Linear Systems with the Exact Solution for Numerical Tests

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Introduction

We discuss the accuracy of approximate solution of

$$Ax = b, \quad A \in \mathbb{F}^{n\times n}, \quad b \in \mathbb{F}^n, \quad \det(A) \neq 0.$$

$\mathbb{F}$: set of floating-point numbers as defined in IEEE 754.

$\tilde{x}$: approximate solution.

Introduction

The residual $A\tilde{x} - b$ is used for checking the accuracy of the approximation $\tilde{x}$.

However,

$$\|\tilde{x} - A^{-1}b\| \leq \|A^{-1}\| \, \|A\tilde{x} - b\|$$

is satisfied.

It indicates that there may be a case;

the residual is small but the error is big

Introduction

Let $x = (1, 1)^T$ be the exact solution of the linear system $Ax = b$:

$$A = \begin{pmatrix} 1 & 1 \\ 1 & 1.0001 \end{pmatrix}, \quad b = \begin{pmatrix} 2 \\ 2.0001 \end{pmatrix}$$

$$\tilde{x} = (2, 0)^T \implies \|A\tilde{x} - b\|_2 = 1.0 * 10^{-4}$$

$$\tilde{x} = (1.0001, 1)^T \implies \|A\tilde{x} - b\|_2 = 1.414 * 10^{-4}$$

Introduction

- Difference between $\|A\tilde{x} - b\|$ and $\|\tilde{x} - x\|$

  $A \in \mathbb{F}^{n\times n}$ and $x, b \in \mathbb{F}^n$ are nice for numerical tests

- is the vector b obtained by $b := Ax$?
  $\longrightarrow$ rounding error may occur in the evaluation of Ax
  $\longrightarrow Ax \notin \mathbb{F}^n$

Notation

- $\mathbf{u}$: roundoff unit ($\mathbf{u} = 2^{-53}$ for binary64)
- $\mathrm{fl}(\cdots)$: result of numerical computations
- $A \in \mathbb{F}^{n\times n}$ and $x \in \mathbb{F}^n$ are given
- $\tilde{x}$ is an approximate solution

Related Work

For given A and x, Miyajima, Ogita, Oishi (2005) proposed a method which produces $A'x' = b$.

For $a, b \in \mathbb{F}$, we can obtain $x, y \in \mathbb{F}$ such that

$$ab = x + y, \ \ x = \mathrm{fl}(ab).$$

$$Ax = \sum_{i=1}^{k} b^{(i)}, \quad b^{(i)} \in \mathbb{F}^n, \quad k \in \mathbb{N}. \tag{1}$$

Related Work

Let $I \in \mathbb{F}^{(k-1)\times(k-1)}$ be the identity matrix and $O \in \mathbb{F}^{(k-1)\times(k-1)}$ be the zero matrix. Setting

$$B = [-b^{(2)}, \ldots, -b^{(k)}] \in \mathbb{F}^{n\times(k-1)}, \quad e = (1, \ldots, 1)^T \in \mathbb{F}^{k-1},$$

$A' \in \mathbb{F}^{(n+k-1)\times(n+k-1)}$, $x' \in \mathbb{F}^{n+k-1}$ and $b' \in \mathbb{F}^{n+k-1}$ are obtained by

$$A' = \begin{pmatrix} A & B \\ O & I \end{pmatrix}, \; x' = \begin{pmatrix} x \\ e \end{pmatrix}, \; b' = \begin{pmatrix} b^{(1)} \\ e \end{pmatrix}.$$

Advantage and Disadvantage

- Ill-conditioned matrix is treatable
- Setting arbitrary x
- The size is increased
- Structure of the matrix is changed

$$A' = \begin{pmatrix} A & B \\ O & I \end{pmatrix}$$

Proposed Method

- Ill-conditioned matrix is not treatable
- Setting arbitrary x is not possible
- The size is not changed
- Structure of the matrix is not changed
  $(a_{ij} = a_{kl},\ a_{ij} = 0)$

$$A = A' + \Delta$$

$$A' \approx A$$

Strategy

A is divided into

$$A = A' + \Delta, \quad A', \Delta \in \mathbb{F}^{n \times n}$$

in order to satisfy

$$A'x = \mathrm{fl}(A'x), \quad A' \approx A.$$

The Proposed Method

For given $A \in \mathbb{F}^{n\times n}$ and $x \in \mathbb{F}^n$, we explain how to obtain A' and b such that

$$A'x = b, \quad A' \in \mathbb{F}^{n\times n}, \quad b \in \mathbb{F}^n \tag{2}$$

Assume that A is non-singular and x is not zero vector.

Each element of the vector θ satisfies

$$\theta_j = 2^k,\ k \in \mathbb{Z}, \quad x_j \in \theta_j\mathbb{Z}, \quad x_j \notin 2\theta_j\mathbb{Z}.$$

The Proposed Method

The vector σ is defined as

$$\sigma_i := 2^{\beta} \cdot 2^{g_i}, \quad \beta = \lceil \log_2 n \rceil.$$

We set the vector g

$$g_i := \begin{cases} \lceil \log_2 \alpha_i \rceil, & \alpha_i = 0 \\ 1 & \text{otherwise} \end{cases}, \qquad \alpha_i := \max_{1 \le j \le n} |a_{ij} x_j|$$

The Proposed Method

The vector σ is defined as

$$\sigma_i := 2^{\beta} \cdot 2^{g_i}, \quad \beta = \lceil \log_2 n \rceil.$$

If the structure is preserved, then we set the vector g

$$g_i := \begin{cases} \lceil \log_2 \alpha \rceil, & \alpha = 0 \\ 1 & \text{otherwise} \end{cases}, \quad \alpha := \max_{1 \le i,j \le n} |a_{ij} x_j|$$

The Proposed Method

We set the σ'

$$\sigma' = \frac{2}{\min\limits_{\theta_j \neq 0} \theta_j} \cdot \sigma. \tag{3}$$

The matrix A' is obtained by

$$a'_{ij} := \mathrm{fl}((a_{ij} + \sigma'_i) - \sigma'_i). \tag{4}$$

Here, $\mathrm{fl}(A'x) = A'x$ is satisfied.

MATLAB Code, $x = (1, \ldots, 1)^T$

```
function [A2, b] = str_one(A)
  n = length(A);
  y = max(abs(A(:)));
  σ = 2^ceil(log2(n)) * 2.^ceil(log2(y));
  T = repmat(σ, n, n);
  A2 = (A + T) - T;
  b = A2 * ones(n, 1);    %no rounding error
end
```

MATLAB Code for Sparse

```
function [A2, b] = str_one(A)
  n = length(A);
  y = max(abs(A(:)));
  σ = 2^ceil(log2(n)) * 2.^ceil(log2(y));
  T = σ * spones(A);
  A2 = (A + T) - T;
  b = A2 * ones(n, 1);     %no rounding error
end
```

Iterative Refinement

If we set smaller σ', the $Ax = b$ may be satisfied.

If we take small σ' until

$$\mathrm{fl}_{\nabla}(A'x) \neq \mathrm{fl}_{\triangle}(A'x)$$

- fl_{∇}: numerical results with rounding downward mode
- $\mathrm{fl}_{\triangle}$: numerical results with rounding upward mode

Iterative Refinement

n	original A'	after the refinement
100	2.2552e-13	2.0687e-14
500	1.1593e-12	7.9412e-14
1000	2.9518e-12	9.2558e-14
5000	2.8430e-11	4.1641e-13
10000	6.2564e-11	4.7524e-13

Table 1: The maximum of $\dfrac{|a_{ij} - a'_{ij}|}{|a_{ij}|}$

Tests for VNC

We check the tightness of the verified numerical computations.

$$\|\tilde{x} - A^{-1}b\|_\infty \leq \frac{\|R(A\tilde{x} - b)\|_\infty}{1 - \|RA - I\|_\infty} =: \alpha$$

is well known. We set $\tilde{x}$ and check $\dfrac{\alpha}{\|\tilde{x} - A^{-1}b\|_\infty}$.

Test for VNC

S. Oishi, T. Ogita, T. Ohta, Numerical Verification Method for Systems of Linear Equations Using Accurate Computation of Dot Product, Simulation, 25(3), 2006 (in Japanese).

$$\|\tilde{x} - A^{-1}b\|_\infty \leq \frac{\|R(A\tilde{x} - b)\|_\infty}{1 - \|RA - I\|_\infty} =: \alpha$$

We check $\dfrac{\alpha}{\|\tilde{x} - A^{-1}b\|_\infty}$ for $x = (1, 1, \ldots, 1)^T$ and

$\tilde{x} = (c, c, \ldots, c)^T, c \in \mathbb{F}$.

Test for VNC

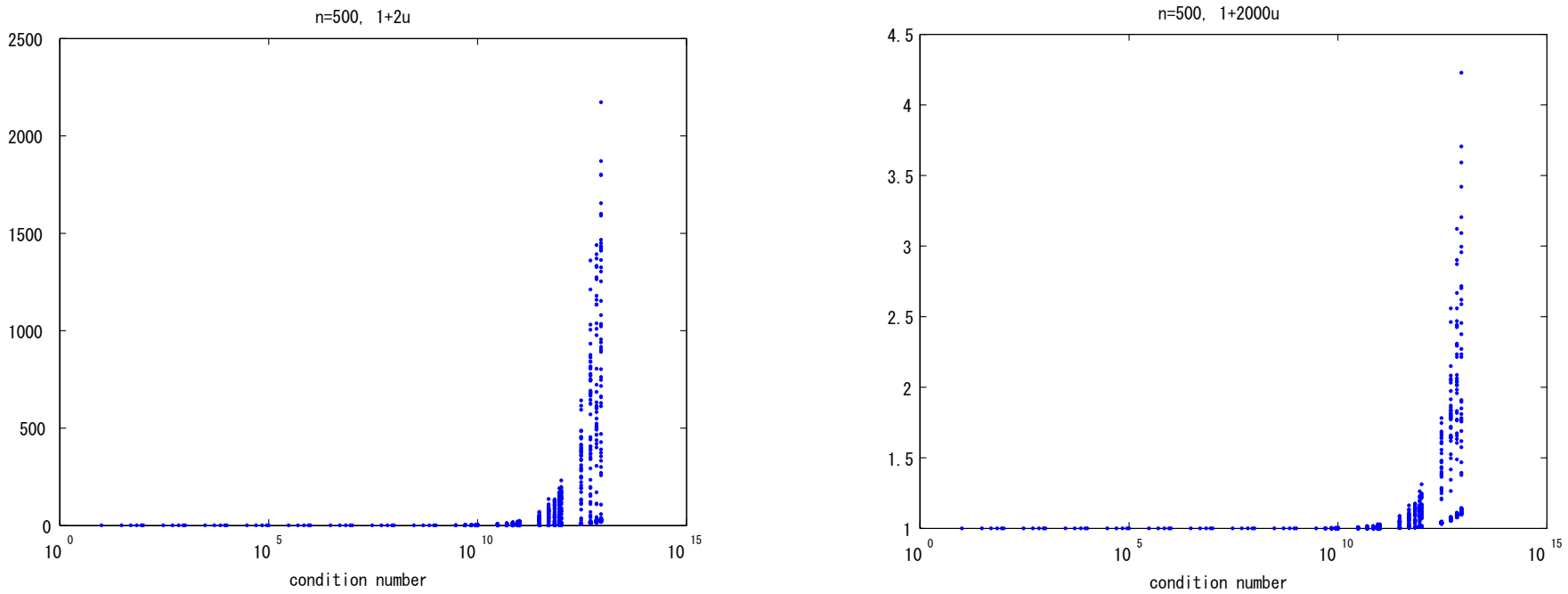


Figure 1: $c = 1 + 2\mathbf{u}$ (left) and $c = 1 + 2000\mathbf{u}$ (right)

Test for CG method

If the exact solution is known in advance, we check the behavior of iterative methods exactly.

We check

$$\|A\tilde{x} - b\|_2, \quad \|r_{k+1}\|_2 = \|r_k - \alpha_k A p_k\|_2, \quad \|x - \tilde{x}\|_2$$

using conjugate gradient (CG) method.

$r_0 = b - Ax_0;$

$p_o = r_0;$

`while` 1

$\alpha_k = (r_k^T r_k)/(p_k^T A p_k);$

$x_{k+1} = x_k + \alpha_k p_k;$

$r_{k+1} = r_k - \alpha_k A p_k;$

`if` $\|r_{k+1}\|_2 < 1e-10,$ `break;` , `end`

$\beta_k = (r_{k+1}^T r_{k+1})/(r_k^T r_k);$

$p_{k+1} = r_{k+1} + \beta_k p_k;$

`end`

Test for CG method

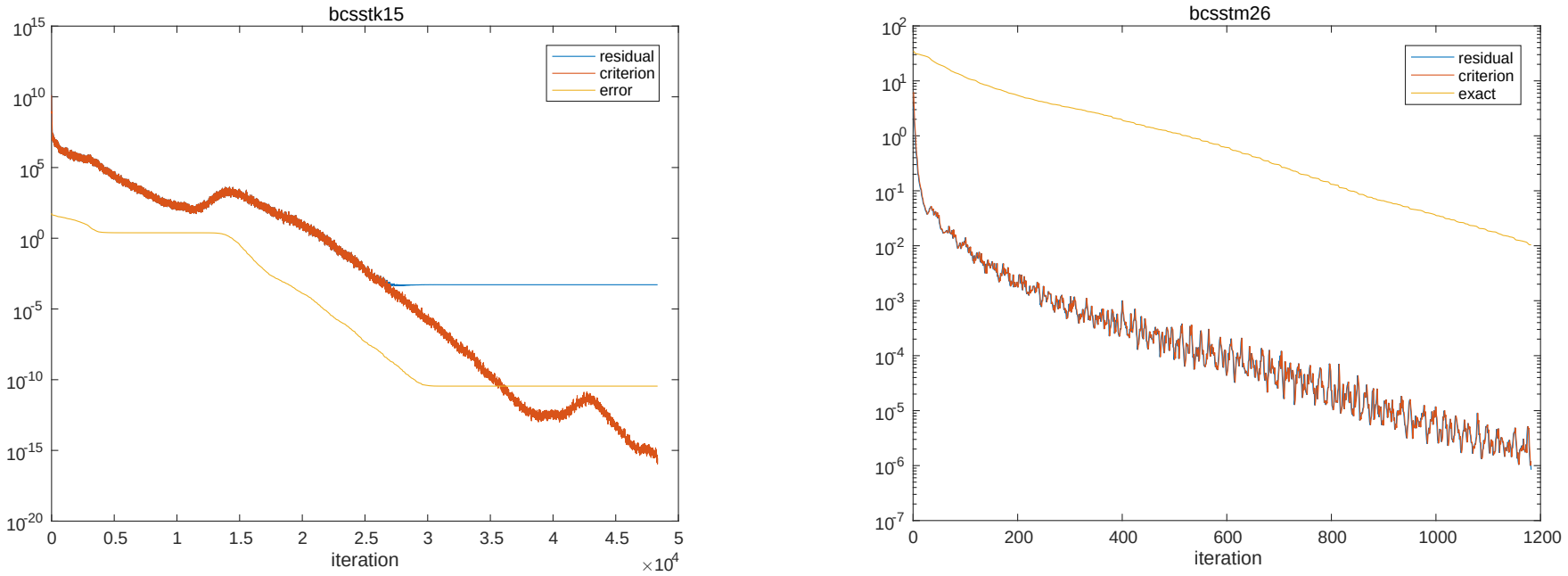


Figure 2: bcsstk15 and bcsstm26 from Matrix Market

Test for CG method

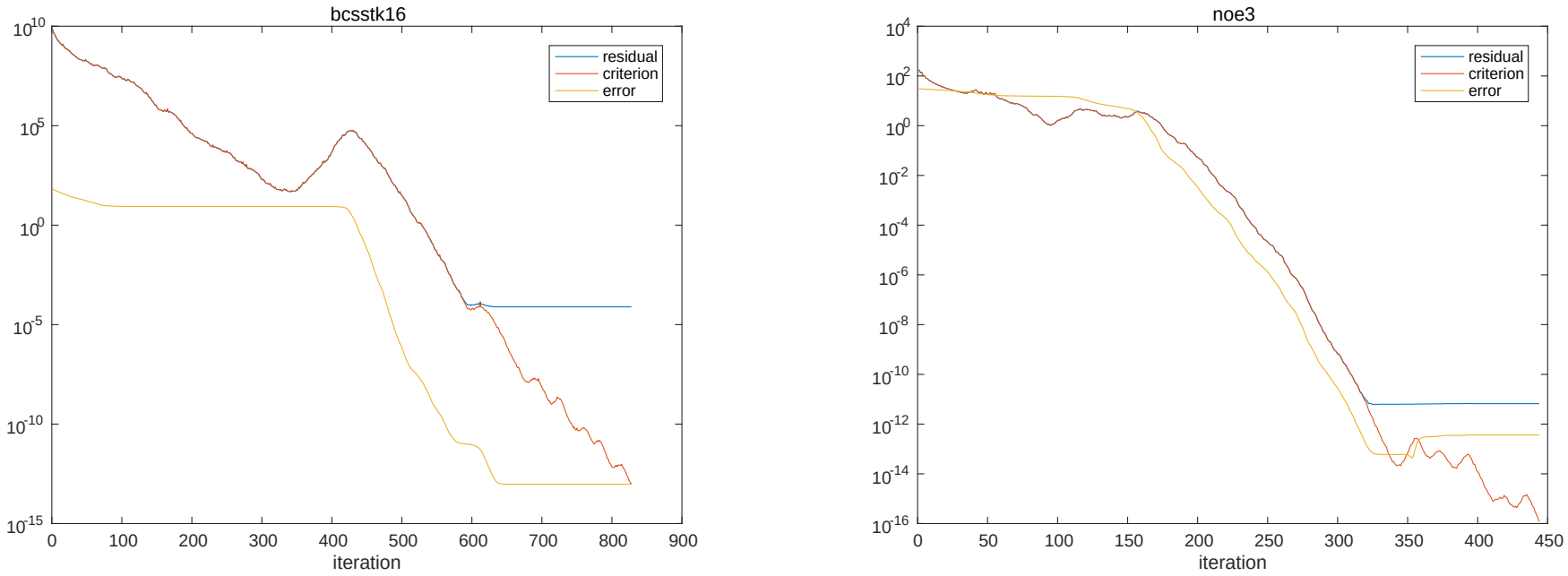
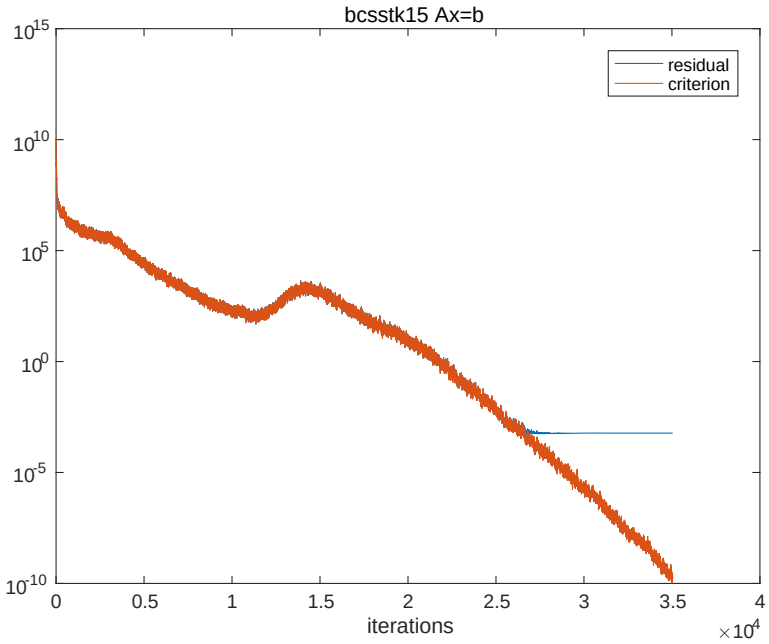


Figure 3: bcsstk16 and nos3 from Matrix Market

Test for CG method (bcsstk15)



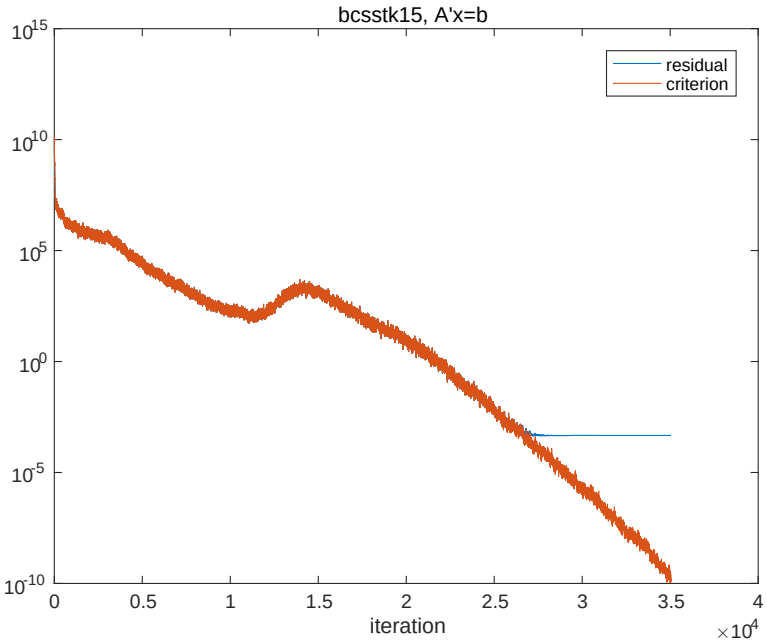


Figure 4: $Ax = b$ (left) and $A'x = b$ (right)

Test for CG method (bcsstm26)

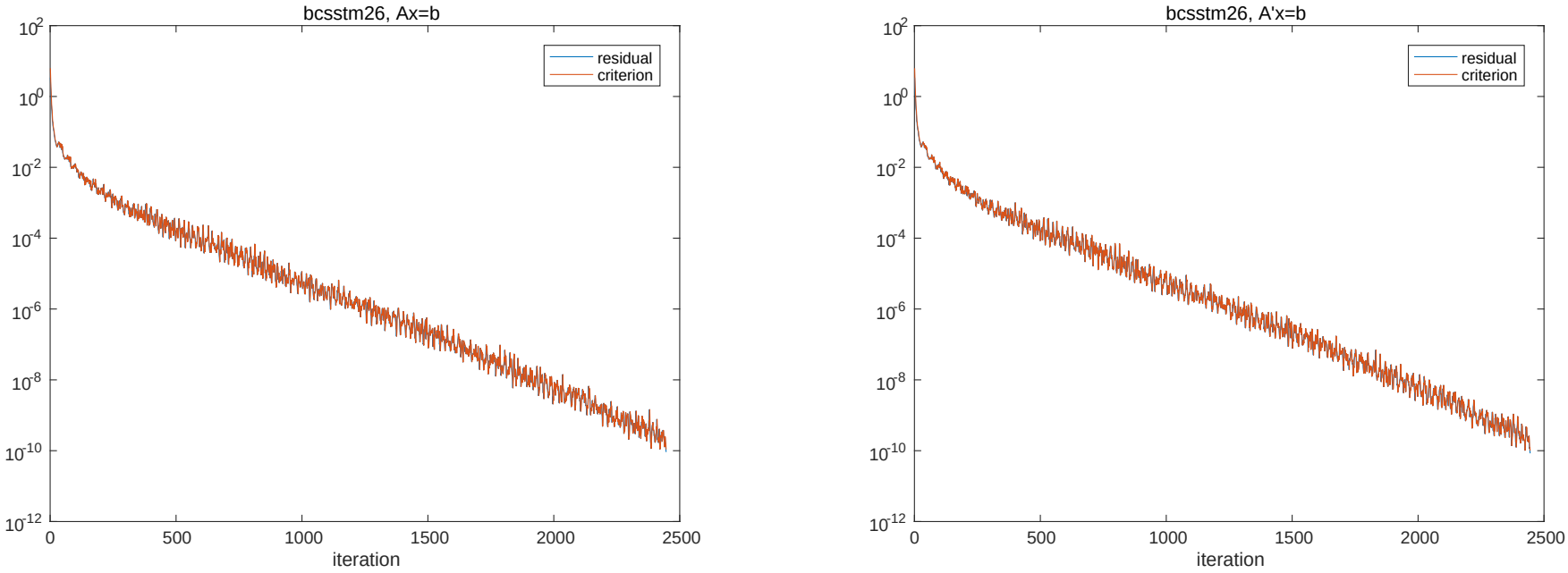


Figure 5: $Ax = b$ (left) and $A'x = b$ (right)

Conclusion

- We proposed a method which produces linear systems with the exact solution.
- We can develop alternative method using bit operations.
- However, the method introduced in this talk based on matrix operation, so that it is easy to implement.

Thank you very much for your attention!