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Rational Krylov methods for inverse problems

Volker Grimm

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Outline

Inverse problems and discrete inverse problems

- Ill-posed problems

Regularisation schemes

- Multiplication operator
- Order-optimal regularisation schemes

Rational Krylov subspace method

- SINE algorithm
- Convergence
- Regularisation properties

Ill-posed problems

We consider

$$Tx = y$$

where T 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 ($y \mapsto x$ 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.

Moore–Penrose pseudoinverse

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

$$x^+ = T^+ b \qquad \text{of} \qquad Tx = y\,,$$

where $T^+ : \mathcal{D}(T^+) = \mathcal{R}(T) \oplus \mathcal{R}(T)^\perp \to \mathcal{N}(T)^\perp$ is the Moore–Penrose pseudoinverse.

Lemma

The set of all least-squares solutions

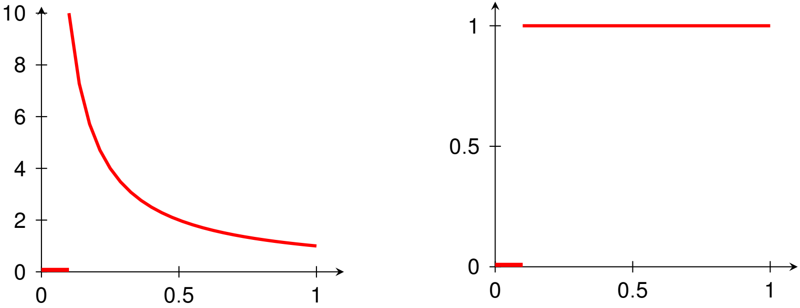
$$\mathrm{Ls} := \{x \in \mathcal{X} \mid T^*Tx = T^*y\} = \mathrm{argmin}_{x\in\mathcal{X}} \|y - Tx\|$$

is not empty for $y \in \mathcal{D}(T^+)$ and the minimum norm solution x^+ can be characterised as

$$x^+ \in \mathrm{Ls} \qquad \text{and} \qquad x^+ \perp \mathcal{N}(T)^\perp$$

Multiplication operator

- T^+ bounded if and only if $\mathcal{R}(T)$ is closed.
- $Tx = y$ ill-posed problem if and only if T^+ is unbounded.
- $T : L_2(0,1) \to L_2(0,1)$, $(Tx)(t) := t \cdot x(t)$



The problem with ill-posed problems

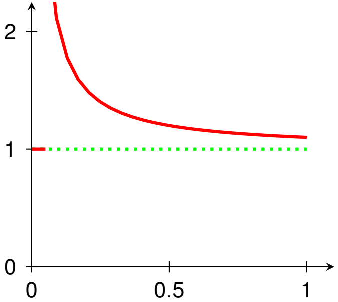
Instead of right-hand side y only perturbed data with noise-level δ

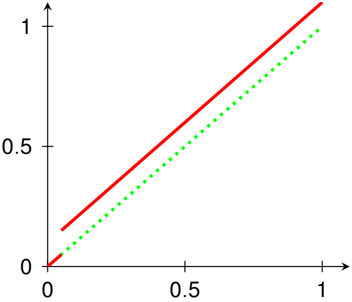
$$y^\delta = y + e, \qquad \|e\| \leq \delta$$

known. Exact solution

$$x^{\delta,+} = T^+ y^\delta$$

not existent or useless due to ill-posedness.





(Iterative) Regularisation schemes

Let $\{R_m\}_{m\in\mathbb{N}_0}$ be a family (sequence) of continuous linear or nonlinear operators from $\mathcal{Y}$ to $\mathcal{X}$ with $R_m 0 = 0$. If there exists a mapping $m : \mathbb{R}^+ \times \mathcal{Y} \to \mathbb{N}_0$ such that for any $x^+ \in \mathcal{N}(T)^\perp$

$$\limsup_{\delta\to 0}\{\|R_{m(\delta,y^\delta)}y^\delta - x^+\| \mid y^\delta \in \mathcal{Y}, \|y^\delta - Tx^+\| \leq \delta\} = 0$$

holds true, then the pair $(R_m, m(\delta, y^\delta))$ is called a (convergent) regularisation scheme for T.

The mapping m is called parameter choice or stopping rule.

Dicrepancy principle: Choose a fixed $\tau > 1$ and set:

$$m(\delta, y^\delta) := \min\{m \in \mathbb{N}_0 \mid \|y^\delta - Tx_m^\delta\| \leq \tau\delta\}\,, \tag{1}$$

where $x_m^\delta := R_m y^\delta$.

Functional calculus

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Spectral families

$$
\begin{aligned}
E_\lambda &= \mathbf{1}_{(-\infty,\lambda]}(T^*T) \\
F_\lambda &= \mathbf{1}_{(-\infty,\lambda]}(TT^*)
\end{aligned}
$$

Operator functions

$$
\begin{aligned}
f(T^*T) &= \int_{-\infty}^{\infty} f(\lambda)\, dE_\lambda \\
f(TT^*) &= \int_{-\infty}^{\infty} f(\lambda)\, dF_\lambda
\end{aligned}
$$

Scalar products

$$
\begin{aligned}
(f(T^*T)x, y) &= \int_{-\infty}^{\infty} f(\lambda)\, d(E_\lambda x, y) \\
\|f(T^*T)x\|^2 &= \int_{-\infty}^{\infty} f^2(\lambda)\, d\|E_\lambda x\|^2
\end{aligned}
$$

Convergence rates

- source set $\mathcal{X}_{\mu,\rho} := \{x \in \mathcal{X} \mid x = (T^*T)^\mu w,\ \|w\| \leq \rho\}$, $\mu > 0$
- For the multiplication operator $(Tx)(t) = t \cdot x(t)$, we have $((T^*T)^\mu x)(t) = t^{2\mu} \cdot x(t)$.

Definition

Regularisation schemes $(R_m, m(\delta, y^\delta))$ of optimal order in $\mathcal{X}_{\mu,\rho}$ if

$$\sup\{\|R_{m(\delta,y^\delta)} y^\delta - x^+\| \mid x^+ \in \mathcal{X}_{\mu,\rho}, \|y^\delta - Tx^+\| \leq \delta\} \leq C_\mu \delta^{\frac{2\mu}{2\mu+1}} \rho^{\frac{1}{2\mu+1}},$$

where C_μ neither depends on δ nor on ρ.

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Rational Krylov subspace and SINE

Shift-and-invert or resolvent Krylov subspace

$$\begin{aligned}\mathcal{Q}_m &= \mathcal{K}_m((\gamma I + T^*T)^{-1}, T^*y^\delta)\\ &= \operatorname{span}\left\{T^*y^\delta, (\gamma I + T^*T)^{-1}T^*y^\delta, \ldots, (\gamma I + T^*T)^{-m+1}T^*y^\delta\right\}\\ &= \left\{\frac{p_m(T^*T)}{(\gamma + T^*T)^m}T^*y^\delta \,\middle|\, p_m \in \mathcal{P}_m\right\}\end{aligned}$$

Shift-and-invert on the normal equation (SINE)
Determine

$$x_m^\delta \in \mathcal{Q}_m \qquad \text{such that} \qquad \|r_m\| = \|y^\delta - Tx_m\| = \min_{x \in \mathcal{Q}_m} \|y^\delta - Tx\|$$

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

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

Set $x_0 = 0$, $r_0 = y^\delta - Tx_0$, $w_0 = T^* r_0$.
for $j = 0, 1, 2, \ldots$ **do**

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

end for

Properties

Lemma

As long as $q_{m-1} \neq 0$: $(r_m, q_j) = (T^* r_m, w_j) = 0, j = 0, \ldots, m-1$

Lemma

If the algorithm breaks down in step κ with $q_\kappa = 0$, then $x_\kappa = x^+ = T^+ y^\delta$.

Proof

$$\begin{aligned} 0 &= (r_\kappa, q_\kappa) = (T^* r_\kappa, w_\kappa) = (T^* r_\kappa, t_\kappa - \beta_{\kappa-1} w_{\kappa-1}) = (T^* r_\kappa, t_\kappa) \\ &= ((I + T^* T/\gamma) t_\kappa, t_\kappa) = (t_\kappa, t_\kappa) + \frac{1}{\gamma}(T t_\kappa, T t_\kappa) \\ &= \|t_\kappa\|^2 + \frac{1}{\gamma}\|T t_\kappa\|^2 . \end{aligned}$$

Hence we have $0 = (I + T^* T/\gamma) t_\kappa = T^* r_\kappa$ in all cases. This means

$$T^* T x_\kappa = T^* y^\delta, \qquad x_\kappa \in \mathcal{Q}_\kappa \subseteq \mathcal{N}(T)^\perp,$$

which characterises the least-squares solution, that is $x_\kappa = x^+$.

Properties

Lemma

The iterates x_m of SINE satisfy $\|r_m\| = \min_{x \in \mathcal{Q}_m} \|y^\delta - Tx\|$.

Proof

Let $z_m \in \mathcal{Q}_m = \operatorname{span}\{w_0, \ldots, w_{m-1}\}$. Since $x_m \in \mathcal{Q}_m$, we can write

$$z_m - x_m = \sum_{j=0}^{m-1} \xi_j w_j, \qquad \xi_j \in \mathbb{R}.$$

Hence

$$\begin{aligned} \|y^\delta - Tz_m\|^2 &= \|y^\delta - Tx_m\|^2 - 2\sum_{j=0}^{m-1} \xi_j (Tw_j, r_m) + \|T\sum_{j=0}^{m-1} \xi_j w_j\|^2 \\ &\geq \|y^\delta - Tx_m\|^2 - 2\sum_{j=0}^{m-1} \xi_j (q_j, r_m) = \|y^\delta - Tx_m\|^2 \end{aligned}$$

Convergence

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Theorem

The sequence of the SINE approximations $\{x_n\}$ w.r.t. $T \in \mathcal{L}(\mathcal{X}, \mathcal{Y})$ and $y \in \mathcal{D}(T^+)$ with $x_0 \in \mathcal{X}$ converges to $T^+y + \mathcal{P}_{\mathcal{N}(T)}x_0$.

Idea of proof:

- $r_m = r_m(TT^*)y$, $r_m(\lambda) = \frac{p_m(\lambda)}{(1-\lambda/\gamma)^{m-1}}$, $p_m(\lambda) = \Pi_{j=1}^m \left(1 - \frac{\lambda}{\lambda_{j,m}}\right)$
- $\|r_m\| \leq \|F_{\lambda_{1,m}}\varphi_m(TT^*)y\| \leq \max_{0\leq\lambda\leq\lambda_{1,m}} \sqrt{\lambda\varphi_m^2(\lambda)} \quad \|E_{\lambda_{1,m}}x^+\|$.
- $\varphi_m(\lambda) := r_m(\lambda)\left(\frac{\lambda_{1,m}}{\lambda_{1,m}-\lambda}\right)^{\frac{1}{2}}, \qquad 0 \leq \lambda \leq \lambda_{1,m}$
- For $0 < \epsilon \leq \lambda_{1,m}$, we split

$$\|x^+ - x_m\| = \|r_m(T^*T)x^+\| \leq \|E_\epsilon r_m(T^*T)x^+\| + \|(I - E_\epsilon)r_m(T^*T)x^+\|$$

SINE order-optimal regularisation method

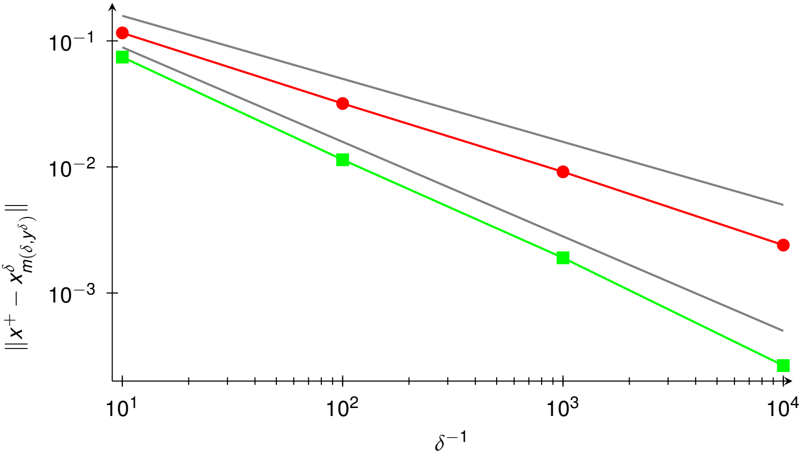
Theorem

If $y \in \mathcal{R}(T)$ *and if* SINE *is stopped according to the discrepancy principle with* $m(\delta, y^\delta)$, *then* SINE *is an order-optimal regularisation method, i.e., if* $T^+ y \in \mathcal{X}_{\mu,\rho}$, *then*

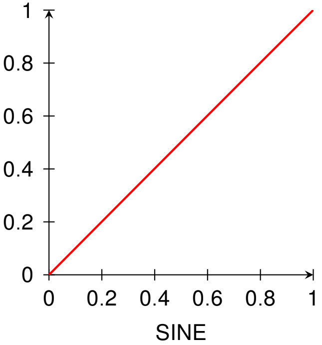
$$\| T^+ y - x^\delta_{m(\delta, y^\delta)} \| \leq c \rho^{\frac{1}{2\mu+1}} \delta^{\frac{2\mu}{2\mu+1}} .$$

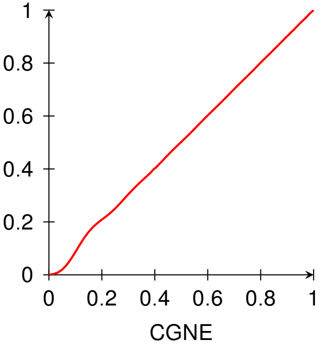
- Proof similar to convergence, including estimate from discrepancy principle
- SINE always stops after finite time

Rate for multiplication operator



SINE vs CGNE





Summary and outlook

- Review of some standard idas in dealing with inverse problems
- SINE is an optimal order regularisation scheme for ill-posed problems with bounded $T \in \mathcal{L}(\mathcal{X}, \mathcal{Y})$, $\mathcal{X}$, $\mathcal{Y}$ Hilbert spaces.
- First to stop amount all methods that use $\mathcal{Q}_m$
- Properties analogous to CGNE in standard Krylov subspace
- Study convergence including discretisation

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