Arnoldi for matrix functions

$A \in \mathbb{C}^{m\times m}$ large, sparse $b \in \mathbb{C}^m$

How to compute $f(A)b$?

Krylov space:

$$K_n(A,b) = \text{span}\{b, Ab, \dots A^{n-1}b\}$$

$V_n \in \mathbb{C}^{m\times n}$ whose columns are an orthonormal basis for $K_n(A,b)$.

<u>Lemma</u>: if $p(x)$ is a polynomial of degree $d<n$

$$A_n = V_n^* A V_n \in \mathbb{C}^{n\times n}$$

$$\underbrace{V_n}_{m\times n}\underbrace{p(A_n)}_{\substack{p\\ n\times n}} V_n^* b = \underbrace{p(A)}_{\substack{p\\ m\times m}} b$$

For a general function f, we can take

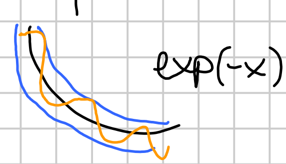
$$c = V_n \underbrace{f(A_n)}_{n\times n} V_n^* b \quad \text{as an approximation of} \quad \underbrace{f(A)}_{m\times m} b$$

<u>Theorem</u>: let $A\in\mathbb{C}^{m\times m}$ <u>Hermitian</u>, and set

$$I = [\lambda_{min}, \lambda_{max}] = \text{hull}(\Lambda(A)).$$

Let $a(x)$ be the best-approximation polynomial for f on I, i.e., the polynomial of degree $d<n$ such that

$$\delta = \max_{x\in I} |f(x) - a(x)| \quad \text{is the smallest possible.}$$



Then, $\|f(A)b - c\| \le 2\delta \|b\|$.

Recall that $c = p_n(A)b$ for a certain polynomial of degree $d<n$ (the interpolating polynomial for f on $\Lambda(A_n)$)

<u>Proof</u>: sum and subtract $a(A)b = V_n\, a(A_n) V_n^* b$

$$\|f(A)b - c\| = \|(f-a)(A)b - V_n (f-a)(A_n) V_n^* b\|$$

$$\leq \underbrace{\|(f-a)(A)\|}_{=\delta} \cdot \|b\| + \underbrace{\|V_n\|}_{=1} \, \underbrace{\|(f-a)(A_n)\|}_{=\delta} \cdot \underbrace{\|V_n^*\|}_{=1} \cdot \|b\| = 2\delta \|b\|.$$

claim → δ δ ← claim

$$\|(f-a)(A)\| \leq \|(f-a)(Q\Lambda Q^*)\| = \left\|Q \begin{bmatrix} (f-a)(\lambda_1) & & \\ & \ddots & \\ & & (f-a)(\lambda_n) \end{bmatrix} Q^*\right\|$$

$$= \max_i |(f-a)(\lambda_i)| \leq \delta \quad \text{because } \lambda_i \in I$$

We would like to use the same argument for the second term:

$$\|(f-a)(A_n)\| = \max_{\mu_i \in \Lambda(A_n)} |(f-a)(\mu_i)| \leq \delta$$

for the last inequality to hold, we need to check that $\Lambda(A_n) \subset I$

Let $A_n x = x\mu$ be an eigenpair for A_n,

$$\mu = \frac{x^* A_n x}{x^* x} = \frac{x^* V_n^* A V_n x}{x^* V_n^* V_n x} = \frac{y^* A y}{y^* y} \qquad \text{with } V_n x = y$$

Rayleigh quotient for A_n Rayleigh quotient on A

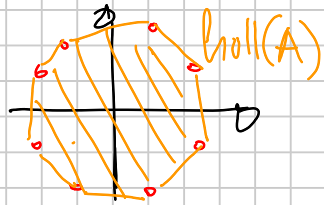
$$\frac{y^* A y}{y^* y} = \frac{y^* Q^* \Lambda Q y}{y^* Q^* Q y} = \frac{z^* \Lambda z}{z^* z} = \frac{\sum |z_i|^2 \lambda_i}{\sum |z_i|^2}.$$

$=$ linear comb. of $\lambda_i \in I$ by convexity

This concludes the proof. $\square$

This also works for normal matrices, if we replace $[\lambda_{min}, \lambda_{max}]$ with the convex hull $\text{hull}(\Lambda(A))$

which in general is a polygon $\in \mathbb{C}$.



We would like to generalize this result to non-normal A as well.

Two steps do not work:

1. $\Lambda(A_n) \subseteq \text{hull}(\Lambda(A))$
2. $\|f(A)\| = \max_{\lambda \in \Lambda(A)} |f(\lambda)|$.

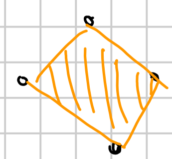
only true for normal A.

Two technical tools

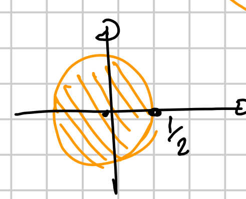
Def: the numerical radius or field of values of A is the set of all possible values of the Rayleigh quotient

$$W(A) = \left\{ \frac{x^* A x}{x^* x} : x \in \mathbb{C}^m \setminus \{0\} \right\}$$

Ex: 1. If A normal, $W(A) = \text{hull}(\Lambda(A))$



2. $A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$ has $W(A) = B(0, \frac{1}{2})$



3. $\Lambda(A) \subseteq W(A) \subseteq B(0, \|A\|)$

Euclidean norm $\sigma_{max}(A)$

Since the Rayleigh quotients of A_n are Rayleigh quotients for A,

$$W(A_n) \subseteq W(A) \qquad \frac{x^* A_n x}{x^* x} = \frac{y^* A y}{y^* y} \quad y = V_n x$$

Theorem: (CROUZEIX-PALENCIA 2017) Let $\boxed{\gamma} = 1+\sqrt{2}$, then for every $A \in \mathbb{C}^{n\times n}$, and every f holomorphic on $W(A)$, we have

$$\|f(A)\| \leq \gamma \max_{z\in W(A)} |f(z)|$$

Conjecture (CROUZEIX's conjecture): $\boxed{\gamma}=2$ works as well

Theorem: let $A \in \mathbb{C}^{n\times n}$, f holomorphic on $W(A)$, let $a(z)$ be the best-approx. polynomial to f in $W(A)$ i.e. the polynomial of degree $d<n$ that achieves minimum

$$\delta = \max_{z\in W(A)} |f(z)-a(z)|$$

Then, $\| f(A)b - c\| \leq 2\boxed{\gamma}\delta \|b\|$.

Proof:

$$\|f(A)b - c\| = \| (f-a)(A)b - V_n (f-a)(A_n) V_n^* b\|$$

$$\leq \underbrace{\|(f-a)(A)\|}_{\leq \gamma\delta} \cdot \|b\| + \underbrace{\|V_n\|}_{1} \cdot \underbrace{\|(f-a)(A_n)\|}_{\leq\gamma\delta} \cdot \underbrace{\|V_n^*\|}_{1} \cdot \|b\|.$$

by the theorem on $f-a$

by the same theorem, since $W(A_n) \subset W(A)$

$f(A)b = p(A)b$ $\quad$ p interpolates f on blue xs

$c = p_n(A)b$ $\quad$ p_n interpolates f on red Os

Idea (from the power method): if we want only the eigenvalues on the rightmost part of $\Lambda(A)$, we use V_n not from $K_n(A,b)$, but from $K_n\left((A-\alpha I)^{-1}, b\right)$ where α is a suitable value right of $\Lambda(A)$

Shift-and-invert Arnoldi : cost: 1 sparse factorization
n sparse solves

$$\operatorname{span} V_n = \left\{ r(A)b \;:\; r(x) = \frac{p(x)}{(x-\alpha)^n}, \deg(p) < n \right\}$$

$$K_n = \left\{ p(A)b \quad \dots \right\}$$

The same results hold with $Q(z)$ being the best approximating rational function with denominator $(x-\alpha)^n$

Generalization: rational Arnoldi:

choose an arbitrary polynomial at the denominator,

$$q(x) = (x-\alpha_1)(x-\alpha_2)\cdots\cdots(x-\alpha_n)$$

one can compute a basis for

$$K_{q,n} = \left\{ r(A)b \;:\; r(z) = \frac{p(z)}{q(z)}, \deg p \leq \deg q \right\}.$$

(Güttel 2013 review of rational Arnoldi for matrix functions)

$$\left\{ \frac{p(z)}{q(z)} : \deg p \leq \deg q \right\} = \operatorname{span}\left(\frac{1}{z-\alpha_1}, \frac{1}{z-\alpha_2} \cdots \frac{1}{z-\alpha_n} \right)$$