Square regularization matrices for large linear discrete ill-posed problems

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Outline

1. Tikhonov regularization
2. Range restricted Arnoldi and GMRES
3. Square regularization matrices
4. Boundary conditions
5. Numerical results

Large discrete ill-posed problems

$$\mathbf{b} = A\mathbf{x} + \mathbf{e}$$

- $A \in \mathbb{R}^{n \times n}$ large and severely ill-conditioned
- $\mathbf{b} \in \mathbb{R}^n$ known, measured data
- $\mathbf{e} \in \mathbb{R}^n$ noise,

Goal: compute approximation of the noise free solution $\mathbf{x}$.

Tikhonov regularization

$$\min_{\mathbf{x}\in\mathbb{R}^n}\{\|A\mathbf{x}-\mathbf{b}\|^2+\mu\|L\mathbf{x}\|^2\} \tag{1}$$

with solution

$$\mathbf{x}_\mu=(A^TA+\mu L^TL)^{-1}A^T\mathbf{b},$$

where we assume that

$$\mathcal{N}(A)\cap\mathcal{N}(L)=\{\mathbf{0}\}.$$

- $\mu>0$ regularization parameter
- L regularization matrix

Regularization matrices

Common choices of regularization matrices $L \in \mathbb{R}^{k \times n}$, $1 \leq k \leq n$, are the identity matrix and scaled finite difference matrices, such as

$$L = \frac{1}{4} \begin{bmatrix} -1 & 2 & -1 & & & & 0 \\ & -1 & 2 & -1 & & & \\ & & \ddots & \ddots & \ddots & & \\ 0 & & & & -1 & 2 & -1 \end{bmatrix} \in \mathbb{R}^{(n-2) \times n}, \qquad (2)$$

$$\mathcal{N}(L) = \mathrm{span}\{[1, 1, \dots, 1]^T, [1, 2, \dots, n]^T\}.$$

Null space of regularization matrices is important!

Vectors in the $\mathcal{N}(L)$ are not damped in Tikhonov regularization problem (1).

Standard form

Tikhonov regularization problems (1) are said to be

- $L = I \rightarrow$ in standard form
- $L \neq I \rightarrow$ in general form

Large-scale Tikhonov regularization problems in standard form

First reduce to a small problem by a few steps of Lanczos bidiagonalization, then determine an approximate solution $\mathbf{y}_\mu$ of the small problem, and finally compute an approximation $\mathbf{x}_\mu$ of (1) [O'Leary and Simmons '81, Björck '88, Golub and von Matt '97].

Reduction in standard form

The A-weighted pseudoinverse of L is [Eldén '82]

$$L_A^{\dagger} = \left(I - (A(I - L^{\dagger}L))^{\dagger} A \right) L^{\dagger} \in \mathbb{R}^{n \times k}.$$

The Tikhonov regularization problem (1) is equivalent to

$$\min_{\bar{\mathbf{x}} \in \mathbb{R}^k} \{ \| A L_A^{\dagger} \bar{\mathbf{x}} - \bar{\mathbf{b}} \|^2 + \mu \| \bar{\mathbf{x}} \|^2 \}. \tag{3}$$

Matrix-vector products with the matrices $L_A^{\dagger}$ and $AL_A^{\dagger}$ can be evaluated quite inexpensively provided that:

1. $\mathcal{N}(L)$ is of small dimension and has an explicitly known basis,
2. matrix-vector product with $L^{\dagger}$ is inexpensive to compute.

Range restricted Arnoldi process

When A is square, reduction to a small problem can also be achieved by few steps of a (range restricted) Arnoldi-type process instead of Lanczos bidiagonalization.
Regularization operators with the Arnoldi process:

- rectangular operators in [Hansen and Jensen '06]
- need to evaluate the norm of the residual

$$\Downarrow$$

L has to be square!

Range restricted GMRES (RR-GMRES)

The solution can be approximated by truncated iteration of RR-GMRES where the ℓth iterated, $\mathbf{x}_\ell$, satisfies

$$\mathbf{x}_\ell = \underset{\mathbf{x} \in \mathcal{K}_\ell(A, A\mathbf{b})}{\operatorname{argmin}} \|A\mathbf{x} - \mathbf{b}\|,$$

with $\mathbf{x}_0 = \mathbf{0}$ and

$$\mathcal{K}_\ell(A, A\mathbf{b}) = \operatorname{span}\{A\mathbf{b}, A^2\mathbf{b}, \ldots, A^\ell\mathbf{b}\}.$$

Preconditioning

- The A-weighted pseudoinverse $L_A^\dagger$ is a popular preconditioner for discrete ill-posed problems [Hanke '92].
- If L is inventible then $L_A^\dagger = L^{-1}$.

Our Goal

L square such that:

1. $\mathcal{N}(L)$ has an explicitly known basis and it contains the main components of the signal,
2. matrix-vector product with $L^\dagger$ is inexpensive to compute.

Square regularization matrices in literature

1. Appending rows to the differential operator [Calvetti et al. '04]

$$\begin{bmatrix} 1 & -1 & 0 & \dots & 0 \\ & 1 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & & 1 & -1 \\ 0 & \dots & 0 & 0 & 10^{-8} \end{bmatrix}, \quad \begin{bmatrix} 1 & -1 & 0 & \dots & 0 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ 0 & \dots & 0 & -1 & 2 \end{bmatrix}$$

2. Orthogonal projectors: $L = I - WW^T$, [Morigi et al. '07].
3. $L = (\hat{C}_2^{\dagger} D_{\delta}^{-1})^{\dagger}$, where $\hat{C}_2$ is the Laplacian circulant matrix with the two smallest eigenvalues changed in zero and $D_\delta = \mathrm{diag}([\delta, 1, \dots, 1, \delta]^T)$, $\delta = 10^{-8}$, [Reichel and Ye '09].

Boundary condition for Laplacian

G. Strang '99:

"The discrete case has a new level of variety and complexity, often appearing in the boundary conditions".

- The boundary conditions affect only the first and the last row.
- Consider a vector $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{x} = (x_0, \ldots, x_{n-1})^T$, corresponding to the approximation of the solution x.

$$\begin{bmatrix} -1 & 2 & -1 & & & 0 \\ & -1 & 2 & -1 & & \\ & & \ddots & \ddots & \ddots & \\ 0 & & & -1 & 2 & -1 \end{bmatrix}_{n\times(n+2)} \begin{bmatrix} x_{-1} \\ x_0 \\ \vdots \\ x_{n-1} \\ x_n \end{bmatrix}$$

Dirichlet boundary conditions

$$u_{-1} = 0 \qquad \text{and} \qquad u_n = 0,$$

$$\Downarrow$$

$$L_D = \begin{bmatrix} 2 & -1 & 0 & \dots & 0 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ 0 & \dots & 0 & -1 & 2 \end{bmatrix},$$

$$\mathcal{N}(L_D) = \{\mathbf{0}\}.$$

Neumann boundary conditions

Midpoint symmetry $u_{-1} = u_0$ and $u_n = u_{n-1}$,

$$\Downarrow$$

$$L_R = \begin{bmatrix} 1 & -1 & 0 & \dots & 0 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ 0 & \dots & 0 & -1 & 1 \end{bmatrix}.$$

$$\mathcal{N}(L_R) = \mathrm{span}\{[1, 1, \dots, 1]^T\}$$

Mixed boundary conditions $\Rightarrow \mathcal{N}(L) = \{\mathbf{0}\}$.

Antireflective boundary conditions

[Serra Capizzano '03]

$$u_{-1} - u_0 = u_0 - u_1 \qquad \text{and} \qquad u_n - u_{n-1} = u_{n-1} - u_{n-2},$$

$$\Downarrow$$

$$L_A = \begin{bmatrix} 0 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ 0 & \dots & 0 & 0 & 0 \end{bmatrix}. \tag{4}$$

$$\mathcal{N}(L_A) = \mathrm{span}\{[1, 1, \dots, 1]^T, [1, 2, \dots, n]^T\}.$$

AR Spectral decomposition

Let h be a cosine real-valued polynomial of degree at most n-3. Then

$$A = AR_n(h) = T_n \mathrm{diag}(h(\hat{\mathbf{y}}))\, T_n^{-1},$$

where $\hat{\mathbf{y}} = [0,\, \tilde{\mathbf{y}}^T,\, 0]^T$, $\tilde{\mathbf{y}} = [\frac{j\pi}{n-1}]_{j=1}^{n-2}$ and

$$T_n = \left[1 - \frac{\mathbf{y}}{\pi},\, \sin(\mathbf{y}),\, \ldots,\, \sin((n-2)\mathbf{y}),\, \frac{\mathbf{y}}{\pi}\right],$$

with $\mathbf{y} = [0,\, \tilde{\mathbf{y}}^T,\, \pi]^T$.

[Aricò et al. '11]

Algebraic interpretation

Eigenvalues and eigenvectors

Let $\mathbf{y}$ be a uniform sampling in $[0, \pi]$:

- $h(0) = 0$ with multiplicity 2 (Laplacian: $h(z) = 2 - 2\cos(z)$)
- $\mathcal{N}(L_A) = \mathrm{span}\{\pi - \mathbf{y}, \mathbf{y}\} \Rightarrow$ preserve linear functions.
- eigenvector $\sin(k\mathbf{y})$ with eigenvalue $\sin\left(\frac{k\pi}{n-1}\right)$, $k = 1, \ldots, n-2$.

G. Strang '99

"We hope that the eigenvector approach will suggest more new transforms, and that one of them will be fast and visually attractive.".

High order BC with cosine basis

Let h be a cosine real-valued polynomial of degree at most n-3. Then

$$A_C(h) = C_n \mathrm{diag}(h(\hat{\mathbf{y}}))C_n^{-1},$$

where $\hat{\mathbf{y}} = [0, \tilde{\mathbf{y}}^T, 0]^T$, $\tilde{\mathbf{y}} = \left[\frac{(j-1)\pi}{n-2}\right]_{j=1}^{n-2}$ and

$$C_n = [\mathbf{h_1}, \cos(0\mathbf{y}), \ldots, \cos((n-3)\mathbf{y}), \mathbf{h_2}],$$

with $\mathbf{y} = \left[\frac{(2i-1)\pi}{2n-4}\right]_{j=0}^{n-1}$.

[D., '10]

Laplacian with high order BC

$$L_H = C_n \mathrm{diag}(2 - 2\cos(\hat{\mathbf{y}}))C_n^{-1},$$

there is not a geometrical interpretation!

Eigenvalues and eigenvectors

- $h(0) = 0$ with multiplicity 3
- $\mathcal{N}(L_H) = \mathrm{span}\{\mathbf{1}, \mathbf{h_1}, \mathbf{h_2}\}$
- eigenvector $\cos(k\mathbf{y})$ with eigenvalue $\cos\left(\frac{k\pi}{n-2}\right)$,
  $k = 1, \ldots, n-3$, $\mathbf{y}$ is a uniform sampling in $[0, \pi]$.

Numerical Experiments

- Truncated iteration preconditioned RR-GMRES
- The minimal error

$$\|\hat{\mathbf{x}} - \mathbf{x}_{k^*}\| = \min_{k \geq 0} \|\hat{\mathbf{x}} - \mathbf{x}_k\|$$

  and the index k^*.
- Examples from Hansen's "Regularization Tools" Matlab Toolbox.
- Add white Gaussian noise with level $\nu = \frac{\|\mathbf{e}\|}{\|\hat{\mathbf{b}}\|}$, where $\hat{\mathbf{b}}$ is the noise-free rhs.
- Comparisons only with the best choice in literature.

Example 1 (deriv2)

Fredholm integral equation of the first kind

$$\int_0^1 k(s,t)x(t)\mathrm{d}t = g(s), \qquad 0 \le s \le 1,$$

where

$$k(s,t) = \begin{cases} s(t-1), & s < t, \\ t(s-1), & s \ge t, \end{cases}$$

$$g(s) = \exp(s) + (1-\mathrm{e})s - 1,$$

and the solution is

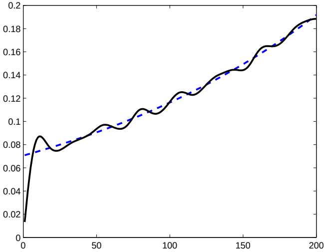
$$x(t) = \exp(t).$$

Discretization

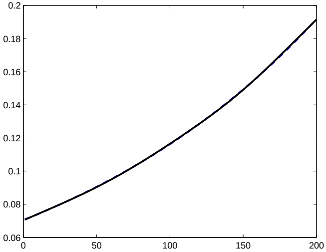
- Discretize the integral equation by a Galerkin method with orthonormal box functions
- symmetric indefinite matrix $A \in \mathbb{R}^{200\times 200}$
- add noise with $\nu = 10^{-3}$

Preconditioner	$\|\hat{\mathbf{x}} - \mathbf{x}_{k^*}\|$	k^*
L_{DR}	9.7e-2	34
L_A	1.6e-3	13
L_H	6.1e-4	17

Restorations



L_{DR}



L_A

Example 2

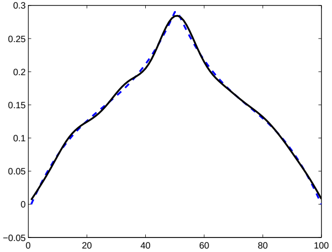
$$g(s) = \begin{cases} (4s^3 - 3s)/24, & s < \frac{1}{2} \\ (-4s^3 + 12s^2 - 9s + 1) & s \geq \frac{1}{2} \end{cases},$$

and the solution is

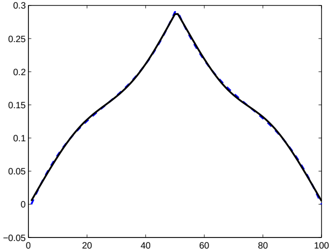
$$x(t) = \begin{cases} t, & t < \frac{1}{2} \\ 1 - t & t \geq \frac{1}{2} \end{cases}.$$

We define a new solution $\hat{\mathbf{x}} = 10\tilde{\mathbf{x}} - \cos(\pi(2\mathbf{t} - 1)) - c$, where $\mathbf{t}$ is a uniform grid in $[0, 1]$ and c is a constant such that $\hat{\mathbf{x}}$ is zero at the boundary.

Restorations

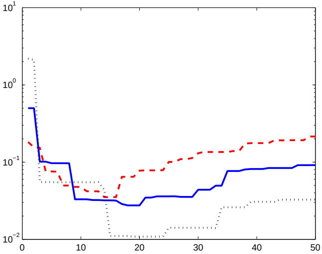


L_D



L_H

Error norm



Prec.	$\|\hat{\mathbf{x}} - \mathbf{x}_{k^*}\|$	k^*
L_D	3.5e-2	13
L_A	2.7e-2	17
L_H	1.0e-2	18

$\|\hat{\mathbf{x}} - \mathbf{x}_k\|$ varying k. The dashed curve is L_D, the solid curve is L_A, and the dotted curve is L_H.

Example 3 (phillips)

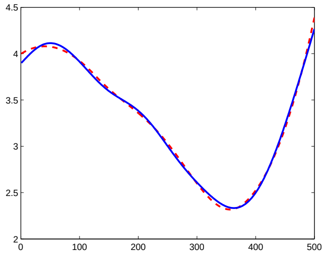
$$\int_{-6}^{6} x(s-t)x(t)\mathrm{d}t = g(s), \qquad -6 \le s \le 6,$$

with

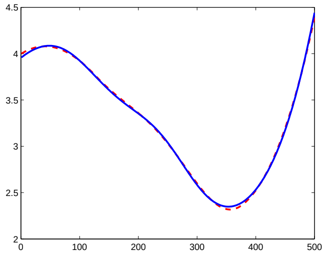
$$x(t) := \begin{cases} 1+\cos(\frac{\pi}{3}t), & \text{if } |t| < 3, \\ 0, & \text{otherwise.} \end{cases}$$

- We define a new solution $\hat{\mathbf{x}} = \tilde{\mathbf{x}} + 3\cos(\pi\mathbf{s}) + \exp(\mathbf{s})^2$, where $\mathbf{s}$ is a uniform grid in $[0,1]$.
- Noise with $\nu = 10^{-2}$.
- We compare $(\hat{C}_2^\dagger D_\delta^{-1})^\dagger$ for $\delta = 10^{-8}$, L_A, and L_H where $\mathbf{h_1} = \mathbf{s}$ and $\mathbf{h_2} = \exp(\mathbf{s})$.

Restorations



$(\hat{C}_2^{\dagger} D_{\delta}^{-1})^{\dagger}$



L_H

Preconditioner	$\lVert \hat{\mathbf{x}} - \mathbf{x}_{k^*} \rVert$	k^*
$(\hat{C}_2^{\dagger} D_{\delta}^{-1})^{\dagger}$	9.3e-3	4
L_A	9.8e-3	4
L_H	4.8e-3	4

Conclusions

- The use of boundary conditions is a simple and general framework to combine fast trigonometric transforms with the selection of a specific subspace that we want to preserve (the signal space).
- If no prior information about the solution are available:
  1. compute a first restoration with antireflective boundary conditions,
  2. if this is not satisfactory, an approximation of the signal space can be deduced from the shape of the computed solution and such approximation can be used to define the eigenvectors $\mathbf{h_1}$ and $\mathbf{h_2}$ for computing a second improved restoration by high order boundary conditions.