Krylov subspace methods and GMRES

(Generalized Minimal Residuals)

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Recap:

- What is Krylov subspace?
- $\mathcal{K}_k(A, u) = < u, Au, A^2u, \ldots, A^{k-1}u >$, $u \in \mathbb{R}^n$.
- How does one represent a vector in such space with its basis shown above?
- If $x_k \in \mathcal{K}_k$,

  $x_k = \alpha_0 u + \alpha_1 Au + \alpha_2 A^2 u + \cdots + \alpha_{k-1} A^{k-1} u = \sum_{i=0}^{k-1} \alpha_i A^i u$, for some coefficients $\alpha_i \in \mathbb{R}$.
- How does one write the above vector in terms of a matrix polynomial?
- $x_k = p^{(k-1)}(A)u$, where $p^{(k-1)}(t) = \sum_{i=0}^{k-1} \alpha_i t^i$, is a polynomial of degree $k - 1$.
- Given $Ax = b$, what vector is usually chosen as u ?

Recap:

- Why one does not choose columns of matrix$K = [b \,|\, Ab \,|\, A^2 b \,|\, \ldots \,|\, A^{k-1} b]$ as the basis of$\mathcal{K}_k(A, b)$
- Its usually ill-conditioned.
- What is the remedy?
- An orthonormal matrix $Q_k \to \mathcal{K}_k(A, b)$.
- How to find such Q_k ?
- Arnoldi iteration.

Recap:

- What is a complete reduction of a matrix A to its Heisenberg form?

- $A = QHQ^* \rightarrow AQ = QH$

- What is a partial reduction of A to its Heisenberg form?

- $AQ_k = Q_{k+1}\tilde{H}_k$, where

$$\tilde{H}_k = \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1k} \\ h_{21} & h_{22} & \cdots & h_{2k} \\ & \ddots & \ddots & \vdots \\ & & h_{k,k-1} & h_{kk} \\ & & & h_{k+1,k} \end{bmatrix} \in \mathbb{R}^{(k+1)\times k}$$

Recap:

- What is the $(j+1)$-term recurrence relation for q_{j+1}?

- $Aq_j = h_{1j}q_1 + h_{2j}q_2 + \cdots + h_{jj}q_j + h_{j+1,j}q_{j+1}$
  $\rightarrow q_{j+1} = (Aq_j - h_{1j}q_1 - h_{2j}q_2 - \cdots - h_{jj}q_j)/h_{j+1,j}$

- How does one find $h_{i,j}$, $i = 1, \cdots, j$ above?

- Via orthogonality of $q_j's$

Recap:

$$\tilde{H}_k = \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1k} \\ h_{21} & h_{22} & \cdots & h_{2k} \\ & \ddots & \ddots & \vdots \\ & & h_{k,k-1} & h_{kk} \\ & & & h_{k+1,k} \end{bmatrix} \in \mathbb{R}^{(k+1)\times k}$$

- What quantity does the off-diagonal entry $h_{j+1,j}$ equal to?
- $h_{j+1,j} = \|q'_{j+1}\|,$ the length of the "leftover" vector of $A^j b$ being "peeled" off against previous $q'_i s$.

$$\tilde{H}_k = \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1k} \\ h_{21} & h_{22} & \cdots & h_{2k} \\ & \ddots & \ddots & \vdots \\ & & h_{k,k-1} & h_{kk} \\ & & & 0 \end{bmatrix} \in \mathbb{R}^{(k+1)\times k}$$

- What if there is a breakdown, i.e., $h_{k+1,k} = 0$?
- $q_{k+1} = q'_{k+1}/h_{k+1,k}$ cannot be formed.
- Will this situation cause unwanted results?

If $h_{k+1,k} = 0$

- What will happen to $AQ_k = Q_{k+1}\tilde{H}_k$?

$$A[q_1 \,|\, q_2 \,|\, \cdots \,|\, q_k] = [q_1 \,|\, q_2 \,|\, \cdots \,|\, q_k \,|\, \cancel{q_{k+1}}] \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1k} \\ h_{21} & h_{22} & \cdots & h_{2k} \\ & \ddots & \ddots & \vdots \\ & & h_{k,k-1} & h_{kk} \\ & & & \cancel{h_{k+1,k}} \end{bmatrix}$$

- Will there be any effect on the right-hand side corresponding to Aq_1 ?
- What about $Aq_2, \cdots, Aq_{k-1}$?
- What about Aq_k ?
- $Aq_k = h_{1k}q_1 + h_{2k}q_2 + \cdots + h_{kk}q_k + h_{k+1,k}\cancel{q_{k+1}}$
- $AQ_k = Q_kH_k$

If there is breakdown of the Arnoldi iteration, i.e., $h_{k+1,k} = 0, AQ_k = Q_k H_k$

- For any vector $v \in \mathcal{K}_k$, what subspace will A map it to? In other words, what subspace does Av live in?
- $v = \sum_{i=1}^{k} \alpha_i q_i$, for some coefficients $\alpha' s$.
- $Av = A \sum_{i=1}^{k} \alpha_i q_i$
- $= \sum_{i=1}^{k} \alpha_i A q_i$
- $= \sum_{i=1}^{k-1} \alpha_i A q_i + \alpha_k A q_k$
- $= \sum_{i=1}^{k-1} \alpha_i (h_{1i} q_1 + h_{2i} q_2 + \cdots + h_{ii} q_i + h_{i+1,i} q_{i+1}) + \alpha_k A q_k$
- $= \sum_{i=1}^{k-1} \alpha_i (\sum_{j=1}^{i+1} h_{ji} q_j) + \alpha_k (h_{1k} q_1 + h_{2k} q_2 + \cdots + h_{kk} q_k) \in \; < q_1, \cdots, q_k > \; = \mathcal{K}_k$

$\mathcal{K}_k$ is an invariant subspace of A, i.e.,

$A\mathcal{K}_k \subseteq \mathcal{K}_k$ or

For any $v \in \mathcal{K}_k$, one has $Av \in \mathcal{K}_k$.

If there is breakdown of the Arnoldi iteration, i.e., $h_{k+1,k} = 0, AQ_k = Q_k H_k$

- Can one expend $\mathcal{K}_k = < q_1, \cdots, q_k >$ more by $A^k b, A^{k+1} b, \ldots$?
- $\mathcal{K}_k = < q_1, \cdots, q_k > = < b, Ab, \cdots, A^{k-1} b >$
- $< q_1, \cdots, q_k, A^k b > = < b, Ab, \cdots, A^{k-1} b, A^k b > := \mathcal{K}_{k+1}$
- $A^k b = A(A^{k-1} b)$
- $= A(\sum_{i=1}^{k} \beta_i q_i)$, for some coefficient $\beta_i' s$.
- $= \sum_{i=1}^{k} \beta_i A q_i$
- $= \sum_{i=1}^{k-1} \beta_i A q_i + \beta_k A q_k$
- $= \sum_{i=1}^{k-1} \beta_i A q_i + \beta_k (h_{1k} q_1 + h_{2k} q_2 + \cdots + h_{kk} q_k) \in < q_1, \cdots, q_k > = \mathcal{K}_k$

$\mathcal{K}_k = \mathcal{K}_{k+1}$

If there is breakdown of the Arnoldi iteration, i.e., $h_{k+1,k} = 0$, $AQ_k = Q_k H_k$

$$\mathscr{K}_k = \mathscr{K}_{k+1} = \mathscr{K}_{k+2} = \cdots$$

- Any relationship between eigenvalues of H_k and eigenvalues of A?
- Suppose $H_k y = \lambda y$.
- $Q_k H_k y = Q_k \lambda y$
- $Q_k H_k y = \lambda Q_k y$
- $AQ_k y = \lambda Q_k y$
- $A(Q_k y) = \lambda(Q_k y)$
- $\rightarrow$ if (λ, y) is an eigenpair of H_k, then $(\lambda, Q_k y)$ is an eigenpair of A.

If there is breakdown of the Arnoldi iteration, i.e., $h_{k+1,k} = 0, AQ_k = Q_k H_k$

- Since $\mathscr{K}_k = \mathscr{K}_{k+1} = \mathscr{K}_{k+2} = \cdots$, one cannot expand the dimension more than k by definition.
- Is the solution one seeks in $\mathscr{K}_k$ good enough to solve the minimizing problem: Find $y \in \mathbb{R}^k$ s.t. $\|AQ_k y - b\|$ is minimum? ($x_k = Q_k y$)
- We assume A^{-1} exists and $x_* = A^{-1}b$.
- Suppose $x_* \notin \mathscr{K}_k$
- $Ax_* = b$
- $A^k A x_* = A^k b \in < q_1, \cdots, q_k > = \mathscr{K}_k$
- $x_* = \sum_{i=1}^{k} c_i q_i + \sum_{j=1}^{m} d_j w_j$, where $< w_1, \cdots, w_m >$ some basis linearly independent of $< q_1, \cdots, q_k >$.

- $A^{k+1}x_* = A^{k+1}(\sum_{i=1}^{k} c_i q_i + \sum_{j=1}^{m} d_j w_j)$
- $A^{k+1}x_* = \sum_{i=1}^{k} c_i A^{k+1} q_i + \boxed{\sum_{j=1}^{m} d_j A^{k+1} w_j} \rightarrow \notin \mathcal{K}_k$
- WLOG, assume $Aw_1 \in \mathcal{K}_k$
- $Aw_1 = \sum_{i=1}^{k} t_i q_i$
- $w_1 = A^{-1} \sum_{i=1}^{k} t_i q_i$
- $w_1 = p(A) \sum_{i=1}^{k} t_i q_i$, for some matrix polynomial p of A.
- Since for any $v \in \mathcal{K}_k$, one has $Av \in \mathcal{K}_k$. $\rightarrow w_1 \in \mathcal{K}_k$. Contradiction.

- $A^{k+1}x_* = A^{k+1}(\sum_{i=1}^{k} c_i q_i + \sum_{j=1}^{m} d_j w_j)$

- $A^{k+1}x_* = \boxed{\sum_{i=1}^{k} c_i A^{k+1} q_i} + \boxed{\sum_{j=1}^{m} d_j A^{k+1} w_j} \rightarrow \notin \mathscr{K}_k$

$\in < q_1, \cdots, q_k > = \mathscr{K}_k$

- $A^{k+1}x_* = A^k b \notin \mathscr{K}_k$ **Contradiction.**

- $x_* \in \mathscr{K}_k$

If there is breakdown of the Arnoldi iteration, i.e., $h_{k+1,k} = 0, AQ_k = Q_k H_k$

- True solution
  $x_* = A^{-1}b \in \mathscr{K}_k$
- We can stop the iteration.
- This is a good breakdown.

From now on, we assume Arnoldi iteration does not break down.

- What is $Q_k^* Q_{k+1}$?
- $Q_k^* Q_{k+1} = I_{k\times(k+1)}$
- What effect does $I_{k\times(k+1)}$ has on a given matrix $M \in \mathbb{R}_{(k+1,m)}$?
- $I_{k\times(k+1)}$ eliminates the last row of M.
- $$\tilde{H}_k = \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1k} \\ h_{21} & h_{22} & \cdots & h_{2k} \\ & \ddots & \ddots & \vdots \\ & & h_{k,k-1} & h_{kk} \\ & & & h_{k+1,k} \end{bmatrix}$$
- $Q_k^* Q_{k+1} \tilde{H}_k = ?$
- $Q_k^* Q_{k+1} \tilde{H}_k = H_k$

- $AQ_k = Q_{k+1}\tilde{H}_k$
- $Q_k^* A Q_k = Q_k^* Q_{k+1}\tilde{H}_k = H_k$
- What is the interpretation of H_k?
- Since Q_k has orthonormal columns, $Q_k Q_k^*$ is the orthogonal projector from $\mathbb{R}^n$ to the column space of Q_k.
- Let $v \in \mathbb{R}^n$.
- $v_p := Q_k Q_k^* A v \ \rightarrow Q_k w = Q_k Q_k^* A Q_k y$
- $v_p = Q_k w$ w.r.t. the basis of columns of Q_k
- $v = Q_k y$ w.r.t. the basis of columns of Q_k

- $Q_k w = Q_k Q_k^* A Q_k y$
- $Q_k w = Q_k H_k y$ w.r.t. the standard basis $< e_1, e_2, \cdots, e_n >$
- $w = H_k y$ w.r.t. the basis $< q_1, q_2, \cdots, q_k >$
- H_k is the orthogonal projector that project a vector in $A\mathscr{K}_k$ to $\mathscr{K}_k$ w.r.t. the basis of column of Q_k.

GMRES method

- Original problem: Find $x_* \in \mathbb{R}^n$ s.t. $Ax_* = b$
- Minimizing problem: Find $x \in \mathscr{V}$ of dimension $k \ll n$ s.t. $\|Ax - b\|$ is minimum.
- Minimizing problem: Find $y \in \mathbb{R}^k$ s.t. $\|AQ_k y - b\|$ is minimum.
- Once y is found, $x_k = Q_k y$ is the best estimate of x_*.

- $\|AQ_k y - b\|$
- $AQ_k = ?$
- $AQ_k = Q_{k+1}\tilde{H}_k$
- $\|AQ_k y - b\| = \|Q_{k+1}\tilde{H}_k y - b\|$
- $= \|Q_{k+1}^*(Q_{k+1}\tilde{H}_k y - b)\|?$
- $= \|\tilde{H}_k y - Q_{k+1}^* b\|$
- What is q_1?
- $q_1 = b/\|b\|$
- $\rightarrow b = \|b\|q_1 := \beta q_1$

- $\|\tilde{H}_k y - Q_{k+1}^* b\| = \|\tilde{H}_k y - Q_{k+1}^* \beta q_1\|$
- $= \|\tilde{H}_k y - \beta Q_{k+1}^* q_1\|$
- What is $Q_{k+1}^* q_1$?
- $Q_{k+1}^* q_1 = [1,0,\cdots,0]^T := e_1$
- $\|\tilde{H}_k y - \beta Q_{k+1}^* q_1\| = \|\tilde{H}_k y - \beta e_1\|$
- Minimizing problem: Find $y \in \mathbb{R}^k$ s.t. $\|\tilde{H}_k y - \beta e_1\|$ is minimum.

Assignment 2: Write a Matlab code for GMRES algorithm.

- Hint:
- $q_1 = b/\|b\|$.
- For $i = 1,2,\cdots$
    - The i^{th} step of Arnoldi iteration
    - Find y that minimizes $\|\tilde{H}_k y - \beta e_1\|$
    - $x_i = Q_i y$
- What method could you apply to minimize $\|\tilde{H}_k y - \beta e_1\|$?
- Think about a stopping criterion.