Topics in Numerical Analysis II
Computational Inverse Problems

Lecturer: Bangti Jin (btjin@math.cuhk.edu.hk)

Chinese University of Hong Kong

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Outline

Review

linear inverse problems

$$Ax = y$$

- The Landweber method

$$x_{k+1} = x_k - \beta A^*(Ax_k - y)$$

- the method is convergent for exact data: $x_k \to x^\dagger$
- the method is stable for fixed k

$$\|x_k^\delta - x_k\| \leq \sqrt{k}\delta$$

- convergence rate under source condition $x^\dagger = A^* w$

$$\|x_k - x^\dagger\| \leq (2k+2)^{-1/2}\|w\|$$

- the discrepancy principle can be applied and is optimal

Review

Landweber method can be very slow ...

- How to accelerate the computation ...
  - it takes many iterations
  - each iteration requires A, A^*
- What are the remedies ?
  - simple: Anderson acceleration
  - simple: Kaczmarz / stochastic gradient descent
  - complex: conjugate gradient, MINRES
  - ...

Anderson acceleration for fixed point equation: $x_{n+1} = T(x_n)$

- let $g(x) = T(x) - x$, $g_k = g(x_k)$
- set x_0 and $m \geq 1$ (memory parameter)

D. G. Anderson. Iterative Procedures for Nonlinear Integral Equations. J. the ACM. 1965; 12 (4): 547–560

$x_1 = T(x_0)$
for $k = 1, 2, \ldots$ **do**
$\quad m_k = \min(m, k)$
$\quad G_k = [g_{k-m_k} \;\; \ldots \;\; g_k]$
$\quad \alpha_k = \arg\min_{\sum_{i=0}^{m_k} \alpha_i = 1} \|G_k \alpha\|$
$\quad x_{k+1} = \sum_{i=0}^{m_k} (\alpha_k)_i f(x_{k-m_k+i})$
end for

very effective, but no analysis of the regularizing property!

Old idea: Kaczmarz method starts from initial guess x_0,

$$x_{k+1} = x_k + \frac{y_i - (a_i, x_k)}{\|a_i\|^2} a_i, \quad i = (k \bmod n) + 1,$$

orthogonal projection into hyperplanes ...

- Kaczmarz method was proposed in 1937 by Polish mathematician Stefan Kaczmarz.
- It was re-invented by Gordon et al. (1970) under the name algebraic reconstruction technique (ART), for image reconstruction in computed tomography:
  randomized version works better ! Natterer 1986
- randomized version first analyzed by Vershynin-Strohmer 2009

Kaczmarz method

Consider the linear system

$$Ax = y$$

with $A \in \mathbb{R}^{m \times n}$, $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^m$. We write the system matrix A in the form

$$A = \begin{bmatrix} A_1 \\ A_2 \\ \vdots \\ A_\ell \end{bmatrix}, \quad A_j \in \mathbb{R}^{k_j \times n}, j = 1, \ldots, \ell,$$

with $k_1 + \ldots + k_\ell = m$, and each submatrix has k_j linearly indep. row vectors, i.e., $\mathrm{rank}(A_j) = k_j \leq n$, and A_j is surjective from $\mathbb{R}^n$ to $\mathbb{R}^{k_j}$.

Similarly, we decompose $y \in \mathbb{R}^m$ into ℓ subvectors

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_\ell \end{bmatrix}, \quad y_j \in \mathbb{R}^{k_j}, j = 1, \ldots, \ell.$$

The original equation can be given as the system

$$A_j x = y_j, \quad j = 1, \ldots, \ell$$

The jth problem is composed of $k_j \leq n$ linearly indep. linear eq., and the solution space

$$X_j = \{x \in \mathbb{R}^n : A_j x = y_j\}$$

is an $(n - k_j)$ dimensional hyperplane in $\mathbb{R}^n$. This hyperplane is a subspace iff $y_j = 0$.

- define an orthogonal projection $P_j : \mathbb{R}^n \to X_j$ by requiring

$$P_j z \in X_j \quad \text{and} \quad (I - P_j)z \perp (w_1 - w_2), \quad \forall z \in \mathbb{R}^n, w_1, w_2 \in X_j$$

  $P_j z$ is the point closest to z in X_j.
- define sequential proj. $P : \mathbb{R}^n \to \mathbb{R}^n$ by

$$P = P_\ell P_{\ell-1} \dots P_2 P_1$$

- The Kaczmarz sequence $\{x_k\}_{k=0}^\infty$ is defined by Stephan Kaczmarz 1937

$$x_{k+1} = P x_k, \quad x_0 = 0$$

Theorem

If $X = \cap_{j=1}^{\ell} X_j \neq \emptyset$, then the Kaczmarz sequence $\{x_k\}_{k=0}^{\infty}$ converges to the minimum norm solution $x^\dagger = A^\dagger y$ as $k \to \infty$, i.e.

$$\lim_{k\to\infty} x_k = x^\dagger.$$

The proof is quite lengthy

Algebraic reconstruction technique (ART)

Consider the special case where the original problem $Ax = y$, $A \in \mathbb{R}^{m\times n}$, is partitioned into m subproblems, i.e.,

$$A_j x = a_j^\top x = y_j, \quad j = 1, \dots, m,$$

- $a_j^\top$: the jth row of A.
- $A_j : \mathbb{R}^n \to \mathbb{R}$ is a surjection $\forall j \Leftrightarrow A$ has no empty rows

This version of Kaczmarz method is called algebraic reconstruction technique (ART). ART is used extensively in X-ray tomography.

Richard Gordon, Robert Bender, Gabor Herman 1970

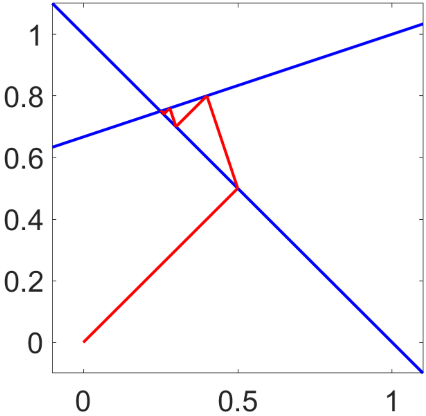
ART iteration

$$A = \begin{bmatrix} 1 & 1 \\ -1 & 3 \end{bmatrix}, \quad y = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

A is invertible and the hyperplanes in $\mathbb{R}^2$ are given by

$$X_1 = \{(x_1, x_2) : x_1 + x_2 = 1\}$$
$$X_2 = \{(x_1, x_2) : -x_1 + 3x_2 = 2\}$$

ART converges to the unique solution $x = (\frac{1}{4}, \frac{3}{4})$. We visualize each projection P_j, $j = 1, 2$, not just the sequential projection P.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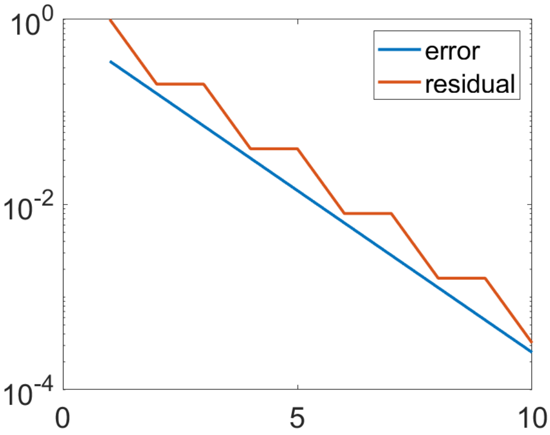
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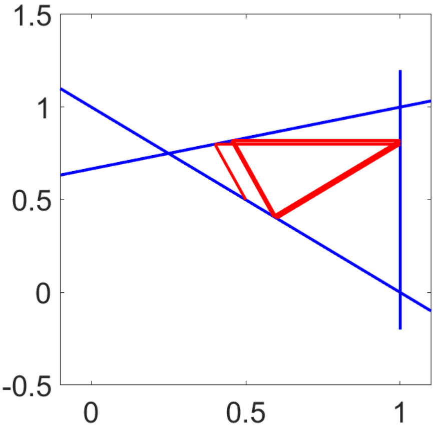
error
residual

ART iteration

$$A = \begin{bmatrix} 1 & 1 \\ -1 & 3 \\ 1 & 0 \end{bmatrix}, \quad y = \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix}$$

added the third hyperplane $X_3 = \{x_1 = 1\}$

the linear system is inconsistent and does not have a solution. ART appears convergent to a solution.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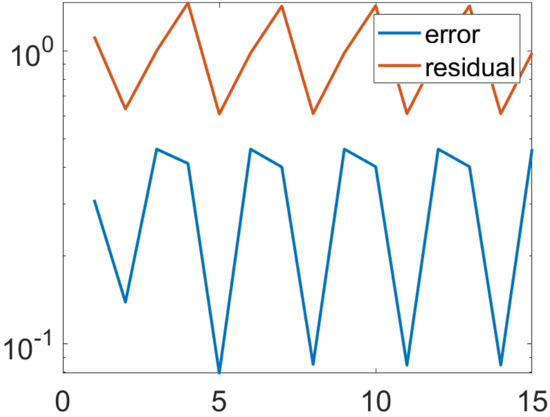
error with respect to the least-squares solution ...



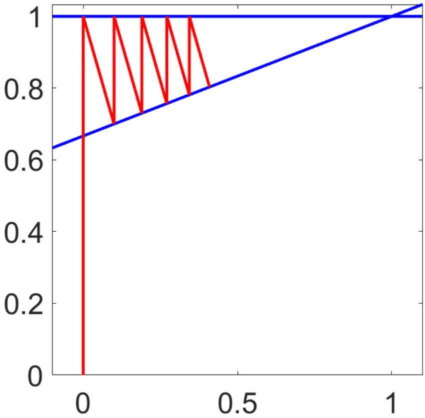
ART iteration

$$A = \begin{bmatrix} 0 & 1 \\ -1 & 3 \end{bmatrix}, \quad y = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

A is invertible and the hyperplanes in $\mathbb{R}^2$ are given by

$$\begin{aligned} X_1 &= \{(x_1, x_2) : x_2 = 1\} \\ X_2 &= \{(x_1, x_2) : -x_1 + 3x_2 = 2\} \end{aligned}$$

ART converges to the unique solution $x = (1, 1)$, but extremely slowly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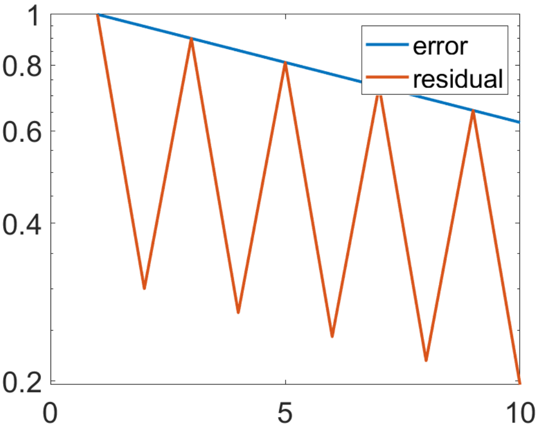
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0.2
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5
10
error
residual

The computation of the projection P_j:

$$A = \begin{bmatrix} A_1 \\ A_2 \\ \vdots \\ A_\ell \end{bmatrix}, \quad A_j \in \mathbb{R}^{k_j \times n}, \quad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_\ell \end{bmatrix}, \quad y_j \in \mathbb{R}_{k_j}, \quad j = 1, \dots, \ell,$$

with each A_j being surjective

- X_j: the hyperplane composed of the solutions to $A_j x = y_j$
- $P_j : \mathbb{R}^n \to X_j$: orthogonal projection onto X_j
- $Q_j : \mathbb{R}^n \to \ker(A_j)$: orthogonal projection onto the kernel of A_j
  $\Rightarrow I - Q_j : \mathbb{R}^n \to \ker(A_j)^\perp = \operatorname{range}(A_j^\top)$: orthogonal projection
- the identity

$$P_j x = z + Q_j(x - z), \quad \forall x \in \mathbb{R}^n, z \in X_j$$

This formula is indep. of the choice of z

Lemma

The projection P_j can be written explicitly as

$$P_j x = x + A_j^\top (A_j A_j^\top)^{-1}(y_j - A_j x), \quad \forall x \in \mathbb{R}^n.$$

- $A_j A_j^\top \in \mathbb{R}^{k_j \times k_j}$ is invertible: $A_j : \mathbb{R}^n \to \mathbb{R}^{k_j}$ surjective $\Rightarrow A_j^\top$ injective $\Rightarrow A_j A_j^\top$ injective:

$$A_j A_j^\top z = 0 \Rightarrow z^\top A_j A_j^\top z = 0 \Rightarrow \|A_j^\top z\|^2 = 0 \Rightarrow z = 0$$

  $\Rightarrow$ injective square matrix $A_j A_j^\top$ is invertible.

- Fix any $x \in \mathbb{R}^n$, let

$$P_j x = z + Q_j(x - z), \quad \text{with } z \in X_j$$

$\Rightarrow$

$$\begin{aligned} x - P_j x &= (x - z) - Q_j(x - z) \\ &= (I - Q_j)(x - z) \in \ker(A_j)^\perp = \mathrm{range}(A_j^\top) \end{aligned}$$

- there exists $w \in \mathbb{R}^{k_j}$ s.t.

$$A_j^\top w = x - P_j x$$

- $+ \; P_j x \in X_j \Rightarrow$

$$A_j A_j^\top w = A_j x - A P_j x = A_j x - y_j$$

- Solving for w and substitution:

$$A_j^\top (A_j A_j^\top)^{-1} (A_j x - y_j) = x - P_j x.$$

implementation of ART:

- when the submatrices $A_j = a_j^\top$, $j = 1, \dots, m$, are rows of the original system matrix A, y_j, $j = 1, \dots, m$, are the components of y, the inverse is just real numbers

$$(A_j A_j^\top)^{-1} = (a_j^\top a_j)^{-1} = 1/\|a_j\|^2$$

- update

$$P_j x = x + (y_j - (a_j, x)) \frac{a_j}{\|a_j\|^2}$$

discrepancy principle for Kaczmarz method

- the measurement y^δ is a noisy version of exact data $y^\dagger$ with

$$\|y^\delta - y^\dagger\| = \delta > 0$$

- The Morozov's discrepancy principle works for the Kaczmarz iteration as follows: choose the smallest k s.t.

$$\|y^\delta - Ax_k^\delta\| \leq \delta$$

if such k exists.

remark

- Unlike truncated SVD and Landweber method, the condition

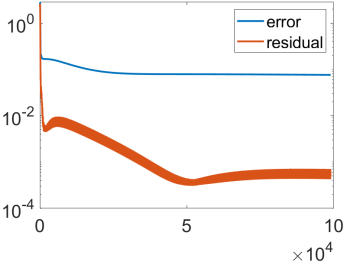
$$\delta > \|y^\delta - Py^\delta\|$$

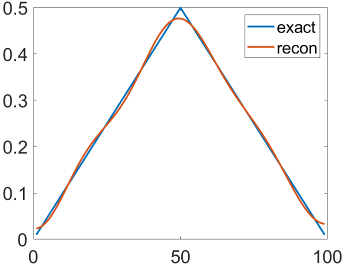
  where P is the projection onto the range of A, is insufficient to guarantee the existence of a stopping index k
- The evaluation of the full residual is costly ...

Example: discretized inverse heat conduction

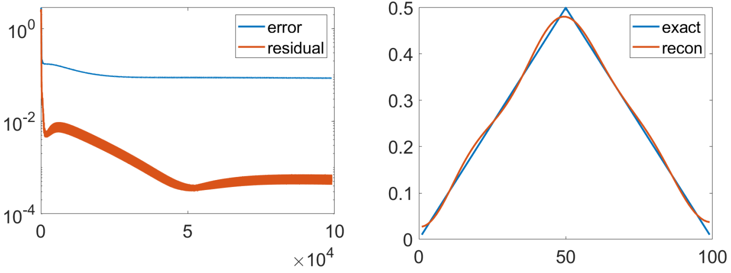
- simulate the data, add some noise, same value δ
- use discrepancy principle for early stopping
-

heat example with exact data





heat example with 1% noise



Randomized Kaczmarz method

Thomas Stromer, Roman Vershynin 2009: randomized Kaczmarz method

- choose the ith equation with probability prop. to $\|a_i\|^2$
- the method is a version of stochastic gradient descent

Let $x^\dagger$ be a solution to $Ax = y$. Then randomized Kaczmarz converges to x in expectation:

$$\mathbb{E}[\|x_k - x^\dagger\|^2] \leq (1 - \kappa(A)^{-2})^k \|x_0 - x^\dagger\|^2$$

with

$$\kappa(A) = \|A\|_F \|A^{-1}\|$$

The method converges exponentially fast to $x^\dagger$, and the convergence rate depends only on scaled condition number $\kappa(A)$

- there holds the inequality

$$\sum_{j=1}^{m} |(z, a_j)|^2 \geq \frac{\|z\|^2}{\|A^{-1}\|^2}, \quad \forall z \in \mathbb{R}^n$$

- the identity $\|A\|_F^2 = \sum_{j=1}^m \|a_j\|^2$ + $\kappa(A) = \|A\|_F \|A^{-1}\| \Rightarrow$

$$\sum_{j=1}^{m} \frac{\|a_j\|^2}{\|A\|_F^2} \left(z, \frac{a_j}{\|a_j\|}\right)^2 \geq \kappa(A)^{-2} \|z\|^2$$

  LHS is the expectation of some random variable.

- The solution space of jth equation is $\{x : (x, a_j) = y_j\}$, with normal $\frac{a_j}{\|a_j\|}$

- define a random variable z whose values are these normals:

$$Z = \frac{a_j}{\|a_j\|} \quad \text{with probability } \frac{\|a_j\|^2}{\|A\|_F^2}, \quad j = 1, \ldots, m$$

- there holds the fundamental inequality

$$\mathbb{E}[(z, Z)^2] \geq \kappa(A)^{-2}\|z\|^2, \quad \forall z \in \mathbb{R}^n$$

- The orthogonal projection P onto the sol. space of a random eq. of $Ax = y$ is given by

$$Pz = z - (z - x^\dagger, Z)Z$$

- the approx. x_k is computed from x_{k-1} via $x_k = P_k x_{k-1}$, with $P_1, P_2, \ldots$ are indep. realization of the random projection P
- The vector $x_k - x_{k-1}$ in the kernel of P_{i_k}: orthogonal to the sol. space of $(a_{i_k}, x) = y_{i_k}$ onto which projects $\Rightarrow$

$$\|x_k - x^\dagger\|^2 = \|x_{k-1} - x^\dagger\|^2 - \|x_{k-1} - x_k\|^2$$

  (Pythagorean theorem)
- by the definition of x_k

$$x_{k-1} - x_k = (x_{k-1} - x^\dagger, Z_k) Z_k$$

  Z_k: indep. realizations of the random vector Z
- Z_k unit norm $\Rightarrow$ error reduction

$$\|x_k - x^\dagger\|^2 = \left(1 - \left(\frac{x_{i-1} - x^\dagger}{\|x_{k-1} - x^\dagger\|}, Z_k\right)^2\right) \|x_{k-1} - x^\dagger\|^2$$

- taking conditional expectation on both sides

$$\mathbb{E}_k[\|x_k - x^\dagger\|^2] = (1 - \mathbb{E}\Big(\frac{x_{i-1} - x^\dagger}{\|x_{k-1} - x^\dagger\|}, Z_k\Big)^2)\|x_{k-1} - x^\dagger\|^2$$

- independence + the fundamental inequality

$$\mathbb{E}_k[\|x_k - x^\dagger\|^2] \leq (1 - \kappa(A)^{-2})\|x_{k-1} - x^\dagger\|^2$$

- taking full conditional yields

$$\mathbb{E}[\|x_k - x^\dagger\|^2] \leq (1-\kappa(A)^{-2})\mathbb{E}[\|x_{k-1} - x^\dagger\|^2] \leq (1-\kappa(A)^{-2})^k\|x_0 - x^\dagger\|^2$$

convergence analysis via SVD

- error $e_k = x_k - x^*$
- error recursion

$$e_{k+1} = \left(I - \frac{a_{i_k} a_{i_k}^t}{\|a_{i_k}\|^2} \right) e_k. \tag{1}$$

$I - \frac{a_{i_k} a_{i_k}^t}{\|a_{i_k}\|^2}$ is an orthogonal projection operator

- $\sigma_{\min} \|e\| \leq \|Ae\| \leq \sigma_1 \|e\|$

$$\begin{aligned}\|e_{k+1}\|^2 &= \|e_k\|^2 - \frac{2}{\|a_{i_k}\|^2}\langle a_{i_k}, e_k\rangle\langle a_{i_k}, e_k\rangle + \langle a_{i_k}, e_k\rangle^2 \frac{\|a_{i_k}\|^2}{\|a_{i_k}\|^4} \\ &= \|e_k\|^2 - \frac{2}{\|a_{i_k}\|^2}\langle a_{i_k}, e_k\rangle\langle a_{i_k}, e_k\rangle + \langle a_{i_k}, e_k\rangle^2 \frac{1}{\|a_{i_k}\|^2}\end{aligned}$$

Upon noting the identity $\sum_{i=1}^{n} a_i a_i^t = A^t A$, taking expectation

$$\mathbb{E}[\|e_{k+1}\|^2 | e_k] \leq \|e_k\|^2 - \frac{2}{\|A\|_F^2}\langle e_k, A^t A e_k\rangle + \frac{\|Ae_k\|^2}{\|A\|_F^2} = \|e_k\|^2 - \frac{\|Ae_k\|^2}{\|A\|_F^2}$$

+ $\|Ae\| \geq \sigma_{\min}\|e\| \Rightarrow$

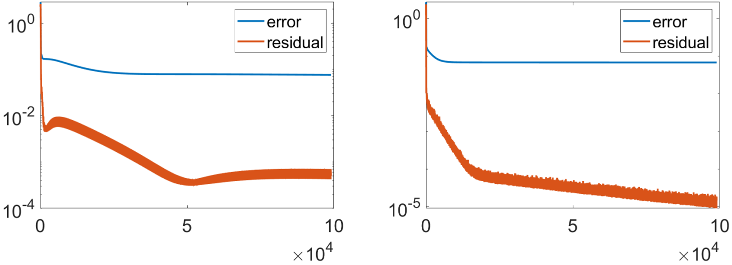
$$\mathbb{E}[\|e_{k+1}\|^2 | e_k] \leq \|e_k\|^2 - \frac{\sigma_{\min}^2 \|e_k\|^2}{\|A\|_F^2} = (1 - \kappa(A)^{-2})\|e_k\|^2$$

Theorem

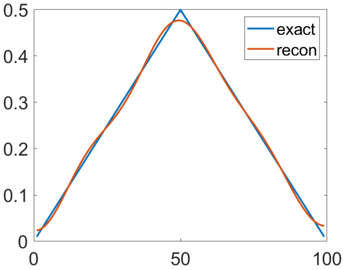
Let $c_1 = \frac{\sigma_L^2}{\|A\|_F^2}$ *and* $c_2 = \frac{\sum_{i=L+1}^{r}\sigma_i^2}{\|A\|_F^2}$. *Then there hold*

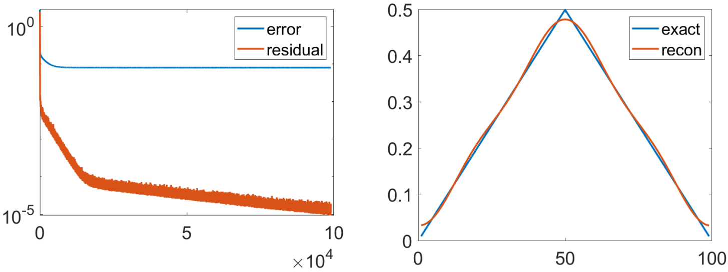
$$\mathbb{E}[\|P_L e_{k+1}\|^2 | e_k] \le (1 - c_1)\|P_L e_k\|^2 + c_2\|P_H e_k\|^2,$$
$$\mathbb{E}[\|P_H e_{k+1}\|^2 | e_k] \le c_2\|P_L e_k\|^2 + (1 + c_2)\|P_H e_k\|^2.$$

heat example with exact data



heat example with exact data




error
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