

# Krylov subspace method with sparse matrix

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## Linear equation sparse matrix for partial differential eqs.

linear equation with sparse matrix  $A \in \mathbb{R}^{N \times N}$  and RHS  $\vec{b} \in \mathbb{R}^N$

$$\text{to find } \vec{x} \in \mathbb{R}^N \quad A \vec{x} = \vec{b}$$

obtained from discretization of PDE by finite element/finite volume/finite difference methods

Laplace equation

$$-\Delta u = \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = f \text{ in } \Omega, \quad u = 0 \text{ on } \partial\Omega$$

square region  $\Omega = (0, 1) \times (0, 1)$  and its boundary

$$\begin{aligned} \partial\Omega = & \{(x, 0); 0 \leq x \leq 1\} \cup \{(1, y); 0 \leq y \leq 1\} \cup \\ & \{(x, 1); 0 \leq x \leq 1\} \cup \{(0, y); 0 \leq y \leq 1\} \end{aligned}$$

discretization with uniform mesh  $\Delta x = \Delta y = h$  with  $(n+1)h = 1$

$$\frac{-u_{i-1,j} + 2u_{i,j} - u_{i+1,j}}{\Delta x^2} + \frac{-u_{i,j-1} + 2u_{i,j} - u_{i,j+1}}{\Delta y^2} = f_{i,j}$$

for unknown value  $u_{i,j} \sim u(x, y)$  at  $(x, y) = (i\Delta x, j\Delta y)$ .

numbering of two dimensional grid by

$\lambda: \{1, \dots, n\} \times \{1, \dots, n\} \rightarrow \{1, \dots, n^2\}$  with  $\lambda(i, j) = i + nj$

## sparse matrix with five stencil

$$\begin{array}{cccccccc} 2 & -1 & & & & & & -1 \\ -1 & 4 & -1 & & & & & -1 \\ & -1 & 4 & -1 & & & & -1 \\ & & \ddots & \ddots & \ddots & & & \ddots \\ & & & -1 & 4 & -1 & & -1 \\ & & & & -1 & 2 & & -1 \\ -1 & & & & & 2 & -1 & \\ & -1 & & & & -1 & 4 & -1 \\ & & -1 & & & & -1 & 4 & -1 \\ & & & \ddots & & & \ddots & \ddots & \ddots \\ & & & & -1 & & & -1 & 4 & -1 \\ & & & & & -1 & & & -1 & 2 \end{array}$$

penta-diagonal matrix with

$$N = n^2, \text{nnz} = (3n - 2)n + 2n(n - 1) = 5n^2 - 4n$$

- ▶ exploiting five stencil pattern
- ▶ storing by general sparse matrix for unstructured pattern

## Linear equation and variational problem

$A \in \mathbb{R}^{N \times N}$  : sparse matrix,  $\vec{b} \in \mathbb{R}^N$

$$\text{find } \vec{x} \in \mathbb{R}^N \quad A\vec{x} = \vec{b} \text{ in } \mathbb{R}^N$$

variational problem with test vector  $\vec{y} \in \mathbb{R}^N$

$$\text{find } \vec{x} \in \mathbb{R}^N \quad (A\vec{x} - \vec{b}, \vec{y}) = 0 \quad \forall \vec{y} \in \mathbb{R}^N$$

inner product  $(\vec{x}, \vec{y}) = \sum_{1 \leq i \leq N} [\vec{x}]_i [\vec{y}]_i = \vec{x}^T \vec{y}$

$$\ell^2\text{-norm } \|\vec{x}\| = \sqrt{(\vec{x}, \vec{x})} = \left\{ \sum_{1 \leq i \leq N} [\vec{x}]_i^2 \right\}^{1/2}$$

▶  $A\vec{x} - \vec{b} = \vec{0} \Rightarrow (A\vec{x} - \vec{b}, \vec{y}) = 0$

▶  $(A\vec{x} - \vec{b}, \vec{y}) = 0 \forall \vec{y} \Rightarrow$  putting  $\vec{y} = \vec{e}_i \ 1 \leq \forall i \leq N \ [A\vec{x} - \vec{b}]_i = 0 \Rightarrow A\vec{x} - \vec{b} = \vec{0}$

subspace  $V \subset \mathbb{R}^N$

$$\text{find } \vec{x} \in V \quad (A\vec{x} - \vec{b}, \vec{y}) = 0 \quad \forall \vec{y} \in V$$

$$\vec{r} = \vec{b} - A\vec{x} \perp V \Leftrightarrow \text{residual is orthogonal to } V$$

questions

▶  $A$  is invertible in  $V$  ?  $\Leftrightarrow A$  : coercive

▶ how to generate  $V$  ?  $\Leftrightarrow$  Krylov subspace method with preconditioner

$A \in \mathbb{R}^{N \times N}$  is coercive in subspace  $V \Leftrightarrow \exists \alpha > 0 \forall \vec{x} \in V \ (A\vec{x}, \vec{x}) \geq \alpha \|\vec{x}\|^2$

## Linear equation and variational problem

### Theorem

$A \in \mathbb{R}^{N \times N}$  : coercive in  $V \exists \alpha > 0 \forall \vec{x} \in V (A\vec{x}, \vec{x}) \geq \alpha \|\vec{x}\|^2$

$\Rightarrow \exists! \vec{x}$  satisfying  $(A\vec{x} - \vec{b}, \vec{y}) = 0 \forall \vec{y} \in V$

injectivity and surjectivity of  $A$  in  $V$  are obtained as follows

► injectivity

$(A\vec{x}, \vec{y}) = 0 \forall \vec{y} \in V \Rightarrow \vec{x} = \vec{0}$ , putting  $\vec{y} = \vec{x}$ ,

$0 = (A\vec{x}, \vec{x}) \geq \alpha \|\vec{x}\|^2 \geq 0 \Rightarrow \vec{x} = \vec{0}$

► surjectivity

$P$ : orthogonal projection from  $\mathbb{R}^N$  onto  $V$ ,  $\vec{x} \in V \Rightarrow P\vec{x} = P^T \vec{x}$

$(A\vec{x} - \vec{b}, \vec{y}) = 0 \forall \vec{y} \in V \Leftrightarrow (PAP^T)\vec{x} = P\vec{b}$  with  $PAP^T : V \rightarrow V$

direct sum in  $V$  holds as  $\text{Im}(PAP^T) \oplus \text{Ker}(PAP^T)^T = V$

assuming  $\vec{z} \neq \vec{0}$  satisfying  $\vec{z} \in \text{Ker}(PAP^T)^T = \text{Ker}(PA^T P^T)$

then  $(PA^T P^T \vec{z}, \vec{y}) = 0 \forall \vec{y} \in V \Rightarrow (A^T \vec{z}, \vec{y}) = 0$

putting  $\vec{y} = \vec{z}$ ,  $0 = (A^T \vec{z}, \vec{z}) = (\vec{z}, A\vec{z}) \Rightarrow \vec{z} = \vec{0}$  by coercivity

Linear equation with coercive coefficient matrix  $A$  is solved by

- iterative method by incrementally generated subspace  $V_1 \subset \dots \subset V_m$
- direct solver without pivoting (by assuming without rounding-off i.e., theoretical computation)

## LU factorization without pivoting for coercive matrix

iterative process of factorization of  $A$  as  $LU$

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} a_{11} & 0 \\ a_{21} & S_{22} \end{bmatrix} \begin{bmatrix} 1 & a_{11}^{-1}a_{12} \\ 0 & I_2 \end{bmatrix}$$

$S_{22} = A_{22} - a_{21}a_{11}^{-1}a_{12}$  : Schur complement generated by rank-1 update

- ▶  $a_{11} \neq 0$  thanks to  $A$  is invertible in  $V_1 = \text{span}[\vec{e}_1]$
- ▶  $S_{22}$  is coercive on  $V_{m-1} = \text{span}[\vec{e}_2, \vec{e}_3, \dots, \vec{e}_m]$   
by putting  $\vec{x}_1 = -a_{11}^{-1}a_{12}\vec{x}_2$

$$\begin{aligned} 0 &\leq \left( A \begin{bmatrix} -a_{11}^{-1}a_{12}\vec{x}_2 \\ \vec{x}_2 \end{bmatrix}, \begin{bmatrix} -a_{11}^{-1}a_{12}\vec{x}_2 \\ \vec{x}_2 \end{bmatrix} \right) \\ &= \left( \begin{bmatrix} a_{11}(-a_{11}^{-1}a_{12}\vec{x}_2) + a_{12}\vec{x}_2 \\ a_{21}(-a_{11}^{-1}a_{12}\vec{x}_2) + A_{22}\vec{x}_2 \end{bmatrix}, \begin{bmatrix} \vec{x}_1 \\ \vec{x}_2 \end{bmatrix} \right) \\ &= ((A_{22} - a_{21}a_{11}^{-1}a_{12})\vec{x}_2, \vec{x}_2) = (S\vec{x}_2, \vec{x}_2) \end{aligned}$$

## coercivity and other property of matrix

- ▶ coercive :  $\exists \alpha > 0 \forall \vec{x} (A\vec{x}, \vec{x}) \geq \alpha \|\vec{x}\|^2$ .
- ▶ indefinite matrix does not satisfy coercivity, a simple example:

$$\left( \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \end{bmatrix} \right) = 0$$

- ▶ diagonal dominant :  $|a_{ii}| > \sum_{j \neq i} |a_{ij}|$
- ▶  $M$ -matrix :  $Z$ -matrix  $\wedge \operatorname{Re} \lambda_i > 0 (1 \leq i \leq N)$ ,  $\lambda_i$  :  $i$ -th eigenvalue
- ▶  $Z$ -matrix  $a_{ij} < 0 i \neq j$

$M$ -matrix property is obtained from the maximum principle of the Laplace operator. Convergence of Gauss-Seidel method is proven by this property.

## overview of Krylov subspace methods

$A$  : symmetric

- ▶ positive definite : CG (conjugate gradient)
- ▶ indefinite : SYMMLQ, MINRES

$A$  : unsymmetric

- ▶ coercive : FOM (full orthogonalization method)
- ▶ general : GMRES (generalized minimum residual),  
Orthmin, GCR  
BiCG(bi conjugate gradient), CGS , BiCGstab  
QMR, TFQMR

$\vec{r}_0 = b - A\vec{x}_0$  : initial residual from initial guess  $x_0$

subspaces  $V$  and  $W$

find  $\vec{x} \in \vec{x}_0 + V \quad (A\vec{x} - \vec{b}, \vec{y}) = 0 \quad \forall \vec{y} \in V$  : CG, FOM

find  $\vec{x} \in \vec{x}_0 + V \quad (A\vec{x} - \vec{b}, A\vec{y}) = 0 \quad \forall \vec{y} \in V$  : Orthmin, GCR

find  $\vec{x} \in \vec{x}_0 + V \quad \|A\vec{x} - \vec{b}\| \leq \|A\vec{y} - \vec{b}\| \quad \forall \vec{y} \in \vec{x}_0 + V$  : MINRES, GMRES

find  $\vec{x} \in \vec{x}_0 + V \quad (A\vec{x} - \vec{b}, \vec{y}) = 0 \quad \forall \vec{y} \in W$  : BiCG

### Krylov subspaces

$$V = K_n(A, \vec{r}_0) := \text{span}[\vec{r}_0, A\vec{r}_0, A^2\vec{r}_0, \dots, A^{n-1}\vec{r}_0]$$

$$W = K_n(A^T, \vec{r}_0^*) := \text{span}[\vec{r}_0^*, A^T\vec{r}_0^*, (A^T)^2\vec{r}_0^*, \dots, (A^T)^{n-1}\vec{r}_0^*]$$



## Krylov subspace and solution of the linear system : 1/2

- ▶  $A \in \mathbb{R}^{N \times N}$ , invertible,  $\vec{b} \in \mathbb{R}^N$ ,
- ▶  $\vec{x}_0$  : initial guess,
- ▶  $\vec{r}_0 := \vec{b} - A\vec{x}_0$  : initial residual.

### Krylov subspace

$$K_n(A, \vec{r}_0) := \text{span}[\vec{r}_0, A\vec{r}_0, A^2\vec{r}_0, \dots, A^{n-1}\vec{r}_0]$$

### Lemma

$$A^n \vec{r}_0 \in K_n(A, \vec{r}_0) \Rightarrow A^{n+m} \vec{r}_0 \in K_n(A, \vec{r}_0) \quad \forall m > 0$$

proof by induction, suppose that  $A^{n+m} \vec{r}_0 \in K_n(A, \vec{r}_0) \quad m \geq 0$

$$\begin{aligned} A^{n+m} \vec{r}_0 &= \sum_{k=0}^{n-1} \alpha_k A^k \vec{r}_0 \\ A^{n+m+1} \vec{r}_0 &= \sum_{k=0}^{n-2} \alpha_k A^{k+1} \vec{r}_0 + \alpha_{n-1} A^n \vec{r}_0 \\ &= \sum_{k=0}^{n-2} \alpha_k A^{k+1} \vec{r}_0 + \alpha_{n-1} \sum_{k=0}^{n-1} \beta_k A^k \vec{r}_0 \in K_n(A, \vec{r}_0). \end{aligned}$$

dimension of the largest Krylov subspace created by  $A$  and  $\vec{r}_0$ .

$$\text{▶ } n_0 := \min_n \{K_n(A, \vec{r}_0) = K_{n+1}(A, \vec{r}_0)\}$$

$$K_1(A, \vec{r}_0) \subset K_2(A, \vec{r}_0) \subset \dots \subset K_{n_0}(A, \vec{r}_0) = K_{n_0+1}(A, \vec{r}_0) = K_{n_0+2}(A, \vec{r}_0) = \dots$$

$$\dim K_l(A, \vec{r}_0) = l \quad 1 \leq l \leq n_0$$

## Krylov subspace and solution of the linear system : 2/2

### Theorem

$\vec{x}$  : solution of linear system  $A\vec{x} = \vec{b} \Rightarrow \vec{x} \in \vec{x}_0 + K_{n_0}(A, \vec{r}_0)$ .

proof

recalling that  $\vec{r}_0, A\vec{r}_0, A^2\vec{r}_0, \dots, A^{n_0-1}\vec{r}_0$  : linearly independent.

$\alpha_0 \neq 0$  such that  $A^{n_0}\vec{r}_0 = \sum_{k=0}^{n_0-1} \alpha_k A^k \vec{r}_0$ .

$$\alpha_0 = 0 \Rightarrow A^{n_0}\vec{r}_0 = \sum_{k=1}^{n_0-1} \alpha_k A^k \vec{r}_0,$$

by applying  $A^{-1}$

$$A^{n_0-1}\vec{r}_0 = \sum_{k=1}^{n_0-1} \alpha_k A^{k-1}\vec{r}_0,$$

$\Rightarrow \vec{r}_0, A\vec{r}_0, A^2\vec{r}_0, \dots, A^{n_0-1}\vec{r}_0$  : linearly dependent  $\Rightarrow \Leftarrow$

$$\alpha_0 \vec{r}_0 + \sum_{k=1}^{n_0-1} \alpha_k A^k \vec{r}_0 - A^{n_0}\vec{r}_0 = \vec{0} \Leftrightarrow \vec{r}_0 + \sum_{k=1}^{n_0-1} \frac{\alpha_k}{\alpha_0} A^k \vec{r}_0 - \frac{1}{\alpha_0} A^{n_0}\vec{r}_0 = \vec{0}$$

$$\Leftrightarrow (\vec{b} - A\vec{x}_0) + \sum_{k=1}^{n_0} \gamma_k A^k \vec{r}_0 = \vec{0} \Leftrightarrow A \left( \vec{x}_0 - \sum_{k=1}^{n_0} \gamma_k A^k \vec{r}_0 \right) = \vec{b}.$$

$$\vec{x}_0 - \sum_{k=1}^{n_0} \gamma_k A^k \vec{r}_0 \in \vec{x}_0 + K_{n_0}(A, \vec{r}_0) + \text{uniqueness of the solution : } A\vec{x} = \vec{b}.$$

## Krylov subspace and variational solution of the linear system

### Theorem

problem (V) to find  $\vec{x} \in \vec{x}_0 + K_{n_0}(A, \vec{r}_0)$   $(A\vec{x} - \vec{b}, \vec{y}) = 0 \quad \forall \vec{y} \in K_{n_0}(A, \vec{r}_0)$   
has a unique solution and is equivalent to the problem  $A\vec{x} = \vec{b}$ .

proof

- ▶  $\vec{x}_* \in \vec{x}_0 + K_{n_0}(A, \vec{r}_0)$  : solution of (V).
- ▶  $\vec{x}_1$  : solution of  $(A\vec{x} - b, \vec{y}) = 0 \quad \forall \vec{y} \in \mathbb{R}^N \Rightarrow \vec{x}_1 \in \vec{x}_0 + K_{n_0}(A, \vec{r}_0)$ .  
 $(A\vec{x}_1 - b, \vec{y}) = 0 \quad \forall \vec{y} \in K_{n_0}(A, \vec{r}_0) \subset \mathbb{R}^N \Rightarrow \vec{x}_1$  : solution of (V).

to verify uniqueness  $(A(\vec{x}_0 - \vec{x}_*), \vec{y}) = 0 \quad \forall \vec{y} \in K_{n_0}(A, \vec{r}_0) \stackrel{?}{\Rightarrow} \vec{x}_0 - \vec{x}_* = \vec{0}$   
 $A : 1$  to  $1$  on  $K_{n_0}(A, \vec{r}_0)$  is verified as

$$\vec{z} \in K_{n_0}(A, \vec{r}_0) \text{ satisfying } (A\vec{z}, \vec{y}) = 0 \quad \forall \vec{y} \in K_{n_0}(A, \vec{r}_0) \\ \Rightarrow A\vec{z} \in (K_{n_0}(A, \vec{r}_0))^\perp \vee \vec{z} \in \ker A$$

$$\left. \begin{array}{l} \vec{z} \in K_{n_0}(A, \vec{r}_0) \Rightarrow A\vec{z} \in K_{n_0}(A, \vec{r}_0) \\ \exists A^{-1} \Rightarrow \ker A = \{\vec{0}\} \end{array} \right\} \Rightarrow \vec{z} = \vec{0}.$$

### successive computation of variational problems

do  $m = 1, 2, \dots, n_0$

find  $\vec{x} \in \vec{x}_0 + K_m(A, \vec{r}_0)$   $(A\vec{x} - \vec{b}, \vec{y}) = 0 \quad \forall \vec{y} \in K_m(A, \vec{r}_0)$

- ▶ Conjugate Gradient (CG) method  $\Leftarrow A$  : symmetric positive definite
- ▶ Full Orthogonalization Method (FOM)  $\Leftarrow A$  : coercive

## Arnoldi process

$\|\vec{v}_1\| = 1,$   
 $\{\vec{v}_1, A\vec{v}_1, A^2\vec{v}_1, \dots, A^{m-1}\vec{v}_1\} \rightarrow$  orthonormal basis  $\{\vec{v}_1, \vec{v}_2, \dots, \vec{v}_m\}$   
by Gram-Schmidt

Algorithm (Arnoldi process)

do  $j = 1, 2, \dots, m$

$$h_{i,j} = (A\vec{v}_j, \vec{v}_i) \quad 1 \leq i \leq j$$

$$\vec{w}_j = A\vec{v}_j - \sum_{i=1}^j h_{i,j} \vec{v}_i$$

$$h_{j+1,j} = \|\vec{w}_j\|^2$$

$$\vec{v}_{j+1} = \frac{\vec{w}_j}{h_{j+1,j}}$$

from the last line,

$$h_{j+1,j} \vec{v}_{j+1} = A\vec{v}_j - \sum_{i=1}^j h_{i,j} \vec{v}_i,$$

$$A\vec{v}_j = \sum_{i=1}^{j+1} h_{i,j} \vec{v}_i.$$

$$[A\vec{v}_1, \dots, A\vec{v}_m] = [\vec{v}_1, \dots, \vec{v}_m, \vec{v}_{m+1}] \begin{bmatrix} h_{1,1} & h_{1,2} & \cdots & h_{1,m-1} & h_{1,m} \\ h_{2,1} & h_{2,2} & \cdots & h_{2,m-1} & h_{2,m} \\ & h_{3,2} & \cdots & h_{3,m-1} & h_{3,m} \\ & & \ddots & \vdots & \vdots \\ & & & h_{m,m-1} & h_{m,m} \\ & & & & h_{m+1,m} \end{bmatrix}$$

$$AV_m = V_{m+1} \bar{H}_m \quad \bar{H}_m \in \mathbb{R}^{(m+1) \times m} : \text{Hessenberg matrix,}$$

$$V_m^T AV_m = H_m \Leftrightarrow V_m^T V_m = I_m \Leftrightarrow (\vec{v}_j, \vec{v}_i) = \delta_{ij} \quad 1 \leq i, j \leq m$$

## Full Orthogonalization Method

- ▶  $A \in \mathbb{R}^{N \times N}$ , invertible,  $\vec{b} \in \mathbb{R}^N$ ,
- ▶  $\vec{x}_0$  : initial guess,
- ▶  $\vec{r}_0 := \vec{b} - A\vec{x}_0$  : initial residual.
- ▶  $K_n(A, \vec{r}_0) := \text{span}[\vec{r}_0, A\vec{r}_0, A^2\vec{r}_0, \dots, A^{n-1}\vec{r}_0]$  : Krylov subspace

construction of basis of Krylov subspace by Arnoldi process  
starting from  $\vec{v}_1 = \vec{r}_0/\beta$ ,  $\beta = \|\vec{r}_0\|$ ,

$$AV_m = V_{m+1}\bar{H}_m$$

$$V_m^T AV_m = H_m$$

$$V_m^T \vec{r}_0 = V_m^T \beta \vec{v}_1 = \beta \vec{\epsilon}_m^{(1)}, \quad [\vec{\epsilon}_m^{(1)}]_i = \delta_{i1} \quad 1 \leq i \leq m$$

find  $\vec{x}_m \in \vec{x}_0 + K_m(A, \vec{r}_0)$   $(A\vec{x}_m - \vec{b}, \vec{y}) = 0 \quad \forall \vec{y} \in K_m(A, \vec{r}_0)$

$$\vec{x}_m = \vec{x}_0 + V_m \vec{\eta}_m$$

$$\begin{aligned} A\vec{x}_m - \vec{b} &= A\vec{x}_0 - \vec{b} + AV_m \vec{\eta}_m \\ &= -\vec{r}_0 + AV_m \vec{\eta}_m \end{aligned}$$

$$\begin{aligned} V_m^T (A\vec{x}_m - \vec{b}) &= -V_m^T \vec{r}_0 + V_m^T AV_m \vec{\eta}_m \\ &= -\beta \vec{\epsilon}_m^{(1)} + H_m \vec{\eta}_m, \end{aligned}$$

$$\vec{\eta}_m = H_m^{-1} (\beta \vec{\epsilon}_m^{(1)})$$

$H_m$  : invertible?  $A$  is coercive  $\Rightarrow$  yes

## Generalized Minimal Residual (GMRES) Method : 1/3

- ▶  $A \in \mathbb{R}^{N \times N}$ , invertible,  $\vec{b} \in \mathbb{R}^N$ ,
- ▶  $\vec{x}_0$  : initial guess,
- ▶  $\vec{r}_0 := \vec{b} - A\vec{x}_0$  : initial residual.
- ▶  $K_n(A, \vec{r}_0) := \text{span}[\vec{r}_0, A\vec{r}_0, A^2\vec{r}_0, \dots, A^{n-1}\vec{r}_0]$  : Krylov subspace

construction of basis of Krylov subspace by Arnoldi process  
starting from  $\vec{v}_1 = \vec{r}_0/\beta, \beta = \|\vec{r}_0\|$ ,

$$AV_m = V_{m+1}\bar{H}_m,$$

$$\vec{r}_0 = \beta\vec{v}_1 = \beta V_{m+1}\vec{\epsilon}_{m+1}^{(1)}, \quad [\vec{\epsilon}_{m+1}^{(1)}]_i = \delta_{i1} \quad 1 \leq i \leq m+1$$

find  $\vec{x}_m \in \vec{x}_0 + K_m(A, \vec{r}_0)$

$$\|\vec{b} - A\vec{x}_m\| \leq \|\vec{b} - A\vec{y}\| \quad \forall \vec{y} \in \vec{x}_0 + K_m(A, \vec{r}_0)$$

$$\vec{y} = \vec{x}_0 + V_m\vec{\eta}_m$$

$$\vec{b} - A\vec{y} = \vec{b} - A\vec{x}_0 - AV_m\vec{\eta}_m$$

$$= \vec{r}_0 - AV_m\vec{\eta}_m$$

$$= V_{m+1} \left( \beta\vec{\epsilon}_{m+1}^{(1)} - \bar{H}_m\vec{\eta}_m \right)$$

$$\|\vec{b} - A\vec{y}\| = \|\beta\vec{\epsilon}_{m+1}^{(1)} - \bar{H}_m\vec{\eta}_m\| \quad \Leftarrow V_{m+1}^T V_{m+1} = I_{m+1}.$$

find  $\vec{x}_m = \vec{x}_0 + V_m\vec{\eta}_m, \vec{\eta}_m = \underset{\vec{\eta}}{\text{argmin}} \|\beta\vec{\epsilon}_{m+1}^{(1)} - \bar{H}_m\vec{\eta}_m\|$  works for any  $\bar{H}_m$

## Generalized Minimal Residual (GMRES) Method : 2/3

a way to solve minimization problem by QR-factorization with Givens rotation

Givens rotation matrices  $\Omega_i \in \mathbb{R}^{(m+1) \times (m+1)}$

$$\Omega_1 := \begin{bmatrix} c_1 & s_1 & & & & \\ -s_1 & c_1 & & & & \\ & & I_{m-1} & & & \\ & & & & & \\ & & & & & \\ & & & & & \end{bmatrix}, \quad c_1 := \frac{h_{1,1}}{\sqrt{h_{1,1}^2 + h_{2,1}^2}}, \quad s_1 := \frac{h_{2,1}}{\sqrt{h_{1,1}^2 + h_{2,1}^2}}.$$

$$\Omega_1 \bar{H}_m = \begin{bmatrix} h_{1,1}^{(1)} & h_{1,2}^{(1)} & \cdots & h_{1,m-1}^{(1)} & h_{1,m}^{(1)} \\ 0 & h_{2,2}^{(1)} & \cdots & h_{2,m-1}^{(1)} & h_{2,m}^{(1)} \\ & h_{3,2} & \cdots & h_{3,m-1} & h_{3,m} \\ & & \ddots & \vdots & \vdots \\ & & & h_{m,m-1} & h_{m,m} \\ & & & & h_{m+1,m} \end{bmatrix}, \quad \beta \Omega_1 \bar{e}_{m+1}^{(1)} = \beta \Omega_1 \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix} = \beta \begin{bmatrix} c_1 \\ -s_1 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}$$

$$Q_m := \Omega_m \Omega_{m-1} \cdots \Omega_1 \in \mathbb{R}^{(m+1) \times (m+1)},$$

$$Q_{m-1} \bar{H}_m = \begin{bmatrix} h_{1,1}^{(1)} & h_{1,2}^{(1)} & h_{1,3}^{(1)} & \cdots & h_{1,m-1}^{(1)} & h_{1,m}^{(1)} \\ 0 & h_{2,2}^{(2)} & h_{2,3}^{(2)} & \cdots & h_{2,m-1}^{(2)} & h_{2,m}^{(2)} \\ & 0 & h_{3,3}^{(3)} & \cdots & h_{3,m-1}^{(3)} & h_{3,m}^{(3)} \\ & & & \ddots & \vdots & \vdots \\ & & & & \vdots & \vdots \\ & & & & h_{m-1,m-1}^{(m-2)} & h_{m-1,m}^{(m-2)} \\ & & & & 0 & h_{m,m}^{(m-1)} \\ & & & & 0 & h_{m+1,m} \end{bmatrix} \beta \begin{bmatrix} c_1 \\ -c_2 s_1 \\ c_3 s_2 s_1 \\ \vdots \\ \gamma_{m-2} \\ \gamma_{m-1} \\ -s_{m-1} \gamma_{m-1} \\ 0 \end{bmatrix}$$

## Generalized Minimal Residual (GMRES) Method : 3/3

$$Q_m \bar{H}_m = \begin{bmatrix} h_{1,1}^{(1)} & h_{1,2}^{(1)} & h_{1,3}^{(1)} & \cdots & h_{1,m-1}^{(1)} & h_{1,m}^{(1)} \\ 0 & h_{2,2}^{(2)} & h_{2,3}^{(2)} & \cdots & h_{2,m-1}^{(2)} & h_{2,m}^{(2)} \\ & 0 & h_{3,3}^{(3)} & \cdots & h_{3,m-1}^{(3)} & h_{3,m}^{(3)} \\ & & 0 & \ddots & \vdots & \vdots \\ & & & \ddots & h_{m-1,m-1}^{(m-1)} & h_{m,m-1}^{(m-1)} \\ & & & & 0 & h_{m,m}^{(m)} \\ & & & & 0 & 0 \end{bmatrix}, \beta Q_m \bar{e}_{m+1}^{(1)} = \beta \begin{bmatrix} c_1 \\ -c_2 s_1 \\ c_3 s_2 s_1 \\ \vdots \\ \gamma_{m-1} \\ \gamma_m \\ -s_m \gamma_m \end{bmatrix}$$

$\bar{R}_m := Q_m \bar{H}_m$ : upper triangular,

$$\bar{\gamma}_{m+1} := \beta Q_m \bar{e}_{m+1}^{(1)} = [\gamma_1, \gamma_2, \dots, \gamma_{m+1}]^T = [\bar{\gamma}_m^T, \gamma_{m+1}]^T,$$

$$\min \|\beta \bar{e}_{m+1}^{(1)} - \bar{H}_m \bar{\eta}\| = \min \|Q_m (\bar{\gamma}_{m+1} - \bar{R}_m \bar{\eta})\| = |\gamma_{m+1}| = |s_1 s_2 \cdots s_m| \beta.$$

$\bar{\eta}_m = R_m^{-1} \bar{\gamma}_m$  attains the minimum.

- ▶  $\exists R_m^{-1}$  ( $1 \leq m \leq n_0$ ) for invertible matrix  $A \Leftarrow h_{j+1,j} > 0$  ( $1 \leq j < n_0$ )
- ▶ residual  $\|\bar{r}_m\| = \|\bar{b} - A\bar{x}_m\|$  decreases monotonically thanks to  $s_m$ .
- ▶  $h_{m,m}^{(m-1)} = 0 \Rightarrow Q_{m-1} H_m$ : singular, FOM fails  
 $\Rightarrow c_m = 0, s_m = 1$ , GMRES stagnates at  $m$ -th step.
- ▶  $\bar{r}_m^{\text{GMRES}} = s_m^2 \bar{r}_{m-1}^{\text{GMRES}} + c_m^2 \bar{r}_m^{\text{FOM}}$   $s_{n_0} = 0, c_{n_0} = 1 \Leftarrow h_{n_0+1, n_0} = 0$ .



## conjugate gradient method : 1/3

- ▶  $A \in \mathbb{R}^{N \times N}$ , symmetric positive definite,  $\vec{b} \in \mathbb{R}^N$ ,
- ▶  $\vec{x}_0$  : initial guess,
- ▶  $\vec{r}_0 := \vec{b} - A\vec{x}_0$  : initial residual.
- ▶  $K_n(A, \vec{r}_0) := \text{span}[\vec{r}_0, A\vec{r}_0, A^2\vec{r}_0, \dots, A^{n-1}\vec{r}_0]$  : Krylov subspace

### Algorithm(CG)

$\vec{p}_0 = \vec{r}_0$ .

do  $m = 0, 1, \dots$

$$\alpha_m = \|\vec{r}_m\|^2 / (A\vec{p}_m, \vec{p}_m),$$

$$\vec{x}_{m+1} = \vec{x}_m + \alpha_m \vec{p}_m,$$

$$\vec{r}_{m+1} = \vec{r}_m - \alpha_m A\vec{p}_m,$$

if  $\|\vec{r}_{m+1}\| < \epsilon$  exit loop.

$$\beta_m = \|\vec{r}_{m+1}\|^2 / \|\vec{r}_m\|^2,$$

$$\vec{p}_{m+1} = \vec{r}_{m+1} + \beta_m \vec{p}_m.$$

**Lemma** for  $1 \leq m \leq n_0$

$$\text{▶ } (\vec{r}_m, \vec{z}) = 0 \quad \forall \vec{z} \in K_m(A, \vec{r}_0)$$

$$\text{▶ } (A\vec{p}_m, \vec{z}) = 0 \quad \forall \vec{z} \in K_m(A, \vec{r}_0)$$

$$\text{▶ } \text{span}[\vec{r}_0, \vec{r}_1, \dots, \vec{r}_m] = \text{span}[\vec{p}_0, \vec{p}_1, \dots, \vec{p}_m] = K_{m+1}(A, \vec{r}_0)$$

### successive computation of variational problems

do  $m = 1, 2, \dots, n_0$

$$\text{find } \vec{x} \in \vec{x}_0 + K_m(A, \vec{r}_0) \quad (A\vec{x} - \vec{b}, \vec{y}) = 0 \quad \forall \vec{y} \in K_m(A, \vec{r}_0)$$

## conjugate gradient method : 2/3

proof of Lemma by induction

for  $m = 1$

$$(1) \quad (\vec{r}_1, \vec{r}_0) = (\vec{r}_0 - \alpha_0 A\vec{p}_0, \vec{r}_0) = (\vec{r}_0, \vec{r}_0) - \frac{\|\vec{r}_0\|^2}{(A\vec{p}_0, \vec{p}_0)} (A\vec{p}_0, \vec{p}_0) = 0$$

$$(2) \quad (A\vec{p}_1, \vec{r}_0) = (\vec{r}_1 + \beta_0 \vec{p}_0, A\vec{p}_0) \quad \text{by symmetry of } A \\ = (\vec{r}_1 + \beta_0 \vec{p}_0, \frac{1}{\alpha_0}(\vec{r}_0 - \vec{r}_1)) = -\frac{1}{\alpha_0}(\vec{r}_1, \vec{r}_1) + \frac{\beta_0}{\alpha_0}(\vec{p}_0, \vec{r}_0) = 0$$

$$(3) \quad \text{span}[\vec{r}_0, \vec{r}_1] = \text{span}[\vec{p}_0, \vec{p}_1] = K_2(A, \vec{r}_0) \Leftarrow \alpha_0 \neq 0$$

for  $m = k$ ,  $\vec{z} \in K_{k+1}(A, \vec{r}_0)$  : decomposed as  $\vec{z} = \vec{z}_0 + \gamma_k \vec{p}_k$ ,  $\vec{z}_0 \in K_k(A, \vec{r}_0)$

$$(1) \quad (\vec{r}_{k+1}, \vec{z}_0) = (\vec{r}_k - \alpha_k A\vec{p}_k, \vec{z}_0) = (\vec{r}_k, \vec{z}_0) - \alpha_k (A\vec{p}_k, \vec{z}_0) = 0 \\ (\vec{r}_{k+1}, \vec{p}_k) = (\vec{r}_k, \vec{p}_k) - \alpha_k (A\vec{p}_k, \vec{p}_k)$$

$$= (\vec{r}_k, \vec{r}_k + \beta_{k-1} \vec{p}_{k-1}) - \|\vec{r}_k\|^2 = \beta_{k-1}(\vec{r}_k, \vec{p}_{k-1}) = 0$$

$$(2) \quad (A\vec{p}_{k+1}, \vec{z}_0) = (A(\vec{r}_{k+1} + \beta_k \vec{p}_k), \vec{z}_0) = (\vec{r}_{k+1}, A\vec{z}_0) + \beta_k (A\vec{p}_k, \vec{z}_0) = 0 \\ (A\vec{p}_{k+1}, \vec{p}_k) = (\vec{r}_{k+1}, A\vec{p}_k) + \beta_k (A\vec{p}_k, \vec{p}_k)$$

$$= (\vec{r}_{k+1}, \frac{1}{\alpha_k}(\vec{r}_k - \vec{r}_{k+1})) + \beta_k (A\vec{p}_k, \vec{p}_k)$$

$$= -\frac{1}{\alpha_{k+1}} \|\vec{r}_{k+1}\|^2 + \|\vec{r}_{k+1}\|^2 \frac{(A\vec{p}_k, \vec{p}_k)}{\|\vec{r}_k\|^2} = 0$$

$$(3) \quad \text{span}[\vec{r}_0, \dots, \vec{r}_k, \vec{r}_{k+1}] = \text{span}[\vec{r}_0, \dots, \vec{r}_k, \vec{r}_k - \alpha_k A\vec{p}_k] = K_{k+2}(A, \vec{r}_0)$$



## bi-conjugate gradient method : 1/3

- ▶  $A \in \mathbb{R}^{N \times N}$  : invertible,  $\vec{b} \in \mathbb{R}^N$ ,
- ▶  $\vec{x}_0$  : initial guess,
- ▶  $\vec{r}_0 := \vec{b} - A\vec{x}_0$  : initial residual,  $\vec{r}_0^*$  : shadow residual
- ▶  $K_n(A, \vec{r}_0) := \text{span}[\vec{r}_0, A\vec{r}_0, A^2\vec{r}_0, \dots, A^{n-1}\vec{r}_0]$ ,  $K_n(A^T, \vec{r}_0^*)$

### Algorithm(Bi-CG)

$\vec{p}_0 = \vec{r}_0$ ,  $\vec{p}_0^* = \vec{r}_0^*$ .

do  $m = 0, 1, \dots$

$$\alpha_m = (\vec{r}_m, \vec{r}_m^*) / (A\vec{p}_m, \vec{p}_m^*),$$

$$\vec{x}_{m+1} = \vec{x}_m + \alpha_m \vec{p}_m,$$

$$\vec{r}_{m+1} = \vec{r}_m - \alpha_m A\vec{p}_m, \quad \vec{r}_{m+1}^* = \vec{r}_m^* - \alpha_m A^T \vec{p}_m^*,$$

if  $\|\vec{r}_{m+1}\| < \epsilon$  exit loop.

$$\beta_m = (\vec{r}_{m+1}, \vec{r}_{m+1}^*) / (\vec{r}_m, \vec{r}_m^*),$$

$$\vec{p}_{m+1} = \vec{r}_{m+1} + \beta_m \vec{p}_m, \quad \vec{p}_{m+1}^* = \vec{r}_{m+1}^* + \beta_m \vec{p}_m^*,$$

**Lemma** if without breakdown for  $1 \leq m \leq n_0$

- ▶  $(\vec{r}_m, \vec{z}) = 0 \quad \forall \vec{z} \in K_m(A^T, \vec{r}_0^*)$
- ▶  $(A\vec{p}_m, \vec{z}) = 0 \quad \forall \vec{z} \in K_m(A^T, \vec{r}_0^*)$
- ▶  $\text{span}[\vec{r}_0, \vec{r}_1, \dots, \vec{r}_m] = \text{span}[\vec{p}_0, \vec{p}_1, \dots, \vec{p}_m] = K_{m+1}(A, \vec{r}_0)$
- ▶  $\text{span}[\vec{r}_0^*, \vec{r}_1^*, \dots, \vec{r}_m^*] = \text{span}[\vec{p}_0^*, \vec{p}_1^*, \dots, \vec{p}_m^*] = K_{m+1}(A^T, \vec{r}_0^*)$

successive computation of variational problems

do  $m = 1, 2, \dots, n_0$

$$\text{find } \vec{x} \in \vec{x}_0 + K_m(A, \vec{r}_0) \quad (A\vec{x} - \vec{b}, \vec{y}) = 0 \quad \forall \vec{y} \in K_m(A^T, \vec{r}_0^*)$$

## bi-conjugate gradient method : 2/3

Lanczos biorthogonalization process

$$[A\vec{v}_1, \dots, A\vec{v}_m] = [\vec{v}_1, \dots, \vec{v}_m, \vec{v}_{m+1}]$$

$$\begin{bmatrix} \alpha_1 & \beta_2 & & & & \\ \delta_2 & \alpha_2 & \ddots & & & \\ & \delta_3 & \ddots & & & \\ & & \ddots & \ddots & & \\ & & & \delta_m & \beta_m & \\ & & & & \alpha_m & \\ & & & & & \delta_{m+1} \end{bmatrix}$$

$$AV_m = V_m T_m + \delta_{m+1} \vec{v}_{m+1} \vec{\epsilon}_m^{(m)T}$$

$$A^T W_m = W_m T_m^T + \beta_{m+1} \vec{w}_{m+1} \vec{\epsilon}_m^{(m)T}$$

$$W_m^T A V_m = T_m \quad \Leftrightarrow \quad W_m^T V_m = I_m : \text{bi-orthogonality}$$

### two-sided Lanczos algorithm

variational problem with Petrov-Galerkin type

$$\text{find } \vec{x} \in \vec{x}_0 + K_m(A, \vec{r}_0) \quad (A\vec{x} - \vec{b}, \vec{y}) = 0 \quad \forall \vec{y} \in K_m(A^T, \vec{r}_0^*)$$

$$\text{find } \vec{x}_m = \vec{x}_0 + V_m \vec{\eta}_m, \quad \text{by solving } T_m \vec{\eta}_m = \beta \vec{\epsilon}_m^{(1)}$$

Two possibilities of break down

▶  $(A\vec{p}_m, \vec{p}_m^*) = 0 \Rightarrow T_m$  becomes singular

▶  $(\vec{r}_m, \vec{r}_m^*) = 0 \Rightarrow$  breakdown of Lanczos biorthogonalization process

## bi-conjugate gradient method : 3/3

Composite step biconjugate gradient method  
stable factorization of  $T_m$  with  $2 \times 2$  block pivots

Bank-Chan 1993

Quasi-Minimal Residual (QMR) method  
 $V_m$  generated by look-ahead Lanczos process

Freund-Nachtigal 1991  
Parlett-Taylor-Liu 1985

$$\vec{x}_m = \vec{x}_0 + V_m \vec{\eta}_m$$

$$\vec{b} - A\vec{x}_m = \vec{r}_0 - AV_m \vec{\eta}_m$$

$$= V_{m+1}(\beta \vec{\epsilon}_{m+1}^{(1)} - \bar{T}_m \vec{\eta}_m).$$

$V_{m+1}^T V_{m+1} \neq I_{m+1}$  in general.

find  $\vec{\eta}_m \in \mathbb{R}^m$   $\|\beta \vec{\epsilon}_{m+1}^{(1)} - \bar{T}_m \vec{\eta}_m\| \leq \|\beta \vec{\epsilon}_{m+1}^{(1)} - \bar{T}_m \vec{\eta}\| \quad \forall \vec{\eta} \in \mathbb{R}^m$

to avoid transposed matrix-vector operation  
Conjugate Gradient Squared (CGS) method

Sonnenveld 1989

in BiCG with polynomial of degree  $m$ ,  $\vec{r}_m = \phi_m(A)\vec{r}_0$ ,  $\vec{r}_m^* = \phi_m(A^T)\vec{r}_0^*$ ,

$$\alpha_m = \frac{(\phi_m(A)\vec{r}_0, \phi_m(A^T)\vec{r}_0^*)}{(A\vec{p}_m, \vec{p}_m^*)} = \frac{(\phi_m(A)^2\vec{r}_0, \vec{r}_0^*)}{(A\vec{p}_m, \vec{p}_m^*)}$$

new residual  $\vec{r}_m' = \phi_m(A)^2\vec{r}_0$  is computed without multiplication of  $A^T$ .

to stabilize / smooth convergence

Bi-Conjugate Gradient Stabilized (BiCGSTAB)

van der Vorst 1992

residual  $\vec{r}_m' = \psi_m(A)\phi_m(A)\vec{r}_0$  with smoothing polynomial of degree  $m$ ,

$\psi_m(t) = (1 - \omega_m t)\psi_{m-1}(t)$  : polynomial with variable  $t$ .

## preconditioned conjugate gradient method

- ▶  $A, Q \in \mathbb{R}^{N \times N}$ , symmetric positive definite,  $Q \sim A^{-1}$     $\vec{b} \in \mathbb{R}^N$ ,
- ▶  $\vec{x}_0$  : initial guess,
- ▶  $\vec{r}_0 := \vec{b} - A\vec{x}_0$  : initial residual.
- ▶  $K_n(QA, Q\vec{r}_0) := \text{span}[Q\vec{r}_0, QAQ\vec{r}_0, (QA)^2Q\vec{r}_0, \dots, (QA)^{n-1}Q\vec{r}_0]$

### Algorithm(preconditioned CG)

$\vec{p}_0 = Q\vec{r}_0$ .

do  $m = 0, 1, \dots$

$$\alpha_m = (Q\vec{r}_m, \vec{r}_m) / (A\vec{p}_m, \vec{p}_m),$$

$$\vec{x}_{m+1} = \vec{x}_m + \alpha_m \vec{p}_m,$$

$$\vec{r}_{m+1} = \vec{r}_m - \alpha_m A\vec{p}_m,$$

if  $\|\vec{r}_{m+1}\| < \epsilon$  exit loop.

$$\beta_m = (Q\vec{r}_{m+1}, \vec{r}_{m+1}) / (Q\vec{r}_m, \vec{r}_m),$$

$$\vec{p}_{m+1} = Q\vec{r}_{m+1} + \beta_m \vec{p}_m.$$

### Lemma for $1 \leq m \leq n_0$

- ▶  $(\vec{r}_m, \vec{z}) = 0 \quad \forall \vec{z} \in K_m(QA, Q\vec{r}_0)$
- ▶  $(A\vec{p}_m, \vec{z}) = 0 \quad \forall \vec{z} \in K_m(QA, Q\vec{r}_0)$
- ▶  $\text{span}[Q\vec{r}_0, Q\vec{r}_1, \dots, Q\vec{r}_m] = \text{span}[\vec{p}_0, \vec{p}_1, \dots, \vec{p}_m] = K_{m+1}(A, \vec{r}_0)$

### successive computation of variational problems

do  $m = 1, 2, \dots, n_0$

find  $\vec{x} \in \vec{x}_0 + K_m(QA, Q\vec{r}_0) \quad (A\vec{x} - \vec{b}, \vec{y}) = 0 \quad \forall \vec{y} \in K_m(QA, Q\vec{r}_0)$

## preconditioned Kyrlov subspace method : 1/2

$Q \in \mathbb{R}^N$  : preconditioner,  $Q^{-1} \sim A$ .

preconditioned conjugate gradient method can be seen as following variational problem with  $A = A^T$ .

$(V_Q^{(m)})$  find  $\vec{x} \in \vec{x}_0 + K_m(QA, Q\vec{r}_0)$   $(A\vec{x} - \vec{b}, \vec{y}) = 0 \quad \forall \vec{y} \in K_m(QA, Q\vec{r}_0)$

**assumption** :  $A$  : 1 to 1 on  $K_{n_0}(QA, Q\vec{r}_0)$

**Theorem**

Variational problem  $(V_Q^{(n_0)})$  in  $K_{n_0}(QA, Q\vec{r}_0)$  has a unique solution and is equivalent to the problem  $A\vec{x} = \vec{b}$ .

- ▶  $A, Q$  : symmetric positive definite  $\Rightarrow$  assumption for CG is OK
- ▶  $A, Q$  : coercive  $\Rightarrow$  assumption for FOM is OK

**left preconditioned GMRES**  $(QA)\vec{x} = Q\vec{b}$

find  $\vec{x}_m \in \vec{x}_0 + K_m(QA, Q\vec{r}_0)$

$$\|Q\vec{b} - (QA)\vec{x}_m\| \leq \|Q\vec{b} - (QA)\vec{y}\| \quad \forall \vec{y} \in \vec{x}_0 + K_m(QA, Q\vec{r}_0)$$

**right preconditioned GMRES**  $(AQ)\vec{z} = \vec{b}, \quad \vec{x} = Q\vec{z}$

find  $\vec{x}_m \in \vec{x}_0 + QK_m(AQ, \vec{r}_0)$

$$\|\vec{b} - (AQ)Q^{-1}\vec{x}_m\| \leq \|\vec{b} - (AQ)Q^{-1}\vec{y}\| \quad \forall \vec{y} \in \vec{x}_0 + QK_m(AQ, \vec{r}_0)$$



## flexible GMRES

Flexible GMRES as an extension of right preconditioned GMRES

- ▶  $A \in \mathbb{R}^{N \times N}$  : invertible  $\vec{b} \in \mathbb{R}^N$ ,
- ▶  $Q_m$  : right preconditioner at  $m$ -th step,
- ▶  $\vec{x}_0$  : initial guess,
- ▶  $\vec{r}_0 := \vec{b} - A\vec{x}_0$  : initial residual,  $\beta = \|\vec{r}_0\|$ ,  $\vec{v}_1 = \vec{r}_0/\beta$ .

Arnoldi process with modified Gram-Schmidt is used

Algorithm(flexible GMRES)

do  $j = 1, 2, \dots, m$

$$\vec{z}_j = Q_j \vec{v}_j$$

$$\vec{w} = A\vec{z}_j$$

do  $i = 1, \dots, j$

$$h_{i,j} := (\vec{w}, \vec{v}_i)$$

$$\vec{w} := \vec{w} - h_{i,j} \vec{v}_i$$

$$h_{j+1,j} := \|\vec{w}\|$$

$$\vec{v}_{j+1} = \vec{w}/h_{j+1,j}$$

$$Z_m := [\vec{z}_1, \dots, \vec{z}_m]$$

$$\vec{\eta}_m = \operatorname{argmin}_{\vec{\eta}} \|\beta \vec{e}_{(m+1)}^{(1)} - \overline{H}_m \vec{\eta}\|,$$

$$\vec{x}_m = \vec{x}_0 + Z_m \vec{\eta}_m.$$

right preconditioned GMRES

$$AQ[\vec{v}_1, \vec{v}_2, \dots, \vec{v}_m] = V_{m+1} \overline{H}_m$$

flexible GMRES

$$A[Q_1 \vec{v}_1, Q_2 \vec{v}_2, \dots, Q_m \vec{v}_m] = V_{m+1} \overline{H}_m$$

$$\vec{b} - A(\vec{x}_0 + Z_m \vec{\eta}) = \vec{r}_0 - AZ_m \vec{\eta}$$

$$= V_{m+1} (\beta \vec{e}_{m+1}^{(1)} - \overline{H}_m \vec{\eta})$$

$V_{m+1}^T V_{m+1} = I_{m+1}$  then

$$\|\vec{b} - A(\vec{x}_0 + Z_m \vec{\eta}_m)\| \leq \|\beta \vec{e}_{m+1}^{(1)} - \overline{H}_m \vec{\eta}\| \quad \forall \vec{\eta} \in \mathbb{R}^m$$

$\operatorname{span}[Q_1 \vec{v}_1, Q_2 \vec{v}_2, \dots, Q_m \vec{v}_m]$  is no longer a Krylov subspace except the case  $Q_j = Q$  for  $1 \leq j \leq m$

## convergence analysis of CG

- ▶  $A$  : symmetric positive definite,  $\exists \alpha > 0$   $(A\vec{x}, \vec{x}) \geq \alpha \|\vec{x}\|^2 \forall \vec{x} \in \mathbb{R}^N$ .
- ▶  $A = V\Lambda V^T$ ,  $\Lambda$  : eigenvalues,  $V$  : eigenvectors  $V^T V = I_N$
- ▶  $\vec{x}_*$  : solution of  $A\vec{x} = \vec{b}$ ,  $\vec{x}_m$  : approximate solution by CG
- ▶  $\mathbb{P}_m$  : polynomial of degree  $m$ .

$$\begin{aligned}\vec{y}_m - \vec{x}_* &= \vec{x}_0 + q_{m-1}(A)\vec{r}_0 - \vec{x}_* & q_{m-1} &\in \mathbb{P}_{m-1} \\ &= \vec{x}_0 + q_{m-1}(A)(\vec{b} - A\vec{x}_0) - \vec{x}_* = (\vec{x}_0 - \vec{x}_*) + q_{m-1}(A)A(\vec{x}_* - \vec{x}_0) \\ &= (I - q_{m-1}(A)A)(\vec{x}_0 - \vec{x}_*) = r_m(A)(\vec{x}_0 - \vec{x}_*) \quad r_m \in \mathbb{P}_m, r(0) = 1.\end{aligned}$$

Galerkin orthogonality  $(\vec{b} - A\vec{x}_m, \vec{x}_m - \vec{y}_m) = 0 \quad \forall \vec{y}_m \in \vec{x}_0 + K_m(A, \vec{r}_0)$

$$\begin{aligned}\alpha \|\vec{x}_m - \vec{x}_*\|^2 &\leq (A(\vec{x}_* - \vec{x}_m), \vec{x}_* - \vec{x}_m) \leq \|A\| \|\vec{x}_m - \vec{x}_*\| \|\vec{x}_* - \vec{y}_m\| \\ \|\vec{y}_m - \vec{x}_*\| &= \|r_m(A)(\vec{x}_0 - \vec{x}_*)\| = \|V r_m(\Lambda) V^T (\vec{x}_0 - \vec{x}_*)\| \leq \|r_m(\Lambda)\| \|\vec{x}_0 - \vec{x}_*\|\end{aligned}$$

$$\begin{aligned}\min_{r_m \in \mathbb{P}_m, r_m(0)=1} \|r_m(A)(\vec{x}_0 - \vec{x}_*)\| &\leq \min_{r_m \in \mathbb{P}_m, r_m(0)=1} \max_{\lambda \in [\lambda_{\min}, \lambda_{\max}]} |r_m(\lambda)| \|\vec{x}_0 - \vec{x}_*\| \\ &\leq C_m \left( \frac{\lambda_{\max} + \lambda_{\min}}{\lambda_{\max} - \lambda_{\min}} \right)^{-1} \|\vec{x}_0 - \vec{x}_*\|\end{aligned}$$

$C_m(k) = \cosh(k \cosh^{-1}(t)) \quad |t| \geq 1$  : Chebyshev polynomial of the first kind  
 $\kappa = \lambda_{\max}/\lambda_{\min}$  : condition number

$$\|\vec{x}_m - \vec{x}_*\| \leq 2 \frac{\|A\|}{\alpha} \left( \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^m \|\vec{x}_0 - \vec{x}_*\|$$

## short summary on Krylov subspace method

- ▶ CG, FOM, and GMRES are direct method ? yes and no  
if exact arithmetic is possible, CG and FOM for a positive matrix (symmetric positive definite or coercive) can find the exact solution after  $n_0$  iterations
- ▶ Due to numerical round of error, orthogonality of Lanczos process is rapidly lost in practice
- ▶ Since we need approximate solution normally, Krylov subspace method is useful with termination of iteration by certain criteria before  $n_0$  iterations
- ▶ FOM and GMRES require to store Arnoldi basis vector and computational complexity of Arnoldi process is large, but by short iterations realized by good preconditioner, these methods are robust and practical.
- ▶ residual of GMRES decreases monotonically but there is still no convergence estimate for indefinite matrices
- ▶ family of BiCG method has no monotonic decreasing in residual and in the worst case bi-orthogonal Lanczos process breaks, though look-ahead technique is employed

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