

General Minimal Residual (GMRES)

Problem & Approach

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GMRES

Find $x_* \in \mathcal{K}_k (\subseteq \mathbb{C}^n)$ s.t.

$$\|b - Ax_*\|_2 = \min_{x \in \mathcal{K}_k} \|b - Ax\|_2$$

where $\mathcal{K}_k := \text{span}\{b, Ab, \dots, A^{k-1}b\}$.

We hope $Ax_* \approx b$.

Arnoldi Process

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- ▶ Find $\{q_1, \dots, q_{k-1}, q_k\}$
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Use the Gram-Schmidt procedure

$$Aq_{k-1} = h_{1(k-1)}q_1 + h_{2(k-1)}q_2 + \dots + h_{k(k-1)}q_k$$

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Letting $v := Aq_{k-1}$, due to orthogonality of q_1, \dots, q_k

$$h_{j(k-1)} = q_j^* v \quad j = 1, \dots, k-1,$$

$$h_{k(k-1)} = v - h_{1(k-1)}q_1 - \dots - h_{(k-1)(k-1)}q_{k-1}.$$

Arnoldi Process

```
 $q_1 \leftarrow b / \|b\|_2$   
for  $j = 1, \dots, k - 1$  do  
   $v \leftarrow Aq_j$   
  for  $\ell = 1, \dots, j$  do  
     $h_{\ell j} \leftarrow q_\ell^* v$   
     $v \leftarrow v - h_{\ell j} q_\ell$   
  end for  
   $h_{(j+1)j} \leftarrow \|v\|_2$   
   $q_j \leftarrow v / h_{(j+1)j}$   
end for
```

Arnoldi Recurrence

$$A \underbrace{\begin{bmatrix} q_1 & q_2 & \dots & q_{k-1} \end{bmatrix}}_{Q_{k-1}} = \underbrace{\begin{bmatrix} q_1 & q_2 & \dots & q_{k-1} & q_k \end{bmatrix}}_{Q_k} \begin{bmatrix} h_{11} & h_{12} & \dots & h_{1(k-1)} \\ h_{21} & h_{22} & & h_{2(k-1)} \\ 0 & h_{32} & \ddots & h_{3(k-1)} \\ 0 & 0 & \ddots & \ddots \\ \vdots & & & \ddots & h_{kk} \\ 0 & 0 & & & h_{(k+1)k} \end{bmatrix}$$

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- ▶ $Q_k \in \mathbb{C}^{n \times k}$ columns form orthonormal basis for \mathcal{K}_k
- ▶ $H_k \in \mathbb{C}^{(k+1) \times k}$ Hessenberg

The Least Squares Problem

$$\min_{x \in \mathcal{K}_k} \|b - Ax\|_2 = \min_{\alpha \in \mathbb{C}^k} \|b - AQ_k \alpha\|_2$$

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Procedure

1. Form Q_{k+1} and H_{k+1} by the Arnoldi Procedure.
2. Find $\alpha_k \in \mathbb{C}^k$ s.t.

$$\|Q_{k+1}^*b - H_{k+1}\alpha_k\|_2 = \min_{\alpha \in \mathbb{C}^k} \|Q_{k+1}^*b - H_{k+1}\alpha\|_2$$

3. $x_* := Q_k\alpha_k$ is the (approximate) solution.