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Rational Krylov methods for inverse problems

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INSTITUT FÜR ANGEWANDTE UND NUMERISCHE MATHEMATIK

Outline

Inverse problems and discrete inverse problems
- Ill-posed problems
- Discrete ill-posed problems

Regularisation schemes
- Deblurring
- Iterated Tikhonov method

Rational Krylov subspace method
- Rational Krylov regularisation
- Implementation issues

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Ill-posed problems

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We consider

$$Ax = b$$

where A is a bounded operator between Hilbert spaces $\mathcal{X}$ and $\mathcal{Y}$.

An well-posed problem (Hadamard, 1902) is given whenever

- a solution exists
- the solution is unique
- solution depends continuously on the data ($b \mapsto x$ bounded)

otherwise the problem is termed ill-posed.

Inverse problems are typically ill-posed. Often, the term inverse problem is used when ill-posed problem is meant.

Discrete ill-posed problems

Linear system of equations

$$Ax = b$$

where $A \in \mathbb{C}^{m \times n}$, $b \in \mathbb{C}^m$.

An discrete well-posed problem is given whenever

- a solution exists
- the solution is unique
- computing the solution is well-conditioned

otherwise the problem is termed discret ill-posed.

Remarks:

- $\|A\|$ can be scaled to be 1 or at leased assumed to be moderate
- $\|\cdot\|$ designates Euclidean norm or spectral matrix norm

Moore–Penrose pseudoinverse

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First two conditions of “well-posed” always satisfied with the minimum norm solution

$$x^+ = A^+ b \qquad \text{of} \qquad Ax = b\,,$$

where A^+ is the Moore–Penrose pseudoinverse.

Lemma

With the set of all least-squares solutions

$$\mathrm{Ls} := \{x \in \mathbb{C}^n \mid A^* A x = A^* b\} = \operatorname{argmin}_{x \in \mathbb{C}^n} \|b - Ax\|^2$$

the minimum norm solution x^+ can be characterised as

$$x^+ \in \mathrm{Ls} \quad \text{and} \quad \|x^+\| = \min_{x \in \mathrm{Ls}} \|x\|$$

or

$$x^+ \in \mathrm{Ls} \quad \text{and} \qquad x^+ \perp \ker(A)$$

The problem with discrete ill-posed problems

Instead of right-hand side b only perturbed data with noise-leven δ

$$b^\delta = b + e, \qquad \|e\| \leq \delta$$

known. Exact solution

$$x^{\delta,+} = A^+ b^\delta$$

useless due to ill-conditioning.

Deblurring

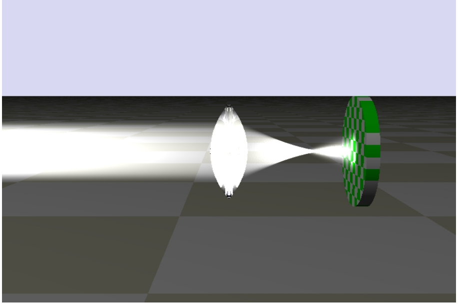
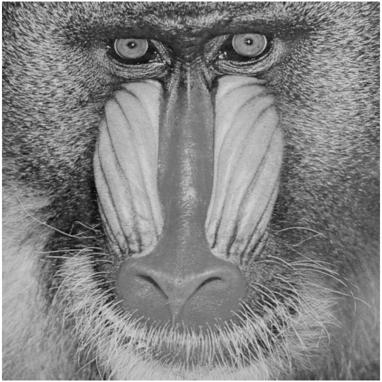
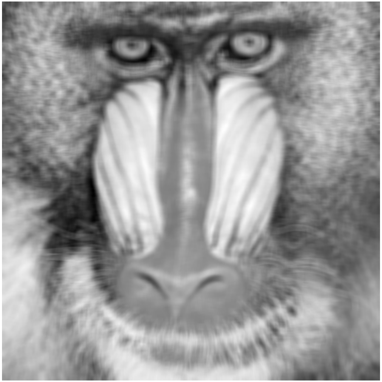
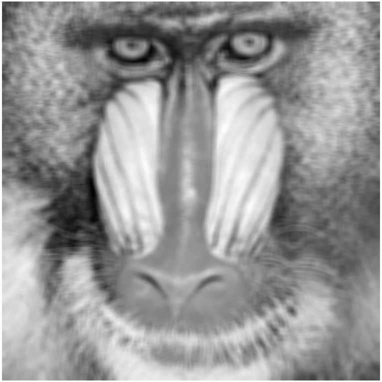


Image and blurred image





Blurred image with noiselevel $\delta < 0.001$



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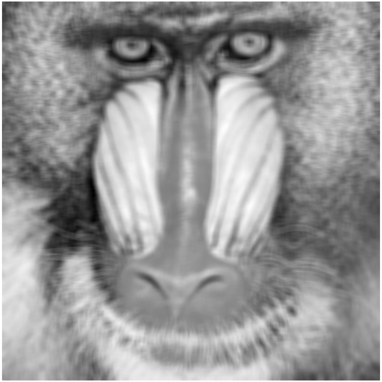
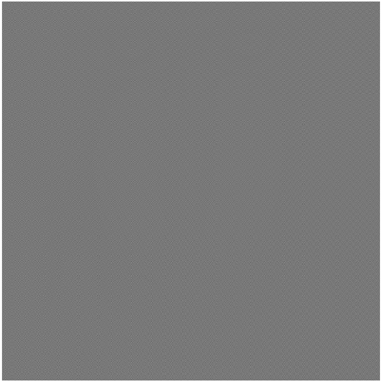




Tikhonov regularisation

Instead of least-squares solution, minimize the Tikhonov functional

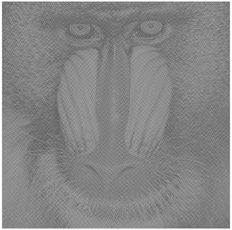
$$\min_{x \in \mathbb{C}^n} \frac{1}{2} \|Ax - b^\delta\|^2 + \frac{\gamma}{2} \|x\|^2$$

with regularisation parameter γ. Unique solution is

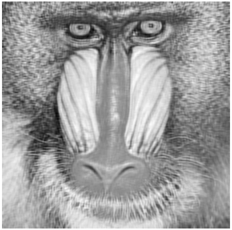
$$x_{\text{Tik}} = (\gamma I + A^* A)^{-1} A^* b$$

Problem: How to choose the regularisation parameter γ?

$\gamma = 0.0000001$



$\gamma = 0.01$



$\gamma = 100$

Iterated Tikhonov method

Given approximation $x_0 \in \mathbb{C}^n$, iterate

$$x_{k+1} = x_k + (\gamma I + A^*A)^{-1} A^*(b^\delta - Ax_k), \qquad k = 0, 1, 2, \ldots$$

Stop, if discrepancy principle

$$\|r_{k+1}\| = \left\| b^\delta - Ax_{k+1} \right\| \leq \tau\delta$$

$\tau > 1$, is satisfied.

If we set $x_0 = 0$ (w.l.o.g), then

$$x_{k+1} = \sum_{\ell=0}^{k} \left(\gamma A^*A(\gamma I + A^*A)^{-1} \right)^{\ell} (\gamma I + A^*A)^{-1} A^* b$$

Rational Krylov subspace

If we choose $x_0 = (\gamma I + A^*A)^{-1}A^*b$, we have

$$x_m \in \mathcal{K}_m((\gamma I + A^*A)^{-1}, A^*b)$$

The space

$$\begin{aligned}
\mathcal{Q}_m &= \mathcal{K}_m((\gamma I + A^*A)^{-1}, A^*b) \\
&= \text{span}\left\{A^*b, (\gamma I + A^*A)^{-1}A^*b, \dots, (\gamma I + A^*A)^{-m+1}A^*b\right\} \\
&= \left\{ \frac{p_m(A^*A)}{(\gamma + A^*A)^m} A^*b \,\middle|\, p_m \in \mathcal{P}_m \right\}
\end{aligned}$$

is an example of a rational Krylov subspace, the shift-and-invert or resolvent Krylov subspace

Rational Krylov subspace method

Determine

$$x_m \in \mathcal{Q}_m \qquad \text{such that} \qquad \|r_m\| = \|b - Ax_m\| = \min_{x \in \mathcal{Q}_m} \|b - Ax\|$$

best choice with respect to $\mathcal{Q}_m$ and the discrepancy principle.

Lemma

The minimizer x_m is unique. If $m = m^*$ is the invariance index of $\mathcal{Q}_m$, then $x_m^* = x^+ = A^+ b$.

Rational Krylov subspace method

Lemma

The minimizer x_m is unique. If $m = m^*$ is the invariance index of $\mathcal{Q}_m$, then $x_m^* = x^+ = A^+ b$.

Proof

We have

$$\mathcal{Q}_m \subseteq \ker(A)^\perp = \ker(A^*A)^\perp$$

and

$$\min_{x \in \mathcal{Q}_m} \|b - Ax\| = \min_{y \in A\mathcal{Q}_m} \|b - y\| = \|b - \Pi_{A\mathcal{Q}_m} b\|$$

Hence, $\Pi_{A\mathcal{Q}_m} b$ is unique, and since $\mathcal{Q}_m \subseteq \ker(A)^\perp$, A is injective on $\mathcal{Q}_m$ and there is a unique x_m such that $Ax_m = \Pi_{A\mathcal{Q}_m} b$.

Rational Krylov subspace method

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Lemma

The minimizer x_m is unique. If $m = m^*$ is the invariance index of $\mathcal{Q}_m$, then $x_m^* = x^+ = A^+ b$.

Proof

If $m = m^*$, we have

$$A^* A \mathcal{Q}_{m^*} \subset \mathcal{Q}_{m^*}$$

and since $\mathcal{Q}_{m^*} \perp \ker(A^* A)$, we can conclude that

$$A^* A \mathcal{Q}_{m^*} = \mathcal{Q}_{m^*}$$

This means, that there is an u_{m^*} such that

$$A^* A u_{m^*} = A^* b$$

Necessarily, $x_{m^*} = u_{m^*} \in \mathrm{Ls}$ is a least-squares solution with $x_{m^*} \in \mathcal{Q}_{m^*} \subset \ker(A)^\perp$. Hence, $x_{m^*} = x^+$.

Computation of x_m

The unique

$$x_m = \operatorname{argmin}_{x \in \mathcal{Q}_m} \|b - Ax\|$$

satisfies

$$(b - Ax_m, Au) = 0 \qquad \forall u \in \mathcal{Q}_m$$
$$(A^*b - A^*Ax_m, u) = 0 \qquad \forall u \in \mathcal{Q}_m$$

Let V_m be an orthonormal basis of $\mathcal{Q}_m$, then

$$V_m^*(A^*b - A^*AV_m y_m) = 0 \qquad \Leftrightarrow \qquad \beta e_1 = S_m y_m$$

where $\beta = \|A^*b\|$. $S_m = V_m^* A^* A V_m$ is positive definite for $m \leq m^*$ (proof necessary) and Hermitian (since A^*A is) and therefore

$$x_m = V_m y_m, \qquad y_m = \beta S_m^{-1} e_1$$

Who does not like CG-like

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Standard rational recurrence

$$
\begin{aligned}
(\gamma I + A^*A)^{-1} V_m &= V_m H_m + h_{m+1,m} v_{m+1} e_m^T \\
S_m &= V_m^* A^* A V_m, \\
x_m &= V_m S_m^{-1} V_m^* A^* b, \qquad V_m^* V_m = I_m
\end{aligned}
$$

CG-like recurrence

$$
\begin{aligned}
(\gamma I + A^*A)^{-1} W_m &= W_m H_m + h_{m+1,m} w_{m+1} e_m^T \\
x_m &= W_m W_m^* A^* b, \qquad W_m^* A^* A W_m = I_m
\end{aligned}
$$

Reasoning, why $x_m = x_m$

We know

$$x_m = \operatorname{argmin}_{x \in \mathcal{Q}_m} \|b - Ax\|$$

uniquely determinded by

$$(A^* b - A^* A x_m, u) = 0 \qquad \forall u \in \mathcal{Q}_m$$

W_m orthonormal basis of $\mathcal{Q}_m$ with respect to $(x, y)_{A^*A} = y^* A^* A x$

$$W_m^*(A^* b - A^* A W_m y_m) = 0 \qquad \Leftrightarrow \qquad W_m^* A^* b - \underbrace{W_m^* A^* A W_m}_{I_m} y_m = 0$$

This leads to

$$x_m = W_m y_m = W_m W_m^* A^* b$$

(Since $\mathcal{Q}_m \perp \ker(A^*A)$, $(\cdot, \cdot)_{A^*A}$ inner product on $\mathcal{Q}_m$)

Shift-and-invert on the normal equations (SINE)

Set $x_0 = 0$, $r_0 = b - Ax_0$, $w_0 = A^* r_0$.
for $j = 0, 1, 2, \ldots$ **do**

$q_j = A w_j$
$\delta_j = (q_j, q_j)$
$\alpha_j = \left(r_j, q_j\right) / \delta_j$
$x_{j+1} = x_j + \alpha_j w_j$
$r_{j+1} = r_j - \alpha_j q_j$
If $\|r_{j+1}\| \leq \tau\delta$, stop (discrepancy principle)
$s_j = A^* q_j$
$t_{j+1} = (\gamma I + A^* A)^{-1} A^* r_{j+1}$
$\beta_j = \left(t_{j+1}, s_j\right) / \delta_j$
$w_{j+1} = t_{j+1} - \beta_j w_j$

end for

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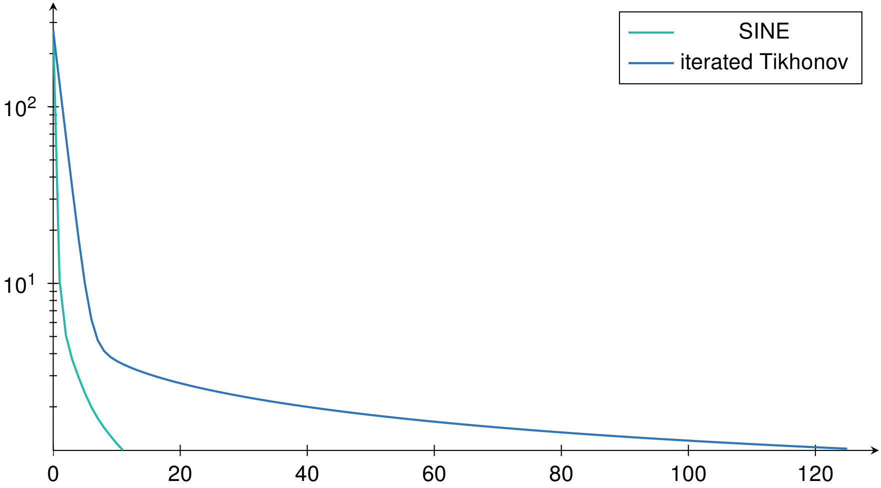
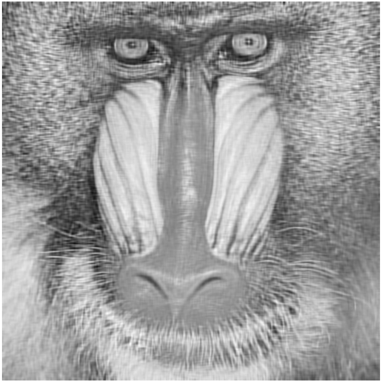
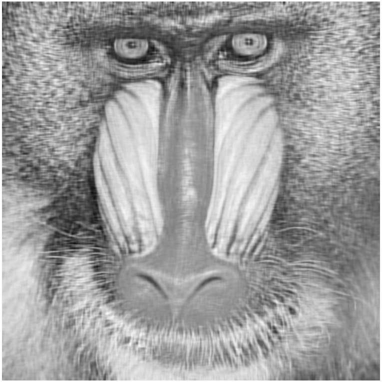
Residuum vs steps



SINE and iterated Tikhonov regularisation





Outlook

- Works similarly for more general rational Krylov subspaces

$$\mathcal{Q}_m = \left\{ \frac{p_m(A^*A)}{q_m(A^*A)} A^* b \,\middle|\, p_m \in \mathcal{P}_m \right\}, \qquad q_m(z) = \prod_{\ell=1}^{m} (z + c_\ell)$$

$c_\ell > 0$, $\ell = 1, \ldots, m$.

  - Uniqueness of bestappoximation in $\mathcal{Q}_m$
  - Needs to save more vectors, but does not need a continuation vector
  - Acceleration of nonstationary iterated Tikhonov

- SINE is an optimal order regularisation scheme for ill-posed problems with bounded $A \in \mathcal{L}(\mathcal{X}, \mathcal{Y})$, $\mathcal{X}$, $\mathcal{Y}$ Hilbert spaces.