

Convergence bounds for CG

Consider case where one eigenvalue λ_n much larger than others.

Construct better polynomial than $T_m\left(\frac{2\lambda-\lambda_n-\lambda_1}{\lambda_n-\lambda_1}\right)/T_m\left(\frac{-\lambda_n-\lambda_1}{\lambda_n-\lambda_1}\right)$ using this information.

For example, “polynomial that is zero at extreme eigenvalue and lower degree Chebyshev over other eigenvalues”.

$$p_m(z) = \left[T_{m-1}\left(\frac{2\lambda-\lambda_{n-1}-\lambda_1}{\lambda_{n-1}-\lambda_1}\right) / T_{m-1}\left(\frac{-\lambda_{n-1}-\lambda_1}{\lambda_{n-1}-\lambda_1}\right) \right] \left(\frac{\lambda_n-\lambda}{\lambda_n}\right)$$

Clearly $p_m(\lambda_n) = 0$ and $|p_m(\lambda_i)| < |T_{m-1}\left(\frac{2\lambda_i-\lambda_{n-1}-\lambda_1}{\lambda_{n-1}-\lambda_1}\right) / T_{m-1}\left(\frac{-\lambda_{n-1}-\lambda_1}{\lambda_{n-1}-\lambda_1}\right)|$, $i < n$

So, new bound $\frac{\|e_m\|_A}{\|e_0\|_A} \leq 2\left(\frac{\sqrt{\kappa_{n-1}}-1}{\sqrt{\kappa_{n-1}}+1}\right)^{m-1}$, where $\kappa_{n-1} = \frac{\lambda_{n-1}}{\lambda_1}$,

versus old bound: $\frac{\|e_m\|_A}{\|e_0\|_A} \leq 2\left(\frac{\sqrt{\kappa_n}-1}{\sqrt{\kappa_n}+1}\right)^m$, where $\kappa_n = \frac{\lambda_n}{\lambda_1}$.

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Convergence bounds for CG and MINRES

Clearly, the trick can be applied if we have multiple outlying eigenvalues (large ones and small ones).

The same convergence bounds obtained for the error in CG can be obtained for the residual in MINRES if A is HPD, since we bound the same polynomial.

MINRES: $\frac{\|r_k\|_2}{\|r_0\|_2} \leq 2\left(\frac{\sqrt{\kappa_n}-1}{\sqrt{\kappa_n}+1}\right)^k$, where $\kappa_n = \frac{\lambda_n}{\lambda_1}$.

However, if A is Hermitian but not definite (MINRES) we need to find a (Tschchebyshev) polynomial that is small on both sides of the origin. This is much harder, which has a significant effect on the convergence (bound).

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Convergence bounds for MINRES (1)

Let A be Hermitian and let $\lambda(A) \subset [a, b] \cup [c, d]$, where $a < b < 0 < c < d$ and $b - a = d - c$.

We need a polynomial that is small over both these intervals.

We proceed more or less the same way as for CG: we construct a polynomial q that maps both intervals into $[-1, 1]$ and define the Chebyshev polynomial in terms of q .

We take $q(z) = 1 + \frac{2(z-b)(z-c)}{ad-bc}$ (2nd degree polynomial)

Check that $q(z)$ maps $[a, b] \cup [c, d]$ into $[-1, 1]$ (draw q).

How would you compute $q(z)$ for more general $[a, b] \cup [c, d]$?

Now we take $p_k(z) = T_l(q(z))/T_l(q(0))$, where $l = \lfloor k/2 \rfloor$ (integral part).

Note that we have Chebyshev polynomials of half the degree we had in the definite case.

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Convergence bounds for MINRES (2)

To compute $\max |p_k(z)|$ we need to compute $T_l(q(0))$.

We have $q(0) = 1 + \frac{2bc}{ad-bc} = \frac{ad+bc}{ad-bc}$.

Set $\mu = \frac{ad+bc}{ad-bc} = \frac{1}{2}(y + y^{-1})$ then $T_l(\mu) = \frac{1}{2}(y^l + y^{-l})$.

Solve $\mu = \frac{1}{2}(y + y^{-1}) \Leftrightarrow \frac{1}{2}y^2 - \mu y + \frac{1}{2} = 0 \quad (y \neq 0)$

$y = \mu \pm \sqrt{\mu^2 - 1}$ (solution are each other's inverse, so same result)

$$y = \frac{ad+bc}{ad-bc} + \sqrt{\frac{(ad+bc)^2}{(ad-bc)^2} - \frac{(ad-bc)^2}{(ad-bc)^2}} = \frac{ad+bc}{ad-bc} + \sqrt{\frac{4adbc}{(ad-bc)^2}} = \frac{ad+bc}{ad-bc} + \frac{2\sqrt{adbc}}{ad-bc} \Leftrightarrow$$

$$y = \frac{(\sqrt{ad} + \sqrt{bc})^2}{(\sqrt{ad} + \sqrt{bc})(\sqrt{ad} - \sqrt{bc})} = \frac{(\sqrt{ad} + \sqrt{bc})}{(\sqrt{ad} - \sqrt{bc})}$$

$$\text{Bound: } \frac{\|r_k\|_2}{\|r_0\|_2} \leq \left(\frac{\sqrt{|ad|} - \sqrt{|bc|}}{\sqrt{|ad|} + \sqrt{|bc|}} \right)^{\lfloor k/2 \rfloor}.$$

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Convergence bounds for MINRES (3)

Let A be Hermitian and let $\lambda(A) \subset [a, b] \cup [c, d]$, where $a < b < 0 < c < d$ and $b - a = d - c$.

$$\text{Bound for MINRES: } \frac{\|r_k\|_2}{\|r_0\|_2} \leq 2 \left(\frac{\sqrt{|ad|} - \sqrt{|bc|}}{\sqrt{|ad|} + \sqrt{|bc|}} \right)^{\lfloor k/2 \rfloor}$$

In the case that $a = -d$ and $b = -c$ (symmetric w.r.t. the origin), we can simplify bound further (but bound does not get better):

$$\frac{\|r_k\|_2}{\|r_0\|_2} \leq 2 \left(\frac{d-c}{d+c} \right)^{\lfloor k/2 \rfloor} = 2 \left(\frac{d/c-1}{d/c+1} \right)^{\lfloor k/2 \rfloor} \quad (\text{note } \kappa = \frac{d}{c})$$

$$\text{In HPD case: } \frac{\|r_k\|_2}{\|r_0\|_2} \leq 2 \left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1} \right)^k.$$

So bound in indefinite case at iteration k is that of the definite case at iteration $k/2$ for matrix with condition number d^2/c^2 .

Dramatic loss of convergence compared with definite case.

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Convergence bounds for MINRES (4)

If we know that A has only a few negative (positive) eigenvalues, we again can improve the bound significantly by taking product $p_s(z)T_{k-s}(z)$, where $p_s = 0$ on negative eigenvalues and T_{k-s} is scaled and shifted Chebyshev polynomial over positive eigenvalues. Product must also satisfy our normalization: $p_s(0)T_{k-s}(0) = 1$.

Let $\lambda_1 < \lambda_2 < \lambda_3 < 0 < \lambda_4 < \dots < \lambda_n$.

$$\text{Possibility: } \tilde{p}_k(z) = (z - \lambda_1)(z - \lambda_2)(z - \lambda_3)T_{k-3}\left(\frac{2z - \lambda_n - \lambda_4}{\lambda_n - \lambda_4}\right)$$

$$\text{Normalize: } p_k(z) = \tilde{p}_k(z)/\tilde{p}_k(0)$$

$$p_k(z) = \frac{(z - \lambda_1)(z - \lambda_2)(z - \lambda_3)}{-\lambda_1\lambda_2\lambda_3} \left[T_{k-3}\left(\frac{2z - \lambda_n - \lambda_4}{\lambda_n - \lambda_4}\right) / T_{k-3}\left(\frac{-\lambda_n - \lambda_4}{\lambda_n - \lambda_4}\right) \right]$$

$$p_k(z) \leq 2C_3 \left(\frac{\sqrt{\kappa_4} - 1}{\sqrt{\kappa_4} + 1} \right)^{k-3}, \quad \text{where } C_3 = \frac{(\lambda_n - \lambda_1)(\lambda_n - \lambda_2)(\lambda_n - \lambda_3)}{-\lambda_1\lambda_2\lambda_3} \text{ and } \kappa_4 = \frac{\lambda_n}{\lambda_4}.$$

Note that $p_k(z)$ may not be good for small k .

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For general matrices we proceed in same way. Now A may have complex eigenvalues. If A real, eigenvalues come in complex-conj. pairs. We assume A diag. ble.

$\|r_m\|_2 = \|q_m^G(A)r_0\|_2$ is minimal, with q_m^G the GMRES residual poly.

So, for any other residual poly, \tilde{q}_m s.t. $\tilde{q}_m(0) = 1$, we have

$$\|r_m\|_2 \leq \|\tilde{q}_m(A)r_0\|_2 \leq \|\tilde{q}_m(A)\|_2 \|r_0\|_2 \iff$$

$$\frac{\|r_m\|_2}{\|r_0\|_2} \leq \|\tilde{q}_m(A)\|_2 \quad \text{substituting } A = V\Lambda V^{-1} \text{ gives}$$

$$\frac{\|r_m\|_2}{\|r_0\|_2} \leq \|V\|_2 \|V^{-1}\|_2 \max_{i=1..n} |\tilde{q}_m(\lambda_i)|, \text{ where } \lambda_i \in \Lambda(A)$$

If $\kappa_2(V)$ very large, this bnd often not so useful, and we

consider other bounds, like those based on FOV or pseudo-spectra. Similar if A not diag. ble. In the latter case, we can also consider polys of Jordan blocks explicitly.

To consider bounds on $\max |\tilde{q}_m(\lambda_i)|$, we assume eig. values contained in region $\Omega \subset \mathbb{C}$ and consider

$$\max \{ |\tilde{q}_m(\lambda_i)| : \lambda_i \in \Omega \}.$$

We use again Chebyshev poly.s $T_m(z) = \cosh(m \operatorname{acosh}(z))$ but now in the complex plane.

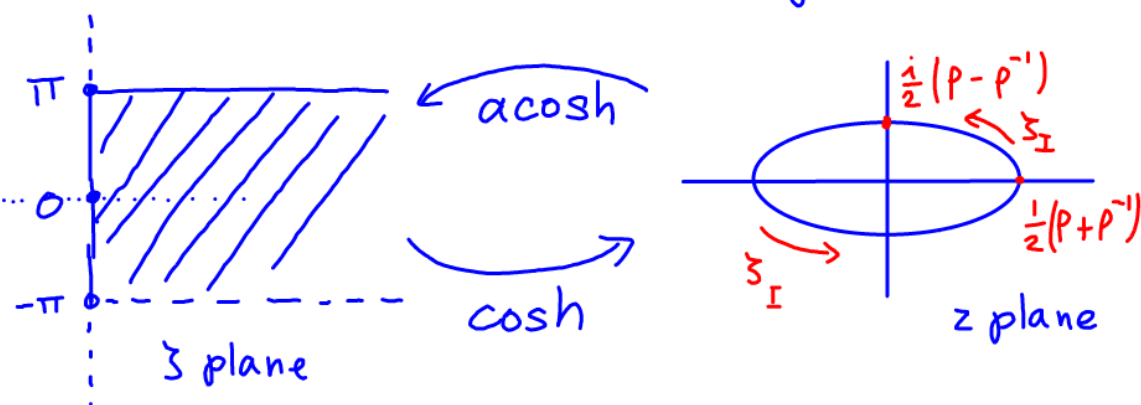
What map does $T_m(z)$ define?

$$\text{Let } \zeta \stackrel{\text{P.V.}}{=} \operatorname{acosh}(z) \Rightarrow z = \cosh \zeta = \frac{1}{2}(e^\zeta + e^{-\zeta}) = \frac{1}{2}(e^{\zeta_R + i\zeta_I} + e^{-\zeta_R - i\zeta_I}) = \frac{1}{2}e^{\zeta_R}(\cos \zeta_I + i \sin \zeta_I) + \frac{1}{2}e^{-\zeta_R}(\cos \zeta_I - i \sin \zeta_I) = \frac{1}{2}(e^{\zeta_R} + e^{-\zeta_R}) \cos \zeta_I + i \frac{1}{2}(e^{\zeta_R} - e^{-\zeta_R}) \sin \zeta_I$$

$$\text{Let } p = e^{\zeta_R} \rightarrow \frac{1}{2}(p + p^{-1}) \cos \zeta_I + i \frac{1}{2}(p - p^{-1}) \sin \zeta_I$$

For fixed p this describes ellipse in complex plane

The real part ζ_R defines length of major and minor axes.



To make mapping 1-to-1 we take $\zeta_R \geq 0$ and $-\pi < \zeta_I \leq \pi$

$$T_m(z) = \cosh(m\zeta) = \frac{1}{2}(e^{m\zeta} + e^{-m\zeta}) = \frac{1}{2}(e^{m\zeta_R} + e^{-m\zeta_R}) \cos(m\zeta_I) + i \frac{1}{2}(e^{m\zeta_R} - e^{-m\zeta_R}) \sin(m\zeta_I)$$

Ellipse with much larger axes. Note that $|T_m(z)|$ is essentially determined by ζ_R and mostly by e^{ζ_R}

since $\zeta_R \geq 0$.

$T_m(z)$ poly of degree m in z ?

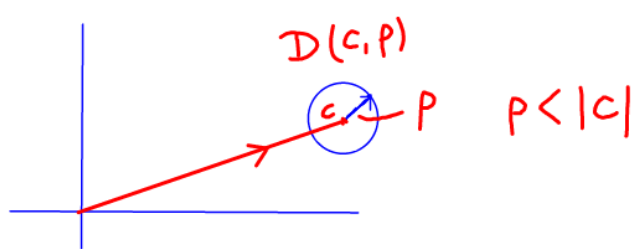
$$\text{Quick test: } z = \frac{1}{2}(e^\zeta + e^{-\zeta}) \rightarrow T_m(z) = \frac{1}{2}(e^{m\zeta} + e^{-m\zeta})$$

$$z^2 = \frac{1}{4}(e^\zeta + e^{-\zeta})(e^\zeta + e^{-\zeta}) = \frac{1}{4}(e^{2\zeta} + 2 + e^{-2\zeta}) \rightarrow T_2(z) = 2z^2 - \frac{1}{2}$$

$$z^3 = \frac{1}{8}(e^{3\zeta} + e^{-3\zeta}) + \frac{3}{8}(e^\zeta + e^{-\zeta}), \text{ etc (we can derive simple recurrence for } T_m)$$

Bounds for some simple regions in \mathbb{C} .

Eigenvalues in disk, $D(c, p)$ with center c and radius p .



Consider $\tilde{q}_m(z) = \left(\frac{z-c}{-c}\right)^m$

Note $\tilde{q}_m(0) = 1$ and for z inside disk:

$|z-c| < p \Rightarrow |\tilde{q}_m(z)|^m \leq \left(\frac{p}{|c|}\right)^m$. So, the smaller p is compared

with $|c|$, the faster convergence the bound suggests

The max modulus is obtained (true in general).
on the boundary. This follows a general principle:

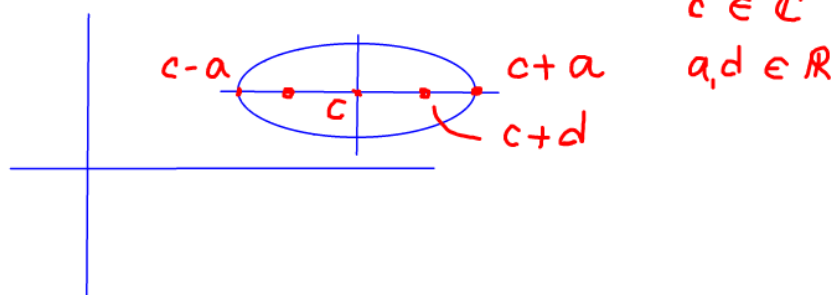
(i) If $f(z)$ analytic in domain D , then $|f(z)|$ cannot have max in D unless $f(z)$ constant.

(ii) If $f(z)$ analytic in bounded region D and $|f(z)|$ continuous in the closed region \bar{D} , then $|f(z)|$ assumes max on boundary of region.

So, for analytic functions, like polys we only need to check the boundary.

Consider eig. vals contained in ellipse in complex plane with major axis aligned with real axis, not containing origin.

Consider ellipse $E(c, d, a)$ with
 center c
 major axis length a
 focal distance d



First map $E(c, d, a)$ to ellipse given by $\hat{z} = \cosh(\zeta)$.

Corresponds to translating and scaling, like we did for real positive case, mapping $[a, b] \rightarrow [-1, 1]$.

Note poly. in shifted and scaled z is still poly in z of same degree.

Consider $\hat{z} = \frac{z-c}{d} \rightarrow E(0, 1, a/d)$, normalized with foci ± 1

$$\frac{1}{2}(p+p^{-1}) = a/d \Leftrightarrow \frac{2a}{d} = p+p^{-1} \Rightarrow p^2 - 2\frac{a}{d}p + 1 = 0 \Rightarrow p_{1,2} = \frac{a}{d} \pm \sqrt{\frac{a^2}{d^2} - 1}$$

$p_1, p_2 = 1$ $\begin{cases} p = p_1 \\ p^{-1} = p_2 \end{cases}$ so choice doesn't matter. Pick p w. max modulus

$$p = \frac{a}{d} + \left(\frac{a^2}{d^2} - 1\right)^{1/2} = e^{\zeta_R} \Rightarrow \zeta_R = \ln\left(\frac{a}{d} + \sqrt{\frac{a^2}{d^2} - 1}\right) \quad (\zeta_R \geq 0)$$

Consider only boundary of ellipse:

$$\hat{z} = \frac{1}{2}(e^{\zeta} + e^{-\zeta}) = \frac{1}{2}(p+p^{-1})\cos \zeta_I + \frac{i}{2}(p-p^{-1})\sin \zeta_I$$

where $p = e^{\zeta_R}$ fixed and $-\pi < \zeta_I \leq \pi$

$$T_m(\hat{z}) = \frac{1}{2}(e^{m\zeta} + e^{-m\zeta})$$

Scale to ensure $\tilde{q}_m(z) = 1 \rightarrow \tilde{q}_m(z) = \frac{T_m\left(\frac{z-c}{d}\right)}{T_m\left(\frac{-c}{d}\right)}$, $-\frac{c}{d}$ image of origin of shift/scale

$$\text{Let } \gamma = -\frac{c}{d}$$

$$\text{Bound } |\tilde{q}_m(z)| \rightarrow \max_{\hat{z}} \frac{|T_m(\hat{z})|}{|T_m(\gamma)|}$$

$$T_m(\hat{z}) = \frac{1}{2}(e^{m\xi_R} + e^{-m\xi_R}) \cos(m\xi_I) + \frac{i}{2}(e^{m\xi_R} - e^{-m\xi_R}) \sin(m\xi_I)$$

$$= \frac{1}{2}(p^m + p^{-m}) \cos(m\xi_I) + \frac{i}{2}(p^m - p^{-m}) \sin(m\xi_I)$$

$$|T_m(\hat{z})|^2 = \frac{1}{4}(p^{2m} + 2 + p^{-2m}) \cos^2(m\xi_I) + \frac{1}{4}(p^{2m} - 2 + p^{-2m}) \sin^2(m\xi_I) =$$

$$\frac{1}{4}(p^{2m} + p^{-2m}) (\underbrace{\cos^2(m\xi_I) + \sin^2(m\xi_I)}_{=1}) + \frac{1}{2} \cos^2(m\xi_I) - \frac{1}{2} \sin^2(m\xi_I)$$

$$|T_m(\hat{z})|^2 \leq \frac{1}{4}(p^{2m} + p^{-2m}) + \frac{1}{2} = \frac{1}{4}(p^{2m} + 2 + p^{-2m}) = \left[\frac{1}{2}(p^m + p^{-m}) \right]^2$$

$$|T_m(\hat{z})| \leq \frac{1}{2}(p^m + p^{-m}) = \frac{1}{2}(e^{\xi_R} + e^{-\xi_R})$$

$$\text{Similarly } |T_m(\gamma)|^2 = \frac{1}{4}(p_y^{2m} + p_y^{-2m}) + \frac{1}{2} \cos^2(m\xi_I) - \frac{1}{2} \sin^2(m\xi_I)$$

$$\text{where } \xi = \text{acosh}(\gamma) = \xi_R + i\xi_I, \gamma = \cosh(\xi), p_y = e^{\xi_R}$$

$$|T_m(\gamma)|^2 \geq \frac{1}{4}(p_y^{2m} + p_y^{-2m}) - \frac{1}{2} = \frac{1}{4}(p_y^{2m} - 2 + p_y^{-2m}) \Rightarrow$$

$$|T_m(\gamma)| \geq \frac{1}{2}(p_y^m - p_y^{-m})$$

$$|\tilde{q}_m(\hat{z})| \leq \frac{\frac{1}{2}(p^m + p^{-m})}{\frac{1}{2}(p_y^m - p_y^{-m})} = \frac{(p^m + p^{-m})}{(p_y^m - p_y^{-m})} \approx \frac{p^m}{p_y^m} = \left(\frac{p}{p_y}\right)^m$$

For sufficiently large m , since $p, p_y > 1$

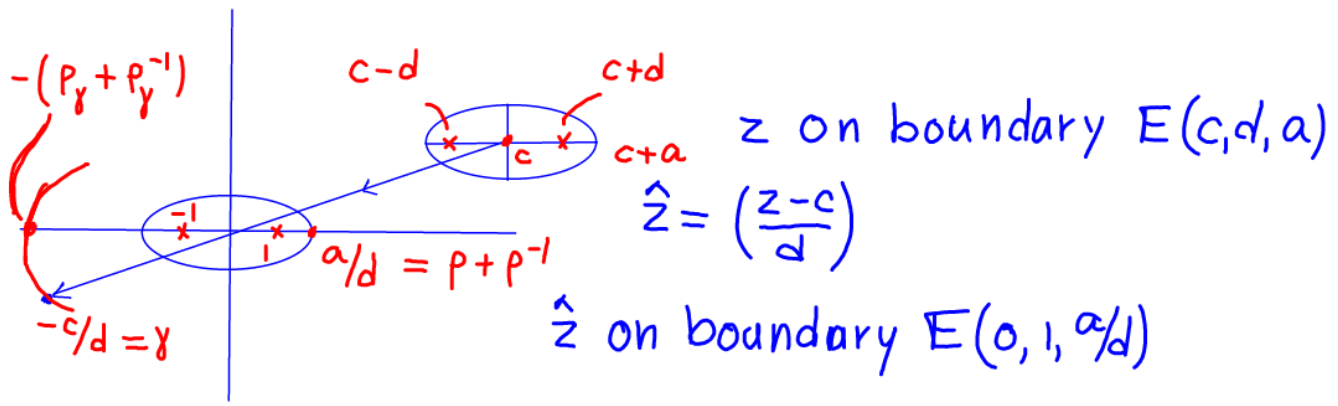
$$p_y? \quad \gamma = -c/d \text{ and } \gamma = \frac{1}{2}(e^{\xi} + e^{-\xi}) = \frac{1}{2}(w + w^{-1}) \Leftrightarrow 2\gamma = w + w^{-1} \Rightarrow$$

$$w^2 - 2\gamma w + 1 = 0 \rightarrow w = \gamma \pm \sqrt{\gamma^2 - 1} \quad (\pm \rightarrow \max |w|)$$

$$p_y = |w| \geq 1 \quad (\text{note } w_1, w_2 = 1)$$

$$= \left| -\frac{c}{d} \pm \sqrt{c^2/d^2 - 1} \right|$$

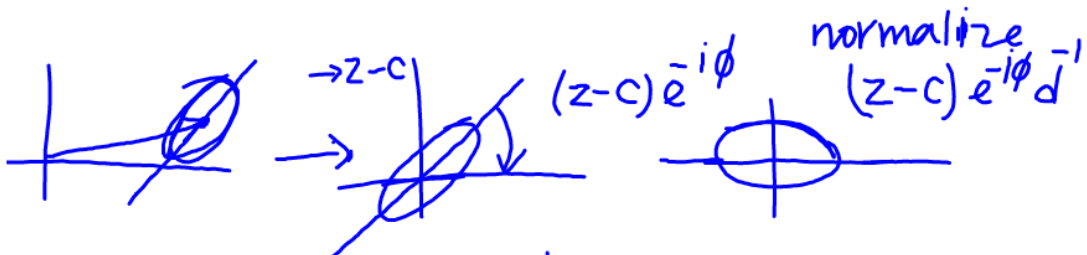
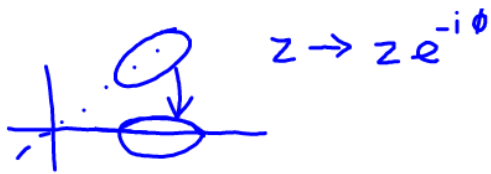
max



T_m maps $E(0, 1, a/d) = E(0, 1, p+p^{-1})$ to $E(0, 1, p^m + p^{-m})$

If origin outside $E(c, d, a)$ then $\gamma = -c/d$ outside $E(0, 1, p+p^{-1})$ and therefore $p_\gamma > p$ and $(p/p_\gamma)^m$ decreases

If $p_\gamma \gg p$ then convergence fast.



$$\frac{1}{2} (e^{j\zeta_R} + e^{-j\zeta_R}) \cos \zeta_I + \frac{j}{2} (e^{j\zeta_R} - e^{-j\zeta_R}) \sin \zeta_I$$

$$\text{local dist: } \frac{1}{4} (e^{2j\zeta_R} + 2 + e^{-2j\zeta_R}) - \frac{1}{4} (e^{j\zeta_R} - 2 + e^{-2j\zeta_R}) = 1$$

$$p + p^{-1} = \frac{a}{d} \Rightarrow p^2 - p \frac{a}{d} + 1 = 0$$

$$p_{1,2} = \frac{a}{2d} \pm \frac{1}{2} \sqrt{\frac{a^2}{d^2} - 4}$$

$$p = \frac{a}{2d} + \frac{1}{2} \sqrt{\frac{a^2}{d^2} - 4}$$

$$p_1 p_2 = \frac{a^2}{4d^2} - \frac{1}{4} \left(\frac{a^2}{d^2} - 4 \right) = 1 \quad p_2 = p_1^{-1}$$

Convergence bounds for GMRES (1)

We will now consider convergence bounds for non-Hermitian problems solved by GMRES. This brings some important changes.

First, \mathbf{A} may not be diagonalizable, and we have to take polynomials over Jordan blocks into account. Second, the eigenvectors (and proper vectors) of \mathbf{A} may not be orthogonal. Third, the eigenvalues may be complex.

Let's assume \mathbf{A} is diagonalizable: $\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1}$

We still have

$$\|\mathbf{r}_k\|_2 \leq \min_{p_k} \|\mathbf{V}p_k(\mathbf{\Lambda})\mathbf{V}^{-1}\mathbf{r}_0\|_2 \leq \kappa(\mathbf{V}) \min_{p_k} \|p_k(\mathbf{\Lambda})\|_2 \|\mathbf{r}_0\|_2 \Rightarrow$$

$$\|\mathbf{r}_k\|_2 / \|\mathbf{r}_0\|_2 \leq \kappa(\mathbf{V}) \min_{p_k} \max_i |p_k(\lambda_i)|$$

Clearly, usefulness of bounding $\min_{p_k} \max_i |p_k(\lambda_i)|$ depends on $\kappa(\mathbf{V})$.

Sharp for normal \mathbf{A} , approach still useful if \mathbf{A} almost normal (\mathbf{V} unitary).

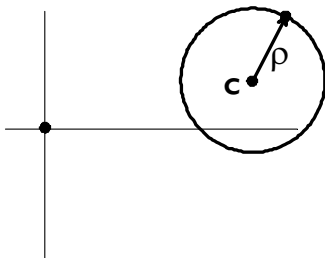
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Convergence bounds for GMRES (2)

Now we must find polynomials that are small over a region in the complex plane. More complicated than Hermitian case. Generally we try to find 'simple' regions containing the eigenvalues, and devise polynomial over such a region (e.g. circle or ellipse).

Eigenvalues in circle $C(c, \rho)$ not containing the origin with center c and radius ρ :

$$\min_{p_k(0)=1} \max_{z \in C(c, \rho)} |p_k(z)| = \left(\frac{\rho}{|c|}\right)^k$$



Obtained for polynomial
 $p_k(z) = \left(\frac{z-c}{0-c}\right)^k = (1 - z/c)^k$

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Convergence bounds for GMRES

We will use minimax polynomials in the complex plane to derive bounds over ellipses (more general regions possible).

Consider the $T_m(z) = \cosh(m \cosh^{-1} z)$ and $z = \cosh \zeta$.

Let $w = e^\zeta$; then $T_m(z) = \frac{1}{2}(w^m + w^{-m})$ where $z = \frac{1}{2}(w + w^{-1})$.

Consider the map $J(w) = \frac{1}{2}(w + w^{-1})$ and the image of the circle $w = \rho e^{i\phi}$.

$$z = \frac{1}{2}(\rho e^{i\phi} + \rho^{-1} e^{-i\phi}) = \frac{1}{2}(\rho + \rho^{-1}) \cos \phi + \frac{1}{2}(\rho - \rho^{-1}) \sin \phi$$

Image is ellipse with semi-axes $\frac{1}{2}(\rho + \rho^{-1})$ and $\frac{1}{2}(\rho - \rho^{-1})$ and foci $-1, 1$.

Inverse map is not unique and so we restrict ourselves to $\rho \geq 1$.

Let E_ρ be the ellipse given above by the Joukowski map $J(w)$.

Now consider the following problem $\min_{q \in \Pi_m, q(\gamma)=1} \max_{z \in E_\rho} |q(z)|$

We use $\min_{\hat{p} \in \Pi_m, \hat{p}(\gamma)=1} \max_{w \in C(0, \rho)} |\hat{p}(w)| = \frac{\rho^m}{|\gamma|^m}$ for $\hat{p}(w) = \frac{p(w)}{p(\gamma)} = \frac{w^m}{\gamma^m}$.

The basic idea is to transform the ellipse to the circle, apply $p(\cdot)$ and transform back, and finally normalize.

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Convergence bounds for GMRES

Consider $J \circ p \circ J^{-1}(z)$ for $z = \frac{1}{2}(w + w^{-1})$ and $w = \rho e^{i\phi}$.

Then $J \circ p \circ J^{-1}(z) = J(\rho^m e^{im\phi}) = \frac{1}{2}(\rho^m e^{im\phi} + \rho^{-m} e^{-im\phi}) \equiv T_m(z)$

Normalization requires $T_m(\gamma) = 1$. So we take $\hat{T}_m(z) = T_m(z)/T_m(\gamma)$.

Let $J^{-1}(\gamma) = w_\gamma = \gamma \pm \sqrt{\gamma^2 - 1}$ (taking max modulus)

$$\left| \frac{T_m(z)}{T_m(\gamma)} \right| = \left| \frac{\rho^m e^{im\phi} + \rho^{-m} e^{-im\phi}}{w_\gamma^m + w_\gamma^{-m}} \right| = \left| \frac{\rho^m e^{im\phi} + \rho^{-m} e^{-im\phi}}{|w_\gamma|^m e^{im\phi_\gamma} + |w_\gamma|^{-m} e^{-im\phi_\gamma}} \right| \simeq \frac{\rho^m}{|w_\gamma|^m} \text{ (large } m \text{)}$$

This gives an upper bound for the minimax polynomial.

It turns out, for large m , $\hat{T}_m(z)$ approximates the optimal polynomial.

Now we can use this for more arbitrary elliptic regions that contain the eigenvalues by scaling, rotating, and translating E_ρ . Notice that a tighter fit around the eigenvalues gives tighter bounds.

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Convergence bounds for GMRES

Consider the eigenvalues contained in the ellipse $E(c, d, a)$ with center c , focal distance d , and major semi-axis a (aligned with x -axis). We want the polynomial normalized such that $\hat{T}_m(0) = 1$ (residual polynomial).

We first translate the polynomial over $-c$ and then scale by d to have focal distance 1. This gives the ellipse $E(0, 1, a/d)$ and the translated and scaled origin gives $\gamma = -c/d$.

So we get $E_\rho = E(0, 1, a/d)$ with $\frac{a}{d} = \frac{1}{2}(\rho + \rho^{-1}) \Rightarrow \rho = a/d + \sqrt{(a/d)^2 - 1}$.

This gives $z \in E_\rho : z = \frac{1}{2}(\rho e^{i\phi} + \rho^{-1} e^{-i\phi}) = J(\rho e^{i\phi})$.

$$|T_m(z)| = \frac{1}{2} |\rho^m e^{im\phi} + \rho^{-m} e^{-im\phi}| \leq T_m(a/d)$$

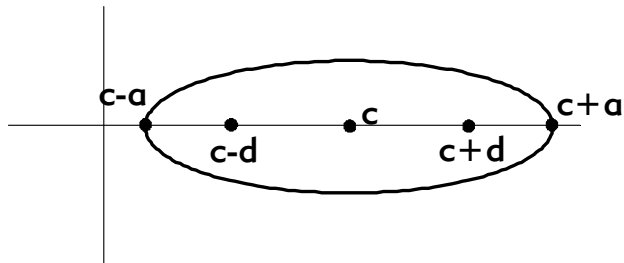
$$|T_m(\gamma)| = \frac{1}{2} |w_\gamma^m + w_\gamma^{-m}| = |T_m(c/d)|$$

$$\text{So finally, we get } |\hat{T}_m(z)| = \frac{|T_m(z)|}{|T_m(c/d)|} \leq \frac{|T_m(a/d)|}{|T_m(c/d)|}$$

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Convergence bounds for GMRES

Eigenvalues in ellipse $E(c, d, a)$ not containing the origin with center c , major semi-axis a , and focal distance d .



$$\|r_m\|_2 / \|r_0\|_2 \leq \kappa(V) \frac{T_m(a/d)}{T_m(c/d)}, \text{ where } T_m(z) = \cosh m \cosh^{-1} z.$$

$$\frac{T_m(a/d)}{T_m(c/d)} = \frac{(a/d + \sqrt{(a/d)^2 - 1})^m + (a/d + \sqrt{(a/d)^2 - 1})^{-m}}{(c/d + \sqrt{(c/d)^2 - 1})^m + (c/d + \sqrt{(c/d)^2 - 1})^{-m}} \approx \frac{(a + \sqrt{a^2 - d^2})^m}{(c + \sqrt{c^2 - d^2})^m}$$

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Convergence bounds for GMRES

Although the eigenvalues often give important information about the convergence of GMRES, we have the following theorem that states this is not generally the case.

Theorem:

Given any set of eigenvalues and any non-increasing convergence curve, a matrix with those eigenvalues and a right hand side can be constructed for which GMRES will display the prescribed convergence curve.

So even with a 'nice' spectrum the convergence can be arbitrarily poor.

This does not have to be the case. Nonnormal matrices are not inherently bad.

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Convergence bounds for GMRES

Consider matrix

$$A = \begin{bmatrix} 0 & 1 & & & \\ & 0 & 1 & & \\ & & \ddots & \ddots & \\ & & & & 1 \\ c_0 & c_1 & c_2 & \cdots & c_{n-1} \end{bmatrix}$$

Eigenvalues are zeros of $p(\lambda) = \lambda^n - c_{n-1}\lambda^{n-1} - c_{n-2}\lambda^{n-2} - \cdots - c_0 = 0$.

Solving $Ax = e_1$ gives no convergence till last step.

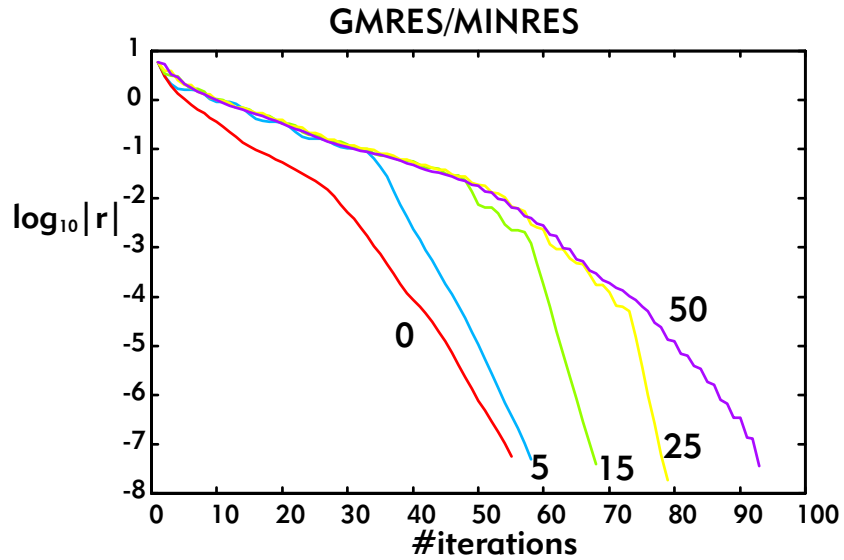
Taking appropriate initial residual yields any convergence curve.

This matrix is rather special, but we get same behavior for any unitarily similar matrix. Note that this matrix is reordered lower triangular matrix, and any matrix is unitarily similar to some lower triangular matrix (Schur decomposition).

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Convergence of Indefinite Problems

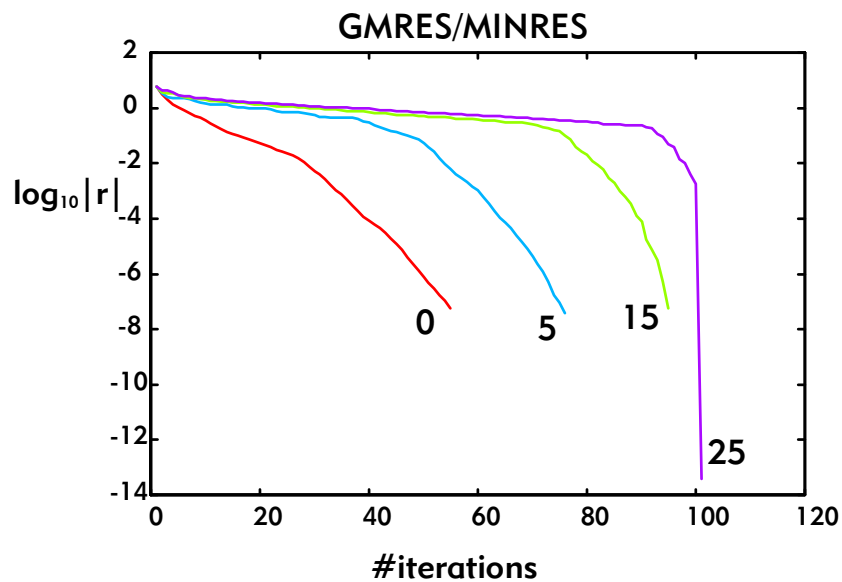
$$A = \text{diag}(-1, -2, \dots, -s, s+1, s+2, \dots, 100)$$



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Convergence of Indefinite Problems

$$A = \text{diag}(1, 2, \dots, 25, -1, -2, \dots, -s, 26+s, \dots, 100)$$



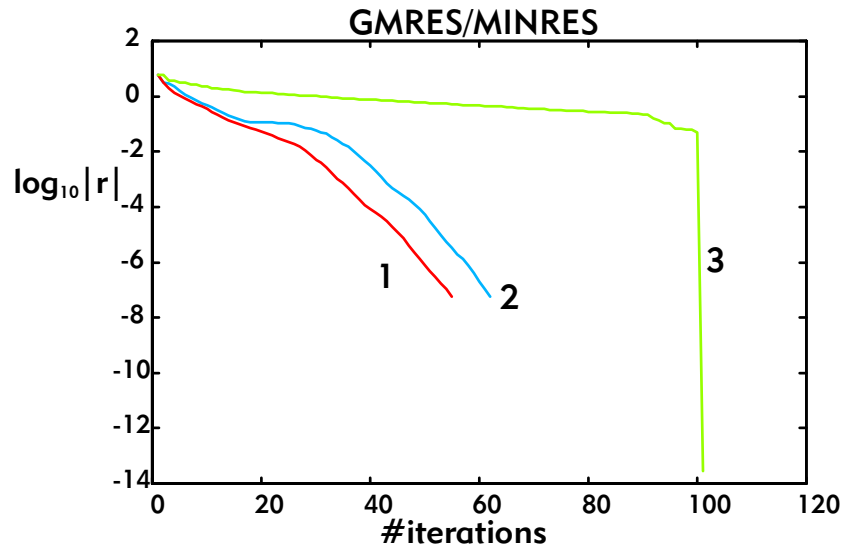
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Convergence of Indefinite Problems

1: $A = \text{diag}(1, 2, 3, \dots, 100)$

2: $A = \text{diag}(-1, -100, 1, 2, \dots, 49, 52, 53, \dots, 100)$

3: $A = \text{diag}(-99, -97, \dots, -1, 1, 3, \dots, 99)$

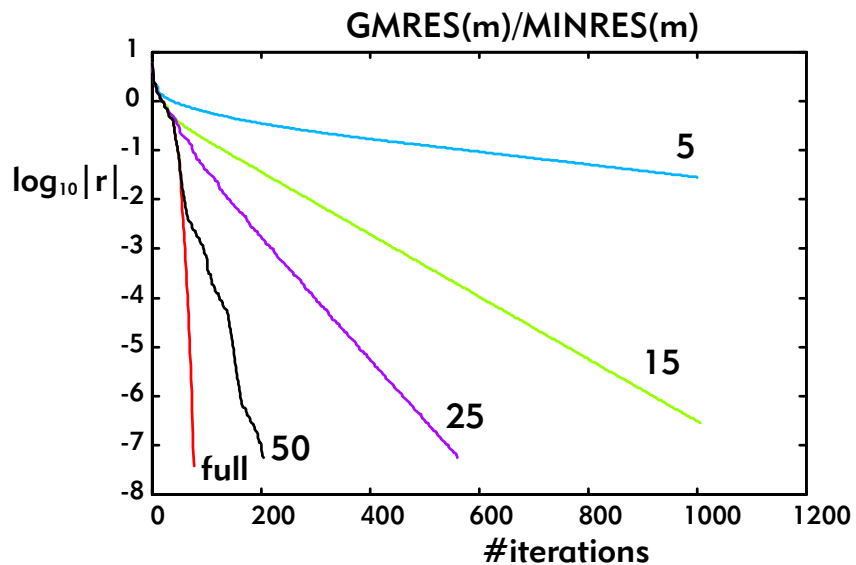


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Convergence of Indefinite Problems

$A = \text{diag}(1, 2, \dots, 25, -1, -2, \dots, -5, 31, 32, \dots, 100)$

GMRES/MINRES without restart takes 76 iterations



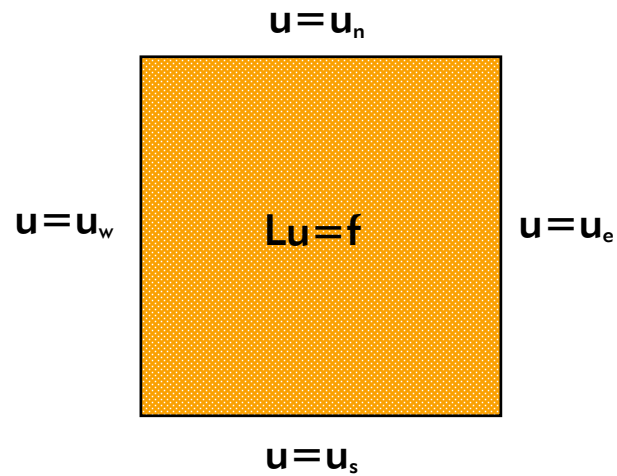
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A Model Problem

Convection-Diffusion(-Reaction) Equation

Dirichlet boundary conditions

$$Lu = -(pu_x)_x - (qu_y)_y + ru_x + su_y + tu = f$$

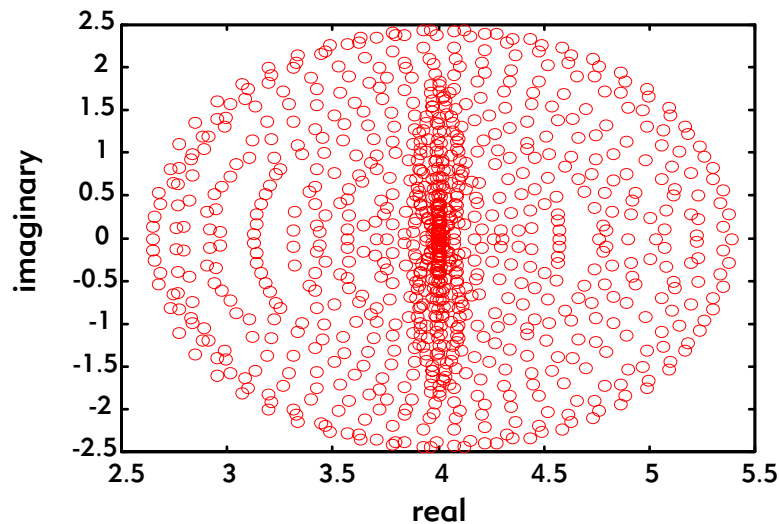


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Eigenvalues

$$p=q=1; r=s=70; h=1/31;$$

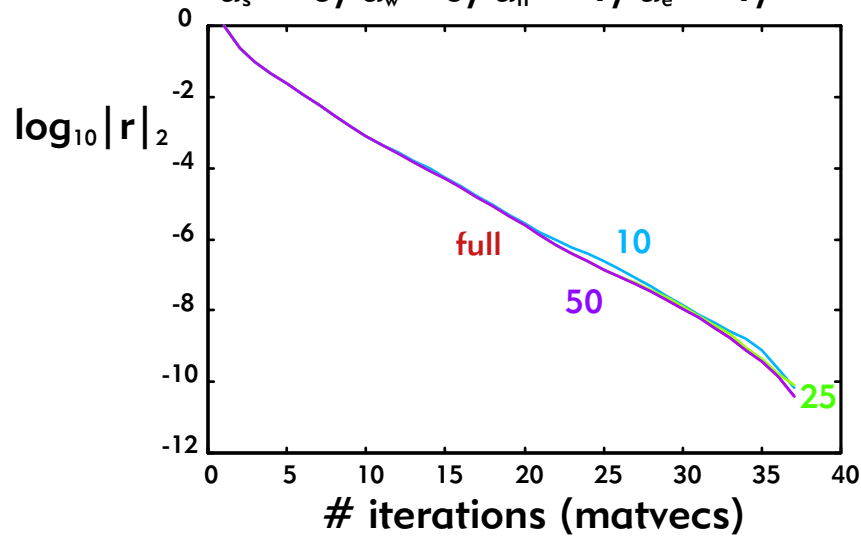
$$u_s=0; u_w=0; u_n=1; u_e=1;$$



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GMRES(m) with $r=s=70$

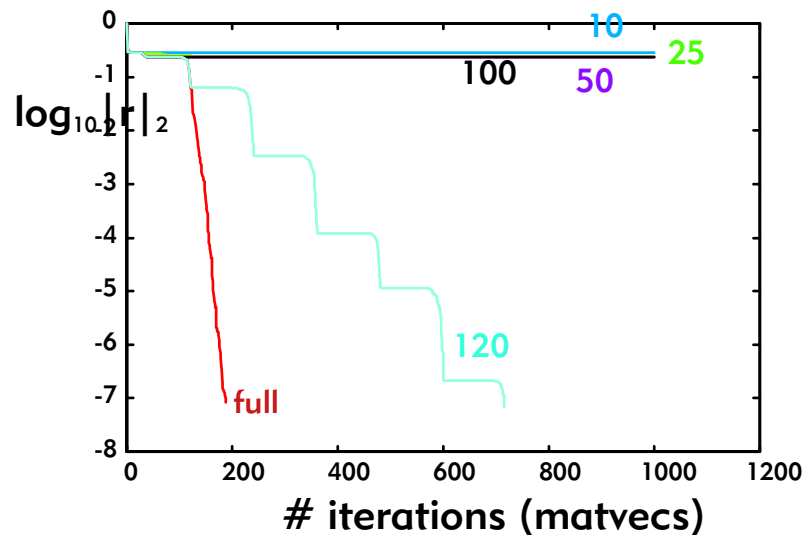
$$p=q=1; r=s=70; h=1/31;$$
$$u_s = 0; u_w = 0; u_n = 1; u_e = 1;$$



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GMRES(m) after shifting spectrum

$$A=A-3.65*I$$
$$p=q=1; r=s=70; h=1/31;$$
$$u_s = 0; u_w = 0; u_n = 1; u_e = 1;$$



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