Lecture 11: Krylov subspace, Generalized minimal residual method



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1. Krylov subspace

• Given $\mathbf{A} \in \mathbb{C}^{m \times m}$ and nonzero $\mathbf{r} \in \mathbb{C}^m$, the jth Krylov subspace generated by \mathbf{A} and \mathbf{r} is defined by

$$\mathcal{K}_j(\mathbf{A}, \mathbf{r}) := \operatorname{span}\{\mathbf{r}, \mathbf{A}\mathbf{r}, \mathbf{A}^2\mathbf{r}, \cdots, \mathbf{A}^{j-1}\mathbf{r}\}.$$

Obviously, $\mathcal{K}_j(\mathbf{A}, \mathbf{r}) \subseteq \mathcal{K}_{j+1}(\mathbf{A}, \mathbf{r})$ and $\dim \mathcal{K}_j(\mathbf{A}, \mathbf{r}) \leq j$.

Proposition 1

Let \mathbb{P}_j denote the set of polynomials of degree $\leq j$. Then

$$\mathcal{K}_j(\mathbf{A}, \mathbf{r}) = \{ p(\mathbf{A})\mathbf{r} \mid p \in \mathbb{P}_{j-1} \}.$$

Proposition 2

If the minimal polynomial of the matrix **A** has degree n, then for any j > n and any nonzero $\mathbf{r} \in \mathbb{C}^m$,

$$\dim \mathcal{K}_i(\mathbf{A}, \mathbf{r}) \leq n.$$

1.1. Arnoldi process

Algorithm: Arnoldi process generating orthonormal basis

Given
$$\mathbf{A} \in \mathbb{C}^{m \times m}$$
 and nonzero $\mathbf{r} \in \mathbb{C}^m$
 $\mathbf{q}_1 = \mathbf{r}/\|\mathbf{r}\|_2$
for $j = 1, 2, 3, \ldots$,
 $\mathbf{v} = \mathbf{A}\mathbf{q}_j$
for $i = 1$ to j
 $h_{ij} = \langle \mathbf{v}, \mathbf{q}_i \rangle = \mathbf{q}_i^* \mathbf{v}$
 $\mathbf{v} = \mathbf{v} - h_{ij} \mathbf{q}_i$
end
 $h_{j+1,j} = \|\mathbf{v}\|_2$
 $\mathbf{q}_{j+1} = \mathbf{v}/h_{j+1,j}$
end

• At the end of step j, we obtain

$$\mathbf{v} = (\mathbf{I} - \mathbf{q}_j \mathbf{q}_j^*) \cdots (\mathbf{I} - \mathbf{q}_2 \mathbf{q}_2^*) (\mathbf{I} - \mathbf{q}_1 \mathbf{q}_1^*) \mathbf{A} \mathbf{q}_j.$$

• We call the Arnoldi process breaks down at step k if $h_{k+1,k} = 0$.

Remark 3

The Arnoldi process is the modified Gram-Schimidt orthogonalization applied to $\{\mathbf{r}, \mathbf{Aq}_1, \mathbf{Aq}_2, \cdots\}$. We have the Arnoldi relation

$$\mathbf{A} \begin{bmatrix} \mathbf{q}_1 & \cdots & \mathbf{q}_j \end{bmatrix} = \begin{bmatrix} \mathbf{q}_1 & \cdots & \mathbf{q}_{j+1} \end{bmatrix} \begin{bmatrix} h_{11} & \cdots & h_{1j} \\ h_{21} & \ddots & \vdots \\ & \ddots & h_{jj} \\ & & h_{j+1,j} \end{bmatrix},$$

that is $\mathbf{AQ}_j = \mathbf{Q}_{j+1}\widetilde{\mathbf{H}}_j$. ($\widetilde{\mathbf{H}}_j$ is an upper Hessenberg matrix.) Let

$$\mathbf{H}_j := \mathbf{Q}_j^* \mathbf{A} \mathbf{Q}_j = \mathbf{Q}_j^* \mathbf{Q}_{j+1} \widetilde{\mathbf{H}}_j = \begin{bmatrix} h_{11} & \cdots & h_{1j} \\ h_{21} & \ddots & \vdots \\ & \ddots & h_{jj} \end{bmatrix}.$$

If the Arnoldi process breaks down at step k, then $\mathbf{AQ}_k = \mathbf{Q}_k \mathbf{H}_k$.

Theorem 4

Suppose the Arnoldi process breaks down at step k. Then,

$$span{\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_j} = \mathcal{K}_j(\mathbf{A}, \mathbf{r}), \quad j = 1, 2, \dots, k,$$

and the set $\{\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_k\}$ is orthonormal.

Corollary 5

The matrices $\{\mathbf{Q}_j\}_{j=1}^k$ generated by the Arnoldi process are Q-factors of reduced QR factorizations of the Krylov matrices,

$$\mathbf{K}_j := \begin{bmatrix} \mathbf{r} & \mathbf{A}\mathbf{r} & \cdots & \mathbf{A}^{j-1}\mathbf{r} \end{bmatrix} = \mathbf{Q}_j\mathbf{R}_j, \quad j = 1, 2, \dots, k.$$

Remark 6

Both \mathbf{K}_j and \mathbf{R}_j are not formed explicitly in the Arnoldi process.

2. Generalized minimal residual method (GMRES)

• Idea of GMRES: Consider a nonsingular linear system

$$\mathbf{A}\mathbf{x} = \mathbf{b}, \quad \mathbf{A} \in \mathbb{C}^{m \times m}, \quad \mathbf{b} \in \mathbb{C}^m.$$

For any initial guess \mathbf{x}_0 , at step j, GMRES finds the jth approximate solution

$$\mathbf{x}_j = \underset{\mathbf{x} \in \mathbf{x}_0 + \mathcal{K}_j(\mathbf{A}, \mathbf{r}_0)}{\operatorname{argmin}} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2,$$

where $\mathbf{r}_0 := \mathbf{b} - \mathbf{A}\mathbf{x}_0$ and

$$\mathcal{K}_j(\mathbf{A}, \mathbf{r}_0) = \operatorname{span}\{\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \dots, \mathbf{A}^{j-1}\mathbf{r}_0\}.$$

For the residual $\mathbf{r}_i = \mathbf{b} - \mathbf{A}\mathbf{x}_i$, we have

$$\|\mathbf{r}_j\|_2 = \min_{\mathbf{x} \in \mathbf{x}_0 + \mathcal{K}_j(\mathbf{A}, \mathbf{r}_0)} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2 \quad \text{and} \quad \mathbf{r}_j \perp \mathbf{A}\mathcal{K}_j.$$

Assume that the Arnoldi process for the orthonormal basis of $\mathcal{K}_j(\mathbf{A}, \mathbf{r}_0)$ breaks down at step k. For $1 \leq j < k$, we have

$$\begin{aligned} \|\mathbf{r}_{j}\|_{2} &= \min_{\mathbf{x} \in \mathbf{x}_{0} + \mathcal{K}_{j}(\mathbf{A}, \mathbf{r}_{0})} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_{2} = \min_{\mathbf{y} \in \mathbb{C}^{j}} \|\mathbf{r}_{0} - \mathbf{A}\mathbf{Q}_{j}\mathbf{y}\|_{2} \\ &= \min_{\mathbf{y} \in \mathbb{C}^{j}} \left\|\mathbf{r}_{0} - \mathbf{Q}_{j+1}\widetilde{\mathbf{H}}_{j}\mathbf{y}\right\|_{2} \quad \text{(by Arnoldi relation)} \\ &= \min_{\mathbf{y} \in \mathbb{C}^{j}} \left\|\|\mathbf{r}_{0}\|_{2}\mathbf{e}_{1} - \widetilde{\mathbf{H}}_{j}\mathbf{y}\right\|_{2}. \end{aligned}$$

For j = k, we have

$$\|\mathbf{r}_{k}\|_{2} = \min_{\mathbf{x} \in \mathbf{x}_{0} + \mathcal{K}_{k}(\mathbf{A}, \mathbf{r}_{0})} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_{2} = \min_{\mathbf{y} \in \mathbb{C}^{k}} \|\mathbf{r}_{0} - \mathbf{A}\mathbf{Q}_{k}\mathbf{y}\|_{2}$$

$$= \min_{\mathbf{y} \in \mathbb{C}^{k}} \|\mathbf{r}_{0} - \mathbf{Q}_{k}\mathbf{H}_{k}\mathbf{y}\|_{2} \quad \text{(by Arnoldi relation)}$$

$$= \min_{\mathbf{y} \in \mathbb{C}^{k}} \|\|\mathbf{r}_{0}\|_{2}\mathbf{e}_{1} - \mathbf{H}_{k}\mathbf{y}\|_{2}.$$

Once \mathbf{y}_i is found, set $\mathbf{x}_i = \mathbf{x}_0 + \mathbf{Q}_i \mathbf{y}_i$.

• The least squares problem about \mathbf{y} can be solved inexpensively with Givens rotations, exploiting the upper Hessenberg structure of $\widetilde{\mathbf{H}}_j$, costing just $\mathcal{O}(j^2)$ or $\mathcal{O}(j)$ instead of $\mathcal{O}(j^3)$.

2.1. Convergence of GMRES

Theorem 7

Assume that the Arnoldi process for the orthonormal basis of $\mathcal{K}_j(\mathbf{A}, \mathbf{r}_0)$ breaks down at step k.

(1) For $1 \le j < k$, the residual \mathbf{r}_j satisfies $(\mathbf{AQ}_j)^* \mathbf{r}_j = \mathbf{0}$, i.e.,

$$\mathbf{r}_j \perp \mathbf{A} \mathcal{K}_j$$
.

(2) For $0 \le j \le k$, the residual \mathbf{r}_j satisfies

$$\|\mathbf{r}_0\|_2 \ge \|\mathbf{r}_1\|_2 \ge \dots \ge \|\mathbf{r}_{k-1}\|_2 > \|\mathbf{r}_k\|_2 = 0.$$

That is to say GMRES converges monotonically and finds the exact solution at step k.

Theorem 8

Suppose **A** is diagonalizable, i.e., $\mathbf{A} = \mathbf{V} \mathbf{\Lambda} \mathbf{V}^{-1}$ for some nonsingular matrix **V** and diagonal matrix **\Lambda**. At step j of the GMRES iteration, the residual \mathbf{r}_j satisfies

$$\frac{\|\mathbf{r}_j\|_2}{\|\mathbf{r}_0\|_2} \le \min_{p \in \mathbb{P}_j, p(0) = 1} \|p(\mathbf{A})\|_2 \le \kappa(\mathbf{V}) \min_{p \in \mathbb{P}_j, p(0) = 1} \max_{\lambda \in \Lambda(\mathbf{A})} |p(\lambda)|,$$

where $\Lambda(\mathbf{A})$ is the set of eigenvalues of \mathbf{A} , and $\kappa(\mathbf{V}) = \|\mathbf{V}\|_2 \|\mathbf{V}^{-1}\|_2$.

• Y. Saad and M.H. Schultz

GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems

SIAM J. Sci. Stat. Comput., 7: 856–869, 1986.

• Y. Saad

A Flexible Inner-Outer Preconditioned GMRES Algorithm SIAM J. Sci. Comput., 14: 461–469, 1993.

• Exercise: Assume the Arnoldi process for $\{A, r_0\}$ breaks down at step k > 1. For $1 \le j < k$, we have the Arnoldi relation

$$\mathbf{A}\mathbf{Q}_j = \mathbf{Q}_{j+1}\widetilde{\mathbf{H}}_j.$$

For $1 \le j < k$, prove the following:

(a) The jth residual \mathbf{r}_i of GMRES can be uniquely expressed as

$$\mathbf{r}_j = p_j(\mathbf{A})\mathbf{r}_0, \qquad \deg(p_j) \le j, \qquad p_j(0) = 1.$$

(b) Let $\mathbf{H}_j = \mathbf{Q}_j^* \mathbf{A} \mathbf{Q}_j$. The unique polynomial p_j in (a) is given by

$$p_j(z) = \prod_{i=1}^{j} \left(1 - \theta_i^{(j)} z\right),$$

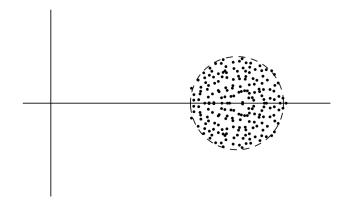
where $\theta_i^{(j)}$, $i=1,2,\ldots,j$, are the eigenvalues of $(\widetilde{\mathbf{H}}_j^*\widetilde{\mathbf{H}}_j)^{-1}\mathbf{H}_j^*$.

2.2. Numerical examples

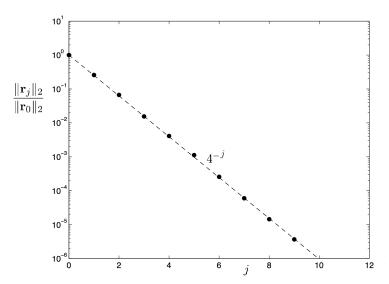
• Example 1: \mathbf{A} , 200×200 entries from real normal distribution of mean 2 and standard deviation $0.5/\sqrt{200}$

$$m = 200; A = 2*eye(m)+0.5*randn(m)/sqrt(m);$$

$$\mathbf{A}\mathbf{x} = \mathbf{b}, \quad \mathbf{x}_0 = \mathbf{0}, \quad \mathbf{b} = \begin{bmatrix} 1 & 1 & \cdots & 1 \end{bmatrix}^{\mathsf{T}}$$



Convergence history of Example 1

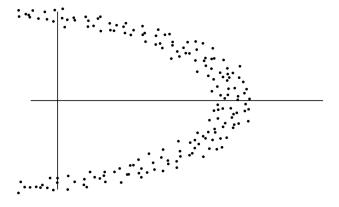


• Example 2:

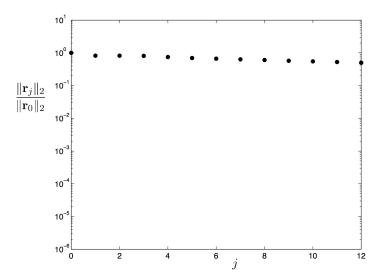
$$m = 200; B = 2*eye(m)+0.5*randn(m)/sqrt(m);$$

A = B + D, D is the diagonal matrix with complex entries

$$d_i = (-2 + 2\sin\theta_i) + i\cos\theta_i, \quad \theta_i = \frac{(i-1)\pi}{m-1}, \quad 1 \le i \le m.$$



Convergence history of Example 2



2.3. Preconditioning (see Lecture 40 of NLA)

- To improve the convergence of Krylov subspace methods, it is important to have a preconditioner (suitable approximation for the original coefficient matrix **A**), denoted by **M**.
- Left preconditioning, i.e.,

$$\mathbf{M}^{-1}\mathbf{A}\mathbf{x} = \mathbf{M}^{-1}\mathbf{b}.$$

• Right preconditioning is often used, i.e.,

$$\mathbf{A}\mathbf{M}^{-1}\mathbf{z} = \mathbf{b}, \quad \mathbf{x} = \mathbf{M}^{-1}\mathbf{z},$$

because it produces the same residual as that of the original system in exact precision arithmetic.

• Note that we never explicitly form \mathbf{M}^{-1} . Only the action of applying the preconditioner solve operation \mathbf{M}^{-1} to a given vector is computed in iterative methods. So $\mathbf{M}^{-1}\mathbf{z}$ must be cheap.

• How to find a good preconditioner? It's problem dependent.

Example. Let
$$\mathcal{A} = \begin{bmatrix} \mathbf{A} & \mathbf{B}^* \\ \mathbf{C} & \mathbf{0} \end{bmatrix}$$
 and $\mathcal{M} = \begin{bmatrix} \mathbf{A} & \mathbf{0} \\ \mathbf{0} & \mathbf{C}\mathbf{A}^{-1}\mathbf{B}^* \end{bmatrix}$, where $\mathbf{A} \in \mathbb{C}^{m \times m}$ is invertible, and $\mathbf{B}, \mathbf{C} \in \mathbb{C}^{n \times m}$ with $m \geq n$. Assume that $-\mathbf{C}\mathbf{A}^{-1}\mathbf{B}^*$ is invertible.

The preconditioned matrix $\mathcal{M}^{-1}\mathcal{A}$ is diagonalizable and has at most three distinct eigenvalues 1, $(1+\sqrt{5})/2$, and $(1-\sqrt{5})/2$.

2.4. Restarted GMRES

- For larger values of j, the cost of GMRES in operations and storage may be prohibitive. In such circumstances a method called l-step restarted GMRES or GMRES(l) is often employed.
- GMRES(l): After l steps, the GMRES iteration is started anew with the current vector \mathbf{x}_l as an initial guess.
- Note that GMRES(l) can be expected fail to converge, whereas GMRES always succeeds for exact arithmetic. (Embree's paper)
- GMRES-IR, GMRES-DR, FGMRES-DR, etc.