Note Title 2023-05-02

Arnoldi method

$$K_n(A,b) = \operatorname{span}(b, Ab, A^2 b, \dots A^{n-1} b)$$

(If at step n $A^n b \in \operatorname{span}(b, Ab, \dots A^{n-1} b)$ for the first time, then $\alpha_{n+1,n} = 0$ and $A V_n = V_n A_n$ is an invariant subspace relation

$$\underset{m\times m}{A}\;\underset{m\times n}{V_n} = \underset{m\times n}{V_n}\;\underset{n\times n}{A_n}$$

$$\boxed{A}\,[\;] = [\;]\,\boxed{A_n}$$

and $f(A) V_n = V_n f(A_n) \quad \forall f$)

Arnoldi produces V_n orthonormal basis of $K_n(A,b)$ and $A_n = V_n^* A V_n$

Theorem:

$$c = \underbrace{V_n}_{\text{coordinates in basis } V_n} \underbrace{f(A_n)}_{\substack{A \text{ restricted to} \\ \text{projected onto } K_n}} \underbrace{V_n^* b}_{\substack{\text{coordinates} \\ \text{of } b \in K_n \\ \text{in basis } V_n}} = f(A) b$$

when f is a polynomial of degree $< n$

Even if f is not a polynomial, c approximates well $f(A)b$

Heuristic reason: $f(A_n) = \tilde{p}(A_n)$, where $\tilde{p}$ is the interpolation polynomial of f in $\Lambda(A_n)$.

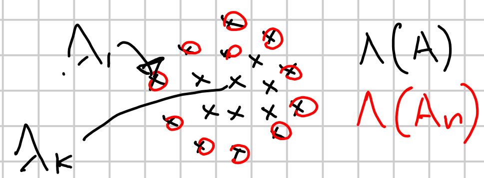
$\tilde{p}$ has degree at most $n-1$, hence

$$c = V_n f(A_n) V_n^* b = V_n \tilde{p}(A_n) V_n^* b = \tilde{p}(A) b$$

$\deg \tilde{p} < n$

Recall that $f(A) = p(A)$, where p is the (degree $< m$) interpolation polynomial in $\Lambda(A)$.

The eigenvalues of A_n approximate well the <u>outer</u> eigenvalues of A



So Arnoldi constructs a polynomial approximant of f which is accurate on the outer eigenvalues

$$|\tilde{p}(\lambda_1) - f(\lambda_1)| \text{ small for eigenvalues } \lambda_1 \text{ "outside"}$$

$$|p(\lambda_k) - f(\lambda_k)| \text{ possibly large for } \lambda_k \in \Lambda(A) \text{ "inside"}$$

(and gives a fast way to evaluate it)

This gives a good approximation of $f(A)$ if the <u>outer</u> eigenvalues are more important than the <u>inner</u> ones.

<u>Ex</u>: matrix exponential of diagonalizable $A = V \cdot \Lambda \cdot V^{-1}$

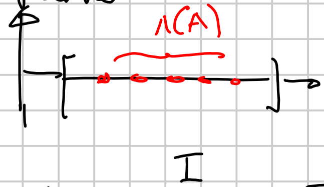
$$\exp(A)b = V \begin{bmatrix} \exp(\lambda_1) & & \\ & \ddots & \\ & & \exp(\lambda_m) \end{bmatrix} \underbrace{V^{-1}b}_{\begin{bmatrix} \gamma_1 \\ \vdots \\ \gamma_m \end{bmatrix}}$$

$$= v_1 \exp(\lambda_1)\gamma_1 + v_2 \exp(\lambda_2)\gamma_2 + \dots + v_m \exp(\lambda_m)\gamma_m$$

The largest summands are usually those with large $\mathrm{Re}(\lambda_i)$, so that $|\exp(\lambda_i)| = \exp(\mathrm{Re}(\lambda_i))$ is large.

Error bound for $c \approx f(A)b$ for <u>Hermitian</u> A

Theorem: Let A be Hermitian, I real interval such that $\Lambda(A) \subset [\lambda_{min}, \lambda_{max}] \subset I$



Let us consider the best approximation polynomial $s(z)$ to f on I, i.e., the one that achieves minimum

$$\delta = \max_{z \in I} |f(z) - s(z)|$$

over all polynomials of degree $< n$.

Then, the approximation provided by Arnoldi $c = V_n f(A_n) V_n^* b$ satisfies

$$\|f(A)b - c\| \leq 2\delta \|b\|.$$

Note that $\|s(A)b - f(A)b\| = \left\| V \begin{bmatrix} s(\lambda_1)-f(\lambda_1) & & \\ & \ddots & \\ & & s(\lambda_m)-f(\lambda_m) \end{bmatrix} V^* b \right\|$

$$\leq \underbrace{\|V\|}_{=1} \underbrace{\left\| \begin{bmatrix} s(\lambda_1)-f(\lambda_1) & & \\ & \ddots & \\ & & s(\lambda_m)-f(\lambda_m) \end{bmatrix} \right\|}_{\leq \delta} \cdot \underbrace{\|V^*\|}_{1} \cdot \|b\| \leq \delta \cdot \|b\|,$$

Hence the approximation $c = \tilde{p}(A)b$ is within a factor 2 of the best possible degree $< n$ polynomial approximation of f.

Proof (of the quasi-optimality theorem):

First, we show that the eigenvalues of A_n are also in I:

$\mu \in A_n$ can be written as a Rayleigh quotient

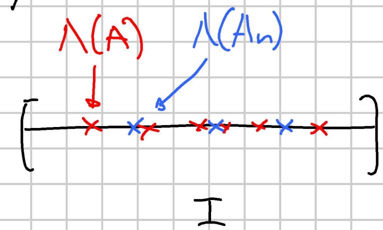
$$\mu = \frac{w^* A_n w}{w^* w} \qquad (w \text{ eigenvector of } A_n,\ A_n w = w\mu)$$

$$= \frac{w V_n^* A V_n w}{w^* V_n^* V_n w} \qquad (V_n \text{ Arnoldi basis matrix, orthonormal})$$

$$= \frac{y^*Ay}{y^*y} = \frac{y^*V\Lambda V^*y}{y^*VV^*y} = \frac{x^*\Lambda x}{x^*x}$$

$$= \frac{\lambda_1|x_1|^2+\lambda_2|x_2|^2+\dots+\lambda_m|x_m|^2}{|x_1|^2+\dots+|x_m|^2}$$

= convex combination of the $\lambda_i \in \Lambda(A) \Rightarrow \mu \in I$.



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

$$= \|f(A)b - s(A)b + V_n s(A_n) V_n^* b - V_n f(A_n) V_n^* b\|$$

$$\leq \|f(A)b - s(A)b\| + \|V_n\left(s(A_n) - f(A_n)\right)V_n^* b\|$$

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

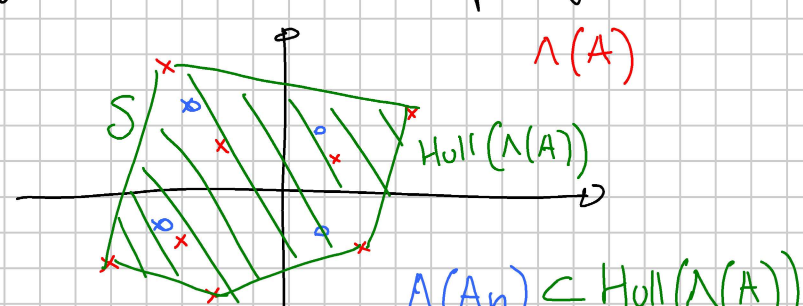
because s satisfies $\delta = \max|f(\lambda)-s(\lambda)|$

because $\Lambda(A_n) \subset I$, too

$$= 2\delta\|b\|. \qquad \square$$

For a <u>normal</u> matrix:

<u>orthogonal</u> V eigenvector matrix, but possibly non-real $\Lambda(A)$



With the same arguments, one can prove the following result:

Let A be $\boxed{\text{normal}}$.

Let $s(z)$ be the best approximation polynomial on $S = \mathrm{Hull}(\Lambda(A))$, i.e. the one with minimum

$$\delta = \max_{z \in S} |s(z) - f(z)|$$

over all polynomials of degree $< n$.

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

What happens if A is <u>not</u> normal?

<u>Def</u>: The <u>numerical range</u> or <u>field of values</u> of $A \in \mathbb{C}^{m \times m}$, possibly non-normal, is

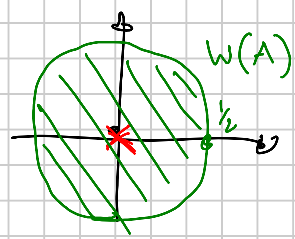
$$W(A) = \left\{ \frac{x^* A x}{x^* x} \; ; \; \text{for } x \in \mathbb{C}^m, \; x \neq 0 \right\}$$

(or $x \in$ unit sphere)

{sets of Rayleigh quotients of A}

For non-normal A, $W(A)$ is <u>bigger</u> than $\mathrm{Hull}(\Lambda(A))$.

<u>Ex</u>. $W\left(\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}\right) = B\left(0, \frac{1}{2}\right)$



<u>Theorem</u> (Crouzeix-Palencia theorem): Let $\gamma = 1 + \sqrt{2} \approx 2.414\ldots$

For any $A \in \mathbb{C}^{m \times m}$ and any f holomorphic on $W(A)$ we have

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

$\uparrow$ Euclidean induced norm $\|\cdot\|_2$, $\|A\| = \sigma_{max}(A)$

Open problem (Crouzeix conjecture): this theorem holds also with $\gamma = 2$.

With this result + the same argument as above:

Theorem: let $A \in \mathbb{C}^{n\times n}$ be any matrix, $s(z)$ best approximation polynomial on $W(A)$, then

$$\| c - f(A) b \| \leq 2 \delta \gamma \|b\|$$

constant in the theorem

$$\delta = \max_{z \in W(A)} |s(z) - p(z)|$$

Proof: same argument as above.

One can extend the results to so-called rational Arnoldi.

Def:

$$K_{q,n}(A,b) = \left\{ r(A)b, \text{ where } r(z) = \frac{p(z)}{q(z)}, \; p \text{ any polynomial of degree} < n \right\}$$

There is a variant of Arnoldi that computes a basis of $K_{q,n}(A,b)$, and many of these results continue to hold replacing "polynomial" with "rational function with fixed denominator".