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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

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

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
$\lambda : \{1, \cdots, n\} \times \{1, \cdots, n\} \to \{1, \cdot n^2\}$ with $\lambda(i,j) = i + n\,j$

sparse matrix with five stencil

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

penta-diagonal matrix with
$N = n^2$, $\mathtt{nnz} = (3n-2)n + 2n(n-1) = 5n^2 - 4n$

- 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, $b \in \mathbb{R}^N$

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

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

ℓ^2-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 $V \subset \mathbb{R}^N$

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

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

questions

- A is invertible in V ? $\;\Leftarrow A$: coercive
- how to generate V ? $\;\Leftarrow$ 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 $PAP^T : V \to V$

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

  assuming $\vec{z} \neq \vec{0}$ satisfying $\vec{z} \in$ Ker$(PAP^T)^T =$ Ker(PA^TP^T)
  then $(PA^TP^T\vec{z}, \vec{y}) = 0\ \forall \vec{y} \in V\ \ \Rightarrow (A^T\vec{z}, \vec{y}) = 0$
  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 $V_1 \subset \cdots \subset V_m$
- 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 $V_1 = \mathrm{span}[\vec{e}_1]$
- S_{22} is coercive on $V_{m-1} = \mathrm{span}[\vec{e}_2, \vec{e}_3, \cdots, \vec{e}_m]$ by putting $\vec{x}_1 = -a_{11}^{-1} a_{12} \vec{x}_2$

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

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

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

- diagonal dominant : $|a_{i\,i}| > \sum_{j \neq i} |a_{i\,j}|$
- M-matrix : Z-matrix $\bigwedge$ Re$\lambda_i > 0 \; 1 \leq i \leq N$, λ_i : i-th eigenvalue
- Z-matrix $a_{i\,j} < 0 \; i \neq j$

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

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

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

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

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

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

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

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

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

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

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

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 $\vec{r}_0, A\vec{r}_0, A^2\vec{r}_0, \cdots, A^{n_0-1}\vec{r}_0$: 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}

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

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

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

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

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

Krylov subspace and variational solution of the linear system

Theorem
problem (V) to find $\vec{x} \in \vec{x}_0 + K_{n_0}(A, \vec{r}_0) \quad (A\vec{x} - \vec{b}, \vec{y}) = 0 \quad \forall \vec{y} \in K_{n_0}(A, \vec{r}_0)$
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 $(A(\vec{x}_0 - \vec{x}_*), \vec{y}) = 0 \quad \forall \vec{y} \in K_{n_0}(A, \vec{r}_0) \overset{?}{\Rightarrow} \vec{x}_0 - \vec{x}_* = \vec{0}$
$A : 1$ to 1 on $K_{n_0}(A, \vec{r}_0)$ is verified as

$$\vec{z} \in K_{n_0}(A, \vec{r}_0) \text{ satisfying } (A\vec{z}, \vec{y}) = 0 \quad \forall \vec{y} \in K_{n_0}(A, \vec{r}_0)$$
$$\Rightarrow A\vec{z} \in (K_{n_0}(A, \vec{r}_0))^{\perp} \vee \vec{z} \in \ker A$$
$$\left.\begin{array}{rcl} \vec{z} \in K_{n_0}(A, \vec{r}_0) & \Rightarrow & A\vec{z} \in K_{n_0}(A, \vec{r}_0) \\ \exists A^{-1} & \Rightarrow & \ker A = \{\vec{0}\} \end{array}\right\} \Rightarrow \vec{z} = \vec{0}.$$

successive computation of variational problems
do $m = 1, 2, \cdots, n_0$
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 (CG) method $\Leftarrow A$: symmetric positive definite
- Full Orthogonization Method (FOM) $\Leftarrow A$: coercive

Arnoldi process

$\|\vec{v}_1\| = 1,$

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

Algorithm (Arnoldi process)

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

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

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

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

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

from the last line,

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

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

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

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

$$V_m^T A V_m = H_m \quad \Leftarrow V_m^T V_m = I_m \Leftrightarrow (\vec{v}_j, \vec{v}_i) = \delta_{i\,j} \;\; 1 \le i, j \le m$$

Full Orthogonizatien 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.
- $K_n(A,\vec{r}_0) :=$ span$[\vec{r}_0, A\vec{r}_0, A^2\vec{r}_0, \cdots, A^{n-1}\vec{r}_0]$: Krylov subspace

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

$$
\begin{aligned}
AV_m &= V_{m+1}\overline{H}_m \\
V_m^T A V_m &= H_m \\
V_m^T \vec{r}_0 &= V_m^T \beta \vec{v}_1 = \beta \vec{\epsilon}_m^{\,(1)}, \quad [\vec{\epsilon}_m^{\,(1)}]_i = \delta_{i\,1}\ 1 \leq i \leq m
\end{aligned}
$$

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

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

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.
- $K_n(A, \vec{r}_0) :=$ span$[\vec{r}_0, A\vec{r}_0, A^2\vec{r}_0, \cdots, A^{n-1}\vec{r}_0]$: Krylov subspace

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

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

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

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

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

$$\begin{aligned}
\vec{y} &= \vec{x}_0 + V_m\vec{\eta}_m \\
\vec{b} - A\vec{y} &= \vec{b} - A\vec{x}_0 - AV_m\vec{\eta}_m \\
&= \vec{r}_0 - AV_m\vec{\eta}_m \\
&= V_{m+1}\left(\beta\vec{\epsilon}^{\,(1)}_{m+1} - \overline{H}_m\vec{\eta}_m\right) \\
\|\vec{b} - A\vec{y}\| &= \|\beta\vec{\epsilon}^{\,(1)}_{m+1} - \overline{H}_m\vec{\eta}_m\| \qquad \Leftarrow V^T_{m+1}V_{m+1} = I_{m+1}.
\end{aligned}$$

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

Generalized Minimal Residual (GMRES) Method : 2/3

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

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

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

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

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

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

Generalized Minimal Residual (GMRES) Method : 3/3

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

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

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

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

$\vec{\eta}_m = R^{-1}_m\vec{\gamma}_m$ attains the minimum.

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

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.
- $K_n(A, \vec{r}_0) :=$ span$[\vec{r}_0, A\vec{r}_0, A^2\vec{r}_0, \cdots, A^{n-1}\vec{r}_0]$: Krylov subspace

Algorithm(CG)

$\vec{p}_0 = \vec{r}_0$.
do $m = 0, 1, \ldots$
  $\alpha_n = \|\vec{r}_m\|^2/(A\vec{p}_m, \vec{p}_m)$,
  $\vec{x}_{m+1} = \vec{x}_m + \alpha_m \vec{p}_m$,
  $\vec{r}_{m+1} = \vec{r}_m - \alpha_m A\vec{p}_m$,
  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 $1 \leq m \leq n_0$

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

successive computation of variational problems

do $m = 1, 2, \cdots, n_0$
  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) $$(\vec{r}_1, \vec{r}_0) = (\vec{r}_0 - \alpha_0 A\vec{p}_0, \vec{r}_0) = (\vec{r}_0, \vec{r}_0) - \frac{\|\vec{r}_0\|}{(A\vec{p}_0, \vec{p}_0)}(A\vec{p}_0, \vec{p}_0) = 0$$

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

$$= (\vec{r}_1 + \beta_0\vec{p}_0, \frac{1}{\alpha_0}(\vec{r}_0 - \vec{r}_1)) = -\frac{1}{\alpha_0}(\vec{r}_1, \vec{r}_1) + \frac{\beta_0}{\alpha_0}(\vec{p}_0, \vec{r}_0) = 0$$

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

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) $$(\vec{r}_{k+1}, \vec{z}_0) = (\vec{r}_k - \alpha_0 A\vec{p}_k, \vec{z}_0) = (\vec{r}_k, \vec{z}_0) - \alpha_k(A\vec{p}_k, \vec{z}_0) = 0$$

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

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

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

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

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

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

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

conjugate gradient method : 3/3

relation with Lanczos process

$A = A^T$: symmetric

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

$AV_m = V_{m+1}\overline{T}_m \quad \overline{T}_m \in \mathbb{R}^{(m+1)\times m}$: tri-diagonal matrix, T_m : symmetric

$V_m^T A V_m = T_m \quad \Leftarrow V_m^T V_m = I_m \;\Leftrightarrow (\vec{v}_j, \vec{v}_i) = 0 \; 1 \leq i, j \leq m$

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

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

$$0 = V_m^T(A\vec{x}_m - \vec{b}) = -V_m^T \vec{r}_0 + V_m^T A V_m \vec{\eta}_m$$

$$= -\beta \vec{\epsilon}_m^{(1)} + T_m \vec{\eta}_m,$$

- A : symmetric positive definite $\Rightarrow T_m$ can be factorized without permutation
- Conjugate Gradient method computes $\vec{x}_m$ without explicit tridiagonal factorization

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

Algorithm(Bi-CG)

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

do $m = 0, 1, \ldots$

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

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

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

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 $1 \leq m \leq n_0$

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

successive computation of variational problems

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

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

$$[A\vec{v}_1, \cdots, A\vec{v}_m] = [\vec{v}_1, \cdots, \vec{v}_m, \vec{v}_{m+1}] \begin{bmatrix} \alpha_1 & \beta_2 & & & \\ \delta_2 & \alpha_2 & \ddots & & \\ & \delta_3 & \ddots & & \\ & & \ddots & \ddots & \beta_m \\ & & & \delta_m & \alpha_m \\ & & & & \delta_{m+1} \end{bmatrix}$$

$$\begin{aligned} AV_m &= V_m T_m + \delta_{m+1} \vec{v}_{m+1} \vec{\epsilon}_m^{(m)\ T} \\ A^T W_m &= W_m T_m^T + \beta_{m+1} \vec{w}_{m+1} \vec{\epsilon}_m^{(m)\ T} \\ W_m^T A\, V_m &= T_m \qquad \Leftarrow W_m^T V_m = I_m \text{ : bi-orthogonality} \end{aligned}$$

two-sided Lanczos algorithm
variational problem with Petrov-Galerkin type

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

find $\vec{x}_m = \vec{x}_0 + V_m \vec{\eta}_m,$ 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
- $(\vec{r}_m, \vec{r}_m^{\,*}) = 0 \quad \Rightarrow$ breakdown of Lanczos biorthogonalization process

bi-conjugate gradient method : 3/3

Composite step biconjugate gradient method — Bank-Chan 1993

stable factorization of T_m with 2×2 block pivots

Quasi-Minimal Residual (QMR) method — Freund-Nachtigal 1991

V_m generated by look-ahead Lanczos process — Parlett-Taylor-Liu 1985

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

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

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

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

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 $\vec{r}_m^{\,\prime} = \phi_m(A)^2\vec{r}_0$ is computed without multiplication of A^T.

to stabilize / smooth convergence

Bi-Conjugate Gradient Stabilized (BiCGSTAB) — van der Vorst 1992

residual $\vec{r}_m^{\,\prime} = \psi_m(A)\phi_m(A)\vec{r}_0$ 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, $Q \sim A^{-1}$ $\quad \vec{b} \in \mathbb{R}^N$,
- $\vec{x}_0$: initial guess,
- $\vec{r}_0 := \vec{b} - A\vec{x}_0$: initial residual.
- $K_n(QA, Q\vec{r}_0) :=$ span$[Q\vec{r}_0, QAQ\vec{r}_0, (QA)^2Q\vec{r}_0, \cdots, (QA)^{n-1}Q\vec{r}_0]$

Algorithm(preconditioned CG)

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

do $m = 0, 1, \dots$

$\alpha_n = (Q\vec{r}_m, \vec{r}_m)/(A\vec{p}_m, \vec{p}_m)$,
$\vec{x}_{m+1} = \vec{x}_m + \alpha_m \vec{p}_m$,
$\vec{r}_{m+1} = \vec{r}_m - \alpha_m A\vec{p}_m$,
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 $1 \leq m \leq n_0$

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

successive computation of variational problems

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

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, $Q^{-1} \sim A$.

- left preconditioner $(Q\,A)\vec{x} = Q\vec{b}$
- right preconditioner $(A\,Q)\vec{z} = \vec{b}, \quad \vec{x} = Q\vec{z}$

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

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

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

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

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

flexible GMRESS

Flexible GMRES as an extension of right preconditioned GMRES

- $A \in \mathbb{R}^{N\times N}$: invertible $\quad \vec{b} \in \mathbb{R}^{N}$,
- 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 $j = 1, 2, \ldots, m$
    $\vec{z}_j = Q_j\vec{v}_j$
    $\vec{w} = A\vec{z}_j$
    do $i = 1, \cdots, j$
        $h_{i,j} := (\vec{w}, \vec{v}_j)$
        $\vec{w} := \vec{w} - h_{i,j}\vec{v}_i$
    $h_{j+1,j} := \|\vec{w}\|$
    $\vec{v}_{j+1} = \vec{w}/h_{j+1,j}$
$Z_m := [\vec{z}_1, \cdots, \vec{z}_m]$
$\vec{\eta}_m = \underset{\vec{\eta}}{\operatorname{argmin}} \|\beta\vec{\epsilon}^{\,(1)}_{(m+1)} - \overline{H}_m\vec{\eta}\|$,
$\vec{x}_m = \vec{x}_0 + Z_m\vec{\eta}_m$.

right preconditioned GMRES

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

flexible GMRES

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

$$\vec{b} - A(\vec{x}_0 + Z_m\vec{\eta}) = \vec{r}_0 - AZ_m\vec{\eta} = V_{m+1}(\beta\vec{\epsilon}^{\,(1)}_{m+1} - \overline{H}_m\vec{\eta})$$

$V^T_{m+1}V_{m+1} = I_{m+1}$ then

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

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

convergence analysis of CG

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

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

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

$$\alpha\|\vec{x}_m - \vec{x}_*\|^2 \leq (A(\vec{x}_* - \vec{x}_m),\ \vec{x}_* - \vec{x}_m) \leq \|A\|\|\vec{x}_m - \vec{x}_*\|\|\vec{x}_* - \vec{y}_m\|$$

$$\|\vec{y}_m - \vec{x}_*\| = \|r_m(A)(\vec{x}_0 - \vec{x}_*)\| = \|Vr_m(\Lambda)V^T(\vec{x}_0 - \vec{x}_*)\| \leq \|r_m(\Lambda)\|\|\vec{x}_0 - \vec{x}_*\|$$

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

$C_m(k) = \cosh(k\cosh^{-1}(t))$ $|t|\geq 1$: 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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