Look-Back GMRES(m) for Solving Large Nonsymmetric Linear Systems

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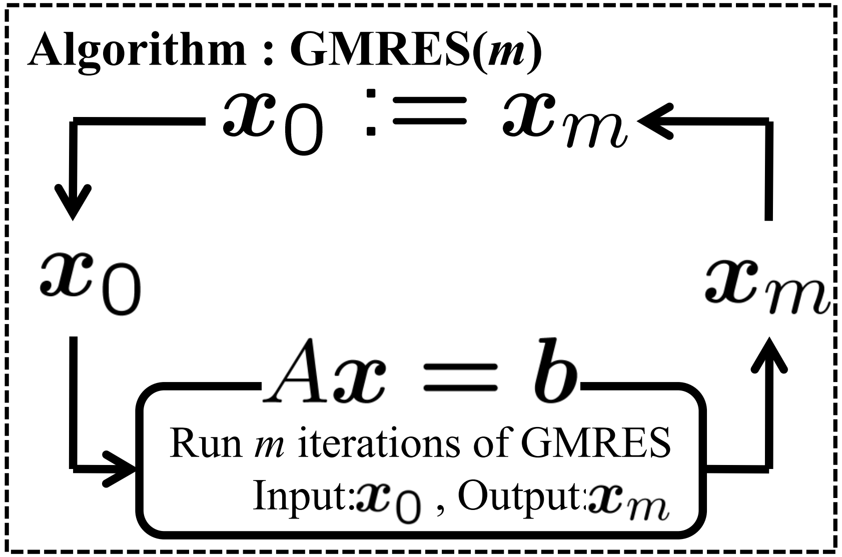
Introduction

- GMRES(m) method [Y. Saad and M. H. Schultz:1986]

  -- Algorithm (focus on restart)



  -- Update the initial guess

$$\boldsymbol{x}_0^{(l)} := \boldsymbol{x}_m^{(l-1)}$$

$$\boldsymbol{r}_0^{(l)} := \boldsymbol{r}_m^{(l-1)}$$

l : number of restart cycle

Introduction

- GMRES(m) method [Y. Saad and M. H. Schultz:1986]

  -- Residual polynomials

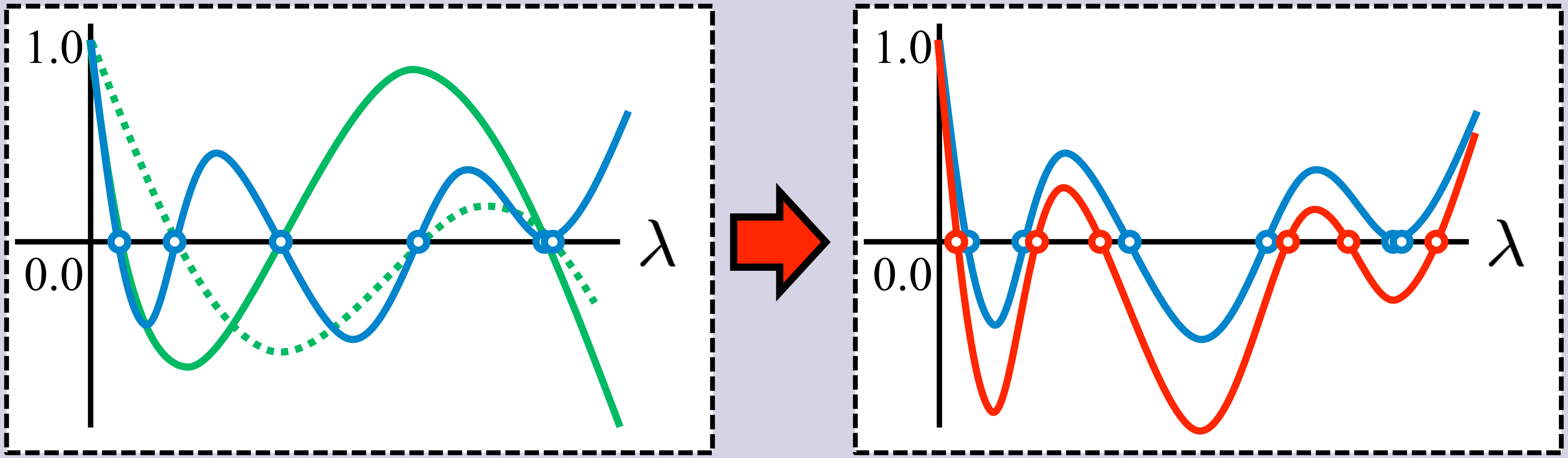
$$\boldsymbol{r}_m^{(l)} = P_m^{(l)}(A)\boldsymbol{r}_0^{(l)}$$
$$= P_m^{(l)}(A)\boldsymbol{r}_m^{(l-1)}$$
$$= P_m^{(l)}(A)P_m^{(l-1)}(A)\cdots P_m^{(1)}(A)\boldsymbol{r}_0^{(1)}$$

$\boldsymbol{r}_0^{(l)} := \boldsymbol{r}_m^{(l-1)}$

l : number of restart

$P_m^{(l)}(\lambda)$: residual polynomial ($P_m^{(l)}(0) = 1$)

Motivation



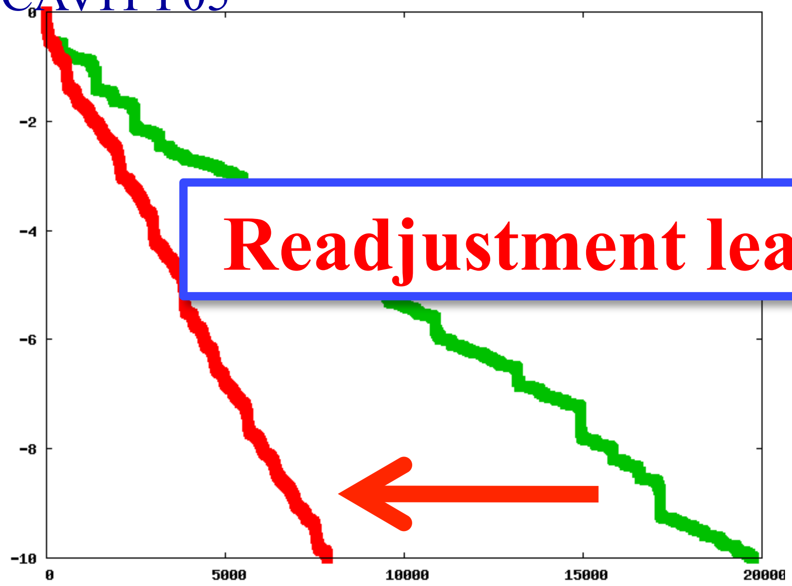
- GMRES(m) method with readjustment

-- Numerical result compared with GMRES(m) method

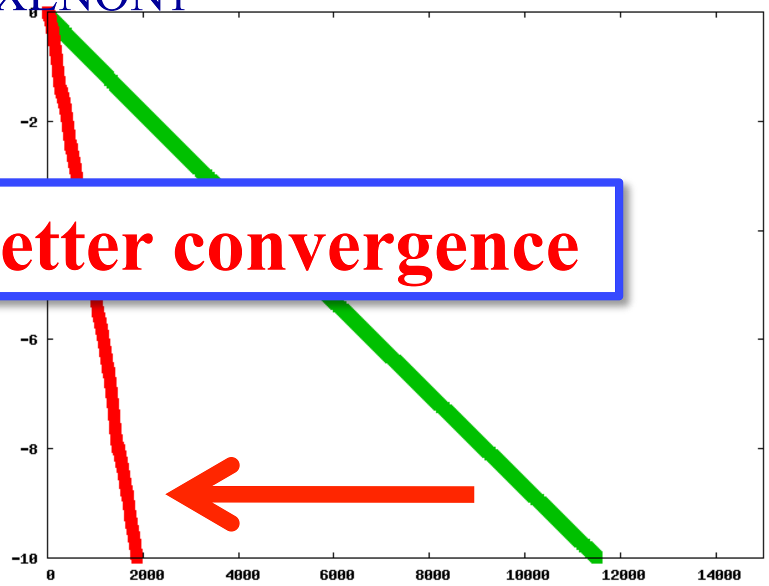
: parameters $b = [1, 1, \ldots, 1]^\top, x_0 = [0, 0, \ldots, 0]^\top, m = 30$

— **GMRES(m)** — **GMRES(m) with readjustment**

CAVITY05



XENON1



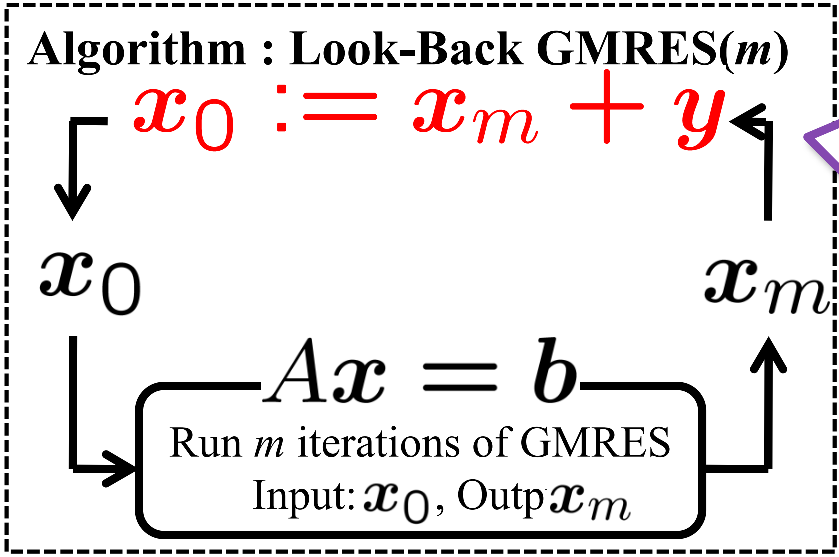
Readjustment leads better convergence

Question

How do we readjust the function s.t. the roots are moved?

- Look-Back GMRES(m) method

  -- Algorithm (focus on update the initial guess)



$$y^{(l)} = \mu^{(l)} w^{(l)},$$

$$\left(\begin{array}{lcl} w^{(l)} & = & z_m^{(l-1)} + y^{(l-1)} + z_m^{(l-2)} \\ \mu^{(l)} & = & \arg\min_{\mu} ||r_m^{(l-1)} - \mu A w^{(l)}||_2 \end{array} \right)$$

We can easily complete the readjustment

Introduction

- Look-Back GMRES(m) method

  -- Extension of the GMRES(m) method

$$\boldsymbol{x}_0^{(l)} := \boldsymbol{x}_m^{(l-1)} \quad \Rightarrow \quad \boldsymbol{x}_0^{(l)} := \boldsymbol{x}_m^{(l-1)} + \boldsymbol{y}^{(l)}$$

→ **Analyze based on error equations**

  -- A Look-Back technique of restart

$$\boldsymbol{y}^{(l)} = \mu^{(l)} \boldsymbol{w}^{(l)}, \quad \begin{pmatrix} \boldsymbol{w}^{(l)} & = & \boldsymbol{z}_m^{(l-1)} + \boldsymbol{y}^{(l-1)} + \boldsymbol{z}_m^{(l-2)} \\ \mu^{(l)} & = & \arg\min_{\mu} ||\boldsymbol{r}_m^{(l-1)} - \mu A \boldsymbol{w}^{(l)}||_2 \end{pmatrix}$$

→ **Analyze based on residual polynomials**

Extension of the GMRES(m) method

- Analysis based on error equations

  -- Introduction of error eq. and iterative refinement scheme

Definition : error equation

Let x and $\widehat{x}$ be the exact solution and the numerical solution respectively. Then the error vector $e := x - \widehat{x}$ can be computed by solving the so-called **error equation**, *i.e.,*

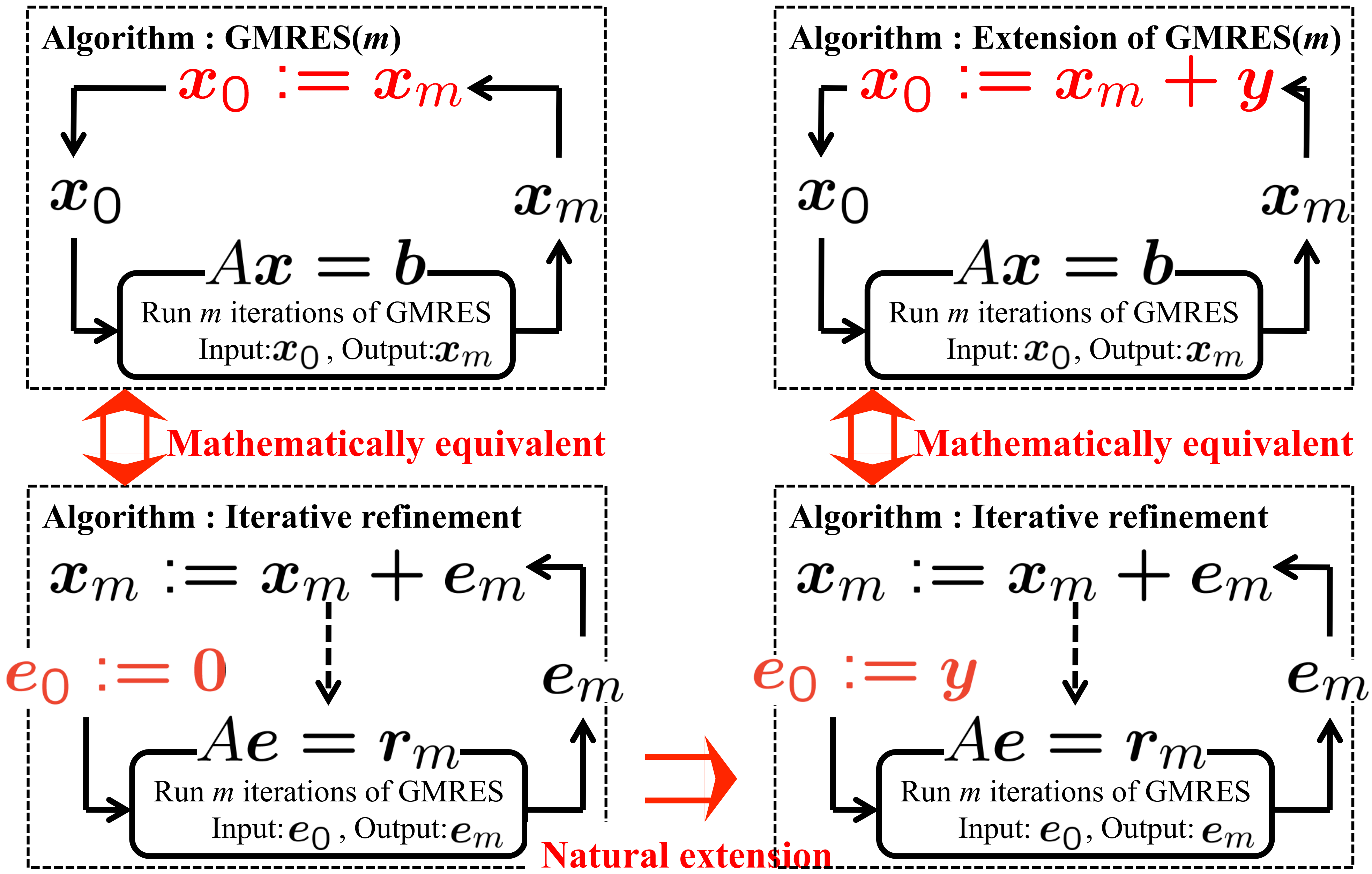
$$Ae = \widehat{r},$$

where $\widehat{r}$ is residual vector corresponding to $\widehat{x}$.

Definition : iterative refinement scheme

The technique based on solving error equations recursively to achieve the higher accuracy of the numerical solution is called the **iterative refinement scheme**.

Extension of the GMRES(m) method



A Look-Back technique of restart

- Difference between GMRES(m) and its Extension

Extension of GMRES(m) method

$$\boldsymbol{x}_0^{(l)} := \boldsymbol{x}_m^{(l-1)} + \boldsymbol{y}^{(l)}$$

l : number of restart

$$\boldsymbol{r}_m^{(l)} = P_m^{(l)}(A)(\boldsymbol{r}_m^{(l-1)} - A\boldsymbol{y}^{(l)})$$

$P_m^{(l)}(\lambda)$: residual polynomial

If we set $\boldsymbol{y}^{(l)} \in \mathcal{K}_n(A, \boldsymbol{r}_0^{(1)})$. Then the rational function $Q^{(l)}(\lambda)$ s.t.

$$Q^{(l)}(A)\boldsymbol{r}_m^{(l-1)} = \boldsymbol{r}_m^{(l-1)} - A\boldsymbol{y}^{(l)}$$

is exist.

$$\boldsymbol{r}_m^{(l)} = P_m^{(l)}(A)Q^{(l)}(A)\boldsymbol{r}_m^{(l-1)}$$

GMRES(m) method

$$\boldsymbol{x}_0^{(l)} := \boldsymbol{x}_m^{(l-1)}$$

$$\boldsymbol{r}_m^{(l)} = P_m^{(l)}(A)\boldsymbol{r}_m^{(l-1)}$$

A Look-Back technique of restart

- Difference between GMRES(m) and its Extension

Extension of GMRES(m) method

$$\boldsymbol{x}_0^{(l)} := \boldsymbol{x}_m^{(l-1)} + \boldsymbol{y}^{(l)}$$

l : number of restart

$$\boldsymbol{r}_m^{(l)} = P_m^{(l)}(A)Q^{(l)}(A)\boldsymbol{r}_m^{(l-1)}$$

$P_m^{(l)}(\lambda)$: residual polynomial

Look-Back GMRES(m) method

$$\boldsymbol{y}^{(l)} = A^{-1}(I - Q^{(l)}(A))\boldsymbol{r}_m^{(l-1)}$$

Set $Q^{(l)}(\lambda)$ by **Look-Back technique**

GMRES(m) method

$$\boldsymbol{x}_0^{(l)} := \boldsymbol{x}_m^{(l-1)}$$

$$\boldsymbol{r}_m^{(l)} = P_m^{(l)}(A)\boldsymbol{r}_m^{(l-1)}$$

A Look-Back technique of restart

- A Look-Back technique

Extension of GMRES(m) method

Look-Back GMRES(m) method

Set $Q^{(l)}(\lambda)$ by **Look-Back technique**

Look-Back strategy

$$\boldsymbol{r}_m^{(l)} = P_m^{(l)}(A)Q^{(l)}(A)\boldsymbol{r}_m^{(l-1)}$$

$$\boldsymbol{r}_m^{(l)} = P_m^{(l)}(A)Q^{(l)}(A)\underbrace{P_m^{(l-1)}(A)Q^{(l-1)}(A)}_{R^{(l)}(A)}\cdots P_m^{(1)}(A)Q^{(1)}(A)\boldsymbol{r}_0^{(1)}$$

Look-Back at the past polynomials and rational functions $R^{(l)}(\lambda)$

→ **Readjust** $R^{(l)}(\lambda)$ s.t. root is moved

A Look-Back technique of restart

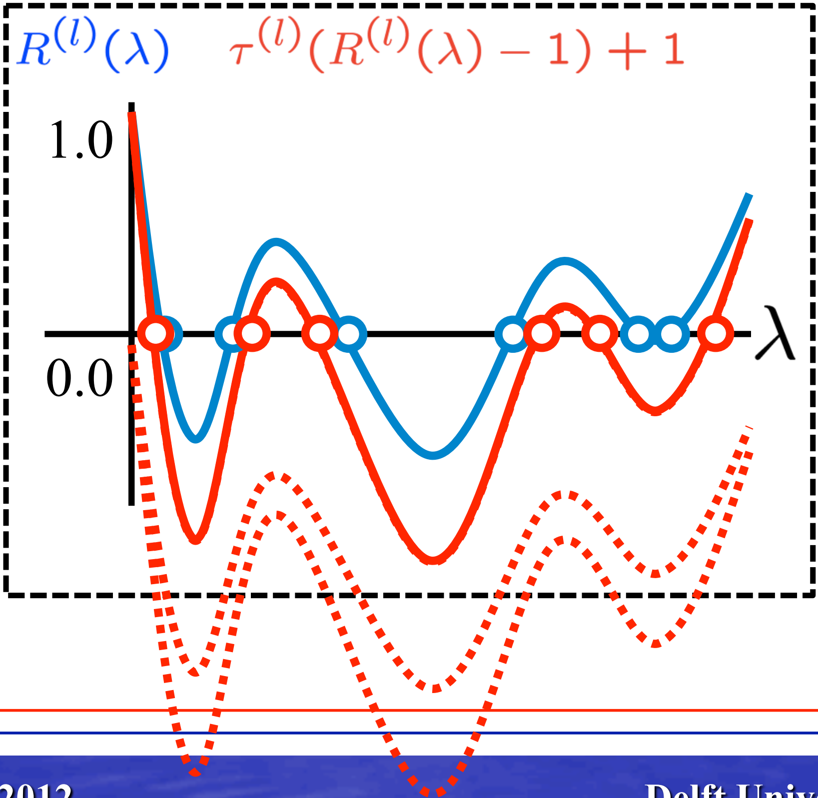
- A Look-Back technique

Extension of GMRES(m) method

Look-Back GMRES(m) method

$Q^{(l)}(\lambda)$ $R^{(l)}(\lambda)$ $= \tau^{(l)} R^{(l)}(\lambda) - (\tau^{(l)} - 1)$

$Q^{(l)}(\lambda) = \tau^{(l)} - (\tau^{(l)} - 1)(R^{(l)}(\lambda))^{-1}$



Motivation

Root of the function is moved (○ → ○)

It is expected that readjustment leads to be high convergence

A Look-Back technique of restart

- A Look-Back technique

Extension of GMRES(m) method

Look-Back GMRES(m) method

$$\boldsymbol{y}^{(l)} = A^{-1}(I - Q^{(l)}(A))\boldsymbol{r}_m^{(l-1)}$$

$$Q^{(l)}(\lambda) = \tau^{(l)} - (\tau^{(l)} - 1)(R^{(l)}(\lambda))^{-1}$$

e.g.

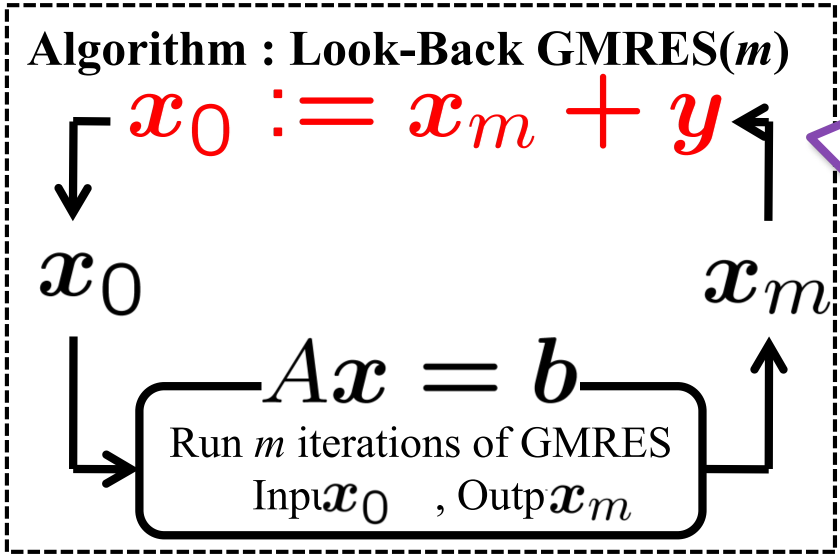
$$R^{(l)}(\lambda) = P_m^{(l-1)}(\lambda)Q^{(l-1)}(\lambda)P_m^{(l-2)}(\lambda)$$

$$\boldsymbol{y}^{(l)} = \mu^{(l)}\boldsymbol{w}^{(l)}, \quad \begin{pmatrix} \boldsymbol{w}^{(l)} & = & \boldsymbol{z}_m^{(l-1)} + \boldsymbol{y}^{(l-1)} + \boldsymbol{z}_m^{(l-2)} \\ \mu^{(l)} & = & \arg\min_{\mu} ||\boldsymbol{r}_m^{(l-1)} - \mu A\boldsymbol{w}^{(l)}||_2 \end{pmatrix}$$

A Look-Back technique of restart

- Proposal of Look-Back GMRES(m) method

  -- Algorithm (focus on update the initial guess)



$$y^{(l)} = \mu^{(l)} w^{(l)},$$

$$\left(\begin{array}{lcl} w^{(l)} & = & z_m^{(l-1)} + y^{(l-1)} + z_m^{(l-2)} \\ \mu^{(l)} & = & \arg\min_{\mu} ||r_m^{(l-1)} - \mu A w^{(l)}||_2 \end{array} \right)$$

  -- extra costs for Look-Back technique

  : 1 matrix-vector multiplication per 1 restart

Numerical experiments

- Test problems [obtained from UF Sparse Matrix Collection]

  -- CAVITY05, CAVITY16, CHIPCOOL0, MEMPLUS, NS3DA, RAJAT03, RDB5000, XENON1, XENON2.

- Compared methods (without preconditioner)

  -- **GMRES(*m*) method**

  -- **Look-Back GMRES(*m*) method**

  (m = 30, 100)

- Parameters

  -- right-hand-side : $\boldsymbol{b} = [1, 1, \ldots, 1]^{\mathsf{T}}$

  -- initial guess : $\boldsymbol{x}_0 = [0, 0, \ldots, 0]^{\mathsf{T}}$

  -- stopping criterion : $\|\boldsymbol{r}\|_2 / \|\boldsymbol{b}\|_2 \leq 10^{-10}$

- Experimental conditions

  -- AMD Phenom II X4 940 (3.0GHz);

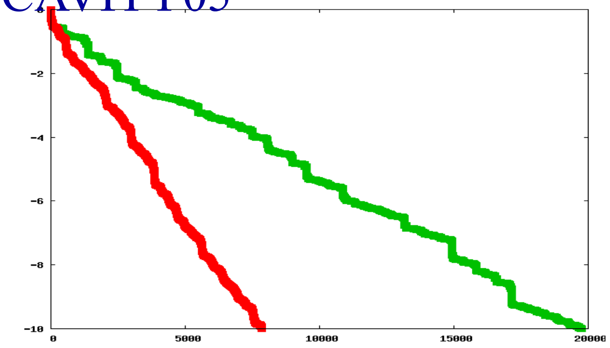
  -- Standard Fortran 77 using double precision.

Numerical experiments

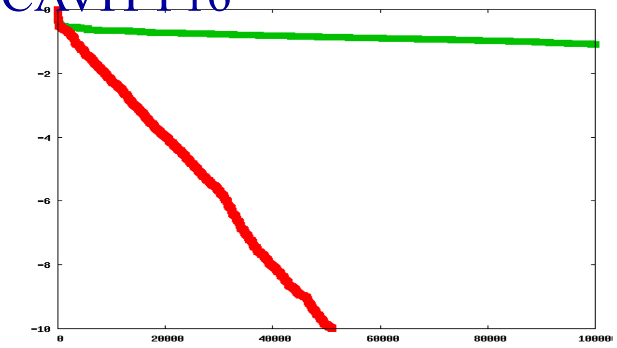
— **GMRES(*m*)** — **Look-Back GMRES(*m*)**

- Numerical results for $m = 30$

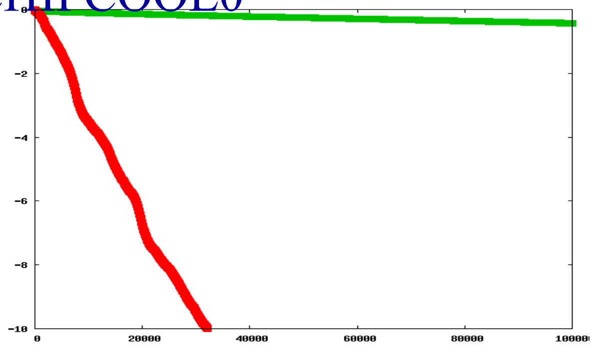
CAVITY05



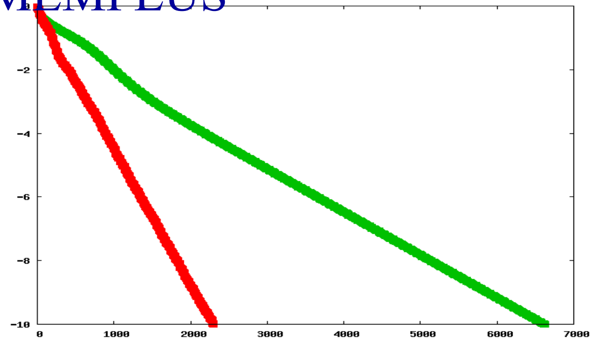
CAVITY16



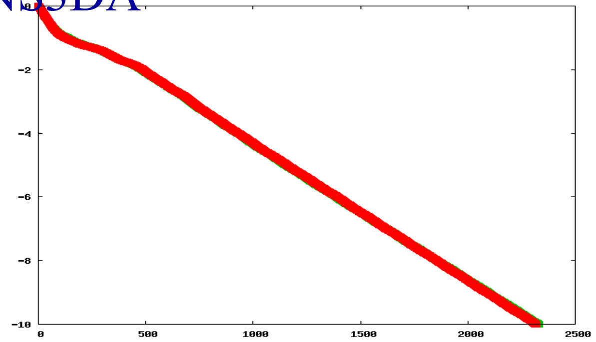
CHIPCOOL0



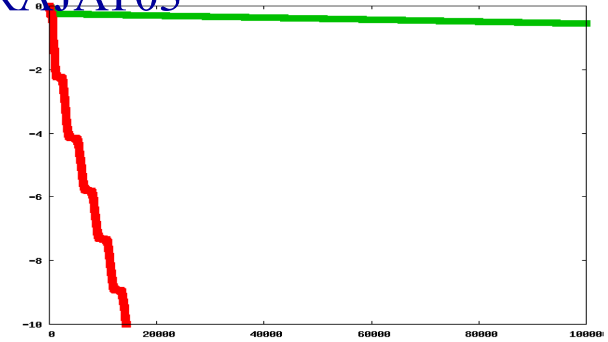
MEMPLUS



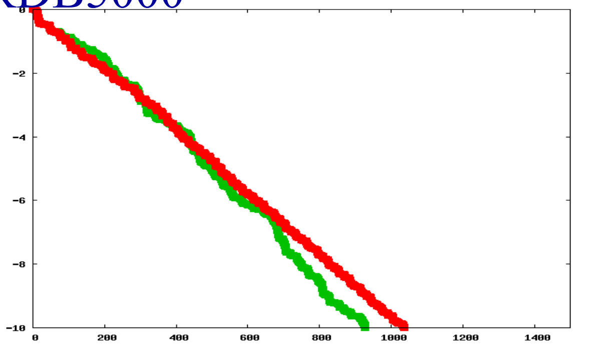
NS3DA



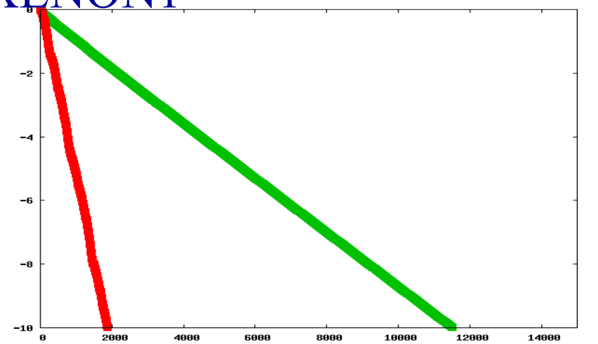
RAJAT03



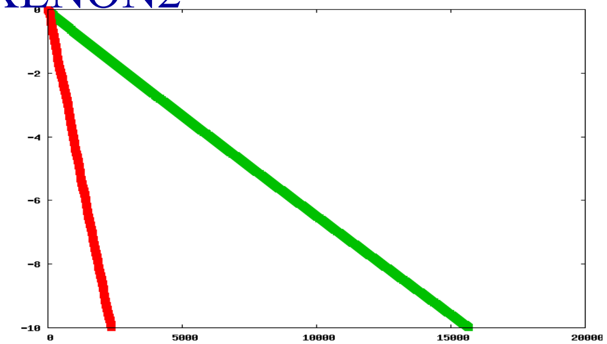
RDB5000



XENON1



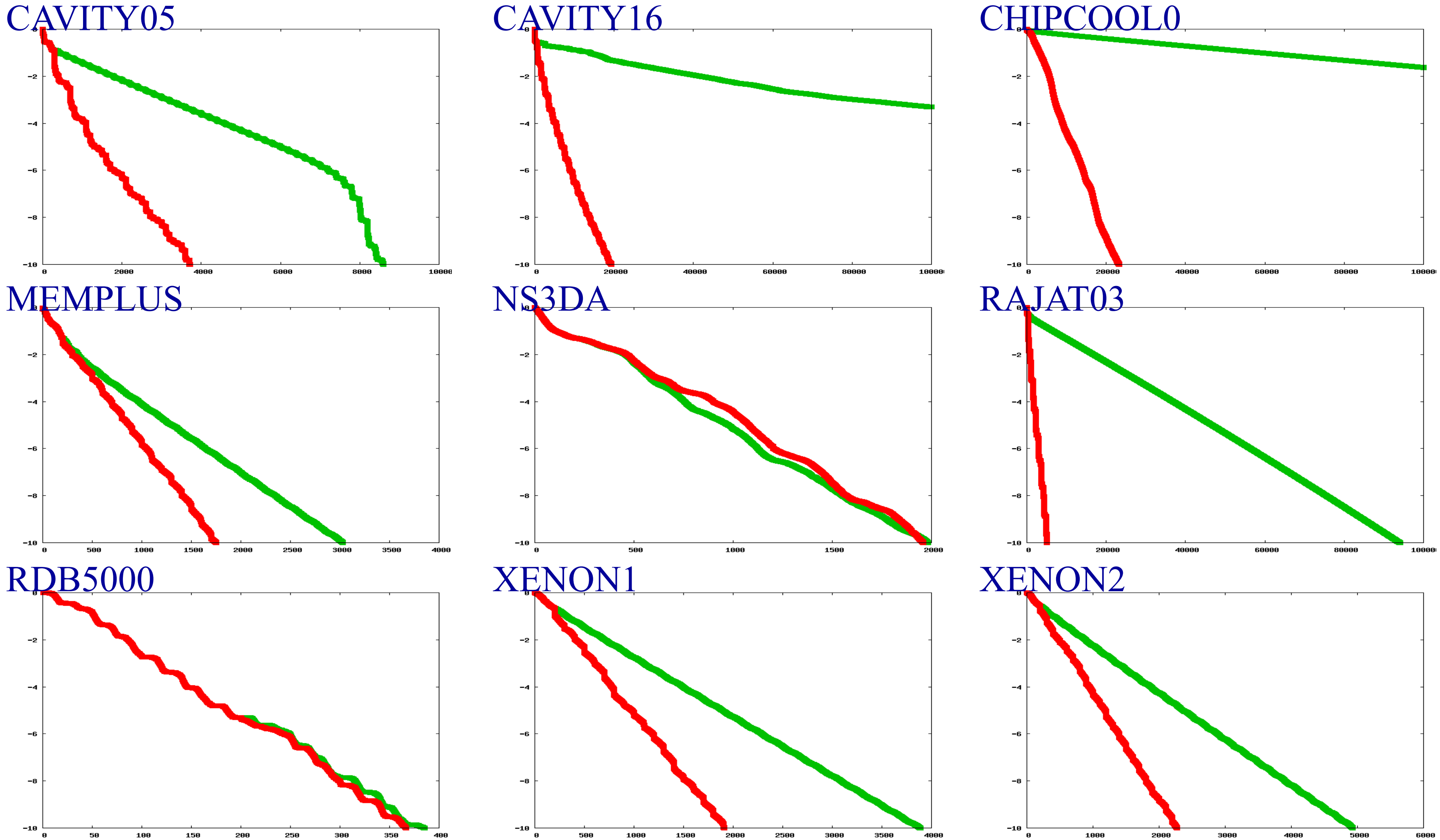
XENON2



Numerical experiments

— **GMRES(*m*)** — **Look-Back GMRES(*m*)**

- Numerical results for $m = 100$



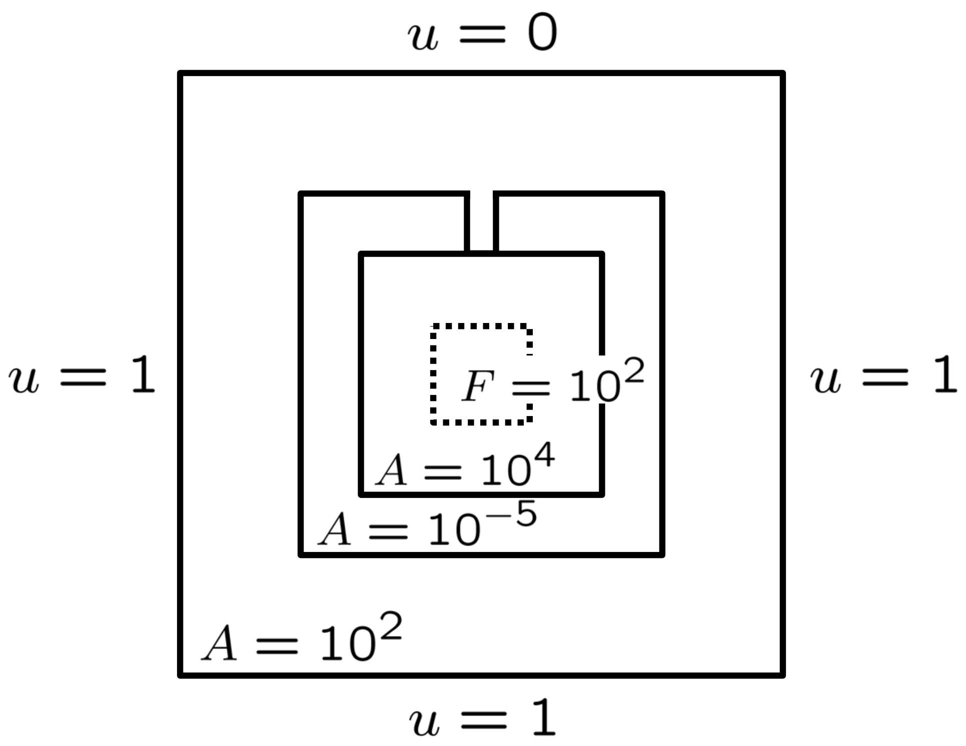
Numerical experiments

- Test problems

  -- From discretization of partial differential equation of the form

$$-(A(x,y)u_x)_x-(A(x,y)u_y)_x+\alpha\,\mathrm{exp}(2(x^2+y^2))u_x = F(x,y)$$

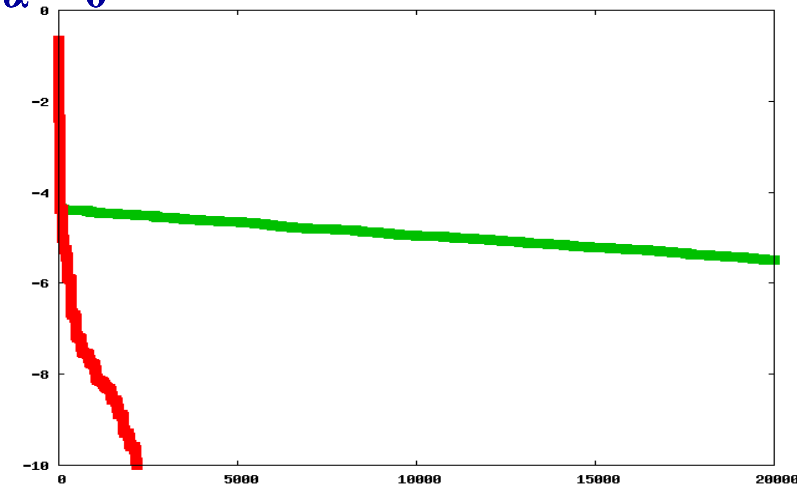
over the unit square $(x,y) \in (0,1) \times (0,1)$.



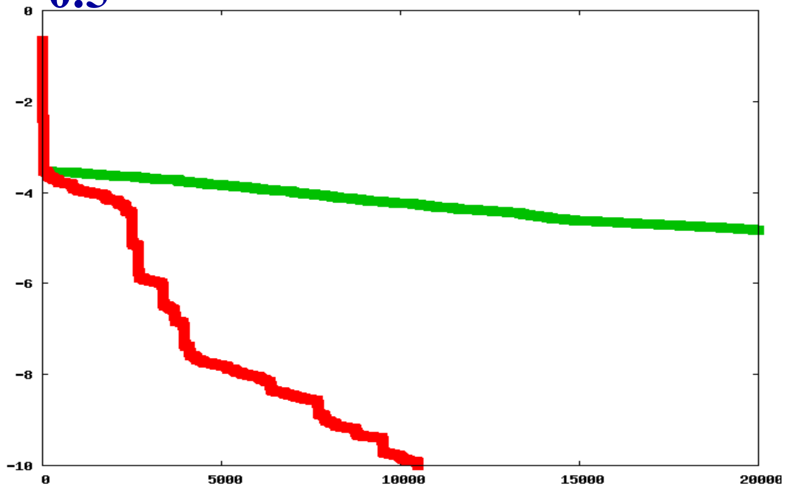
Numerical experiments

- Numerical results (m=10) — **GMRES(*m*)** — **Look-Back GMRES(*m*)**

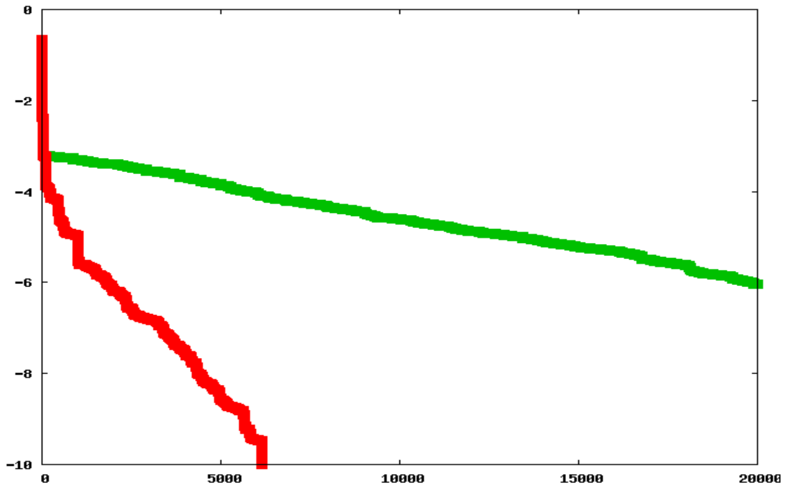
$\alpha = 0$



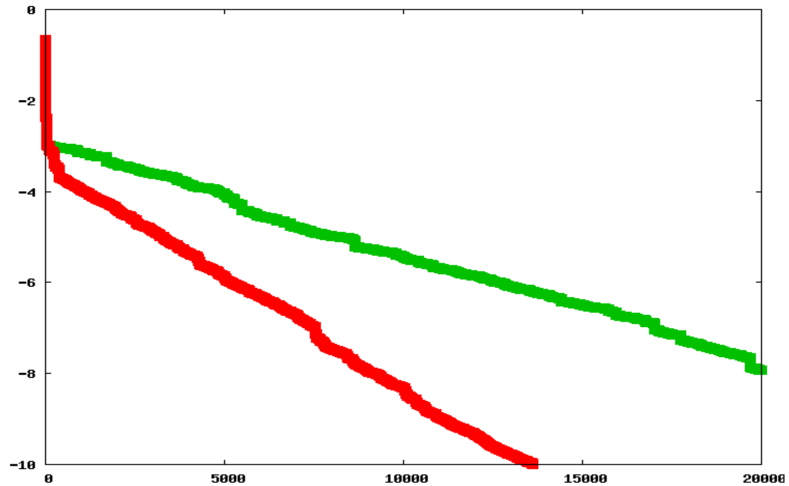
$\alpha = 0.5$



$\alpha = 1.0$



$\alpha = 2.0$



Conclusion and Future works

- Conclusion

  -- In this talk, from analysis based on residual polynomials, we proposed the Look-Back GMRES(m) method.

  -- From our numerical experiments, we learned that the Look-Back GMRES(m) method shows a good convergence than the GMRES(m) method in many cases.

  -- Therefore the Look-Back GMRES(m) method will be an efficient variant of the GMRES(m) method.

- Future works

  -- Analyze details of the Look-Back technique.
  -- Compare with other techniques for the GMRES(m) method.