2 n^2 + \mathcal{O}(n)$$

Results for $m(s) = e^{-\frac{1}{s^\alpha}}$

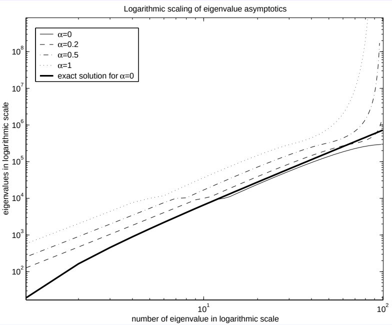

Figure: Computed eigenvalues of Sturm-Liouville problem $-(au')' = \lambda u$ for $n = 100$ in logarithmic scales

$$\lambda_n^{\text{approx}}(A) = f(\alpha)n^2 + \mathcal{O}(n)$$

Galerkin method for integral equations

$$[B(x)](s) = \int_0^1 k(s,t)x(t)dt, \quad 0 \leq s \leq 1, \quad 0 \leq t \leq 1$$

- singular value expansion for square integrable kernels:

$$k(s,t) = \sum_{j=1}^{\infty} \sigma_j u_j(t) v_j(s), \; 0 \leq s \leq 1, \; 0 \leq t \leq 1.$$

- algebraic singular value decomposition of $A \in \mathbb{R}^{n,n}$:

$$A = U\Sigma V^T = \sum_{j=1}^{n} s_j \mathbf{u}_j \mathbf{v}_j^T,$$

- $\|B\|_{HS}^2 := \sum_{j=1}^{\infty} \sigma_j^2 < \infty$, $\|A\|_F^2 := \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij}^2 = \sum_{j=1}^{n} s_j^2$.

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Algorithm for Galerkin's method

- Choose $\{\Psi_j\}$ and $\{\Phi_j\}$ orthonormal sets of basis functions in $I_t = (0,1)$, $I_s = (0,1)$.
- Determine matrix $A \in \mathbb{R}^{n,n}$ with

$$a_{ij} = \langle B\Phi_j, \Psi_i \rangle_{L^2(0,1)} \quad i,j = 1,\dots,n.$$

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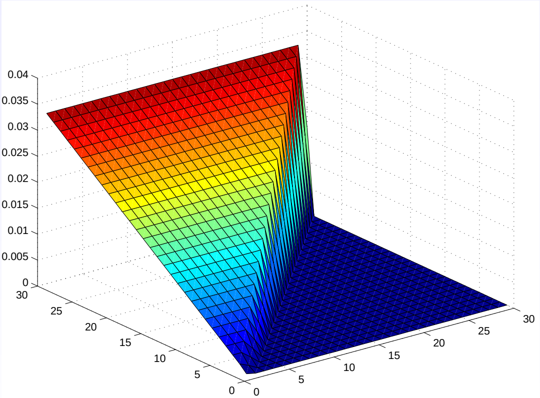
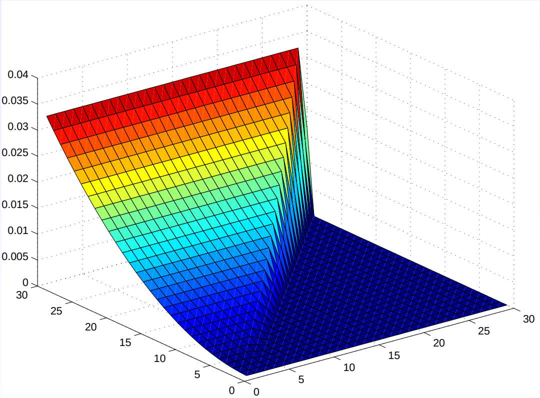
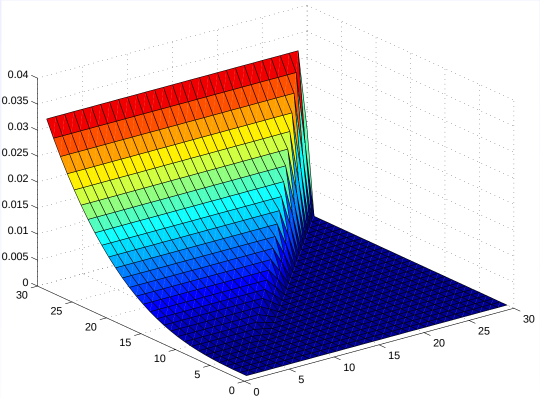
Matrix structure for $m(s) = s$



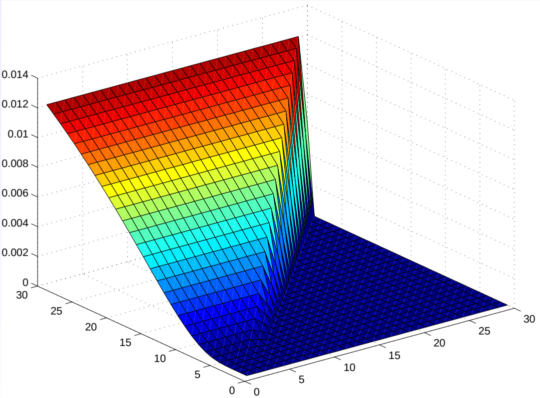
Matrix structure for $m(s) = s^2$



Matrix structure for $m(s) = s^3$



Matrix structure for $m(s) = e^{-\frac{1}{s}}$



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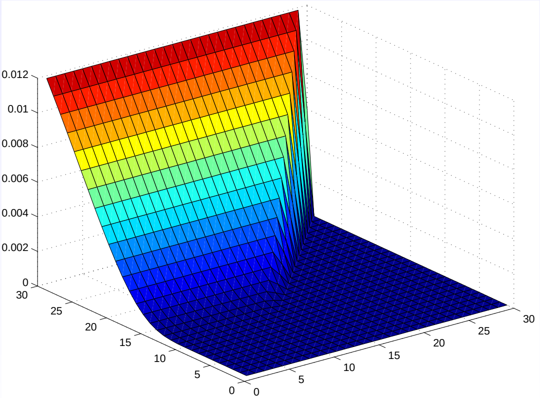


Approximation properties

Proposition Let

$$\|B\|^2 := \int_0^1 \int_0^1 |k(s,t)|^2 dtds = \sum_{i=1}^{\infty} \sigma_i^2.$$

Then

$$s_i^{(n)} \leq s_i^{(n+1)} \leq \sigma_i, \quad i = 1, \ldots, n.$$

The errors of the approximate singular values $s_i^{(n)}$ are bounded by

$$0 \leq \sigma_i - s_i^{(n)} \leq \delta_n, \quad i = 1, \ldots, n,$$

where $\delta_n^2 = \|B\|^2 - \|A\|_F^2$. Furthermore

$$s_i^{(n)} \leq \sigma_i \leq [(s_i^{(n)})^2 + \delta_n^2]^{\frac{1}{2}}, \quad i = 1, \ldots, n.$$

Results for $m(s) = s^\alpha$

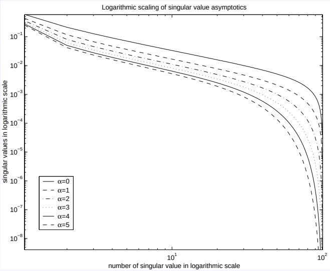
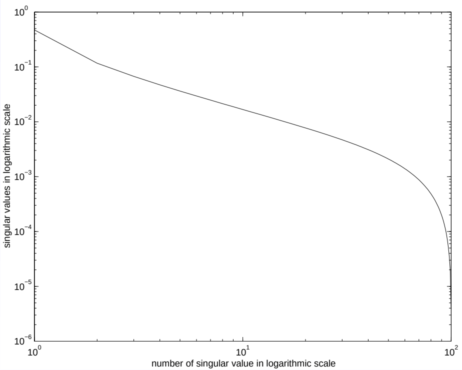


Figure: Computed singular values of integral equation $Bv = \sigma u$ for $n = 100$ in logarithmic scales

$$\sigma_n^{approx}(B) \sim \frac{1}{(\alpha+1)\pi n}$$

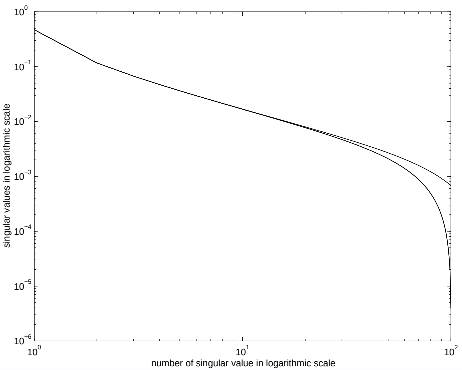
Discrete singular values for $n \longrightarrow \infty$

$$m(s) = s, \quad n = 100$$



Discrete singular values for $n \longrightarrow \infty$

$$m(s) = s, \quad n = 150$$



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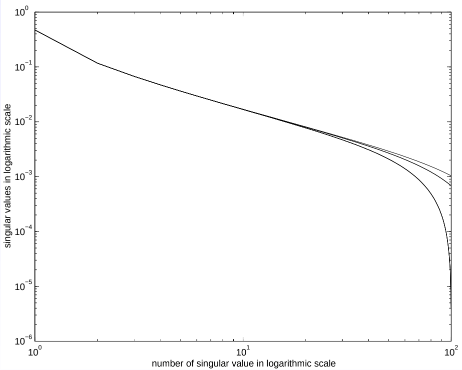
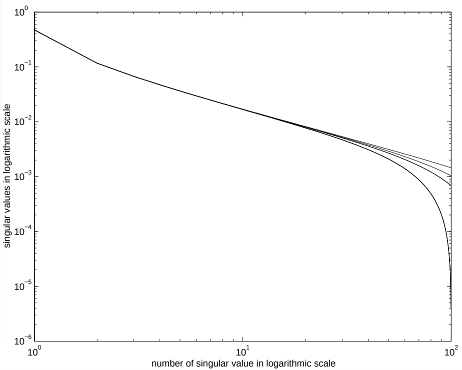


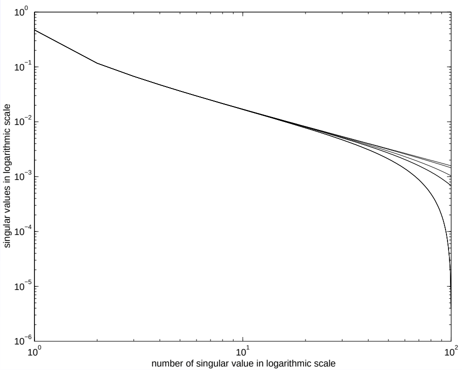
Discrete singular values for $n \longrightarrow \infty$

$$m(s) = s, \quad n = 400$$



Discrete singular values for $n \longrightarrow \infty$

$$m(s) = s, \quad n = 1000$$



Results for $m(s) = e^{-\frac{1}{s^\alpha}}$

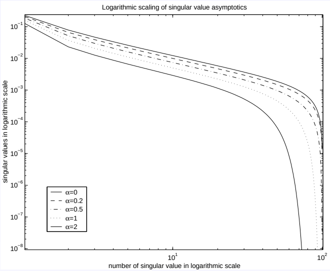


Figure: Computed singular values of integral equation $Bv = \sigma u$ for $n = 100$ in logarithmic scales

$$\sigma_n^{approx}(B) \sim \frac{1}{g(\alpha)n}$$

Discrete singular values for $n \longrightarrow \infty$

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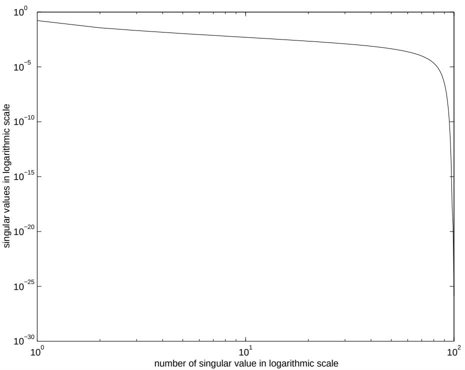

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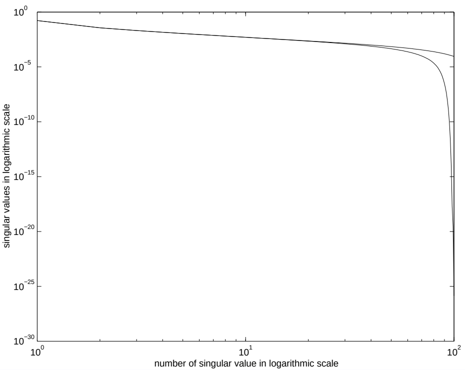

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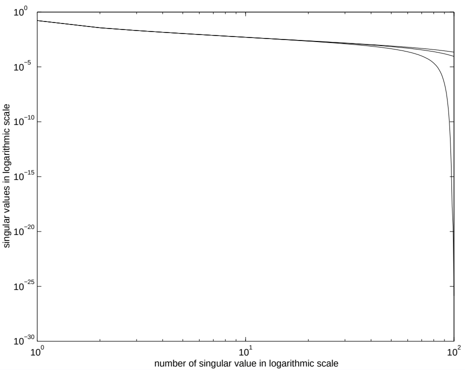

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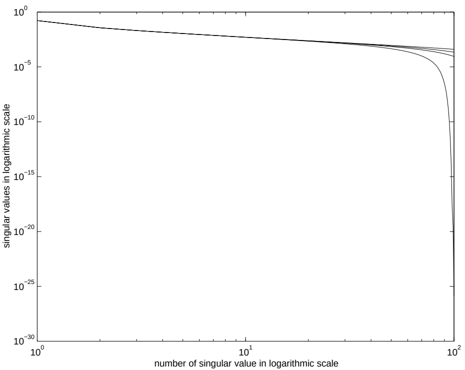

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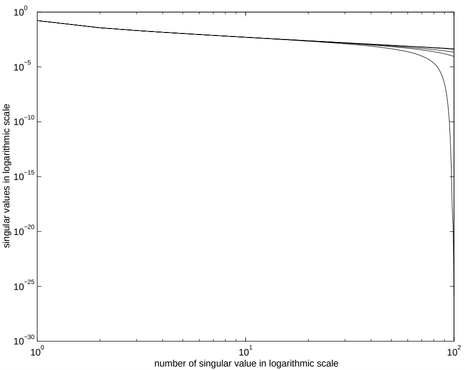

Further numerical approaches and summary

- Rayleigh-Ritz method for symmetric kernel B^*B
- Orthonormal/Non-orthonormal basis functions
- Generalized singular value problem/Generalized eigenproblem
- Combination of analytical and numerical results:

$$\underline{C} n^{-1} = \sigma_n^{\text{approx}}(B) \leq \sigma_n^{\text{exact}}(B) \leq \overline{C} n^{-1}, \quad n \to \infty$$

- Comparison yields

$$\sigma_n(B) = \int_0^1 m(s)ds \cdot \sigma_n(J) = \int_0^1 m(s)ds \cdot \frac{2}{\pi(2n-1)},$$

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- relationship between ill-posedness of nonlinear problems and its linearizations
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Regularization

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$$x_{mn} = A^{\dagger} y$$

  as stable and exact as possible

- apply regularization operator R_α to the approximated given data y_δ:

$$x_\alpha^\delta = R_\alpha y_\delta$$

- estimate the total regularization error

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Tikhonov regularization I

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$$\alpha(\delta) \to 0 \quad \text{and} \quad \frac{\delta^2}{\alpha(\delta)} \to 0 \quad \text{for} \quad \delta \to 0$$

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- Convergence rates

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where ε depends on $\int_0^1 (1 - m(t))^2 dt$.

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Conclusions

- provided several analytical tools in order to derive the degree of ill-posedness of $F'(x_0) = M \circ J$
- stated the problems if $m(t)$ has got a zero
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Thanks for your attention.