On efficient numerical approximation of the scattering amplitude

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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**
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- **Signal processing (the scattering amplitude)**
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  - $\mathbf{A}x = b$ 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*.

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- **Optimization (the primal linear output)**
- **Nuclear physics, quantum mechanics, other disciplines**

Krylov subspace methods approach

Projection of the original problem onto Krylov subspaces

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

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- If $\mathbf{A}$ is HPD and $c = b$, there are several efficient methods.
  [Golub & Meurant '94, '97, Axelsson & Kaporin '01, Strakoš & T. '02, '05]

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  [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 scattering amplitude
3. Numerical experiments

Outline

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

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- Some Krylov subspace methods can be interpreted as methods that solve the Vorobyev moment problem.
- Useful formulation for understanding approximation properties of Krylov subspace methods (matching moments properties).

Non-Hermitian Lanczos

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,

$$\mathbf{T}_n = \begin{bmatrix} \gamma_1 & \eta_2 & & \\ \delta_2 & \gamma_2 & \ddots & \\ & \ddots & \ddots & \eta_n \\ & & \delta_n & \gamma_n \end{bmatrix}.$$

Arnoldi algorithm

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

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,

$$\mathbf{H}_n = \begin{bmatrix} h_{1,1} & h_{1,2} & \cdots & h_{1,n} \\ h_{2,1} & h_{2,2} & \ddots & \vdots \\ & \ddots & \ddots & h_{n-n,n} \\ & & h_{n,n-1} & h_{n.n} \end{bmatrix}.$$

Vorobyev moment problem,

Non-Hermitian Lanczos and Arnoldi

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

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

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Matching moments property:

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

$k = 0, \ldots, 2n-1$ for Lanczos, $k = 0, \ldots, n-1$ 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]

Outline

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

General framework, Strakoš & T. '09

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

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

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

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Examples:

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

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

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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

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

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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,

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- BiCG can be used for computing $c^* \mathbf{A}_n^{-1} b$!

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- 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

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

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Consequently,

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

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

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

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Finally,

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Saylor-Smolarski approach

For diagonalizable matrices

[Saylor & Smolarski '01] introduce

- formally orthogonal polynomials,
- complex Gauss quadrature,

as a tool for approximating the quantity $c^* \mathbf{A}^{-1} b$. Motivated by [Freund & Hochbruck '93], [Golub & Meurant '94, '97].

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Non-Hermitian Lanczos $\rightarrow \hat{\mathbf{T}}_n$ (complex) symmetric. Define

$$c^* \mathbf{A}^{-1} b \approx G\left(\lambda^{-1}\right) \equiv \sum_{j=1}^{n} \frac{\omega_j}{\zeta_j},$$

ζ_j ... eigenvalues of $\hat{\mathbf{T}}_n$, ω_j ... scaled and squared first components of the normalized eigenvectors of $\hat{\mathbf{T}}_n$.

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[Warnick '00] showed:

$$G\left(\lambda^{-1}\right) = c^* x_n \,.$$

Yet another approach

Hybrid BiCG methods

We know that

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

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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.

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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 $c^* x_n$?

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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. '09],

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

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
- from the BiCG coefficients, or, in BiCG using

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

Outline

Numerical experiments

Diffraction of light on periodic structures, RCWA method

[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 nodes used for approximation of the electric and magnetic fields as well as the material properties.

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

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

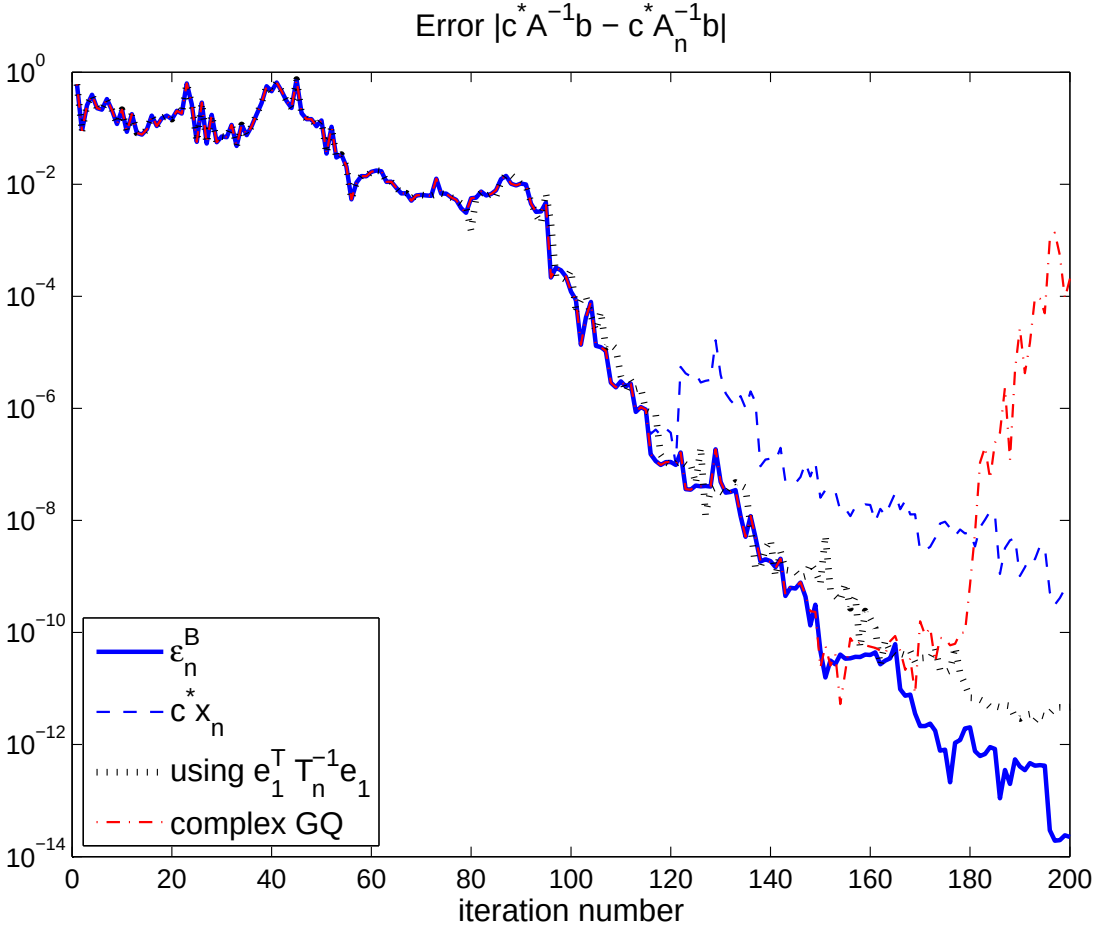
Typically, one needs only the dominant $(M+1)$st component

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

In our experiments $M = 20$, i.e. $\mathbf{A} \in \mathbb{C}^{164\times164}$. [Strakoš & T. '09]

Non-Hermitian Lanczos approach

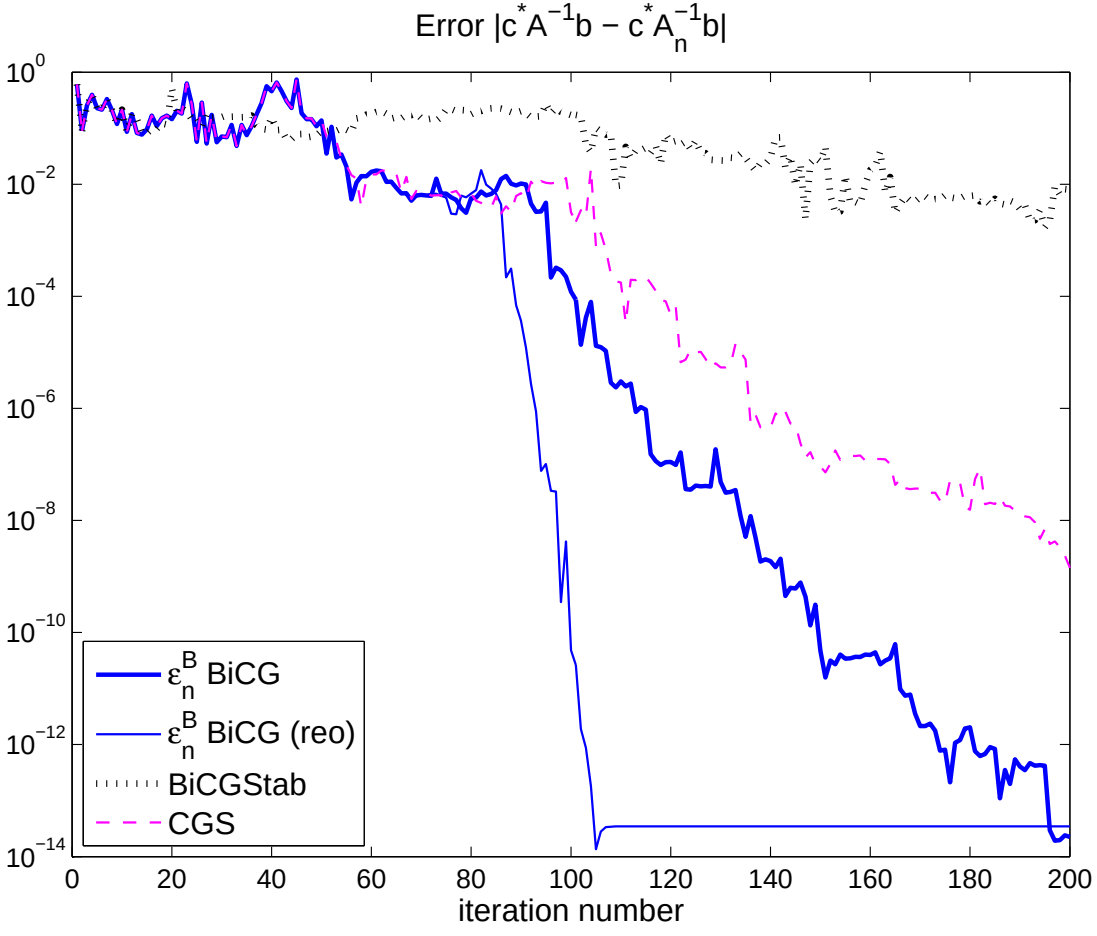
Mathematically equivalent estimates I



Comparison of mathematically equivalent approximations based on BiCG and non-Hermitian Lanczos.

Non-Hermitian Lanczos approach

Mathematically equivalent estimates II



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
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- In finite precision arithmetic, the identities need not hold. A justification is needed (e.g. local biorthogonality).

Related papers

- Z. Strakoš and P. Tichý, [On efficient numerical approximation of the scattering amplitude $c^* \mathbf{A}^{-1} b$ via matching moments, 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

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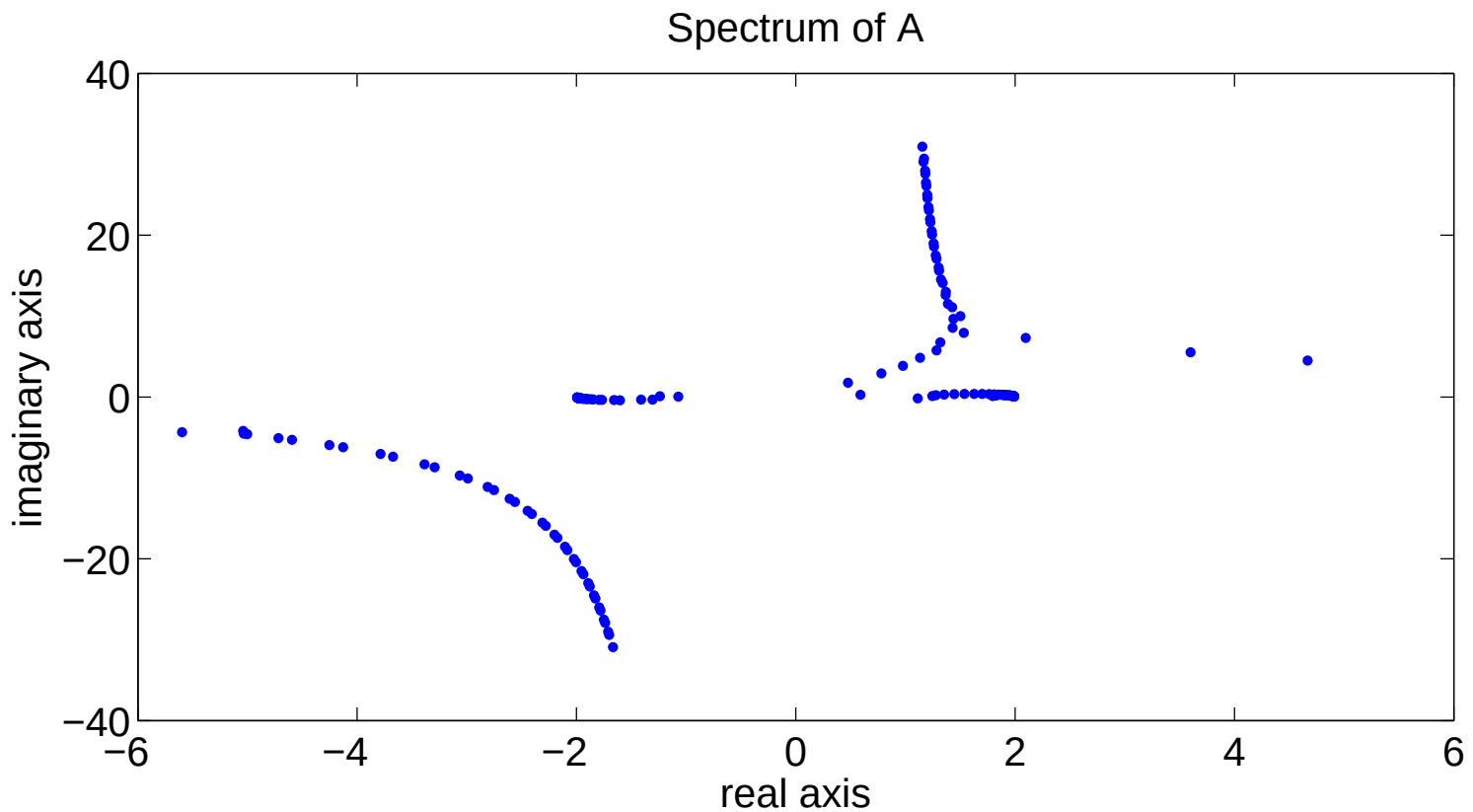
Thank you for your attention!

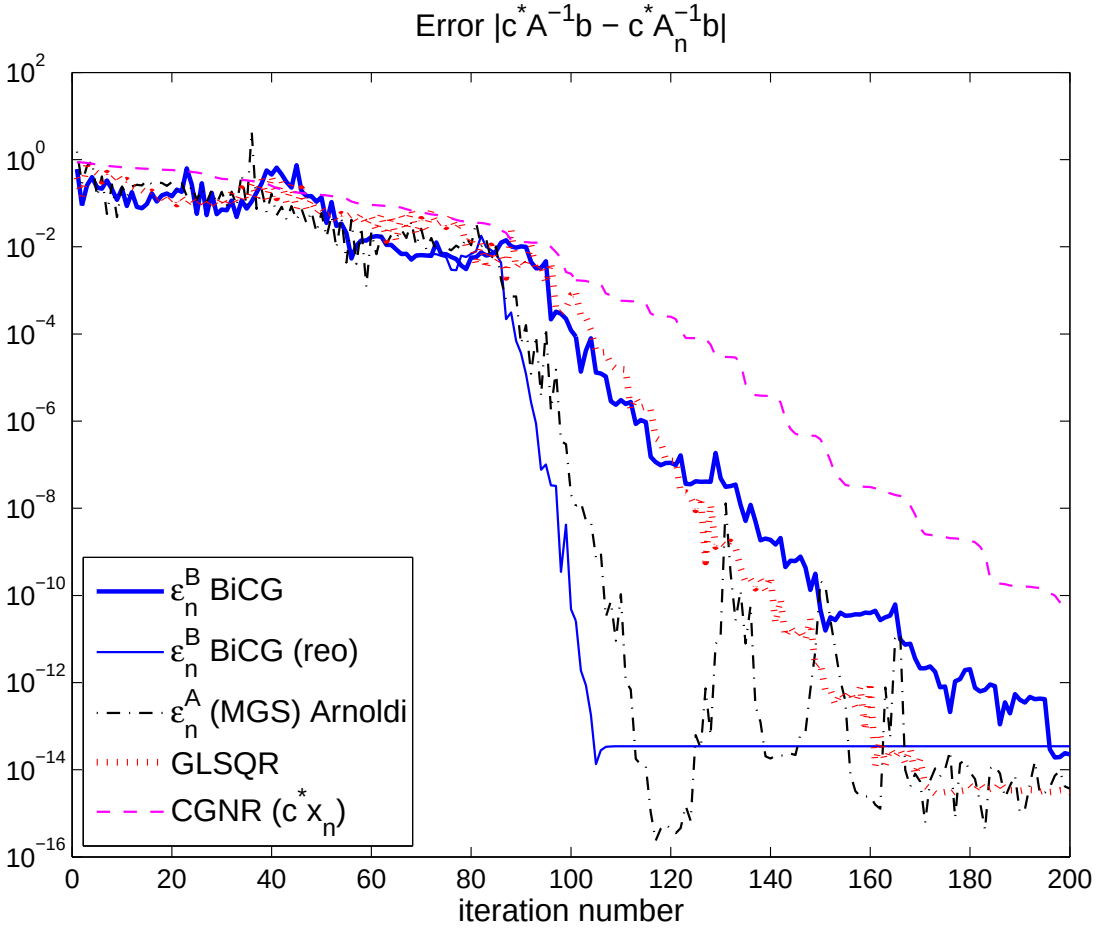
The matrix $\mathbf{A}$

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