Discretization Methods

Must replace the problem of computing the unknown function f with a discrete problem that we can solve on a computer.

Linear integral equation $\Rightarrow$ system of linear algebraic equations.

Quadrature Methods.

Compute approximations $\tilde{f}_j = \tilde{f}(t_j)$ to the solution f at the abscissas $t_1, t_2, \ldots, t_n$.

Expansions Methods.

Compute an approximation of the form

$$f^{(f)}(t) = \sum_{j=1}^{n} \zeta_j \, \phi_j(t),$$

where $\phi_1(t), \ldots, \phi_n(t)$ are expansion/basis functions.

Quadrature Discretization

Recall the quadrature rule

$$\int_0^1 \varphi(t)\, dt = \sum_{j=1}^{n} w_j \, \varphi(t_j) + E_n \ ,$$

where E_n is the quadrature error, and

$$w_j = \text{weights} \ , \quad t_j = \text{abscissas} \ , \qquad j = 1, \ldots, n \ .$$

Now apply this rule *formally* to the integral,

$$\Psi(s) = \int_0^1 K(s,t)\, f(t)\, dt = \sum_{j=1}^{n} w_j \, K(s,t_j)\, f(t_j) + E_n(s) \ .$$

Quadrature Discretization + Collocation

Now enforce the collocation requirement that Ψ equals the right-hand side g at n selected points:

$$\Psi(s_i) = g(s_i) \ , \qquad i = 1, \ldots, n \ ,$$

where $g(s_i)$ are sampled/measured values of the function g.

Must neglect the error term $R_n(s)$, and thus replace $f(t_j)$ by $\tilde{f}_j$:

$$\sum_{j=1}^{n} w_j \, K(s_i, t_j) \, \tilde{f}_j = g(s_i), \quad i = 1, \ldots, n \ .$$

Could use $m > n$ collocation points $\rightarrow$ overdetermined system.

The Discrete Problem in Matrix Form

Write out the last equation to obtain

$$\begin{pmatrix} w_1 K(s_1, t_1) & w_2 K(s_1, t_2) & \cdots & w_n K(s_1, t_n) \\ w_1 K(s_2, t_1) & w_2 K(s_2, t_2) & \cdots & w_n K(s_2, t_n) \\ \vdots & \vdots & & \vdots \\ w_1 K(s_n, t_1) & w_2 K(s_n, t_2) & \cdots & w_n K(s_n, t_n) \end{pmatrix} \begin{pmatrix} \tilde{f}_1 \\ \tilde{f}_2 \\ \vdots \\ \tilde{f}_n \end{pmatrix} = \begin{pmatrix} g(s_1) \\ g(s_2) \\ \vdots \\ g(s_n) \end{pmatrix}$$

or simply

$$\boxed{A\,x = b}$$

where A is $n \times n$ with

$$\left. \begin{aligned} a_{ij} &= w_j \, K(s_i, t_j) \\ x_j &= \tilde{f}(t_j) \\ b_i &= g(s_i) \end{aligned} \right\} \qquad i, j = 1, \ldots, n \ .$$

The midpoint rule $t_j = \frac{j-0.5}{n}$ gives $a_{ij} = n^{-1} K(s_i, t_j)$.

Discretization: the Galerkin Method

Select two sets of functions ϕ_i and ψ_j, and write

$$\begin{aligned} f(t) &= f^{(n)}(t) + E_f(t), \qquad f^{(n)}(t) \in \mathrm{span}\{\phi_1, \ldots, \phi_n\} \\ g(s) &= g^{(n)}(s) + E_g(s), \qquad g^{(n)}(s) \in \mathrm{span}\{\psi_1, \ldots, \psi_n\} \ . \end{aligned}$$

Write $f^{(n)}$ as the expansion

$$f^{(n)}(t) = \sum_{j=1}^{n} \zeta_j \, \phi_j(t)$$

and define the function

$$\begin{aligned} \vartheta(s) &= \int_0^1 K(s,t) \, f^{(n)}(t) \, dt = \sum_{j=1}^{n} \zeta_j \int_0^1 K(s,t) \, \phi_j(t) \ dt \\ &= \vartheta^{(n)}(s) + E_\vartheta(s) \ , \qquad \vartheta^{(n)} \in \mathrm{span}\{\psi_1, \ldots, \psi_n\} \ . \end{aligned}$$

Note that, in general, ϑ does not lie in the same subspace as $g^{(n)}$.

Computation of the Galerkin Solution

The best we can do is to require that $\vartheta^{(n)}(s) = g^{(n)}(s)$ for $s \in [0, 1]$.

This is equivalent to requiring that the residual $g(s) - \vartheta(s)$ is orthogonal to $\mathrm{span}\{\psi_1, \ldots, \psi_n\}$, which is enforced by

$$\langle \psi_i \, , \, g \rangle = \langle \psi_i \, , \, \vartheta \rangle = \left\langle \psi_i \, , \int_0^1 K(s,t) \, f^{(n)}(t) \, dt \right\rangle , \qquad i = 1, \ldots, n.$$

Inserting the expansion for $f^{(n)}$, we obtain the $n \times n$ system

$$\boxed{A \, x = b}$$

with $x_i = \zeta_i$ and

$$\begin{aligned} a_{ij} &= \int_0^1 \int_0^1 \psi_i(s) \, K(s,t) \, \phi_j(t) \, ds \, dt \\ b_i &= \int_0^1 \psi_i(s) \, g(s) \, ds \ . \end{aligned}$$

The Singular Value Decomposition

Assume that A is $m \times n$ and, for simplicity, also that $m \geq n$:

$$A = U \, \Sigma \, V^T = \sum_{i=1}^{n} u_i \, \sigma_i \, v_i^T .$$

Here, Σ is a diagonal matrix with the *singular values*, satisfying

$$\Sigma = \mathrm{diag}(\sigma_1, \ldots, \sigma_n) \ , \qquad \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0 \ .$$

The matrices U and V consist of *singular vectors*

$$U = (u_1, \ldots, u_n) \ , \qquad V = (v_1, \ldots, v_n)$$

and both matrices have orthonormal columns: $U^T U = V^T V = I_n$.

Then $\|A\|_2 = \sigma_1$, $\|A^{-1}\|_2 = \|V \, \Sigma^{-1} U^T\|_2 = \sigma_n^{-1}$, and

$$\mathrm{cond}(A) = \|A\|_2 \, \|A^{-1}\|_2 = \sigma_1 / \sigma_n .$$

SVD Software for Dense Matrices

Software package	Subroutine
ACM TOMS	`HYBSVD`
EISPACK	`SVD`
IMSL	`LSVRR`
LAPACK	`_GESVD`
LINPACK	`_SVDC`
NAG	`F02WEF`
Numerical Recipes	`SVDCMP`
Matlab	`svd`, `ssvd`

Complexity of SVD algorithms: $\mathcal{O}(m \, n^2)$.

Important SVD Relations

Relations similar to the SVE

$$A\,v_i = \sigma_i\,u_i, \qquad \|A\,v_i\|_2 = \sigma_i, \qquad i = 1,\ldots,n.$$

Also, if A is nonsingular, then

$$A^{-1}u_i = \sigma_i^{-1}\,u_i, \qquad \|A^{-1}v_i\|_2 = \sigma_i^{-1}, \qquad i = 1,\ldots,n.$$

These equations are related to the (least squares) solution:

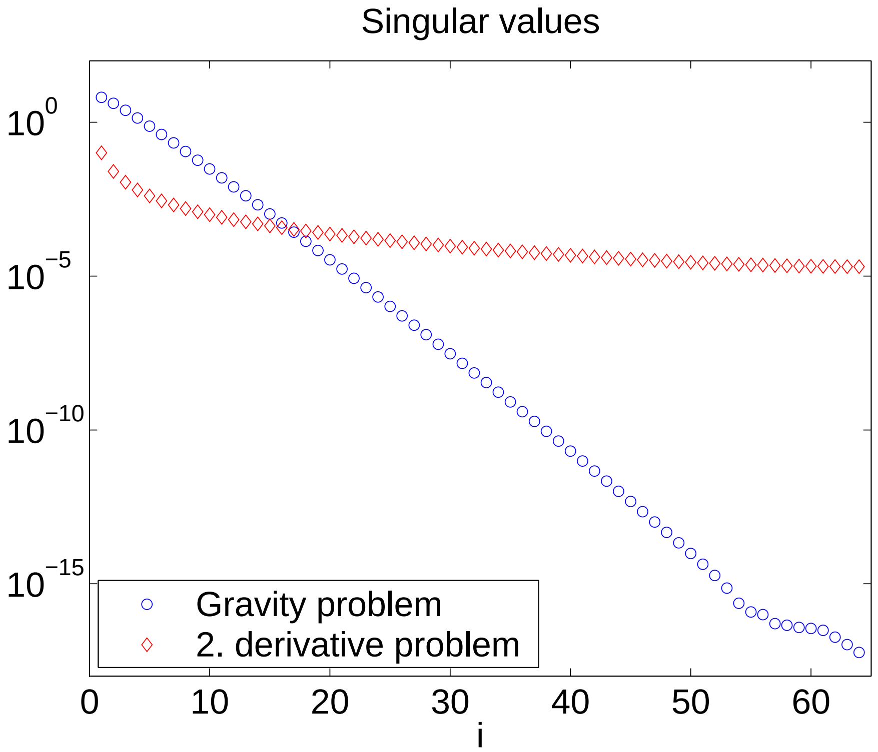
$$\begin{aligned} x &= \sum_{i=1}^{n} (v_i^T x)\,v_i \\ A\,x &= \sum_{i=1}^{n} \sigma_i\,(v_i^T x)\,u_i\ , \quad b = \sum_{i=1}^{n} (u_i^T b)\,u_i \\ A^{-1}b &= \sum_{i=1}^{n} \frac{u_i^T b}{\sigma_i}\,v_i\ . \end{aligned}$$

What the SVD Looks Like

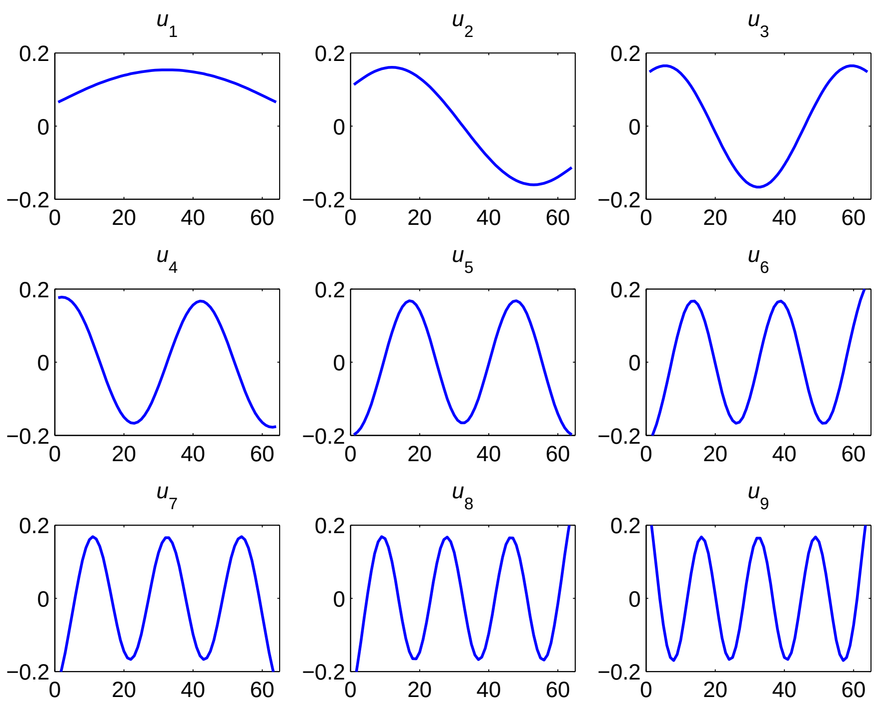
The following figures show the SVD of the 64×64 matrix A, computed by means of `csvd` from Regularization Tools:

```
>> help csvd
 CSVD Compact singular value decomposition.

  s = csvd(A)
  [U,s,V] = csvd(A)
  [U,s,V] = csvd(A,'full')

  Computes the compact form of the SVD of A:
     A = U*diag(s)*V',
  where
     U  is  m-by-min(m,n)
     s  is  min(m,n)-by-1
     V  is  n-by-min(m,n).

  If a second argument is present, the full U and V are returned.
```

The Singular Values



The Left and Right Singular Vectors

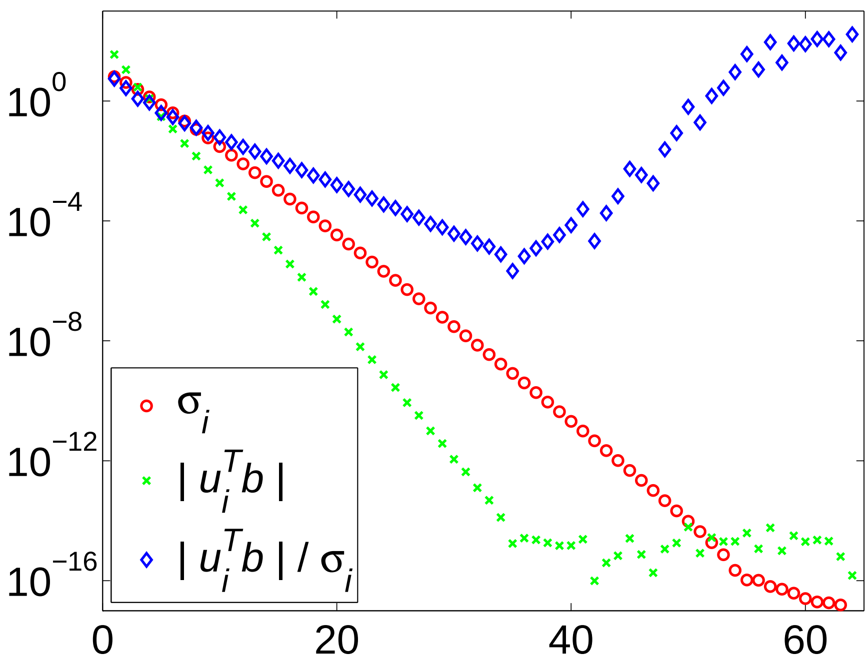


Some Observations

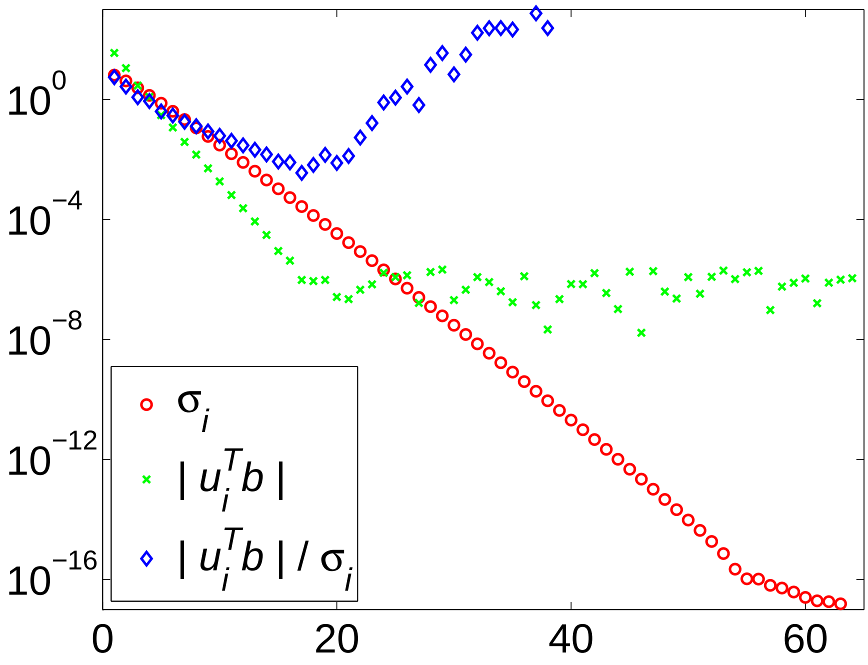
- The singular values decay gradually to zero.
- No gap in the singular value spectrum.
- Condition number cond(A) = "∞."
- Singular vectors have more oscillations as i increases.
- In this problem, # sign changes = $i - 1$.

The following pages: Picard plots with increasing noise.

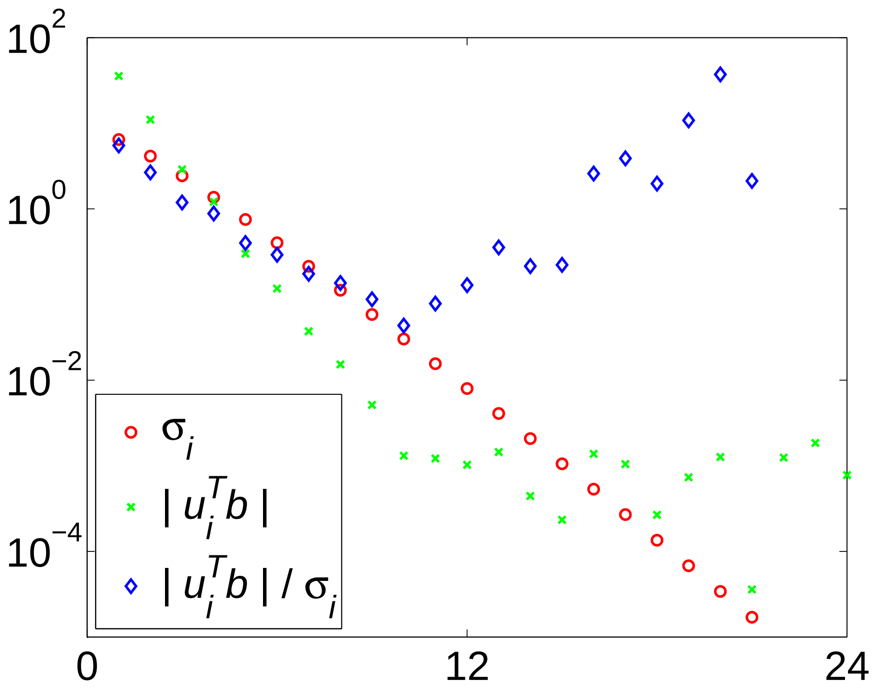
The Discrete Picard Plot



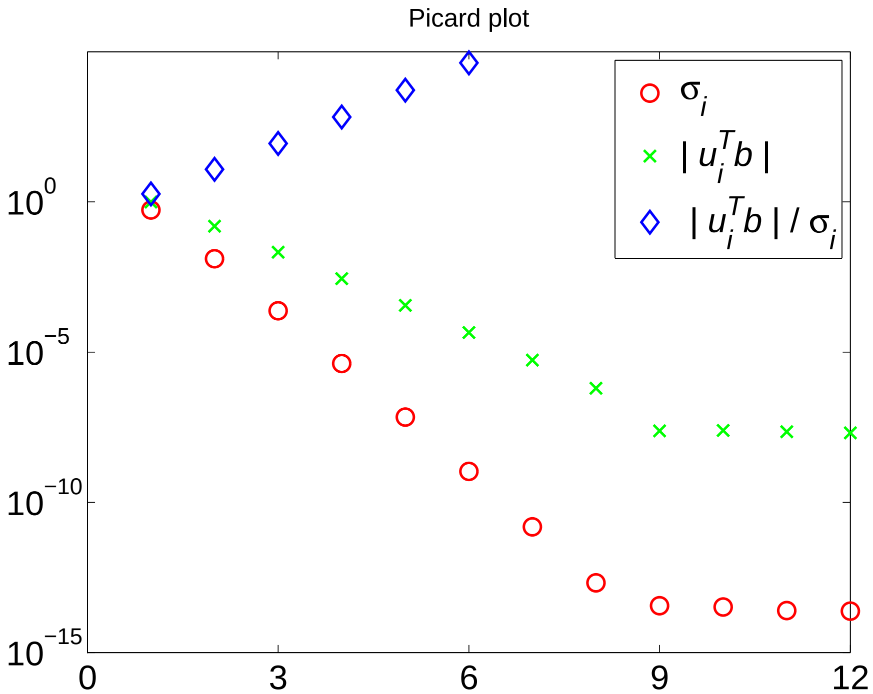
Discrete Picard Plot with Noise



Discrete Picard Plot – More Noise



The Ursell Problem



The Discrete Picard Condition

The relative decay of the singular values σ_i and the right-hand side's SVD coefficients $u_i^T b$ plays a major role!

The Discrete Picard Condition is satisfied if the coefficients $|u_i^T b^{\mathrm{exact}}|$, on the average, *decay* to zero faster than the corresponding singular values σ_i.

Computation of the SVE

Based on the Galerkin method with orthonormal ϕ_i and ψ_j.

1. Discretize K to obtain $n \times n$ matrix A, and compute its SVD.
2. Then $\sigma_j^{(n)} \rightarrow \mu_j$ as $n \rightarrow \infty$.
3. Define the functions

$$\begin{aligned} u_j^{(n)}(s) &= \sum_{i=1}^{n} u_{ij}\, \psi_i(s) , \qquad j = 1, \ldots, n \\ v_j^{(n)}(t) &= \sum_{i=1}^{n} v_{ij}\, \phi_i(t) , \qquad j = 1, \ldots, n . \end{aligned}$$

   Then $u_j^{(n)}(s) \rightarrow u_j(s)$ and $v_j^{(n)}(t) \rightarrow v_j(t)$ as $n \rightarrow \infty$.

4. Finally, the right-hand side coefficients satisfy

$$u_j^T b = \langle u_j^{(n)}, g^{(n)} \rangle \rightarrow \langle u_j, g \rangle \quad \text{as} \quad n \rightarrow \infty.$$

More Precise Results

Let

$$\|K\|_2^2 \equiv \int_0^1 \int_0^1 |K(s,t)|^2\, ds\, dt , \qquad \delta_n^2 \equiv \|K\|_2^2 - \|A\|_{\mathrm{F}}^2 .$$

Then for $i = 1, \ldots, n$

$$0 \le \mu_i - \sigma_i^{(n)} \le \delta_n$$

$$\sigma_i^{(n)} \le \sigma_i^{(n+1)} \le \mu_i$$

Also it can be shown that

$$\max \{ \|u_1 - u_1^{(n)}\|_2 \, , \, \|v_1 - v_1^{(n)}\|_2 \} \le \left(\frac{2\, \delta_n}{\mu_1 - \mu_2} \right)^{1/2} .$$

Similar, but more complicated, results hold for the remaining singular functions.

Noisy Problems

Real problems have noisy data! Recall that we consider problems

$$\boxed{A\,x = b} \qquad \text{or} \qquad \boxed{\min_x \|A\,x - b\|_2}$$

with a very ill-conditioned coefficient matrix A,

$$\text{cond}(A) \gg 1.$$

Noise model:

$$b = b^{\text{exact}} + e, \qquad \text{where} \qquad b^{\text{exact}} = A\,x^{\text{exact}}\ .$$

The ingredients:

- x^{exact} is the exact (and unknown) solution,
- b^{exact} is the exact data, and
- the vector e represents the noise in the data.

Statistical Issues

Let $\text{Cov}(b)$ be the covariance for the right-hand side.

Then the covariance matrix for the (least squares) solution is

$$\text{Cov}(x) = A^{-1}\,\text{Cov}(b)\,A^{-T}.$$

$$\text{Cov}(x_{\text{LS}}) = (A^T A)^{-1} A^T\,\text{Cov}(b)\,A\,(A^T A)^{-1}.$$

Unless otherwise stated, we assume for simplicity that b^{exact} and e are uncorrelated, and that

$$\text{Cov}(b) = \text{Cov}(e) = \eta^2 I,$$

then

$$\text{Cov}(x) = \text{Cov}(x_{\text{LS}}) = \eta^2 (A^T A)^{-1}.$$

$\text{cond}(A) \gg 1 \Rightarrow$

$\text{Cov}(x)$ and $\text{Cov}(x_{\text{LS}})$ are likely to have very large elements.

Need for Stabilization = Noise Reduction

Recall that the (least squares) solution is given by

$$x = \sum_{i=1}^{n} \frac{u_i^T b}{\sigma_i} \, v_i .$$

Must get rid of the "noisy" SVD components. Note that

$$u_i^T b = u_i^T b^{\mathrm{exact}} + u_i^T e \approx \begin{cases} u_i^T b^{\mathrm{exact}}, & |u_i^T b^{\mathrm{exact}}| > |u_i^T e| \\ u_i^T e, & |u_i^T b^{\mathrm{exact}}| < |u_i^T e| . \end{cases}$$

Hence, due to the DPC:

- "noisy" SVD components are those for which $|u_i^T b^{\mathrm{exact}}|$ is small,
- and therefore they correspond to the smaller singular values σ_i.