On efficient numerical approximation of the bilinear form $c^* \mathbf{A}^{-1} b$

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joint work with

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Formulation of the problem

Given a nonsingular matrix $\mathbf{A}$ and vectors b and c.

We want to approximate

$$c^*\mathbf{A}^{-1}b\,.$$

Equivalently, we look for an approximation to

$$c^*x \qquad \text{such that} \qquad \mathbf{A}x = b\,.$$

Motivation

- **Approximation of the jth component of the solution**
  - i.e., we want to approximate $e_j^T \mathbf{A}^{-1} b$.
- **Signal processing (the scattering amplitude)**
  - b and c represent incoming and outgoing waves, respectively, and the operator $\mathbf{A}$ relates the incoming and scattered fields on the surface of an object,
  - $\mathbf{A}x = b$ determines the field x from the signal b. The signal is received on an antenna c. The signal received by the antenna is then c^*x. The value c^*x is called *the scattering amplitude*.
- **Optimization**
- **Nuclear physics, quantum mechanics, other disciplines**

Krylov subspace methods approach

Projection of the original problem onto Krylov subspaces

$$\mathcal{K}_n(\mathbf{A}, b) = \operatorname{span}\{b, \mathbf{A}b, \dots \mathbf{A}^{n-1}b\}.$$

A possible approach: compute x_n using a Krylov subspace method,

$$c^*\mathbf{A}^{-1}b \;=\; c^*x \;\approx\; c^*x_n\,.$$

- Due to finite precision arithmetic, the explicit numerical computation of c^*x_n can be *highly inefficient*.
  [HPD case: Strakoš & T. '02, '05]
- If $\mathbf{A}$ is HPD and $c = b$, there are several efficient methods.
  [Golub & Meurant '94, '97, Axelsson & Kaporin '01, Strakoš & T. '02, '05]
- How to generalize ideas from the HPD case to a general case?

Outline

1. Vorobyev moment problem
2. Approximation of the bilinear form $c^*\mathbf{A}^{-1}b$
3. Numerical experiments

Vorobyev moment problem, Vorobyev '58, '65

Popularized by Brezinski '97, Strakoš '08

Find a linear operator $\mathbf{A}_n$ on $\mathcal{K}_n(\mathbf{A}, v)$ such that

$$\begin{aligned} \mathbf{A}_n\, v &= \mathbf{A}\, v, \\ \mathbf{A}_n^2\, v &= \mathbf{A}^2\, v, \\ &\vdots \\ \mathbf{A}_n^{n-1}\, v &= \mathbf{A}^{n-1}\, v, \\ \mathbf{A}_n^n\, v &= \mathbf{Q}_n \mathbf{A}^n\, v\,, \end{aligned}$$

where $\mathbf{Q}_n$ is a given linear projection operator.

- Some Krylov subspace methods can be identified with the Vorobyev moment problem.
- Useful formulation for understanding approximation properties of Krylov subspace methods.

Non-Hermitian Lanczos and Arnoldi algorithms

Given a nonsingular $\mathbf{A}$, v and w.

Non-Hermitian Lanczos algorithm is represented by

$$\begin{aligned}\mathbf{A}\mathbf{V}_n &= \mathbf{V}_n\mathbf{T}_n + \delta_{n+1} v_{n+1} e_n^T,\\ \mathbf{A}^*\mathbf{W}_n &= \mathbf{W}_n\mathbf{T}_n^* + \eta_{n+1}^* w_{n+1} e_n^T,\end{aligned}$$

where $\mathbf{W}_n^*\mathbf{V}_n = \mathbf{I}$ and $\mathbf{T}_n = \mathbf{W}_n^*\mathbf{A}\mathbf{V}_n$ is tridiagonal.

Arnoldi algorithm is represented by

$$\mathbf{A}\mathbf{V}_n = \mathbf{V}_n\mathbf{H}_n + h_{n+1,n} v_{n+1} e_n^T,$$

where $\mathbf{V}_n^*\mathbf{V}_n = \mathbf{I}$, and $\mathbf{H}_n = \mathbf{V}_n^*\mathbf{A}\mathbf{V}_n$ is upper Hessenberg.

Vorobyev moment problem,

Non-Hermitian Lanczos and Arnoldi

Lanczos: $\mathbf{Q}_n$ projects onto $\mathcal{K}_n(\mathbf{A}, v)$ orthog. to $\mathcal{K}_n(\mathbf{A}^*, w)$,

$$\mathbf{Q}_n = \mathbf{V}_n \mathbf{W}_n^*, \qquad \mathbf{A}_n = \mathbf{V}_n \mathbf{T}_n \mathbf{W}_n^*.$$

Arnoldi: $\mathbf{Q}_n$ projects onto $\mathcal{K}_n(\mathbf{A}, v)$ orthog. to $\mathcal{K}_n(\mathbf{A}, v)$,

$$\mathbf{Q}_n = \mathbf{V}_n \mathbf{V}_n^*, \qquad \mathbf{A}_n = \mathbf{V}_n \mathbf{H}_n \mathbf{V}_n^*.$$

Matching moments property:

$$w^* \mathbf{A}^k v = w^* \mathbf{A}_n^k v,$$

$k = 0, \dots, 2n-1$ for Lanczos, $k = 0, \dots, n-1$ for Arnoldi.

[Gragg & Lindquist '83, Villemagne & Skelton '87]

[Gallivan & Grimme & Van Dooren '94, Antoulas '05]

[a simple proof using the Vorobyev moment problem - Strakoš '08]

Approximation of $c^*\mathbf{A}^{-1}b$

General framework, Strakoš & T. '10

Vorobyev moment problem: $\mathbf{A} \;\rightarrow\; \mathbf{A}_n$

Define approximation: $c^*\mathbf{A}^{-1}b \;\approx\; c^*\mathbf{A}_n^{-1}b$

$\mathbf{A}_n^{-1}$ is the matrix representation of the inverse of the reduced order operator $\mathbf{A}_n$ which is restricted onto $\mathcal{K}_n(\mathbf{A}, b)$.

Examples:

- $\mathbf{A}_n^{-1} \;=\; \mathbf{V}_n\mathbf{T}_n^{-1}\mathbf{W}_n^*$ (Non-Hermitian Lanczos)
- $\mathbf{A}_n^{-1} \;=\; \mathbf{V}_n\mathbf{H}_n^{-1}\mathbf{V}_n^*$ (Arnoldi)

Questions:

- How to compute $c^*\mathbf{A}_n^{-1}b$ efficiently?
- Relationship to the existing approximations?

We concentrate only to non-Hermitian Lanczos approach.

Non-Hermitian Lanczos approach

Define

$$v_1 = \frac{b}{\|b\|}, \qquad w_1 = \frac{c}{c^* v_1}, \qquad \text{i.e.} \qquad w_1^* v_1 = 1\,.$$

Then

$$c^* \mathbf{A}_n^{-1} b \;=\; c^* \mathbf{V}_n \mathbf{T}_n^{-1} \mathbf{W}_n^* b \;=\; (c^* v_1)\, \|b\|\, (\mathbf{T}_n^{-1})_{1,1}\,.$$

Let $x_0 = 0$. We also know that $x_n \;=\; \|b\| \mathbf{V}_n \mathbf{T}_n^{-1} e_1$ is the approximate solution computed via BiCG. Therefore,

$$c^* \mathbf{A}_n^{-1} b \;=\; c^* \|b\| \mathbf{V}_n \mathbf{T}_n^{-1} \mathbf{W}_n^* \mathbf{V}_n e_1 \;=\; c^* x_n\,.$$

- BiCG can be used for computing $c^* \mathbf{A}_n^{-1} b$!
- We used the global biorthogonality !
  Do the identities hold in finite precision computations?

The BiCG method

Simultaneous solving of

$$\mathbf{A}x \;=\; b\,, \qquad \mathbf{A}^*y \;=\; c\,.$$

input $\mathbf{A}$, b, c

$$x_0 = y_0 = 0$$
$$r_0 = p_0 = b,\; s_0 = q_0 = c$$

for $n = 0, 1, \ldots$

$$\alpha_n = \frac{s_n^* r_n}{q_n^* \mathbf{A} p_n}\,,$$
$$x_{n+1} = x_n + \alpha_n\, p_n\,, \qquad y_{n+1} = y_n + {\alpha_n}^*\, q_n\,,$$
$$r_{n+1} = r_n - \alpha_n\, \mathbf{A}p_n\,, \qquad s_{n+1} = s_n - \alpha_n^*\, \mathbf{A}^* q_n\,,$$
$$\beta_{n+1} = \frac{s_{n+1}^* r_{n+1}}{s_n^* r_n}\,,$$
$$p_{n+1} = r_{n+1} + \beta_{n+1}\, p_n\,, \qquad q_{n+1} = s_{n+1} + \beta_{n+1}^*\, q_n$$

end

An efficient approximation based on the BiCG method

How to compute $c^* \mathbf{A}_n^{-1} b$ in BiCG without using the global biorthogonality?

Using local biorthogonality we can show that

$$s_j^* \mathbf{A}^{-1} r_j \; - \; s_{j+1}^* \mathbf{A}^{-1} r_{j+1} \; = \; \alpha_j s_j^* r_j .$$

Consequently,

$$c^* \mathbf{A}^{-1} b \; = \; \sum_{j=0}^{n-1} \alpha_j s_j^* r_j \; + \; s_n^* \mathbf{A}^{-1} r_n \, .$$

Moreover, it can be shown that (using global biorthogonality) that

$$c^* \mathbf{A}^{-1} b \; = \; c^* x_n \; + \; s_n^* \mathbf{A}^{-1} r_n \, .$$

Finally,

$$c^* \mathbf{A}_n^{-1} b \; = \; c^* x_n \; = \; \sum_{j=0}^{n-1} \alpha_j s_j^* r_j \, .$$

Approximations based on the BiCG method

and finite precision arithmetic

It holds that

$$c^*\mathbf{A}^{-1}b \;=\; \sum_{j=0}^{n-1} \alpha_j s_j^* r_j \;\;+\;\; \underbrace{s_n^*\mathbf{A}^{-1} r_n}_{\text{error} \;\sim\; \|y-y_n\|\|r_n\|} \quad .$$

It can be shown that

$$c^*\mathbf{A}^{-1}b \;=\; c^* x_n \;+\; \underbrace{y_n^* r_n \;+\; s_n^*\mathbf{A}^{-1} r_n}_{\text{error} \;\sim\; \|y_n\|\|r_n\|} \, .$$

In exact arithmetic $y_n^* r_n = 0$.

If the global biorthogonality is lost, one can expect that

$$|y_n^* r_n| \;\sim\; \|y_n\|\|r_n\| \, .$$

We know that

$$c^*\mathbf{A}_n^{-1}b \;=\; \sum_{j=0}^{n-1} \alpha_j\, s_j^* r_j \quad \text{and} \quad s_j^* r_j \;=\; (c^*b)\prod_{k=0}^{j-1} \beta_k\,.$$

In hybrid BiCG methods like CGS, BiCGStab, BiCGStab(ℓ), the BiCG coefficients are available, i.e. we can compute the approximation $c^*\mathbf{A}_n^{-1}b$ during the run of these method.

Question: Hybrid BiCG methods produce approximations $\mathbf{x}_n$, better than x_n produced by BiCG.

Is $c^*\mathbf{x}_n$ a better approximation of $c^*\mathbf{A}^{-1}b$ than c^*x_n?

No. We showed that mathematically [Strakoš & T. '10],

$$c^*\mathbf{x}_n = c^*x_n.$$

Summary (non-Hermitian Lanczos approach)

How to compute $c^* \mathbf{A}_n^{-1} b$?

Algorithm of choice:

- non-Hermitian Lanczos
- BiCG
- hybrid BiCG methods

Way of computing the approximation:

- $c^* x_n$
- $(c^* v_1)\, \|b\|\, (\mathbf{T}_n^{-1})_{1,1}$
- complex Gauss quadrature (Saylor-Smolarski approach)
- from the BiCG coefficients, or, in BiCG using

$$\xi_n^B \equiv \sum_{j=0}^{n-1} \alpha_j\, s_j^* r_j \,.$$

[Hench & Strakoš '08]

$$\mathbf{A}\,x \equiv \begin{bmatrix} -\mathbf{I} & \mathbf{I} & e^{\mathbf{i}\sqrt{\mathbf{C}}\varrho} & 0 \\ \mathbf{Y}_I & \sqrt{\mathbf{C}} & -\sqrt{\mathbf{C}}e^{\mathbf{i}\sqrt{C}\varrho} & 0 \\ 0 & e^{\mathbf{i}\sqrt{\mathbf{C}}\varrho} & I & -\mathbf{I} \\ 0 & \sqrt{\mathbf{C}}e^{\mathbf{i}\sqrt{\mathbf{C}}\varrho} & -\sqrt{\mathbf{C}} & -\mathbf{Y}_{\mathrm{II}} \end{bmatrix} x \; = \; b\,,$$

$\mathbf{Y}_{\mathrm{I}},\ \mathbf{Y}_{\mathrm{II}}, \mathbf{C} \in \mathbb{C}^{(2M+1)\times(2M+1)}$, $\varrho > 0$, M is the discretization parameter representing the number of Fourier modes used for approximation of the electric and magnetic fields as well as the material properties.

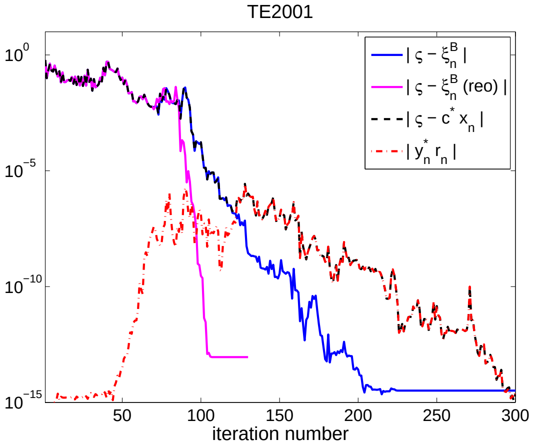
Typically, one needs only the dominant $(M+1)$st component

$$e_{M+1}^{*}\mathbf{A}^{-1}b.$$

In our experiments $M = 20$, i.e. $\mathbf{A} \in \mathbb{C}^{164\times164}$. [Strakoš & T. '10]

Approximations based on the BiCG method

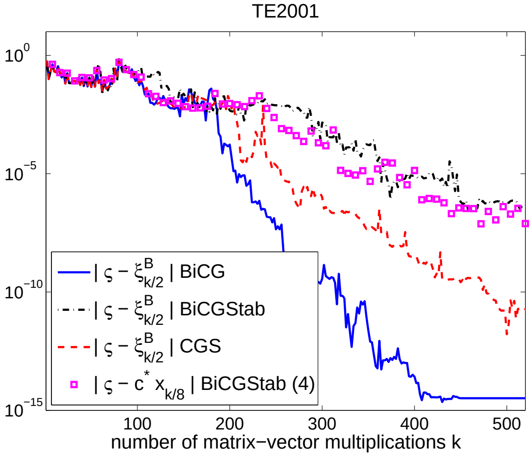
Mathematically equivalent approximations ξ_n^B and $c^* x_n$, $\varsigma \equiv c^* \mathbf{A}^{-1} b$



$$
\begin{aligned}
|c^* \mathbf{A}^{-1} b - c^* x_n| &= |{\color{red} y_n^* r_n} + {\color{blue} s_n^* \mathbf{A}^{-1} r_n}|, \\
|c^* \mathbf{A}^{-1} b - \xi_n^B| &= |{\color{blue} s_n^* \mathbf{A}^{-1} r_n}|.
\end{aligned}
$$

Non-Hermitian Lanczos approach

Mathematically equivalent approximations based on hybrid BiCG methods



The BiCGStab and CGS approximations are significantly more affected by rounding errors than the BiCG approximations.

Conclusions

- Generalization of the HPD case:
  - Via Vorobyev moment problem $\rightarrow$ very natural and general.
    - no assumptions on $\mathbf{A}$, based on approximation properties
  - Complex Gauss Quadrature approach
    - $\mathbf{A}$ has to be diagonalizable, just a formalism
- We proved mathematical equivalence of the existing approximations based on Non-Hermitian Lanczos.
- Preferable approximation

$$\xi_n^B \equiv \sum_{j=0}^{n-1} \alpha_j \, s_j^* r_j \, .$$

  It is simple and numerically better justified.
- In finite precision arithmetic, the identities need not hold. A justification is necessary (e.g. local biorthogonality).

Related papers

- Z. Strakoš and P. Tichý, [On efficient numerical approximation of the bilinear form $c^*\mathbf{A}^{-1}b$, submitted to SISC, 2009].
- G. H. Golub, M. Stoll, and A. Wathen, [Approximation of the scattering amplitude and linear systems, Electron. Trans. Numer. Anal., 31 (2008), pp. 178–203].
- Z. Strakoš and P. Tichý, [On error estimation in the conjugate gradient method and why it works in finite precision computations, Electron. Trans. Numer. Anal., 13 (2002), pp. 56–80].
- P. E. Saylor and D. C. Smolarski, [Why Gaussian quadrature in the complex plane?, Numer. Algorithms, 26 (2001), pp. 251–280].
- G. H. Golub and G. Meurant, [Matrices, moments and quadrature, in Numerical analysis 1993 (Dundee, 1993), vol. 303 of Pitman Res. Notes Math. Ser., Longman Sci. Tech., Harlow, 1994, pp. 105–156].

More details

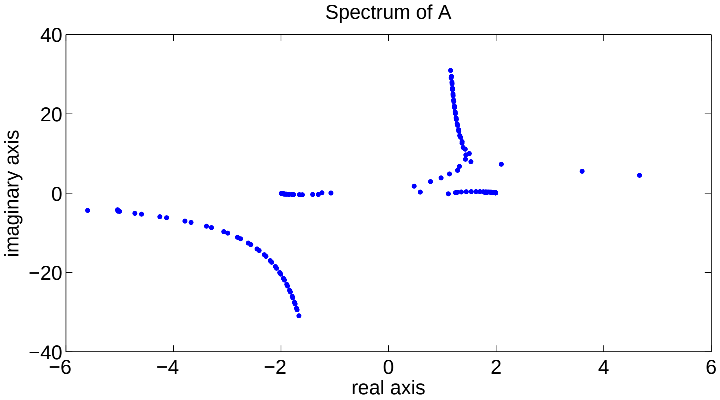
More details can be found at

http://www.cs.cas.cz/strakos
http://www.cs.cas.cz/tichy

Thank you for your attention!

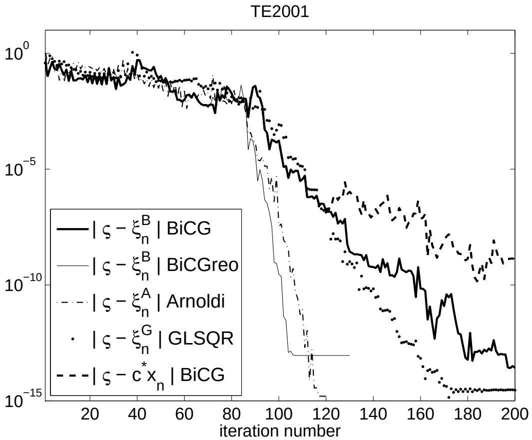
The matrix $\mathbf{A}$

Spectrum of $\mathbf{A}$ computed via the Matlab command `eig`



Some eigenvalues have large imaginary parts in comparison to the real parts, $\kappa(\mathbf{A}) \approx 104$.

Non-Hermitian Lanczos, Arnoldi, GLSQR



GLSQR: [Golub & Stoll & Wathen '08], [Saunders & Simon & Yip '88]

Different approaches with preconditioning

Non-Hermitian Lanczos, Arnoldi, GLSQR