Last time:

- Goal: $A \in \mathbb{C}^{n\times n}$ $(\det A \neq 0)$, $b \in \mathbb{C}^n$, $Ax = b$, find $x \in \mathbb{C}^n$
- Projection method:

  given $x_0 \in \mathbb{C}^n$, find $x_k \in x_0 + \mathcal{K}_k$ s.t.

  $b - Ax_k \perp \mathcal{L}_k$ Petrov–Galerkin condition

  want: $A(x_0 + \tilde{x}) \approx b$. $\tilde{x} \in \mathcal{K}_k$

  $$A\tilde{x} \approx r_0$$

  $$\tilde{x} \approx A^{-1} r_0$$

  need to choose $\mathcal{K}_k$ such that $A^{-1} r_0$ can be well-approximated (Cayley–Hamilton)
- Krylov subspace methods:

  $$\mathcal{K}_k = \mathcal{K}_k(A, r_0) = \operatorname{span}\{r_0, Ar_0, \dots, A^{k-1} r_0\}$$

  $\Rightarrow$ $x_k = x_0 + p_{k-1}(A) r_0$. p_{k-1} is $(k-1)$-degree polynomial

  Different choices of $\mathcal{L}_k$ lead to different methods

- FOM, $\mathcal{L}_k = \mathcal{K}_k$

  Galerkin condition: $r_k = b - Ax_k \perp \mathcal{K}_k$

  – Different formulation

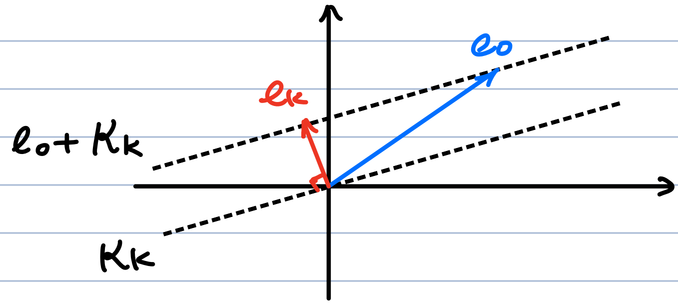
  let $e_k = x_k - x$, then $r_k = A(x - x_k) = -Ae_k$

  If A is Hermitian positive definite,

  $$r_k \perp \mathcal{K}_k \Leftrightarrow e_k \perp_A \mathcal{K}_k$$

  perpendicular under A-inner product

  Since $e_k = x_k - x = x_0 + \tilde{x} - x = e_0 + \tilde{x}$, $\tilde{x} \in \mathcal{K}_k$



we know $\|e_k\|_A = \min_{e \in e_0 + K_k} \|e\|_A$

or $\boxed{\|x_k - x\|_A = \min_{y \in x_0 + K_k} \|y - x\|_A}$

when A is real. same as minimizing $\frac{1}{2} y^T A y - y^T b$ (CG)

$\Rightarrow$ The least-squares problem is uniquely solvable. x_k exists and unique.

For general A, there is no guarantee that x_k exists.
(counterexample last lecture)

- <u>(Generalized) minimal residual method</u> (GMRES / MINRES)

Take $L_k = A K_k$

$$\boxed{\text{Find } x_k \in x_0 + K_k, \text{ s.t. } r_k = b - Ax_k \perp A K_k \quad (*)}$$

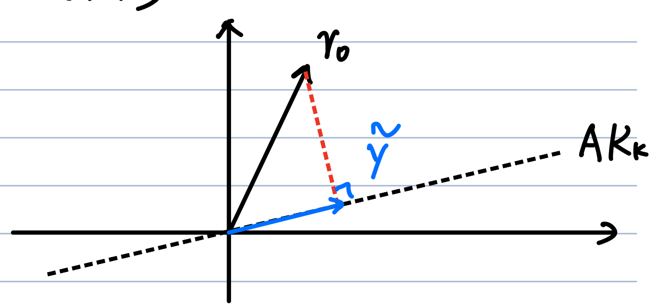
— Equivalent formulation:

$$\boxed{\text{Find } x_k \in x_0 + K_k, \ \|r_k\|_2 = \|b - Ax_k\|_2 = \min_{y \in x_0 + K_k} \|b - Ay\|_2 \quad (\star)}$$

Actually, $\min_{y \in x_0 + K_k} \|b - Ay\|_2$

$\overset{y = x_0 + \tilde{x}}{=} \min_{\tilde{x} \in K_k} \|r_0 - A\tilde{x}\|_2 \quad (**)$

$\overset{\tilde{y} = A\tilde{x}}{=} \min_{\tilde{y} \in AK_k} \|r_0 - \tilde{y}\|_2$



So $x_k \in x_0 + K_k$ minimizes $\|r_k\|_2$

$$\Longleftrightarrow \quad \underbrace{r_0 - \tilde{y}} \perp AK_k$$

since $\tilde{y} = A\tilde{x} = A(x_k - x_0)$

we know $r_0 - \tilde{y} = b - Ax_k = r_k \longleftarrow$ formulation $(*)$

– The least-squares problem $(**)$ is uniquely solvable as long as A is nonsingular. When $k=n$, $x_n = x$. (Why?)

• How to find x_k in $(*)$ or $(☆)$?

– Use Arnoldi to find an orthonormal basis of K_k

$$Q_k = [q_1 \cdots q_k] \in \mathbb{C}^{n\times k}$$

and $H_k \in \mathbb{C}^{k\times k}$, $h_{k+1,k} \in \mathbb{C}$, $q_{k+1} \in \mathbb{C}^n$, $q_{k+1}^* Q_k = 0$

$$\boxed{AQ_k = Q_k H_k + h_{k+1,k}\, q_{k+1} e_k^*} \qquad (AD)$$

and $r_0 = \beta q_1$, $\beta = \|r\|_2$

– let $\bar{H}_k = \begin{bmatrix} H_k \\ h_{k+1,k} e_k^* \end{bmatrix} \in \mathbb{C}^{(k+1)\times k}$

then $AQ_k = Q_{k+1} \bar{H}_k$

– $(☆) \Longleftrightarrow \min\limits_{y \in x_0 + K_k} \|b - Ay\|_2 = \min\limits_{\tilde{x} \in K_k} \|r_0 - A\tilde{x}\|_2$

$$\overset{\tilde{x} = Q_k z}{=} \min_{z \in \mathbb{C}^k} \|\beta q_1 - AQ_k z\|_2$$

$$= \min_{z \in \mathbb{C}^k} \|\beta q_1 - Q_{k+1} \bar{H}_k z\|_2$$

$$= \min_{z \in \mathbb{C}^k} \| Q_{k+1} (\beta \bar{e}_1 - \bar{H}_k z) \|_2 \qquad e_1 = (1, 0, \cdots, 0)^T \in \mathbb{R}^{k+1}$$

$$= \min_{z \in \mathbb{C}^k} \| \beta \bar{e}_1 - \bar{H}_k z \|_2$$

Summary: Find $z_k = \arg\min_{z \in \mathbb{C}^k} \| \beta e_1 - \bar{H}_k z \|_2 \quad (\star\star)$

then $x_k = x_0 + Q_k z_k$

Algorithm (GMRES) Given $x_0 \in \mathbb{C}^n$, $k \geq 1$

Step 1: Compute $r_0 = b - Ax_0$, $\beta = \| r_0 \|_2$,

Step 2: Use Arnoldi to compute $\bar{H}_k \in \mathbb{C}^{(k+1) \times k}$, $Q_k \in \mathbb{C}^{n \times k}$ in (AD)

Step 3: Solve the LS problem $z_k = \arg\min_{z \in \mathbb{C}^k} \| \beta \bar{e}_1 - \bar{H}_k z \|_2$

and form solution $x_k = x_0 + Q_k z_k$

- Solve L-S problem $(\star\star)$
  - For $(\star\star)$ to be uniquely solvable, we need $\mathrm{rank}(\bar{H}_k) = k$.

    This is true as long as $h_{j+1,j} \neq 0$, $j = 1, \cdots, k-1$

    (Hint: what's $\mathrm{rank}(\bar{H}_k)$ if $h_{k+1,k} \neq 0$? If $h_{k+1,k} = 0$, use Arnoldi decomposition)
  - Solve $(\star\star)$ by normal eqn is costly because forming $\bar{H}_k^* \bar{H}_k$ cost $\mathcal{O}(n^3)$ flops.

    We can do better with QR since $\bar{H}_k$ is upper Hessenberg

    that is, compute $z_k = \bar{R}_k^{-1} \bar{Q}_k^* (\beta \bar{e}_1)$, with $\bar{H}_k = \bar{Q}_k \bar{R}_k$ $\quad \bar{Q}_k \in \mathbb{C}^{(k+1) \times k}$, $R_k \in \mathbb{C}^{k \times k}$

$$\bar{H}_k = \begin{bmatrix} \boxed{\times} & \times & \times & \times \\ \boxed{\times} & \times & \times & \times \\ & \times & \times & \times \\ & & \times & \times \\ & & & \times \end{bmatrix} \xrightarrow[\underset{G_1 \in \mathbb{C}^{(k+1)\times(k+1)}}{\begin{bmatrix} \tilde{G}_1 & \\ & I_{k-1} \end{bmatrix}}]{} \begin{bmatrix} \times & \times & \times & \times \\ 0 & \boxed{\times} & \times & \times \\ & \boxed{\times} & \times & \times \\ & & \times & \times \\ & & & \times \end{bmatrix} \xrightarrow[\underset{G_2 \in \mathbb{C}^{(k+1)\times(k+1)}}{\begin{bmatrix} 1 & & \\ & \tilde{G}_2 & \\ & & I_{k-2} \end{bmatrix}}]{} \begin{bmatrix} \times & \times & \times & \times \\ & \times & \times & \times \\ & 0 & \boxed{\times} & \times \\ & & \boxed{\times} & \times \\ & & & \times \end{bmatrix}$$

$(\tilde{G}_i \in \mathbb{C}^{2\times 2}$ Givens$)$

$$\longrightarrow \cdots \longrightarrow \begin{bmatrix} \times & \times & \times & \times \\ & \times & \times & \times \\ & & \times & \times \\ & & & \times \\ \hline & & 0 & \end{bmatrix} = \begin{bmatrix} R_k \\ \hline 0 \end{bmatrix} = \bar{R}_k \in \mathbb{C}^{(k+1)\times k}$$

$R_k \in \mathbb{C}^{k\times k}$

$(\operatorname{rank}(R_k) = \operatorname{rank}(\bar{H}_k))$

Let $\bar{Q}_k^* = G_k G_{k-1} \cdots G_2 G_1 \in \mathbb{C}^{(k+1)\times(k+1)}$, then $\bar{Q}_k^* \bar{H}_k = \bar{R}_k$

Let $\bar{g}_k = \bar{Q}_k^*(\beta \bar{e}_1) = \begin{bmatrix} g_k \\ \gamma_{k+1} \end{bmatrix} \in \mathbb{C}^{k+1}$, $g_k \in \mathbb{C}^k$, $\gamma_{k+1} \in \mathbb{C}$

$$(**) \iff \min_{z \in \mathbb{C}^k} \| \beta \bar{e}_1 - \bar{H}_k z \|_2$$

$$= \min_{z \in \mathbb{C}^k} \| \bar{g}_k - \bar{R}_k z \|_2$$

$$= |\gamma_{k+1}| \qquad \text{minima attained when } z = R_k^{-1} g_k$$

— Lucky breakdown: If $h_{k+1,k} = 0$, then from above $G_k = I$

thus $\gamma_{k+1} = 0$ and $\min\limits_{y \in x_0 + \mathcal{K}_k} \| b - Ay \|_2 = \min\limits_{z \in \mathbb{C}^k} \| \beta \bar{e}_1 - \bar{H}_k z \|_2 = 0$

x_k is an exact solution to $Ax = b$!

- Cost and restarting

$\#\text{flops} = k \times \text{cost computing } Aq$

$\quad + O(k^2 n) \longleftarrow$ Arnoldi

$\quad + O(k^2) \longleftarrow$ solve LS

Memory : $O(kn)$

To keep $k \ll n$, use restart technique to fix the k and use the obtained approximate solution as the initial guess in the next step.

- Even though GMRES provide an output for any k (unlike FOM), there is no guarantee that x_k improves steadily as k increases.

ex. $A = \begin{bmatrix} 0 & \cdots & & 1 \\ 1 & 0 & & \vdots \\ & 1 & 0 & \\ & & \ddots & \ddots \\ & & 1 & 0 \end{bmatrix}$, $b = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$, $x = A^{-1}b = e_n$

Take $x_0 = 0$, by running Arnoldi, $q_i = e_i$, $i = 1, \cdots, k$

$$\underset{\mathbb{R}^{k\times k}}{\underset{\cap}{H_k}} = \begin{bmatrix} 0 & & & \\ 1 & 0 & & \\ & 1 & 0 & \\ & & \ddots & \ddots \\ & & 1 & 0 \end{bmatrix}, \quad \underset{\mathbb{R}^{(k+1)\times k}}{\underset{\cap}{\bar{H}_k}} = \begin{bmatrix} 0 & & & \\ 1 & 0 & & \\ & 1 & 0 & \\ & & \ddots & \ddots \\ & & 1 & 0 \\ & & & 1 \end{bmatrix}, \quad \forall k < n$$

The L-S problem, $\min_{z \in \mathbb{R}^k} \| \beta e_1 - \bar{H}_k z \|_2$

is uniquely solvable, with $z_k = \arg\min_{z \in \mathbb{R}^k} \| \beta e_1 - \bar{H}_k z \|_2 = 0 \quad \forall k < n$

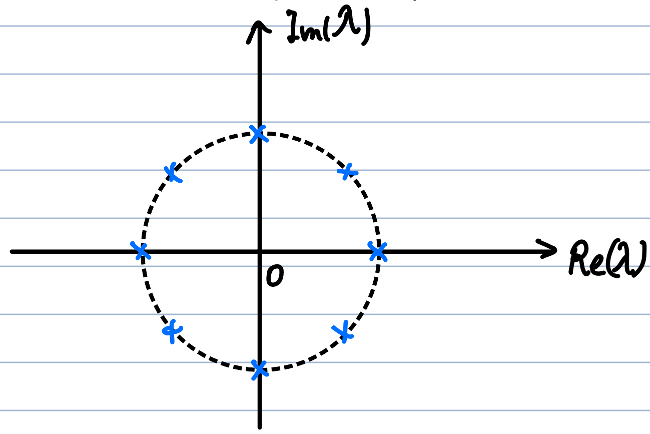
$$\Rightarrow \quad x_k = x_0 + Q_k z_k = 0, \quad \forall k < n$$

So restarted GMRES fails for any $k < n$!

Eigenvalues of A

$\lambda_j = e^{i \frac{2\pi}{n} j}$

$j = 1, \cdots, n$



- When does GMRES have good performance?

Since $x_k \in x_0 + \mathcal{K}_k$, $\exists\, p_{k-1} \in \mathcal{P}_{k-1}(\mathbb{C})$. s.t.

$$x_k = x_0 + p_{k-1}(A) r_0$$

So
$$\begin{aligned}
\|r_k\|_2 &= \|b - Ax_k\|_2 \\
&= \|r_0 - Ap_{k-1}(A) r_0\|_2 \\
&= \|\underbrace{(I - A\,p_{k-1}(A))}_{=:\, q_k(A)} r_0\|_2
\end{aligned}$$

$, \quad q_k(\lambda) = 1 - \lambda\, p_{k-1}(\lambda) \in \mathcal{P}_k(\mathbb{C})$

Since $\|r_k\|_2$ is minimal, as we vary p_{k-1}, we run through all elements in $x_0 + \mathcal{K}_k$, thus

$$\|r_k\|_2 = \min_{\substack{q(0)=1 \\ q \in \mathcal{P}_k(\mathbb{C})}} \|q(A) r_0\|_2$$

Assume that $A = V \Lambda V^{-1}$ diagonalizable.

then $q(A) = V\, p(\Lambda)\, V^{-1}$

so
$$\begin{aligned}
\|r_k\|_2 &= \min_{\substack{q(0)=1 \\ q \in \mathcal{P}_k(\mathbb{C})}} \|V p(\Lambda) V^{-1} r_0\|_2 \\
&\leq \kappa_2(V) \min_{\substack{q(0)=1 \\ q \in \mathcal{P}_k(\mathbb{C})}} \|p(\Lambda)\|_2 \, \|r_0\|_2 \\
&= \kappa_2(V) \|r_0\|_2 \underbrace{\min_{\substack{q(0)=1 \\ q \in \mathcal{P}_k(\mathbb{C})}} \max_{1 \leq i \leq n} |p(\lambda_i)|}_{=:\, \varepsilon_k(A)}
\end{aligned}$$

Remark: if A is singular, there is no convergence for GMRES in general

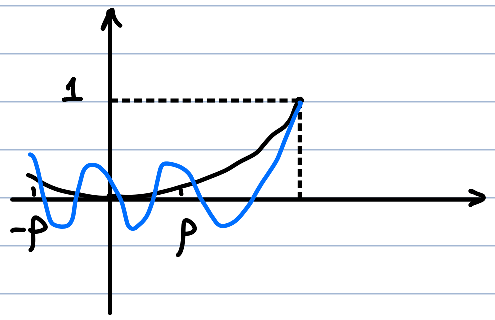
To find an upper bound for $\mathcal{E}_k(A)$,

consider the relaxed version of this min-max problem

Thm (Zarantonello)

Let $B(0,\rho) \subseteq \mathbb{C}$ be a disk centered at 0 with radius $\rho > 0$. Then $\forall\, \gamma \notin B(0,\rho)$

$$\min_{\substack{p(\gamma)=1 \\ p\in P_k}} \max_{\lambda \in B(0,\rho)} |p(\lambda)| = \left(\frac{\rho}{|\gamma|}\right)^k$$



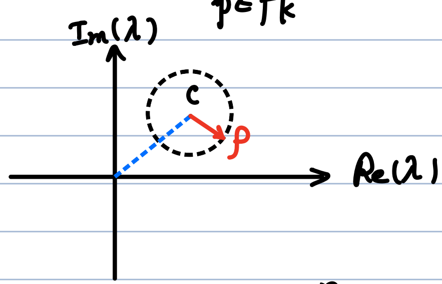
minimum being achieved by $p(\lambda) = \left(\frac{\lambda}{\gamma}\right)^k$ ▨

1) If $\{\lambda_i\}_{i=1}^n \subseteq B(c,\rho)$ with $\rho < |c|$, then

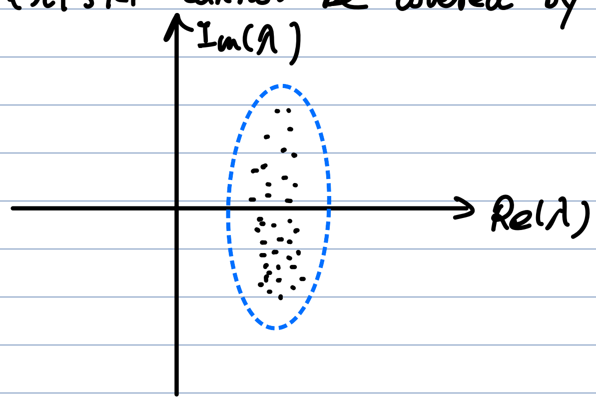
$$\mathcal{E}_k(A) \le \min_{\substack{p(0)=1 \\ p\in P_k}} \max_{\lambda \in B(c,\rho)} |p(\lambda)| = \left(\frac{\rho}{|c|}\right)^k \approx \left(\frac{\kappa_2(A)-1}{\kappa_2(A)+1}\right)^k$$

assume Hermitian positive definite

(CG has better rate, see next lecture notes)



2) We can stretch $B(c,\rho)$ to handle more general case when $\{\lambda_i\}_{i=1}^n$ cannot be covered by a disk away from 0



Can't cover with circle while not intersecting origin

but can do this with ellipse

3) In general, GMRES performs well when eig. values of A cluster away from zero and A is not too far from normality.

- MINRES

When $A^* = A$, we can replace Arnoldi iteration by Lanczos process in GMRES (obtain tridiagonal H_k)

Save flops as well as memory. (See Y. Saad's book)