Krylov subspace methods and GMRES

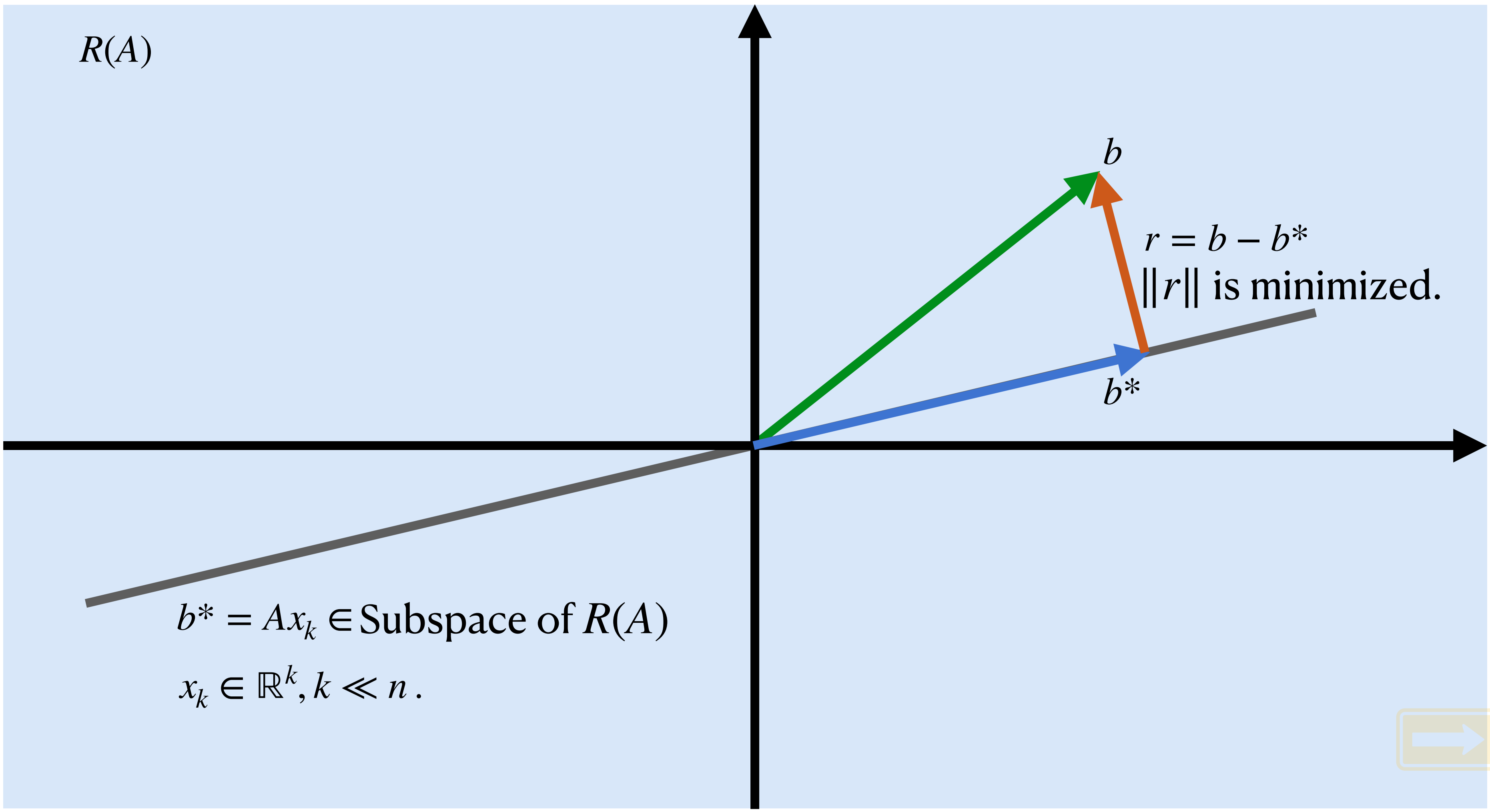
(Generalized Minimal Residuals)

05/02/2024

Preliminary

- $Ax = b$, where $A \in \mathbb{R}^{n\times n}$ is nonsingular, $b \in \mathbb{R}^n$ is known.
- $x_* = A^{-1}b$, the true solution.
- Consider $n \gg 1$.

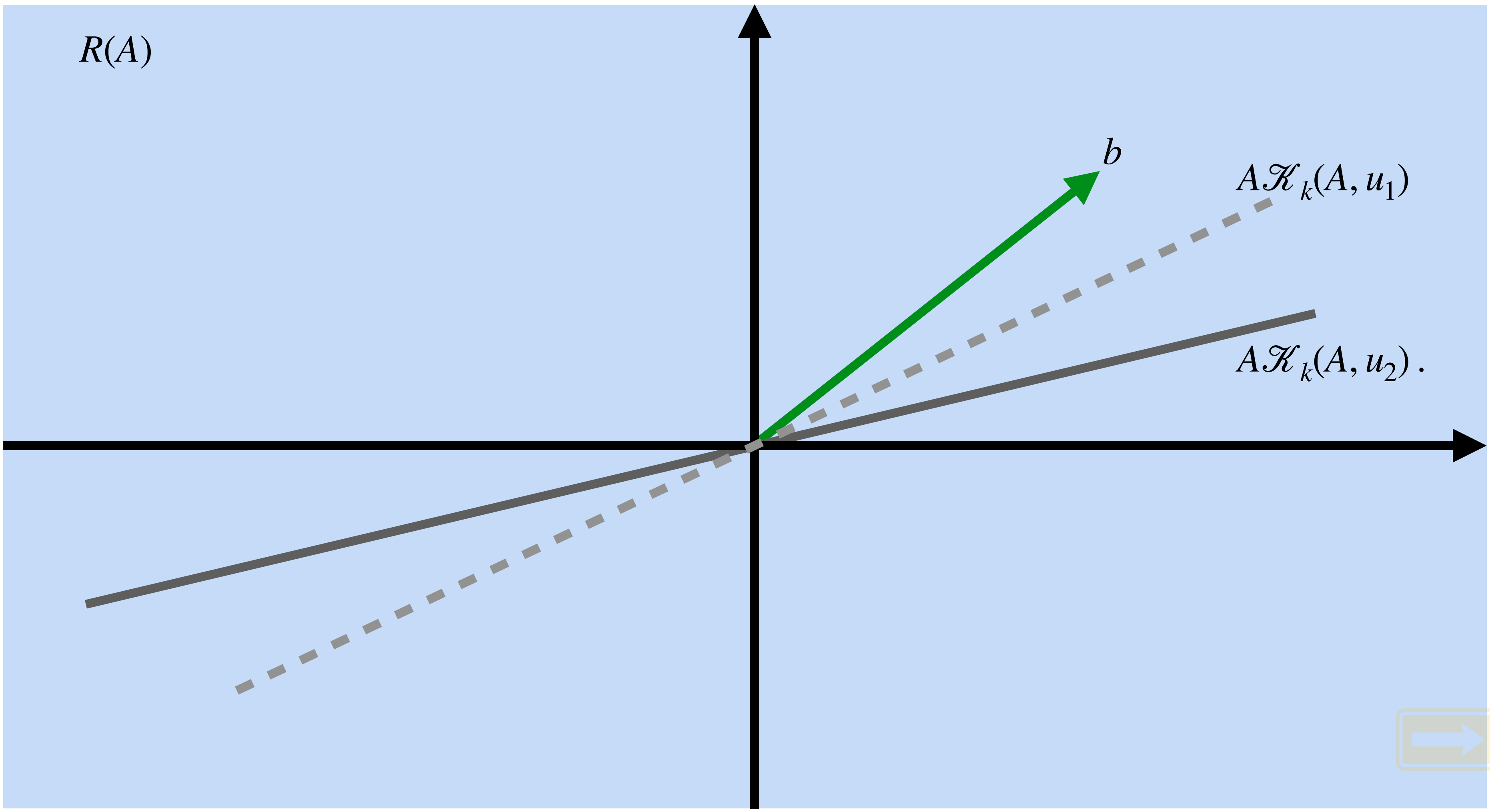
Illustration



Krylov Subspace

- $\mathscr{K}_k(A, u) = < u, Au, A^2u, \ldots, A^{k-1}u >$, $u \in \mathbb{R}^n$.
- If $x_k \in \mathscr{K}_k$, $x_k = \alpha_0 u + \alpha_1 Au + \alpha_2 A^2 u + \cdots + \alpha_{k-1} A^{k-1} u = \sum_{i=0}^{k-1} \alpha_i A^i u$, for some coefficients $\alpha_i \in \mathbb{R}$.
- $x_k = p^{(k-1)}(A)u$, where $p^{(k-1)}(t) = \sum_{i=0}^{k-1} \alpha_i t^i$, is a polynomial of degree $k - 1$.
- How to choose u ?

Illustration



- Cayley-Hamilton theorem: Any matrix satisfies its own characteristic equation $c(A) = 0$.
- $c(z) = \det(zI - A) = \prod_{j=1}^{n} (\lambda_j - z)$ is the characteristic polynomial.
- $$c(A) = (-1)^n A^n + \cdots - \left(\sum_{i=1}^{n} \prod_{j=1, j \neq i}^{n} \lambda_j \right) A + \left(\prod_{j=1}^{n} \lambda_j \right) I = 0$$

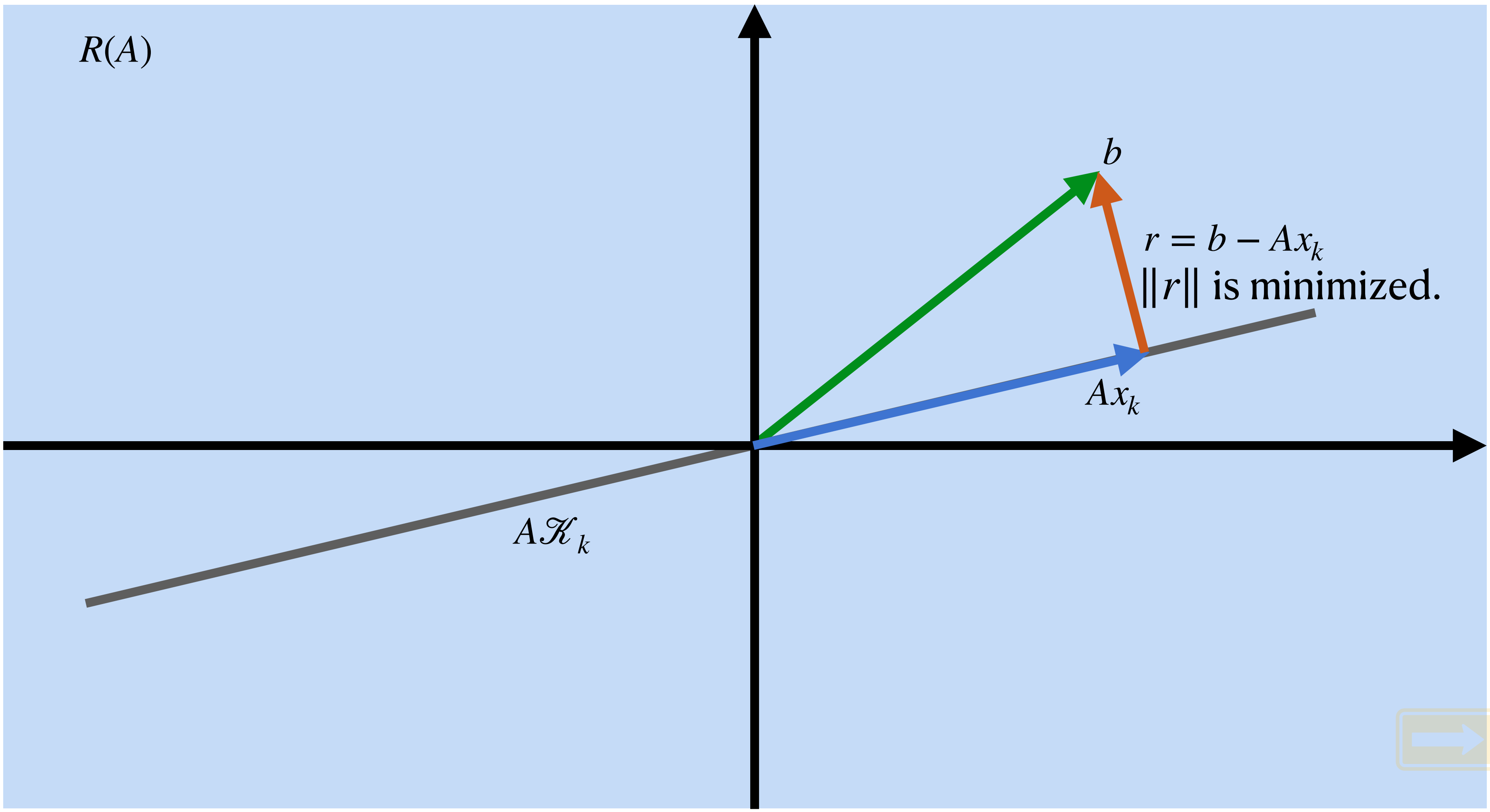
$\det(A) \neq 0$

$$\left((-1)^{n-1} A^{n-1} + \cdots + \left(\sum_{i=1}^{n} \prod_{j=1, j \neq i}^{n} \lambda_j \right) I \right) \Big/ \left(\prod_{j=1}^{n} \lambda_j \right) = A^{-1}$$

$q^{n-1}(A)$

- $x_* = A^{-1}b = q^{n-1}(A)b$
- $x_k = p^{(k-1)}(A)u \rightarrow u = b$
- GMRES is an iterative method, $k = 1,2,\cdots$
- Initial guess x_0
- $\rightarrow r_0 = b - Ax_0$
- $\rightarrow A^{-1}r_0 = x_* - x_0$
- $\qquad\qquad = q^{n-1}(A)r_0$
- $\rightarrow x_* = x_0 + q^{n-1}(A)r_0$
- Usually $x_0 = 0$

Illustration of GMRES



- $\mathscr{K}_k(A, b) = < b, Ab, A^2b, \ldots, A^{k-1}b >$, $b \in \mathbb{R}^n$.
- $K = [b \,|\, Ab \,|\, A^2b \,|\, \ldots \,|\, A^{k-1}b]$ ill-conditioned
- $x_k = \sum_{i=0}^{k-1} \alpha_i A^i b = K\alpha, \text{ where } \alpha = \begin{bmatrix} \alpha_0 \\ \vdots \\ \alpha_{k-1} \end{bmatrix} \in \mathbb{R}^k$.
- Minimizing problem: Find $\alpha \in \mathbb{R}^k$ s.t. $\|AK\alpha - b\|$ is minimum. Numerically unstable
- Once α is found, $x_k = K\alpha$ is the best estimate of x_* in $\mathscr{K}_k(A, b)$.
- What happens if $k = n$?

- An orthonormal matrix $Q_k \to \mathcal{K}_k(A, b)$.
- $x_k = Q_k y$
- 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_*.
- How to find such Q_k ?

Arnoldi iteration

- ~~Complete~~ reduction: $A = QHQ^* \rightarrow AQ = QH$, where Q orthonormal and

$$H = \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1n} \\ h_{21} & h_{22} & \cdots & h_{2n} \\ & \ddots & \ddots & \vdots \\ & & h_{n,n-1} & h_{nn} \end{bmatrix} \in \mathbb{R}^{n\times n} \text{ Hessenberg form.}$$

- $n \gg 1$

- $$A[q_1 \,|\, q_2 \,|\, \cdots \,|\, q_n] = [q_1 \,|\, q_2 \,|\, \cdots \,|\, q_n] \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1n} \\ h_{21} & h_{22} & \cdots & h_{2n} \\ & \ddots & \ddots & \vdots \\ & & h_{n,n-1} & h_{nn} \end{bmatrix}$$

- q_j on the left $\rightarrow q_1, q_2, \cdots, q_j, q_{j+1}$ on the right.

- i.e., $A[q_1 \,|\, q_2 \,|\, \cdots \,|\, q_k] = [q_1 \,|\, q_2 \,|\, \cdots \,|\, q_k \,|\, q_{k+1}] \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1k} \\ h_{21} & h_{22} & \cdots & h_{2k} \\ & \ddots & \ddots & \vdots \\ & & h_{k,k-1} & h_{kk} \\ & & & h_{k+1,k} \end{bmatrix}$
- $\tilde{H}_k = \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1k} \\ h_{21} & h_{22} & \cdots & h_{2k} \\ & \ddots & \ddots & \vdots \\ & & h_{k,k-1} & h_{kk} \\ & & & h_{k+1,k} \end{bmatrix} \in \mathbb{R}^{(k+1)\times k}$ the upper left section H
- Partial reduction: $AQ_k = Q_{k+1}\tilde{H}_k$, where $Q_k = [q_1 \,|\, q_2 \,|\, \cdots \,|\, q_k] \in \mathbb{R}^{n\times k}$

- $$A[q_1 \,|\, q_2 \,|\, \cdots \,|\, q_k] = [q_1 \,|\, q_2 \,|\, \cdots \,|\, q_k \,|\, q_{k+1}] \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1k} \\ h_{21} & h_{22} & \cdots & h_{2k} \\ & \ddots & \ddots & \vdots \\ & & h_{k,k-1} & h_{kk} \\ & & & h_{k+1,k} \end{bmatrix}$$
- $Aq_j = h_{1j}q_1 + h_{2j}q_2 + \cdots + h_{jj}q_j + h_{j+1,j}q_{j+1}$
- $\rightarrow q_{j+1} = (Aq_j - h_{1j}q_1 - h_{2j}q_2 - \cdots - h_{jj}q_j)/h_{j+1,j}$
- q_{j+1} satisfies an $(j+1)$-term recurrence relation → inner loop in coding.

- How to choose q_1 to make sure $q_1 \in \mathcal{K}_k(A, b)$?
- $q_1 = \dfrac{b}{\|b\|}$
- How to find h_{11}, q_2 and h_{21} ?
- $Aq_1 = h_{11}q_1 + h_{21}q_2$
- $q_1^* Aq_1 = q_1^*(h_{11}q_1 + h_{21}q_2) = h_{11}$ due to orthogonality of $q_j's$
- Form q_2 from $Ab \Leftrightarrow Aq_1$
- $\Leftrightarrow Aq_1 := v$ to save computational cost
- $q_2' := \rightarrow v - (v * q_1)q_1$
- $\rightarrow q_2 = q_2'/\|q_2'\|$: Modified Gram-Schmidt iteration

- Compare $q_2' = v - (v * q_1)q_1$ with $q_2 = (Aq_1 - h_{11}q_1)/h_{21}$
- $\rightarrow h_{21} = \|q_2'\|$

First iteration:

1. Form $v = Aq_1$
2. Find h_{11} by orthogonality
3. Find q_2' by G.S.
4. $h_{21} = \|q_2'\|$
5. $q_2 = q_2'/h_{21}$

Second iteration:

1. $v = Aq_2$
2. $h_{j2},\ j = 1{,}2. \ \leftarrow v = h_{12}q_1 + h_{22}q_2 + h_{32}q_3$
3. $q_3' = v - h_{12}q_1 - h_{22}q_2$
4. $h_{32} = \|q_3'\|$
5. $q_3 = q_3'/h_{32}$

j^{th} iteration...

Why $< q_1, q_2, \cdots, q_k > = \mathscr{K}_k(A, b)$?

- $q_1 = \dfrac{b}{\|b\|} \rightarrow < q_1 > = < b >$
- $q_2 = (Aq_1 - h_{11}q_1)/h_{21}$
- $\quad = \left(\dfrac{Ab}{\|b\|} - h_{11}\dfrac{b}{\|b\|} \right)/h_{21}$
- $\rightarrow < q_1, q_2 > = < b, Ab >$
- $q_3 = (Aq_2 - h_{12}q_1 - h_{22}q_2)/h_{32}$
- $\quad = \left(A\left(\dfrac{Ab}{\|b\|} - h_{11}\dfrac{b}{\|b\|} \right)/h_{21} - h_{12}\dfrac{b}{\|b\|} - h_{22}\left(\dfrac{Ab}{\|b\|} - h_{11}\dfrac{b}{\|b\|} \right)/h_{21} \right)/h_{32}$
- $\rightarrow < q_1, q_2, q_3 > = < b, Ab, A^2b >$
- $\rightarrow < q_1, q_2, q_3, \cdots, q_k > = < b, Ab, A^2b, \cdots, A^{k-1}b >$

Assignment 1:

Write pseudocode for Arnoldi iterations for creating $\mathscr{K}_k(A, b)$, where $k \geq 3$ is an arbitrary integer.

Hint:

Follow the pseudocode we just learned ↓

1. $v = Aq_2$
2. $h_{j2}, j = 1{,}2 \leftarrow v = h_{12}q_1 + h_{22}q_2 + h_{32}q_3$
3. $q_3' = v - h_{12}q_1 - h_{22}q_2$
4. $h_{32} = \|q_3'\|$
5. $q_3 = q_3'/h_{32}$