Indefinite inner products in iterative linear system solvers

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The problem

Solve the algebraic linear system

$$Ax = b$$

$A \in \mathbb{C}^{n\times n}$, large dimension ($n \gg 1000$)

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Approximation process: Given x_0 and $r_0 = b - Ax_0$, then

$$x_m \in x_0 + \mathcal{K}_m(A, r_0) = \text{span}\{r_0, Ar_0, \ldots, A^{m-1}r_0\}$$

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Construct sequence of approximation spaces $\mathcal{K}_m \subset \mathcal{K}_{m+1}$ such that

$$\widetilde{x}_m \in \mathcal{K}_m \qquad \text{and} \quad \widetilde{x}_m \to x \qquad \text{as} \quad m \to \infty$$

(in some sense)

Projection process

($x_0 = 0 \Rightarrow r_0 = b$)

Let $\{v_1, \ldots, v_m\}$ be basis of $\mathcal{K}_m(A, b)$, $v_1 = b$. Then

$$x \approx x_m = V_m y_m \qquad V_m = [v_1, \ldots, v_m]$$

What choice for y_m?

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Residual $r_m := b - AV_m y_m$ satisfies

$$r_m \perp_\star \mathcal{L}_m$$

Selection of $\mathcal{L}_m$ and of orthogonality constraint distinguish among several different methods

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Typical (classical) approaches

⋆ A Hermitian positive definite. Galerkin condition:

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Moreover,

$$\|x - x_m\|_A = \min_{\widetilde{x} \in \mathcal{K}_m} !$$

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Arnoldi relation: $(V_m^* V_m = I)$

$$AV_m = V_m H_m + v_{m+1} h_{m+1} e_m^* \qquad \text{Range}(V_m) \subset \text{Range}(V_{m+1})$$

Other typical orthogonality properties

- $\star \quad e_m = x - x_m \;\perp \mathcal{K}_m(A^*, A^*b)$

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- ⋆ $e_m = x - x_m \perp \mathcal{K}_m(A^*, A^*b)$
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- ⋆ Or, in particular,

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minimization of $\|r_m\|_M$ or $\|e_m\|_M$

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⋆ $M = M(m)$ varies with the subspace dimension

An example with M hpd

A positive real,

$A = S + K$, S Hermitian part of A, $S^{-1}A = I + S^{-1}K$

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Concus & Golub, Widlund,...

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This is not the whole story!

Motivations for an indefinite inner product

- Exploit inherent properties of the problem. For instance,

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... to gain in efficiency with (hopefully) no loss in reliability

Indefinite inner products and J-symmetry

⋆ Indefinite inner product $((x, y))$ does not satisfy

$$((x, x)) > 0 \quad \forall x$$

⋆ Given J Hermitian and nonsingular,

- A is J-Hermitian if $A^*J = JA$

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- Note:

  If $A^* J = JA$ and J hpd then A similar to Hermitian matrix

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$$Ax = b$$

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$\star$ Other structure-preserving approaches (e.g., Bunse-Gerstner & Stöver, '99)

Krylov subspace methods using $((\cdot,\cdot))$

Galerkin condition with x^*y replaced by condition with $((x,y)) = x^T y$

$\mathcal{L}_m = \mathcal{K}_m$ and

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BUT

no minimization is carried out

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$A \in \mathbb{C}^{3627 \times 3627}$ $\quad A = K + iC_H$

Stiffness (real) + hysteretic damping matrix

(Structural dynamic problem – ILU Preconditioner)

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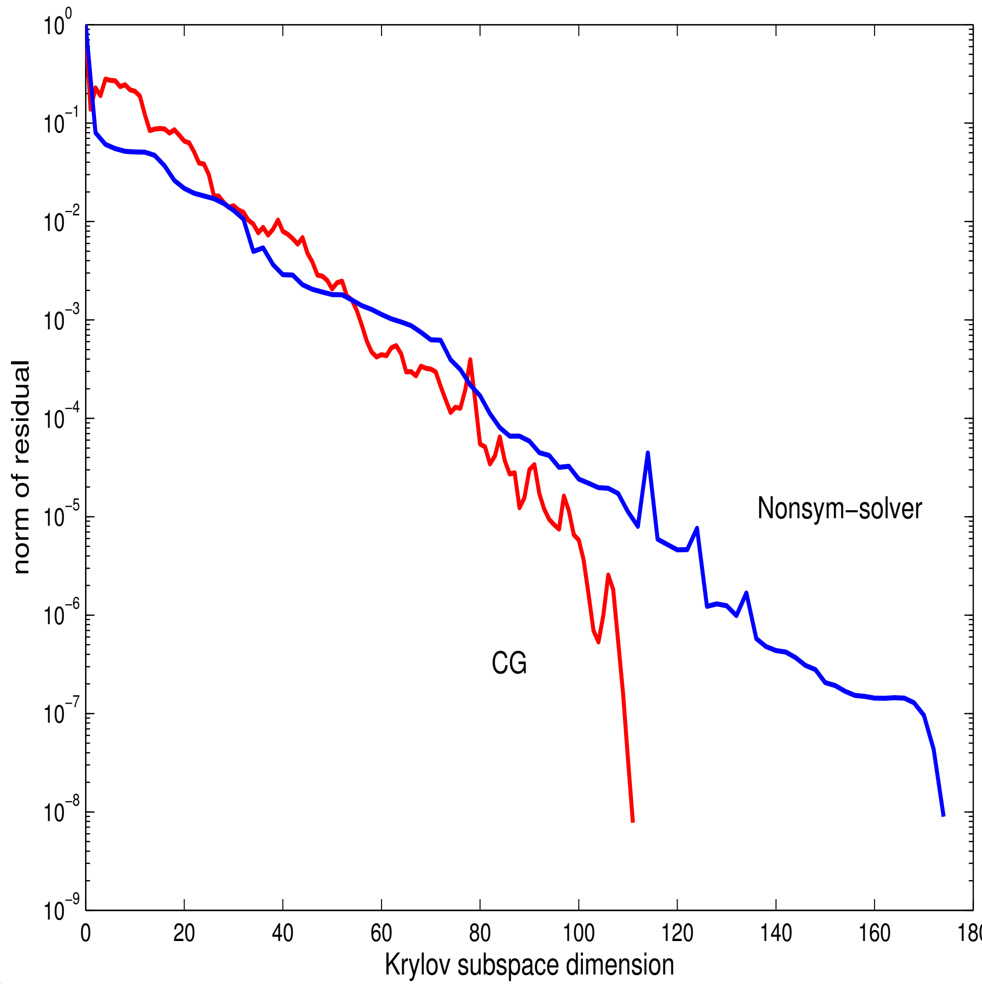

A natural implementation: Two-sided Lanczos

Lanczos method for non-Hermitian matrices:

$$\mathcal{K}_m(A,b), \qquad \mathcal{L}_m = \mathcal{K}_m(A^*, \widehat{b}), \quad \widehat{b} \text{ auxiliary vector}$$

$$V_m, \qquad L_m \quad s.t. \qquad L_m^* V_m = D_m \quad \text{diagonal matrix}$$

$$r_m \perp \mathcal{L}_m \quad \Rightarrow \quad (L_m^* A V_m) y_m = L_m^* b \quad L_m^* A V_m \text{ tridiagonal}$$

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In most implementations now:

$$\mathcal{L}_m = \mathcal{K}_m(A^T, b), \qquad s.t. \quad L_m^T V_m = D_m$$

A complex symmetric $\quad \Rightarrow \quad \mathcal{K}_m(A,b) = \mathcal{L}_m, \qquad L_m^T A V_m$ symmetric

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♣ Two-sided Lanczos provides the setting for convergence analysis

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Two-sided Lanczos and J-inner product

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$$\text{for} \qquad \widehat{b} := Jb$$

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$$\Downarrow$$

No need to generate space $\mathcal{L}_m$ and its basis! (Simplified Lanczos)

Freund & Nachtigal 1995

Disclaimers

- Still in the two-sided Lanczos framework
- Possible breakdown ($L_m^\star V_m$ singular, $\star = T, *$)
- Stability issues
- Specific convergence analysis: open problem

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An application

$$(A + \sigma B)x = b$$

A, B symmetric, B nonsingular $\quad \sigma \in [\alpha, \beta] \subset \mathbb{R}$

Problem: Solve for several (a few hundreds, say) values of σ

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$$(AB^{-1} + \sigma I)\widehat{x} = b \qquad x = B^{-1}\widehat{x}$$

Shift-invariance of Krylov space: $\quad \mathcal{K}_m(AB^{-1} + \sigma I, b) = \mathcal{K}_m(AB^{-1}, b)$

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$\star$ AB^{-1} is B^{-1}-symmetric $\qquad$ (that is, $(AB^{-1})^T B^{-1} = B^{-1}(AB^{-1})$)

$$\Downarrow$$

Simplified Lanczos method with $J = B^{-1}$

(Perotti & Simoncini 2002)

Application to Preconditioning

Saddle-point problem:

$$Ax = b \quad \Leftrightarrow \quad \begin{pmatrix} H & B \\ B^* & -C \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

H, C Hermitian pos. (semi-)definite $\Rightarrow$ A Hermitian indef. (nonsing.)

Recent survey: Benzi & Golub & Liesen, 2005

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⋆ Preconditioning technique: Find nonsingular P s.t.

$$AP^{-1}\widehat{x} = b$$

"easier" to solve, with P cheap to invert (or, $P_1^{-1}AP_2^{-1}\widehat{x} = P_1^{-1}b$)

Various successful choices, mostly problem dependent

For simplicity: $C = 0$

Structured Preconditioners

$$A = \begin{pmatrix} H & B \\ B^* & 0 \end{pmatrix}$$

- Block diagonal (AP^{-1} is P^{-1}-Hermitian – minimization in the "correct" norm)

$$P = \begin{pmatrix} \widetilde{H} & 0 \\ 0^* & S \end{pmatrix} \qquad \widetilde{H} \approx H, \; S \approx B^* H^{-1} B$$

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- Block indefinite (more in the next few slides)

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- Block triangular (AP^{-1} is similar to Hermitian, under conditions on $\widetilde{H}$, S)

$$P = \begin{pmatrix} \widetilde{H} & B \\ 0^* & -S \end{pmatrix} \qquad S \approx B^* H^{-1} B$$

Indefinite (Constraint) Preconditioners

$$P = \begin{pmatrix} \widetilde{H} & B \\ B^* & 0 \end{pmatrix} \qquad\qquad AP^{-1}\widehat{x} = b$$

$\widetilde{H} \approx H$, cheap to solve with

More Indefinite-style preconditioners: Dollar, Gould, Wathen, Schilders, 2005

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* AP^{-1} not symmetrizable!
* However: AP^{-1} is P^{-1}-Hermitian

Use Simplified Lanczos method

Indefinite (Constraint) Preconditioners

$$P = \begin{pmatrix} \widetilde{H} & B \\ B^* & 0 \end{pmatrix} \qquad AP^{-1}\widehat{x} = b$$

$\widetilde{H} \approx H$, cheap to solve with

More Indefinite-style preconditioners: Dollar, Gould, Wathen, Schilders, 2005

* AP^{-1} not symmetrizable!
* However: AP^{-1} is P^{-1}-Hermitian

Use Simplified Lanczos method

What spectral properties?

Spectral properties. I

⋆ Eigenvalues of AP^{-1} are real and positive, in $\lambda \in \{1\} \cup [\alpha_0, \alpha_1]$

⋆ Presence of Jordan blocks

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Jordan blocks do not influence convergence

(with appropriate starting approximate solution)

$$AP^{-1} = \begin{pmatrix} H(I-\Pi)+\Pi & (H-I)B(B^*B)^{-1} \\ 0 & I \end{pmatrix} \qquad r_0 = \begin{pmatrix} * \\ 0 \end{pmatrix}$$

$\Pi = B(B^*B)^{-1}B^*$ Projector

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Axelsson (1979), Ewing Lazarov Lu Vassilevski (1990), Braess Sarazin (1997) Golub Wathen (1998) Vassilevski Lazarov (1996), Lukšan Vlček (1998-1999), Perugia S. Arioli (1999), Keller Gould Wathen (2000), Perugia S. (2000), Gould Hribar Nocedal (2001), Rozloznik S. (2002), Durazzi Ruggiero (2003), Axelsson Neytcheva (2003), Dollar, Gould, Wathen, Schilders (2005),...

Computational Considerations: Exact P vs Inexact P

$$P^{-1} = \begin{pmatrix} \widetilde{H} & B \\ B^* & 0 \end{pmatrix}^{-1} = \begin{pmatrix} I & -B^T \\ O & I \end{pmatrix} \begin{pmatrix} I & O \\ O & -(\mathbf{BB^*})^{-1} \end{pmatrix} \begin{pmatrix} I & O \\ -B & I \end{pmatrix}$$

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3D Magnetostatic problem. Elapsed Time

	SIMPLIFIED LANCZOS		SIMPLIFIED LANCZOS
SIZE	P	$\widehat{P}(2)(it)$	ILDLT(10)
1119	**3.0**(15)	**1.7**(18)	**0.7**
2208	**11.7** (13)	**3.1**(18)	**1.5**
4371	**64.6** (17)	**8.4**(20)	**5.2**
8622	**466.0**(16)	**18.3**(29)	**31.0**
22675	**3745.5**(25)	**63.2**(45)	**246.0**

$BB^* \approx S$ Incomplete Cholesky fact. $\Rightarrow$ $\widehat{P}$ $\quad$ $A\widehat{P}^{-1}\widehat{x} = b$

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Spectral properties. II

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  - $\star$ If $\Im(\lambda) \neq 0$ then

$$(\lambda_{\min}(H) + \lambda_{\min}(\widehat{C})) \leq \Re(\lambda) \leq \frac{1}{2}(\lambda_{\max}(H) + \lambda_{\max}(\widehat{C}))$$

$$|\Im(\lambda)| \leq \sigma_{\max}((I - H)BS^{-\frac{1}{2}}).$$

  - $\star$ If $\Im(\lambda) = 0$ then

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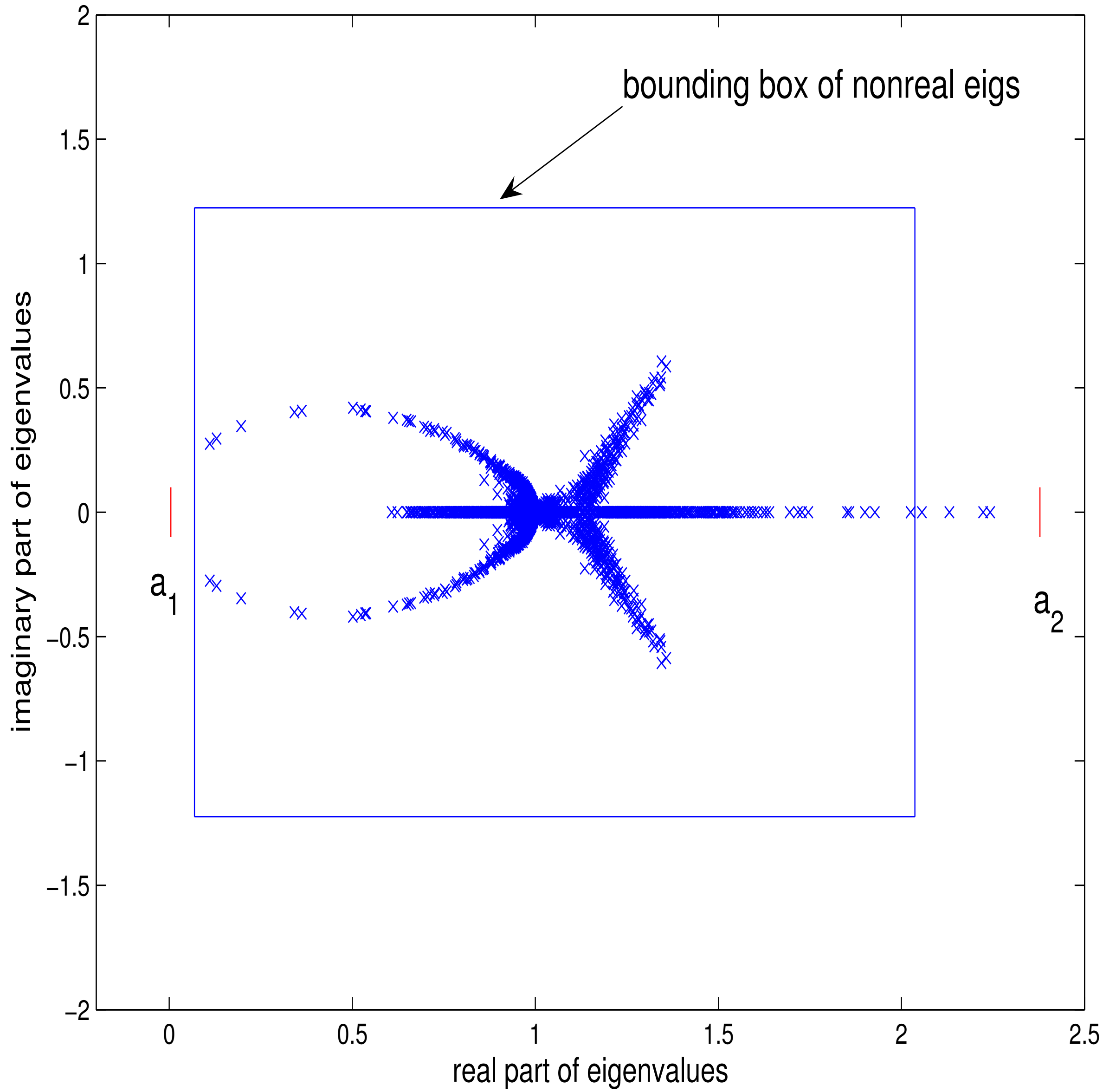
- Eigenvectors: open problem

Spectral bounds



Benzi & Simoncini, 2006

Final Considerations

- Indefinite inner product appropriate
  to exploit inherent problem properties
- Many computational issues still open
- Convergence analysis still very challenging

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“ Recent computational developments in Krylov Subspace Methods for linear systems”

with Daniel Szyld, (Temple University)
To appear J. Numerical Linear Algebra w/Appl.