Preconditioning and iteration for linear systems

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Linear systems:

$$\boldsymbol{Ax} = \boldsymbol{b}, \quad \boldsymbol{A} \in \mathbb{R}^{m \times m}, \boldsymbol{b} \in \mathbb{R}^{m}$$

where $\boldsymbol{A}^{-1}$ exists

and Iterative Methods for their solution

Preconditioning:

$\boldsymbol{M} \in \mathbb{R}^{m \times m}$ which (in a sense I shall make clear later) is an approximation to $\boldsymbol{A}$

it should be feasible/inexpensive/quick to solve systems with $\boldsymbol{M}$

i.e. $\boldsymbol{M}^{-1}$ exists and it's action on a vector should be readily computable

Simple iteration: split $A = M - N$ and for some x_0

$$\text{solve} \quad Mx_k = Nx_{k-1} + b, \quad k = 1, 2, \ldots \qquad (\star)$$

M: splitting matrix or preconditioner (invertible)

Convergence: for any x_0, $\{x_k\}$ converges to the solution
$\Leftrightarrow |\lambda(M^{-1}N)| = |\lambda(I - M^{-1}A)| < 1$; contractive.

Because $Mx = Nx - b$, the error $e_k = x - x_k$ satisfies

$$e_k = M^{-1}Ne_{k-1} = (I - M^{-1}A)e_{k-1} = (I - M^{-1}A)^k e_0$$

Thus simple iteration essentially builds polynomials

$q_k(s) = s^k = p_k(1 - s), k = 1, 2, \ldots$ such that

$$e_k = q_k(I - M^{-1}A)e_0 = p_k(M^{-1}A)e_0$$

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$q_k(s) = s^k = p_k(1 - s), k = 1, 2, \ldots$ with $p_k(0) = 1$ s.t.

$$e_k = q_k(I - M^{-1}A)e_0 = p_k(M^{-1}A)e_0$$

Convergence: note $|\lambda(I - M^{-1}A)| < 1$; contractive is equivalent to $\lambda(M^{-1}A) \subset B(1,1)$, the open unit ball centred at 1.

If ever $M^{-1}A$ has an eigenvalue with negative real part then the simple iteration ($\star$) certainly can not be contractive.

The above applies to any matrix. Now consider A, M real symmetric:

If $A = A^T$: $inertia(A) = (p, n, z)$ where A has $p$ositive, $n$egative, $z$ero eigenvalues

Lemma: if $inertia(A) \neq inertia(M)$ then $M^{-1}A$ has at least one real negative eigenvalue $\Rightarrow$ $(\star)$ not convergent

Proof
$T(\theta) = (1-\theta)A + \theta M$ is real symmetric $\Rightarrow$ real eigenvalues continuous in θ; $T(0) = A, T(1) = M$.

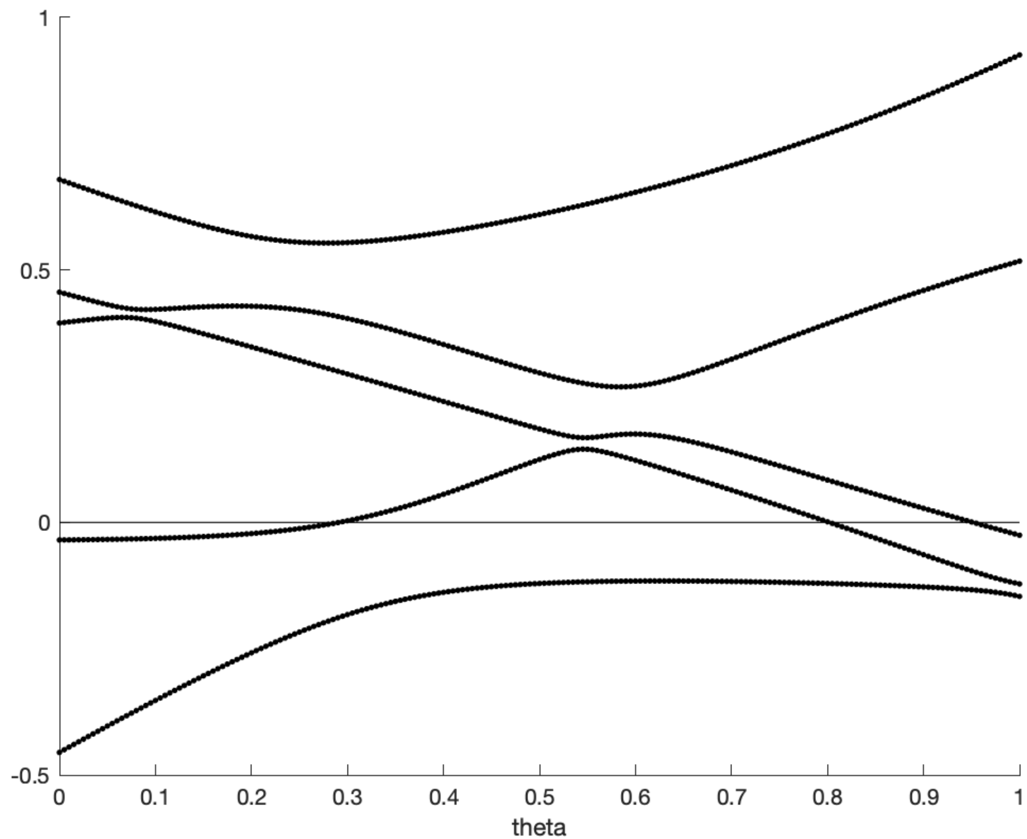
Different inertia $\Rightarrow$ there is $\widehat{\theta} \in (0,1)$ with $T(\widehat{\theta})$ singular.

That is

$$(1-\widehat{\theta})A + \widehat{\theta}M \quad \text{and so} \quad A - \widehat{\theta}/(\widehat{\theta}-1)M$$

is singular i.e. $\widehat{\theta}/(\widehat{\theta}-1) < 0$ is an eigenvalue of $M^{-1}A$. $\square$

Example



$$A = \begin{bmatrix} 0.33 & -.05 & -.29 & 0.01 & 0.01 \\ -.05 & 0.36 & -.11 & -.22 & -.19 \\ -.29 & -.11 & -.32 & 0.11 & -.01 \\ 0.01 & -.22 & 0.11 & 0.49 & -.12 \\ 0.01 & -.19 & -.01 & -.12 & 0.18 \end{bmatrix}, M = \begin{bmatrix} 0.14 & 0.10 & 0.25 & 0.09 & -.28 \\ 0.10 & -.07 & 0.02 & 0.08 & -.11 \\ 0.25 & 0.02 & 0.49 & -.11 & -.23 \\ 0.09 & 0.08 & -.11 & 0.24 & -.34 \\ -.28 & -.11 & -.23 & -.34 & 0.35 \end{bmatrix}$$

$$\lambda_{M^{-1}A} = -0.4098, -4.053, -19.747, 1.7245 \pm 0.8315i$$

Examples:

- A SPD, usually M SPD *(Varga)*
- A SIND, M SPD (eg. block diagonal preconditioning of saddle point problems), inertia unchanged

$$M^{\frac{1}{2}}(M^{-1}A)M^{-\frac{1}{2}} = M^{-\frac{1}{2}}AM^{-\frac{1}{2}}$$

is symmetric and congruent to A so has the same inertia as A (Sylvester's Law of inertia)

- *constraint preconditioning* of saddle point systems

$$M = \begin{bmatrix} W & B^T \\ B & 0 \end{bmatrix}, A = \begin{bmatrix} H & B^T \\ B & 0 \end{bmatrix}$$

$inertia(A) = inertia(M)$ and $\lambda(M^{-1}A)$ all real, positive when W, H SPD *(Keller, Gould, W)*

Multigrid: *Braess-Sarazin*

Note $\boldsymbol{A}$ SIND, $\boldsymbol{M}$ SIND is generally difficult (eigenvalues of $\boldsymbol{M}^{-1}\boldsymbol{A}$ can be complex), but for saddle point problem

$$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{H} & \boldsymbol{B}^T \\ \boldsymbol{B} & \boldsymbol{0} \end{bmatrix},$$

$\boldsymbol{H} \in \mathbb{R}^{n\times n}, \boldsymbol{B} \in \mathbb{R}^{m\times n}$ inertia is $(n, m, 0)$ when $\boldsymbol{H}$ SPD

so eg. *Vanka* splitting for Stokes (Navier-Stokes?) can aim for this inertia

Note: Condition for contraction is necessary, not sufficient eg.

$$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{1} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{-1} \end{bmatrix}, \boldsymbol{M} = \begin{bmatrix} \boldsymbol{-1} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{1} \end{bmatrix}$$

Extensions

If $inertia(A) = (p, n, 0)$, $inertia(M) = (p + r, n - r, 0)$ $(-p \le r \le n)$, then $M^{-1}A$ has $|r| + 2s$ real, negative eigenvalues for some $s \in \{0, 1, 2, \ldots, \lfloor \frac{p+n-r}{2} \rfloor\}$.

$r = -1, s = 1$ in the above example

Positive real eigenvalues: consider

$$S(\theta) = (1 - \theta)A + \theta(-M),$$

$S(0) = A, S(1) = -M$ with

$$inertia(A) = (p, n, 0), inertia(-M) = (n - r, p + r, 0)$$

$M^{-1}A$ has $|p + r - n| + 2t$ real, positive eigenvalues for some $t \in \{0, 1, 2, \ldots, \min\left(\lfloor \frac{2p+r}{2} \rfloor, \lfloor \frac{2n-r}{2} \rfloor\right)\}$.

But not only simple iteration: can build other polynomials!

o Chebyshev (or other) (semi-)iteration: based on polynomials which are small on an interval or set

or

o Krylov subspace methods: implicitly build optimal polynomials:

- Conjugate Gradients (for A,M Symmetric and Positive definite)
- MINRES (for A Symmetric, M Symmetric and Positive definite)
- GMRES (for general A, M)
- . . . and many other methods. . .

- Conjugate Gradients (for A,M Symmetric and Positive definite)

$$e_k = p_k(M^{-1}A)e_0, \quad p_k \in \Pi_k^1,$$

Π_k^1 = degree k polynomials with $p(0) = 1$ such that $\|e_k\|_A^2 = e_k^T A e_k$ is minimised; equivalently

$x_k - x_0 \in$
span$\{M^{-1}r_0, M^{-1}AM^{-1}r_0, \ldots, (M^{-1}A)^k M^{-1}r_0\}$

where $r_k = b - Ax_k = Ae_k$ is the residual for each k

- MINRES (for A Symmetric, M Symmetric and Positive definite)

$$r_k = p_k(M^{-1}A)r_0, \quad p_k \in \Pi_k^1$$

such that $\|r_k\|_{M^{-1}}$ is minimised

- GMRES (for general nonsymmetric A, M) minimises the residual as in MINRES (but requires a full Gram-Schmidt or Arnoldi method to orthogonalize the basis for each Krylov subspace).

Convergence

for diagonalisable $M^{-1}A$: $M^{-1}A = X\Lambda X^{-1}$, Λ diagonal matrix of eigenvalues $\lambda_j, j = 1, \dots, n$

- Conjugate Gradients:

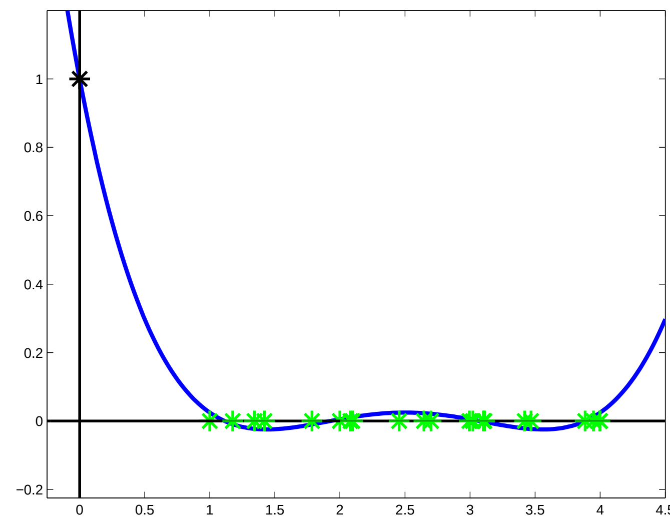
$$\frac{\|e_k\|_A}{\|e_0\|_A} \leq \min_{p\in\Pi_k, p(0)=1} \max_{\lambda\in\sigma(M^{-1}A)} |p(\lambda)|$$

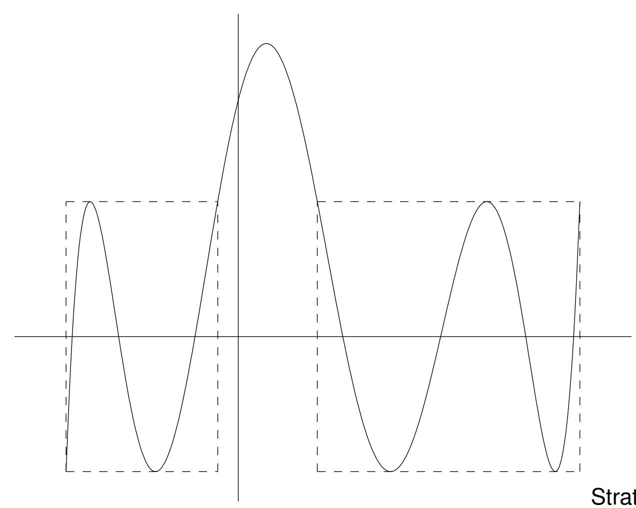
$$\leq 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^k, \quad \kappa = \frac{\lambda_{\max}(M^{-1}A)}{\lambda_{\min}(M^{-1}A)}.$$

- MINRES:

$$\frac{\|r_k\|_{M^{-1}}}{\|r_0\|_{M^{-1}}} \leq \min_{p\in\Pi_k, p(0)=1} \max_{\lambda\in\sigma(M^{-1}A)} |p(\lambda)|$$

Outcome:
convergence in few iterations if $M^{-1}A$ has few eigenvalues/clusters of eigenvalues but convergence for indefinite can be slower





- GMRES:

$$\frac{\|r_k\|_M}{\|r_0\|_M} \leq \|X\|\|X^{-1}\| \min_{p\in\Pi_k, p(0)=1} \max_{\lambda\in\sigma(M^{-1}A)} |p(\lambda)|$$

can be huge even if nicely distributed eigenvalues! In fact significant negative results exists:

Theorem (*Greenbaum, Ptak and Strakos, 1996*)

Given any set of eigenvalues and any monotonic convergence curve, then for any $\mathbf{b}$ there exists a matrix $\mathbf{B}$ having those eigenvalues and an initial guess $\mathbf{x_0}$ such that GMRES for $\mathbf{Bx} = \mathbf{b}$ with $\mathbf{x_0}$ as starting vector will give that convergence curve.

Nevertheless, heuristic ideas abound!

Preconditioning: some examples

A SPD: Domain Decomposition, (Algebraic) Multigrid,...

A SIND: generally hard problems here: Helmholtz:

$$-\nabla^2 u - k^2 u = f,$$

with appropriate boundary conditions

inertia depends on k, discretisation,...

but for saddle point systems: block diagonal/block triangular preconditioners generally based on Schur-complement approximations

A Toeplitz (constant diagonals) or block Toeplitz: Circulant/block circulants

$$y' = ay + f, \qquad y(t_0) = y_0$$

discretise: e.g.

$$\frac{\mathrm{y}^{k+1} - \mathrm{y}^k}{\tau} = \theta a \mathrm{y}^{k+1} + (1-\theta) a \mathrm{y}^k + f^k, \quad \mathrm{y}^0 = y_0,$$

$k = 0, 1, \ldots, \ell$ with $\ell\tau = T$ gives

$$B \underbrace{\begin{bmatrix} \mathrm{y}^1 \\ \mathrm{y}^2 \\ \mathrm{y}^3 \\ \vdots \\ \mathrm{y}^\ell \end{bmatrix}}_{\mathbf{y}} = \underbrace{\begin{bmatrix} \tau f^1 + (1 + a(1-\theta)\tau)\mathrm{y}^0 \\ \tau f^2 \\ \tau f^3 \\ \vdots \\ \tau f^\ell \end{bmatrix}}_{\mathbf{f}},$$

where the $\ell \times \ell$ coefficient matrix B is

$$\begin{bmatrix} b & & & & \\ c & b & & & \\ & c & b & & \\ & & \ddots & \ddots & \\ & & & c & b \end{bmatrix},$$

$b = 1 - a\theta\tau$, $c = -1 - a(1-\theta)\tau$.

Precondition with

$$\begin{bmatrix} b & & & & c \\ c & b & & & \\ & c & b & & \\ & & \ddots & \ddots & \\ & & & c & b \end{bmatrix} \quad \text{periodic!} \Rightarrow \quad \text{FFT}$$

Block preconditioning:

$$\begin{pmatrix} \breve{M}_2 & P_{2\theta} & & G \\ P_{\theta 2} & M_\theta & & \\ D & & M_3 & \\ & -P_{3\theta} & -M_3^\rho & M_3^\Pi \end{pmatrix} \begin{pmatrix} \widehat{\mathbf{u}}' \\ \widehat{\theta}' \\ \widehat{\rho}' \\ \widehat{\Pi}' \end{pmatrix} = \begin{pmatrix} \widehat{\mathbf{R}}_u \\ \widehat{R}_\theta \\ \widehat{R}_\rho \\ \widehat{R}_\Pi \end{pmatrix}$$

Thanks for listening