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

Krylov subspace methods approach

Projection of the original problem onto Krylov subspaces

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

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

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

- The approximation c^*x_n can be highly inefficient!
  How to approximate c^*x without looking for x_n?
- We need a theoretical background
  (find the best possible approximation in some sense).
- Efficient numerical computation and justification
  of the approximation in finite precision arithmetic.

Outline

1. Symmetric, positive definite case
2. Matching moments
3. Approximation of the scattering amplitude
4. Preconditioning
5. Transformation to the Hermitian positive definite case
6. Numerical experiments

The CG method

Let $\mathbf{A}$ be symmetric, positive definite

Solve $\mathbf{A}x = b$.

input $\mathbf{A}$, b

$x_0 = 0$

$r_0 = p_0 = b$

for $k = 0, 1, \ldots$

$\alpha_k = \frac{\|r_k\|^2}{p_k^* \mathbf{A} p_k}$,

$x_{k+1} = x_k + \alpha_k \, p_k$,

$r_{k+1} = r_k - \alpha_k \, \mathbf{A} p_k$,

$\beta_{k+1} = \frac{\|r_{k+1}\|^2}{\|r_k\|^2}$,

$p_{k+1} = r_{k+1} + \beta_{k+1} \, p_k$,

end

The Lanczos algorithm

Let $\mathbf{A}$ be symmetric

Compute orthonormal basis of $\mathcal{K}_n(\mathbf{A}, b)$.

input $\mathbf{A}$, b

$$v_1 = b/\|b\|,\ \delta_1 = 0\,,$$

for $k = 1, 2, \ldots$

$$\gamma_k = v_k^T(\mathbf{A}v_k - \delta_k v_{k-1})\,,$$
$$w = \mathbf{A}v_k - \gamma_k v_k - \delta_k v_{k-1}\,,$$
$$\delta_{k+1} = \|w\|\,,$$
$$v_{k+1} = w/\delta_{k+1}\,,$$

end

The Lanczos algorithm is represented by

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

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

CG versus Lanczos

Let $\mathbf{A}$ be symmetric, positive definite

$$\mathbf{T}_n = \begin{bmatrix} \gamma_1 & \delta_2 & & \\ \delta_2 & \ddots & & \\ & & \ddots & \delta_n \\ & & \delta_n & \gamma_n \end{bmatrix} = \mathbf{L}_n \mathbf{L}_n^T$$

where

$$\mathbf{L}_n = \begin{bmatrix} \frac{1}{\sqrt{\alpha_0}} & & & \\ \sqrt{\frac{\beta_1}{\alpha_0}} & \ddots & & \\ & \ddots & \ddots & \\ & & \frac{\sqrt{\beta_{n-1}}}{\alpha_{n-2}} & \frac{1}{\sqrt{\alpha_{n-1}}} \end{bmatrix} .$$

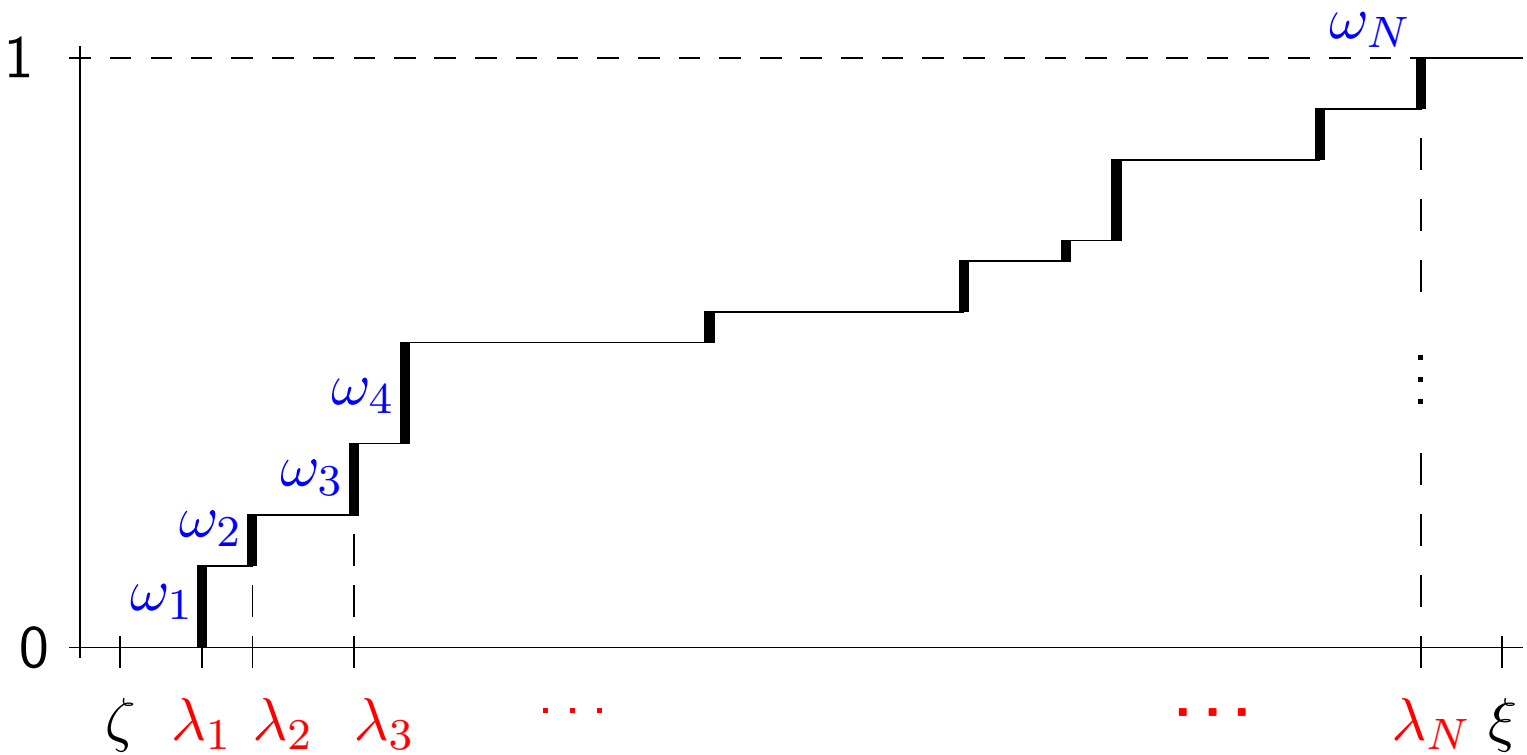
The CG approximation is the given by

$$\mathbf{T}_n y_n = \|b\| e_1, \qquad x_n = x_0 + \mathbf{V}_n y_n \, .$$

Distribution function $\omega(\lambda)$

Without loss of generality $\|b\| = 1$

(λ_i, u_i) ... eigenpair of $\mathbf{A}$, $\omega_i = (b^T u_i)^2$.



$$\int_\zeta^\xi f(\lambda)\, d\omega(\lambda) \;=\; \sum_{i=1}^{N} \omega_i\, f(\lambda_i)\,.$$

The Conjugate gradient method and Gauss Quadrature

Symmetric, positive definite case

At any iteration step n, CG (implicitly) determines weights and nodes of the n-point Gauss quadrature

$$\int_{\zeta}^{\xi} f(\lambda)\, d\omega(\lambda) \;=\; \sum_{i=1}^{n} \omega_i^{(n)} f(\theta_i^{(n)}) \;+\; R_n(f)\,.$$

$\mathbf{T}_n$ . . . the corresponding Jacobi matrices,
$\theta_i^{(n)}$ . . . eigenvalues of $\mathbf{T}_n$, $\omega_i^{(n)}$ . . . scaled and squared first components of the normalized eigenvectors of $\mathbf{T}_n$.

- Behind CG is Gauss Quadrature
- CG can be seen as a procedure for computing Gauss Quadrature nodes and weights.

CG and Gauss Quadrature for $f(\lambda) = \lambda^{-1}$

Symmetric, positive definite case

For $f(\lambda) \equiv \lambda^{-1}$ the formula takes the form

$$\int_{\zeta}^{\xi} \lambda^{-1} \, d\omega(\lambda) \;=\; \sum_{i=1}^{n} \frac{\omega_i^{(n)}}{\theta_i^{(n)}} \;+\; R_n(\lambda^{-1})$$

or, equivalently [Golub & Strakoš '94],

$$\frac{\|x\|_{\mathbf{A}}^2}{\|b\|^2} \;=\; n\text{-th Gauss quadrature} \;+\; \frac{\|x - x_n\|_{\mathbf{A}}^2}{\|b\|^2} \,.$$

We can approximate

$$\|x\|_{\mathbf{A}}^2 \;=\; x^T \mathbf{A} x \;=\; b^T x \;=\; b^T \mathbf{A}^{-1} b$$

using Gauss quadrature.

CG and Gauss Quadrature for $f(\lambda) = \lambda^{-1}$

Mathematically equivalent formulas (multiplied by $\|b\|^2$)

Gauss Quadrature based formula:

$$\|x\|_{\mathbf{A}}^2 \quad = \quad \|b\|^2 \, C_n \; + \; \|x - x_n\|_{\mathbf{A}}^2 \, ,$$

C_n is continued fraction corresponding to $\omega^{(n)}(\lambda)$

[Golub & Strakoš '94, Golub & Meurant '94, '97, '10]

Formulas based on algebraic manipulations

$$\begin{aligned} \|x\|_{\mathbf{A}}^2 &= b^T x_n + \|x - x_n\|_{\mathbf{A}}^2 \\ \|x\|_{\mathbf{A}}^2 &= \sum_{i=0}^{n-1} \alpha_i \|r_i\|^2 + \|x - x_j\|_{\mathbf{A}}^2 . \end{aligned}$$

The first one derived by [Warnick '00], the second one independently by [Hestenes & Stiefel '52, Deufelhard '93, Axelsson & Kaporin '01, Strakoš & T. '02]

CG and the approximation of $b^T \mathbf{A}^{-1} b$

Mathematically equivalent approximations

Approximation based on the formula

$$\|x\|_{\mathbf{A}}^2 \;=\; \|b\|^2 \; n\text{-th Gauss quadrature} \;+\; \|x - x_n\|_{\mathbf{A}}^2 \,.$$

If $\|x - x_n\|_{\mathbf{A}}^2$ is small then

$$b^T \mathbf{A}^{-1} b \;\approx\; \|b\|^2 \; n\text{-th Gauss quadrature}$$

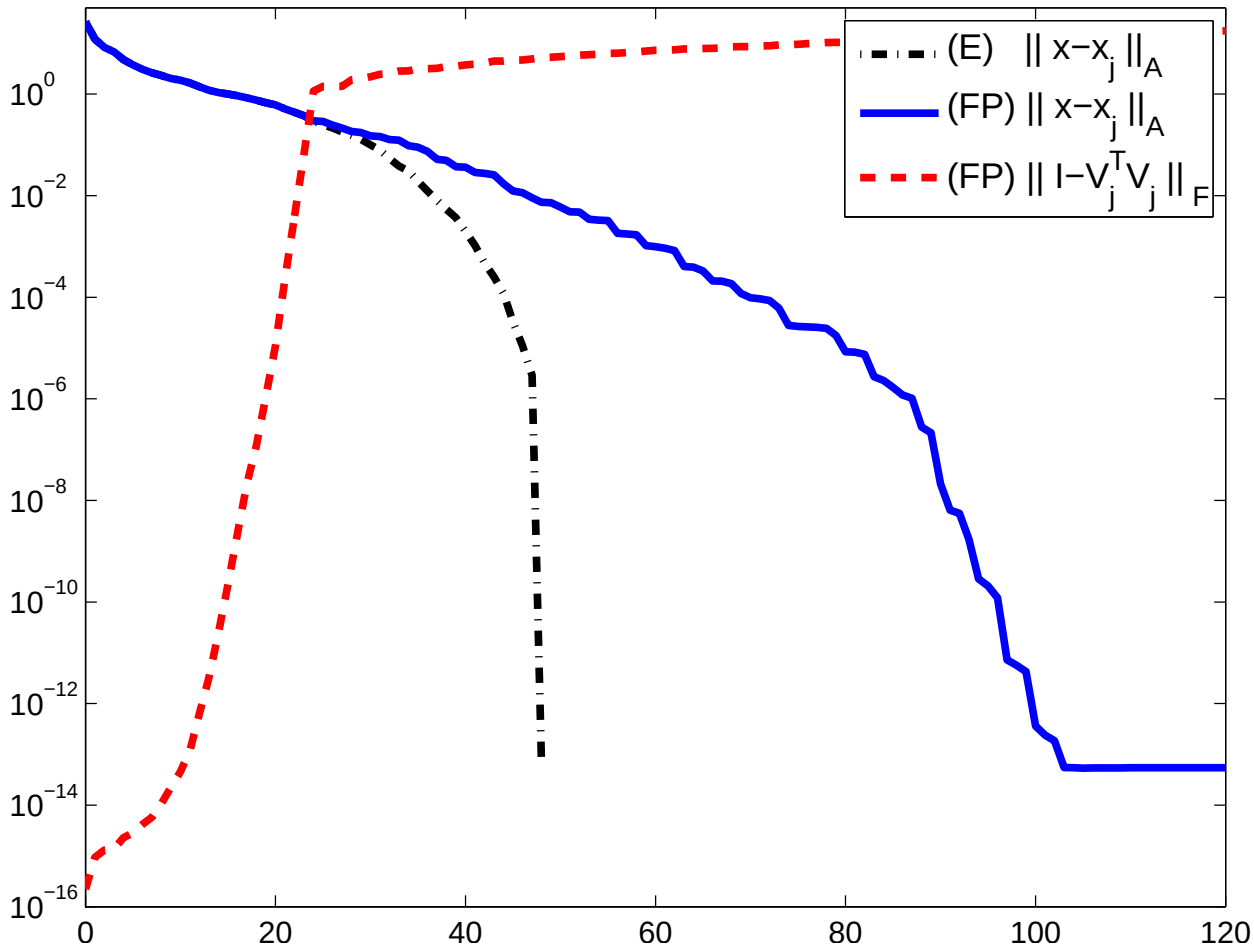
Mathematically equivalent approximations:

$$\|b\|^2 \, C_n, \qquad b^T x_n \qquad \text{and} \qquad \sum_{i=0}^{n-1} \alpha_i \|r_i\|^2 .$$

Finite precision arithmetic

CG behavior

Orthogonality is lost, convergence is delayed!



Identities need not hold in finite precision arithmetic!

Rounding error analysis

Strakoš & T. 2002

Do the identities hold for computed quantities?

1. $$\|x\|_{\mathbf{A}}^2 \quad = \quad b^T x_n \; + \; \|x - x_n\|_{\mathbf{A}}^2$$

   does not hold for computed quantities - its validity is based on preserving global orthogonality among CG residuals.

2. $$\|x\|_{\mathbf{A}}^2 \quad = \quad \sum_{i=0}^{n-1} \alpha_i \|r_i\|^2 \; + \; \|x - x_n\|_{\mathbf{A}}^2 .$$

   holds also for computed quantities - it is based on preserving local orthogonality between r_{n+1} and p_n.

What is the error $|\,\|x\|_{\mathbf{A}}^2 - \text{approx.}\,|$

in finite precision arithmetic?

Assume $\|b\| = 1$. Since $b^T x = x^T \mathbf{A} x = \|x\|_{\mathbf{A}}^2$,

$$\|x\|_{\mathbf{A}}^2 - b^T x_n = b^T (x - x_n)$$

and it holds that

$$|\, b^T (x - x_n)\,| \;\leq\; \|x - x_n\|\,.$$

Due to loss of orthogonality one can expect that

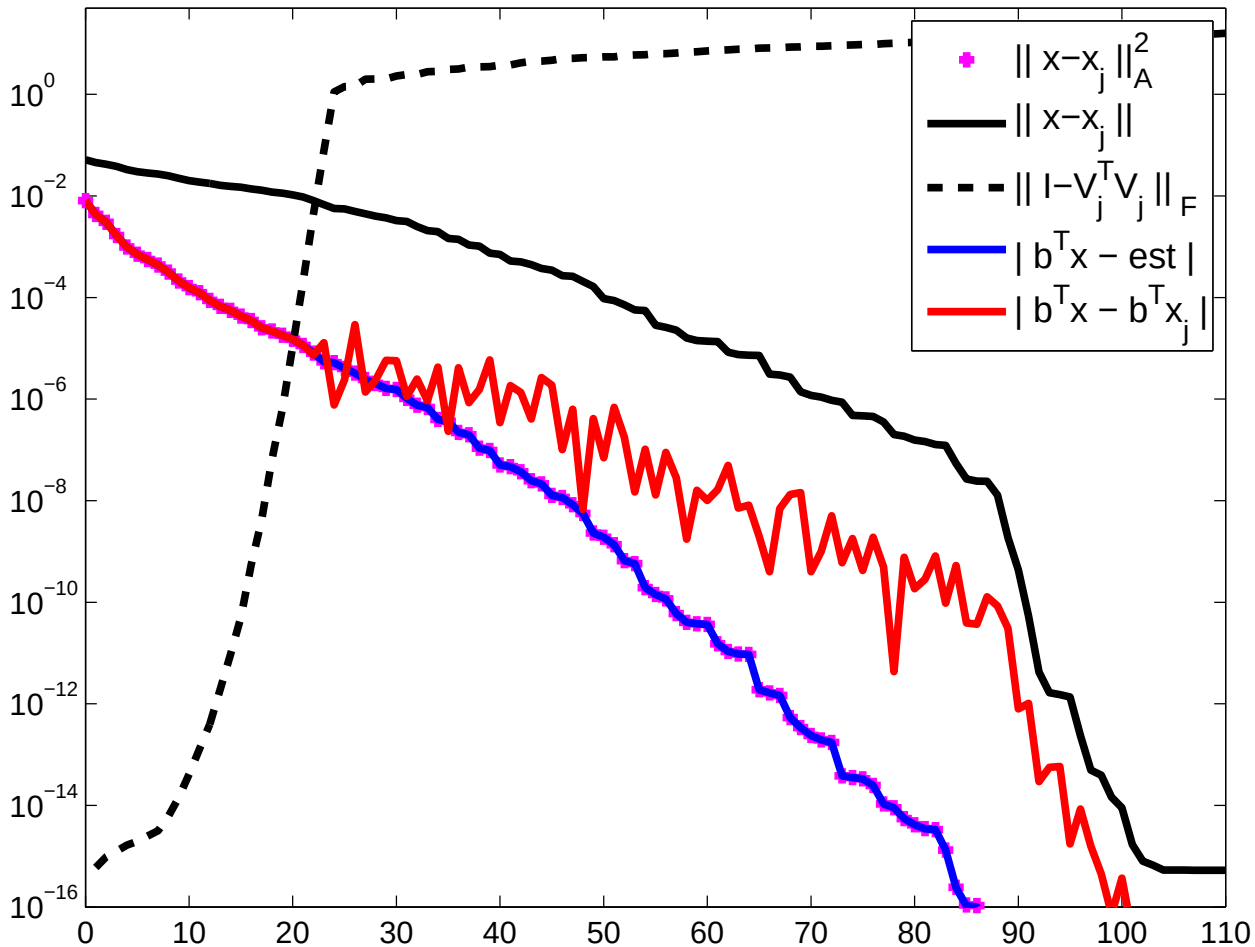
$$|\,\|x\|_{\mathbf{A}}^2 - b^T x_n\,| \quad\sim\quad \|x - x_n\| \quad\sim\quad \|x - x_n\|_{\mathbf{A}}$$

while

$$\|x\|_{\mathbf{A}}^2 - \sum_{i=0}^{n-1} \alpha_i \|r_i\|^2 \quad = \quad \|x - x_n\|_{\mathbf{A}}^2\,.$$

Behavior in finite precision arithmetic

$b^T x_n$ versus $\sum_{i=0}^{n-1} \alpha_i \|r_i\|^2$



Symmetric, positive definite case, $b \neq c$

Conjugate gradient method and non-symmetric Lanczos

1. Use the polarization identity

$$c^T \mathbf{A}^{-1} b \;=\; (c+b)^T \mathbf{A}^{-1}(c+b) - (c-b)^T \mathbf{A}^{-1}(c-b),$$

   and approximate $u^T \mathbf{A}^{-1} u$ for $u = c + b$ and $u = c - b$.

2. Apply the non-symmetric Lanczos to the SPD matrix $\mathbf{A}$ and approximate $c^T \mathbf{A}^{-1} b$ directly.
   Discussed thoroughly in [Golub & Meurant '94, '10]

For a real matrix $\mathbf{A}$, both approaches require approximately the same number of operations. The second approach can suffer from breakdowns.

For a complex matrix $\mathbf{A}$, the polarization identity is more complicated (it will be discussed later).

Symmetric, positive definite case

Summary I

Theoretical background: Gauss quadrature

$$\frac{b^T \mathbf{A}^{-1} b}{\|b\|^2} \;=\; n\text{-th Gauss quadrature} \;+\; \frac{\|x - x_n\|_{\mathbf{A}}^2}{\|b\|^2}\,.$$

If $c = b$, the best way how to approximate $b^T \mathbf{A}^{-1} b$ is to use the Hestenes-Stiefel estimate

$$b^T \mathbf{A}^{-1} b \;\approx\; \sum_{i=0}^{n-1} \alpha_i \|r_i\|^2\,.$$

If $c \neq b$, one can use the polarization identity

$$c^T \mathbf{A}^{-1} b \;=\; (c+b)^T \mathbf{A}^{-1} (c+b) - (c-b)^T \mathbf{A}^{-1} (c-b)\,.$$

Symmetric, positive definite case

Summary II

- We have seen that due to numerical instabilities, the explicit numerical computation of $c^* x_n$ can be highly inefficient.
  [Strakoš & T. '02, '05]

- If $\mathbf{A}$ is SPD and $c = b$, there are several efficient methods (based on CG or Hermitian Lanczos)
  [Golub & Meurant '94, '97, Axelsson & Kaporin '01, Strakoš & T. '02, '05]

- How to generalize ideas from the SPD case to a general case?
  - We need a theoretical background
    (find the best possible approximation in some sense).
  - Efficient numerical computation and justification
    of the approximation in finite precision arithmetic

Complex Gauss Quadrature?

Saylor-Smolarski approach

Let $\mathbf{A}$ be diagonalizable. [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].

Idea: Use BiCG or the Non-Hermitian Lanczos algorithm to generate (implicitly) formally orthogonal polynomials.

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

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

$\theta_k^{(n)}$ ... eigenvalues of $\hat{\mathbf{T}}_n$, $\omega_k^{(n)}$ ... scaled and squared first components of the normalized eigenvectors of $\hat{\mathbf{T}}_n$.

Moment problem

Classical formulation

Consider a non-decreasing distribution function $\omega(\lambda)$, $\lambda \geq 0$ with the moments given by the Riemann-Stieltjes integral

$$\xi_k = \int_0^\infty \lambda^k \, d\omega(\lambda) \,, \quad k = 0, 1, \ldots \,.$$

Find the distribution function $\omega^{(n)}(\lambda)$ with n points of increase $\lambda_i^{(n)}$ which matches the first $2n$ moments for the distribution function $\omega(\lambda)$, i.e. such that for $k = 0, 1, \ldots, 2n-1$

$$\xi_k = \int_0^\infty \lambda^k \, d\omega^{(n)}(\lambda) \equiv \sum_{i=1}^{n} \omega_i^{(n)} (\lambda_i^{(n)})^k \,.$$

Moment problem

and Gauss-Christoffel quadrature

Clearly,

$$\int_0^\infty \lambda^k \, d\omega(\lambda) \;=\; \sum_{i=1}^{n} \omega_i^{(n)} (\lambda_i^{(n)})^k, \quad k = 0, 1, \ldots, 2n-1$$

represents the n-point Gauss-Christoffel quadrature, see

- C. F. Gauss, [Methodus nova integralium valores per approximationem inveniendi, 1814],
- C. G. J. Jacobi, [Über Gauss neue Methode, die Werthe der Integrale näherungsweise zu finden, 1826],
- and the description given in H. H. J. Goldstine, [A History of Numerical Analysis from the 16th through the 19th Century, 1977].

With no loss of generality we assume $\xi_0 = 1$.

Model reduction via matching moments

Gauss-Christoffel quadrature formulation

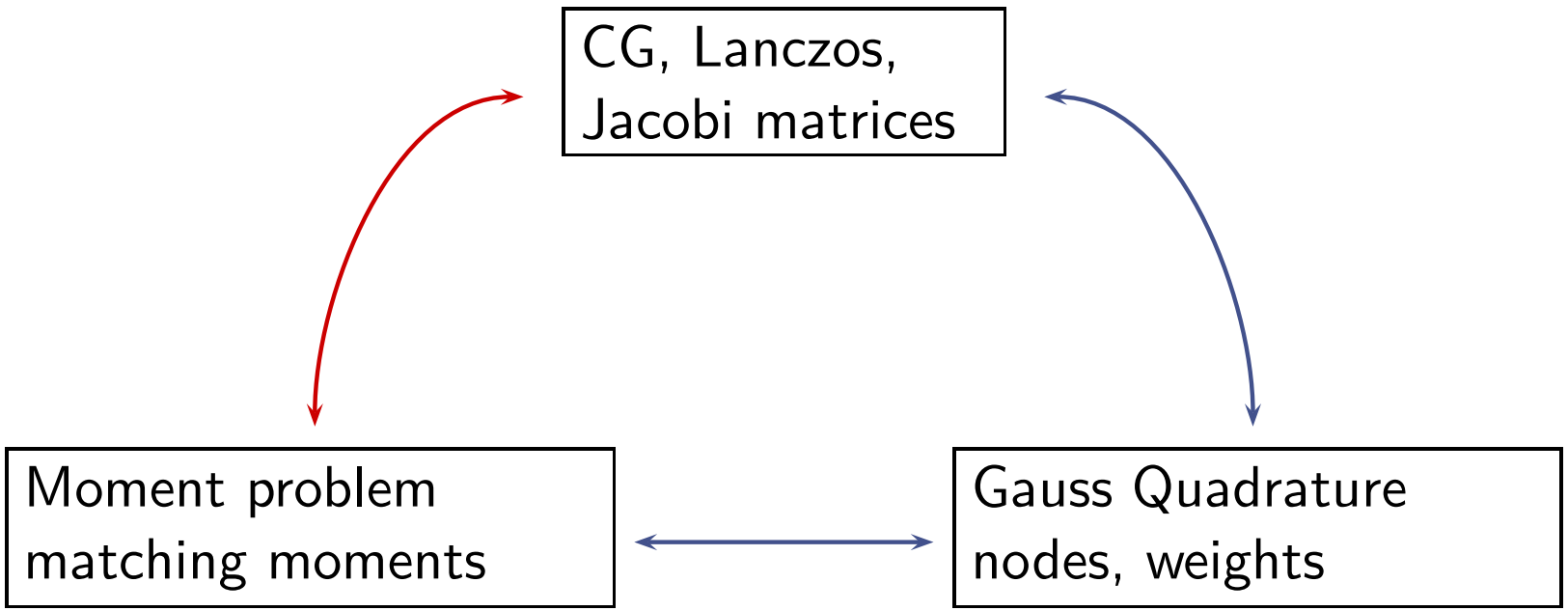
$$\int_0^\infty f(\lambda)\, d\omega(\lambda) \;\approx\; \sum_{i=1}^{n} \omega_i^{(n)} f(\lambda_i^{(n)})\,,$$

where the reduced model given by the distribution function with n points of increase $\omega^{(n)}$ matches the first $2n$ moments

$$\int_0^\infty \lambda^k\, d\omega(\lambda) \;=\; \sum_{i=1}^{n} \omega_i^{(n)} (\lambda_i^{(n)})^k\,, \quad k = 0, 1, \ldots, 2n-1\,.$$

CG, Gauss Quadrature and Matching Moments

Overview



Matching moments

Matrix formulation, without loss of generality $\|b\| = 1$

How to express moments in terms of $\mathbf{A}$, b and $\mathbf{T}_n$?

$$\begin{aligned}
\int_0^\infty \lambda^k \, d\omega(\lambda) &= \sum_{i=1}^{N} \omega_j \, (\lambda_j)^k &&= b^* \, \mathbf{A}^k \, b \,, \\
\int_0^\infty \lambda^k \, d\omega^{(n)}(\lambda) &= \sum_{i=1}^{n} \omega_i^{(n)} \, (\theta_i^{(n)})^k &&= e_1^T \, \mathbf{T}_n^k \, e_1 \,.
\end{aligned}$$

Matching the first $2n$ moments therefore means

$$b^* \, \mathbf{A}^k \, b \equiv e_1^T \, \mathbf{T}_n^k \, e_1 \,, \quad k = 0, 1, \ldots, 2n-1 \,.$$

Model reduction via matching moments

Another view of the CG and Lanczos algorithms

Let $\|b\| = 1$.

CG (Lanczos) reduces for $\mathbf{A}$ HPD at the step n the original model

$$\mathbf{A}x = b \qquad \text{to} \qquad \mathbf{T}_n y_n = e_1$$

such that $2n$ moments are matched,

$$b^* \mathbf{A}^k b = e_1^T \mathbf{T}_n^k e_1, \qquad k = 0, 1, \ldots, 2n-1\,.$$

The Vorobyev moment problem

Vorobyev '58, '65, popularized by Brezinski '97, Strakoš '08

Find a linear HPD 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 $\mathbf{Q}_n$ projects onto $\mathcal{K}_n(\mathbf{A}, b)$ orthogonally to $\mathcal{K}_n(\mathbf{A}, b)$.

Moment problem:

$$\omega(\lambda) \quad \rightarrow \quad \omega^{(n)}(\lambda)\,.$$

Vorobyev moment problem:

$$\mathbf{A},\ v \quad \rightarrow \quad \mathbf{A}_n,\ v\,.$$

Lanczos and the Vorobyev moment problem

Model reduction via matching moments

Let $\mathbf{V}_n$ and $\mathbf{T}_n$ are matrices from the Lanczos algorithm. Then

$$\begin{aligned} \mathbf{Q}_n &= \mathbf{V}_n \mathbf{V}_n^*, \\ \mathbf{A}_n &= \mathbf{V}_n \mathbf{T}_n \mathbf{V}_n^*. \end{aligned}$$

We can identify Lanczos with the Vorobyev moment problem.

Using the Vorobyev moment problem one can show [Strakoš '08]

$$b^* \mathbf{A}^k b \;=\; b^* \mathbf{A}_n^k b \;=\; e_1^* \mathbf{T}_n^k e_1, \qquad k = 0, \ldots, 2n-1\,.$$

The matching moment property of Lanczos (CG) can be shown without using Gauss Quadrature!

This view of Krylov subspace methods appears to be useful when generalizing the ideas from the HPD case.

Vorobyev moment problem

General case

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

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,

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

Non-Hermitian Lanczos

Vorobyev moment problem, matching moments, model reduction

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

- Then

$$\begin{aligned} \mathbf{Q}_n &= \mathbf{V}_n \mathbf{W}_n^* , \\ \mathbf{A}_n &= \mathbf{V}_n \mathbf{T}_n \mathbf{W}_n^* . \end{aligned}$$

- Matching moments property of Non-Hermitian Lanczos:

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

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

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

$$w^* \mathbf{A}^k v = w^* \mathbf{A}_n^k v = e_1^* \mathbf{T}_n^k e_1, \qquad k = 0, \ldots, 2n-1 .$$

- Model reduction

$$\mathbf{A}, v, w \quad \rightarrow \quad \mathbf{T}_n, e_1, e_1 .$$

Arnoldi algorithm

Vorobyev moment problem, matching moments, model reduction

Define $\mathbf{Q}_n$: it projects onto $\mathcal{K}_n(\mathbf{A}, v)$ orthogonally to $\mathcal{K}_n(\mathbf{A}, v)$.

- Then

$$\begin{aligned} \mathbf{Q}_n &= \mathbf{V}_n \mathbf{V}_n^* \,, \\ \mathbf{A}_n &= \mathbf{V}_n \mathbf{H}_n \mathbf{V}_n^* \,. \end{aligned}$$

- Matching moments property of Arnoldi:

$$w^* \mathbf{A}^k v = w^* \mathbf{A}_n^k v = t_n^* \mathbf{H}_n^k e_1, \qquad k = 0, \ldots, n-1 \,,$$

  w is given, $t_n = \mathbf{V}_n^* w$.

- Model reduction

$$\mathbf{A}, v, w \quad \rightarrow \quad \mathbf{H}_n, e_1, t_n \,.$$

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

Theoretical background - 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 $\mathcal{K}_n(\mathbf{A}, b)$,

- $\mathbf{A}_n^{-1} = \mathbf{V}_n \mathbf{T}_n^{-1} \mathbf{W}_n^*$ in Non-Hermitian Lanczos,
- $\mathbf{A}_n^{-1} = \mathbf{V}_n \mathbf{H}_n^{-1} \mathbf{V}_n^*$ in 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 (using global biorthogonality) that

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

Finally,

$$c^* \mathbf{A}_n^{-1} b \; = \; (c^* v_1) \, \|b\| \, (\mathbf{T}_n^{-1})_{1,1} \; = \; c^* x_n \; = \; \sum_{j=0}^{n-1} \alpha_j s_j^* r_j \, .$$

Complex Gauss Quadrature

Saylor-Smolarski approach

Let $\mathbf{A}$ be diagonalizable.

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

$$c^* \mathbf{A}^{-1} b \;\approx\; G\left(\lambda^{-1}\right) \;\equiv\; \sum_{k=1}^{n} \frac{\omega_k}{\theta_k}\,,$$

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

[Warnick '00] showed:

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

where x_n is the nth BiCG approximation. Therefore,

$$c^* \mathbf{A}_n^{-1} b \;=\; c^* x_n \;=\; G\left(\lambda^{-1}\right).$$

Yet another approach

Hybrid BiCG methods

We know that

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

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. '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

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

Preconditioning

General case

Let $\mathbf{P}_L$ and $\mathbf{P}_R$ be a left and a right preconditioner. Then

$$c^* \mathbf{A}^{-1} b = (\underbrace{\mathbf{P}_R^{-*} c}_{\hat{c}})^* \underbrace{(\mathbf{P}_L^{-1} \mathbf{A} \mathbf{P}_R^{-1})^{-1}}_{\hat{\mathbf{A}}^{-1}} (\underbrace{\mathbf{P}_L^{-1} b}_{\hat{b}}) .$$

The approximation techniques can be applied to the problem

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

It is obvious that $\hat{\mathbf{A}}$ need not be formed explicitly.

It is easier to derive the preconditioned algorithm
for approximating the scattering amplitude than
the preconditioned algorithm for solving linear systems.

Transformation to the Hermitian positive definite case

Basic ideas

$$c^* \mathbf{A}^{-1} b = c^* \mathbf{A}^* (\mathbf{A}\mathbf{A}^*)^{-1} b = c^* (\mathbf{A}^* \mathbf{A})^{-1} \mathbf{A}^* b \,,$$

- $\widetilde{c} \equiv \mathbf{A} c$ and approximate $\widetilde{c}^* (\mathbf{A}\mathbf{A}^*)^{-1} b \,,$
- $\widetilde{b} \equiv \mathbf{A}^* b$ and approximate $c^* (\mathbf{A}^* \mathbf{A})^{-1} \widetilde{b} \,.$

Approximate

$$u^* \mathbf{B}^{-1} v \,,$$

where $\mathbf{B}$ is Hermitian and positive definite.

1. Using the polarization identity,
2. BiCG applied to the Hermitian problem,
3. GLSQR approach (Block-Lanczos approach).

Transformation to the Hermitian positive definite case

Using the polarization identity

$$\langle v, u\rangle \;=\; \frac{1}{2}\left(\|v+u\|^2 - (1+\mathbf{i})(\|v\|^2+\|u\|^2) + \mathbf{i}\|v+\mathbf{i}u\|^2\right).$$

Considering $\langle v, u\rangle \equiv u^*\mathbf{B}^{-1}v$, the approximation of $u^*\mathbf{B}^{-1}v$ requires approximation of four terms

$$u^*\mathbf{B}^{-1}u\,,\quad (v+u)^*\mathbf{B}^{-1}(v+u)\,,\quad (v+\mathbf{i}u)^*\mathbf{B}^{-1}(v+\mathbf{i}u)\,,\quad v^*\mathbf{B}^{-1}v\,.$$

One term is always known,

- If $\mathbf{B} = \mathbf{A}\mathbf{A}^*$, $u = \mathbf{A}c$, $v = b$, then $u^*\mathbf{B}^{-1}u = \|c\|^2$.
- If $\mathbf{B} = \mathbf{A}^*\mathbf{A}$, $u = c$, $v = \mathbf{A}^*b$, then $v^*\mathbf{B}^{-1}v = \|b\|^2$.

Methods:

- Use CGNE, CGNR of LSQR.
- The price: *six* matrix-vector multiplications (three with $\mathbf{A}$ and three with $\mathbf{A}^*$) per one iteration step.

Transformation to the Hermitian positive definite case

GLSQR approach - closely connected to Golub-Kahan bi-diagonalization

Apply the block-Lanczos algorithm to the matrix $\mathbf{A}^*\mathbf{A}$ with the starting block $[c, \mathbf{A}^*b]$ or, equivalently, to the augmented matrix

$$\begin{bmatrix} 0 & \mathbf{A} \\ \mathbf{A}^* & 0 \end{bmatrix} \quad \text{with the starting block} \quad \begin{bmatrix} u_1 & 0 \\ 0 & v_1 \end{bmatrix},$$

where $u_1 = b/\|b\|$, $v_1 = c/\|c\|$.

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

The GLSQR method uses the following recurrences

$$\mathbf{A}\mathbf{V}_n = \mathbf{U}_n\mathbf{T}_n + \xi_{n+1}u_{n+1}e_n^T\,,$$
$$\mathbf{A}^*\mathbf{U}_n = \mathbf{V}_n\mathbf{T}_n^* + \theta_{n+1}v_{n+1}e_n^T\,,$$

where $\mathbf{V}_n$ and $\mathbf{U}_n$ are matrices with orthonormal columns, $\mathbf{T}_n$ is tridiagonal. Approximate $c^*\mathbf{A}^{-1}b$ using block Gauss quadrature,

$$c^*\mathbf{A}^{-1}b \qquad \text{by} \qquad \|c\|\|b\|\, e_1^T\mathbf{T}_n^{-1}e_1\,.$$

General case

Summary I

Theoretical background: Model reduction via matching moments .

Several Krylov subspace methods (Lanczos, Arnoldi) can be identified with the Vorobyev moment problem $\mathbf{A} \quad \rightarrow \quad \mathbf{A}_n$.

Approximation:

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

Promising approaches:

$$\text{BiCG} \qquad \text{and} \qquad c^* \mathbf{A}^{-1} b \approx \sum_{j=0}^{n-1} \alpha_j s_j^* r_j \, ,$$

$$\text{Arnoldi} \qquad \text{and} \qquad c^* \mathbf{A}^{-1} b \approx \|b\| \, t_n^* \mathbf{H}_n^{-1} e_1 \, ,$$

where $t_n = \mathbf{V}_n^* c$.

General case – transformation to the HPD case

Summary II

Disadvantage: One can expect slower convergence.

Theoretical background: (block) Gauss quadrature .

Approach based on polarization identity and a CG-like method for normal equations requires six matrix-vector products per iteration.

The most promising approach: GLSQR

- based on block Gauss Quadrature,
- only two matrix-vector products per iteration,
- approximate $c^* \mathbf{A}^{-1} b$ by

$$\|c\| \|b\| \, e_1^T \mathbf{T}_n^{-1} e_1 \, ,$$

  where $\mathbf{T}_n$ is tridiagonal.

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.

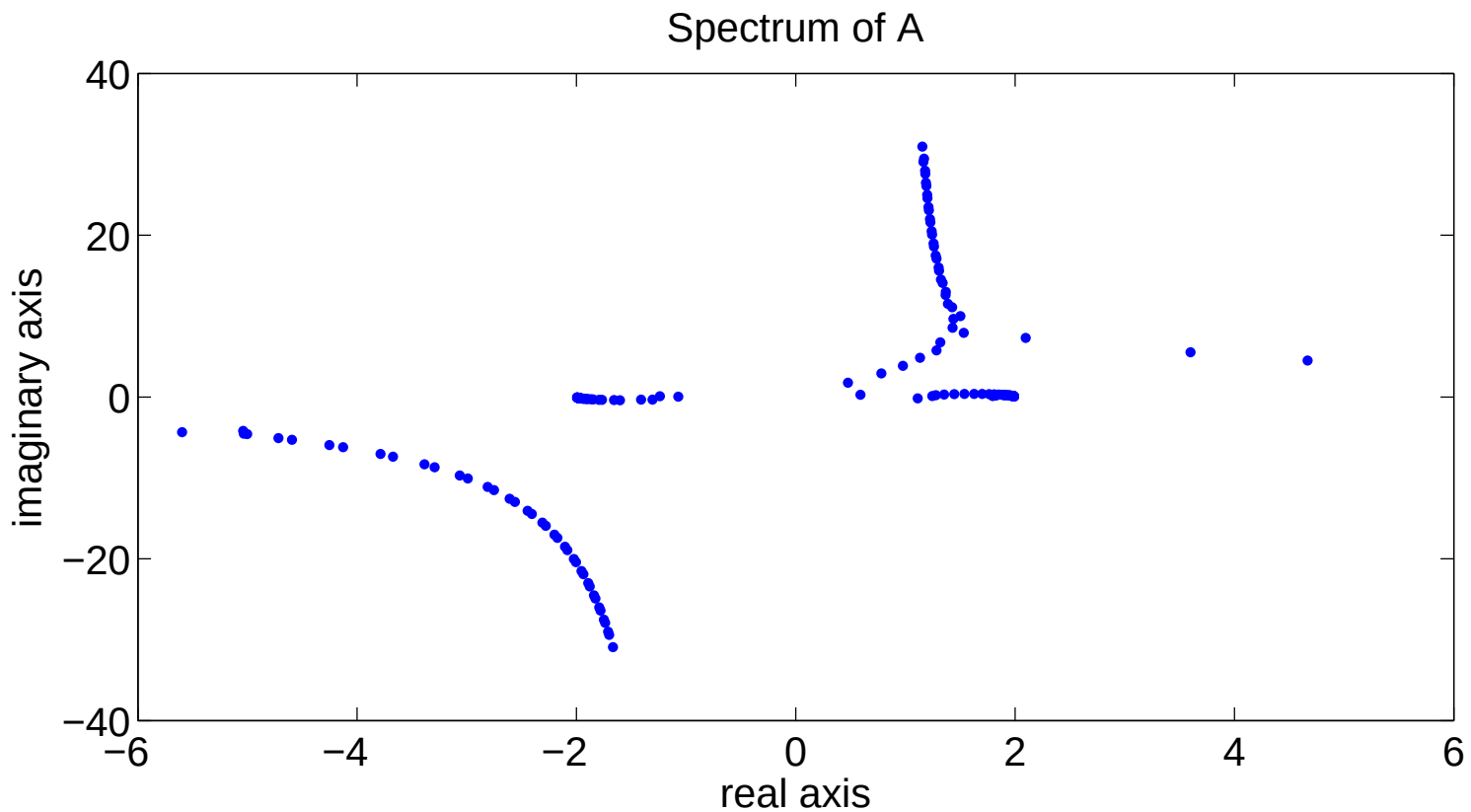
Typically, one needs only the dominant $(M+1)$st component

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

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

The matrix $\mathbf{A}$

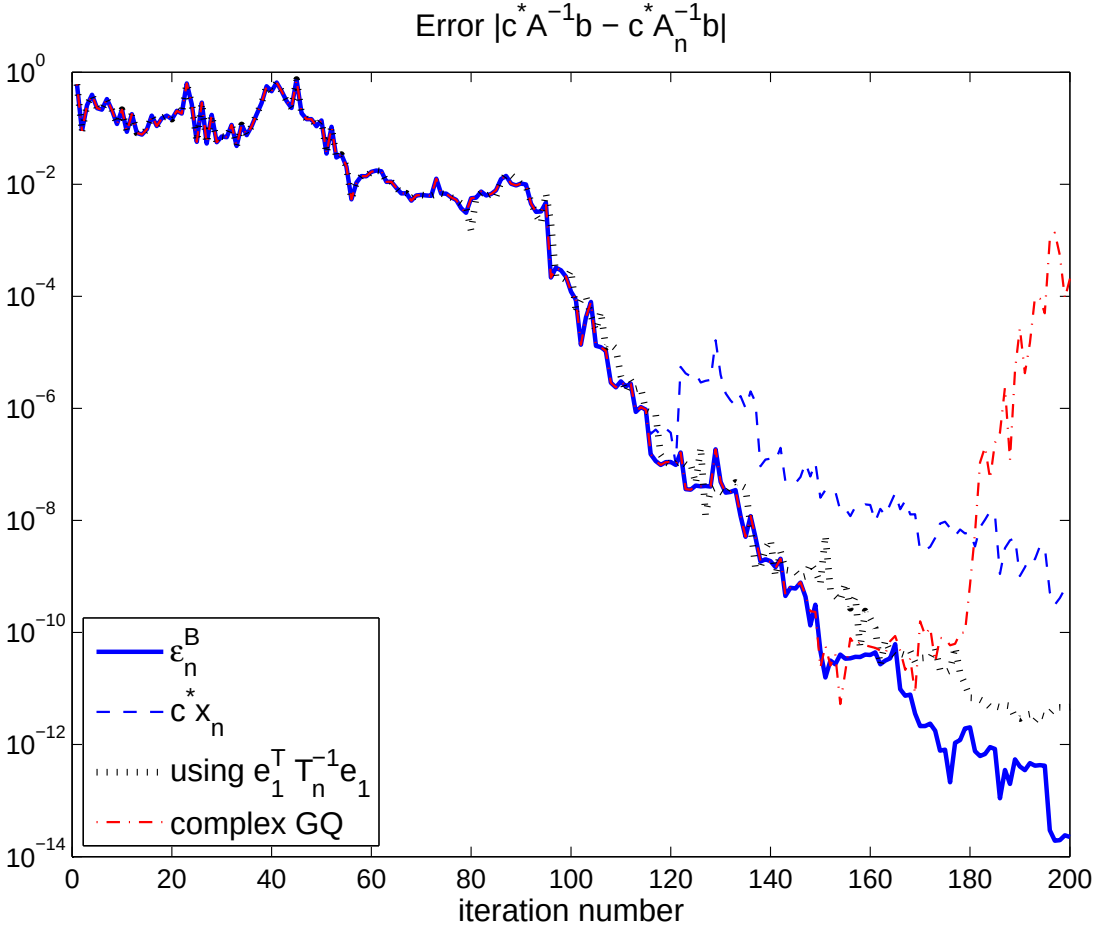
Spectrum of $\mathbf{A}$ computed via the Matlab command `eig`



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

Non-Hermitian Lanczos approach

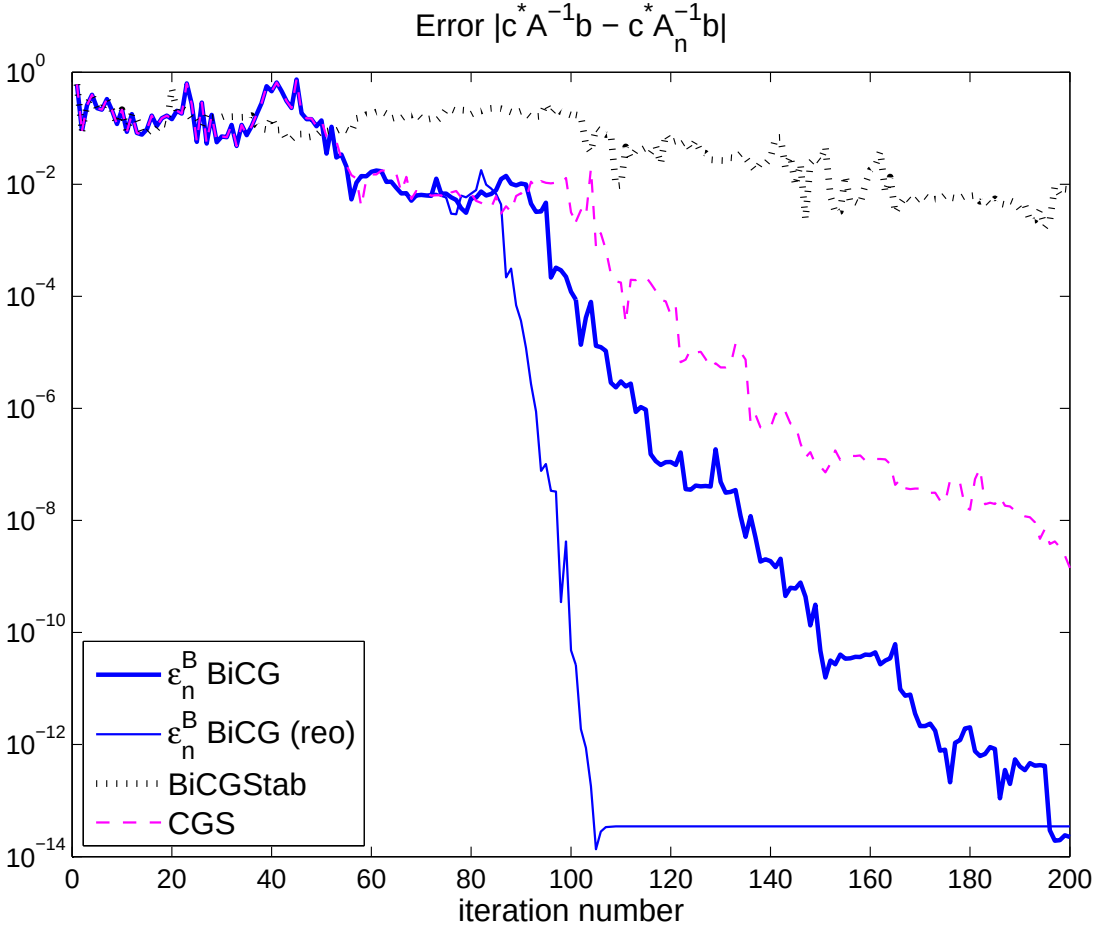
Mathematically equivalent estimates I



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

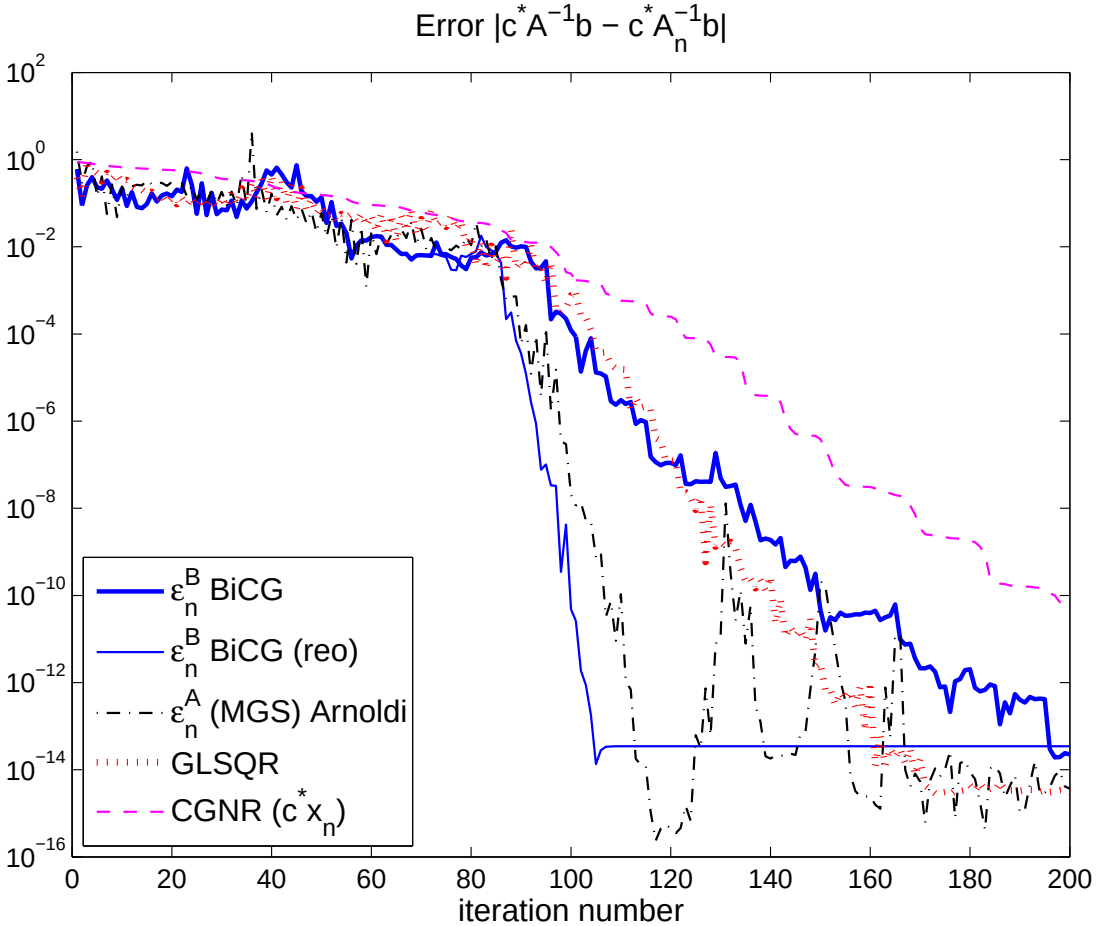
Non-Hermitian Lanczos approach

Mathematically equivalent estimates II



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

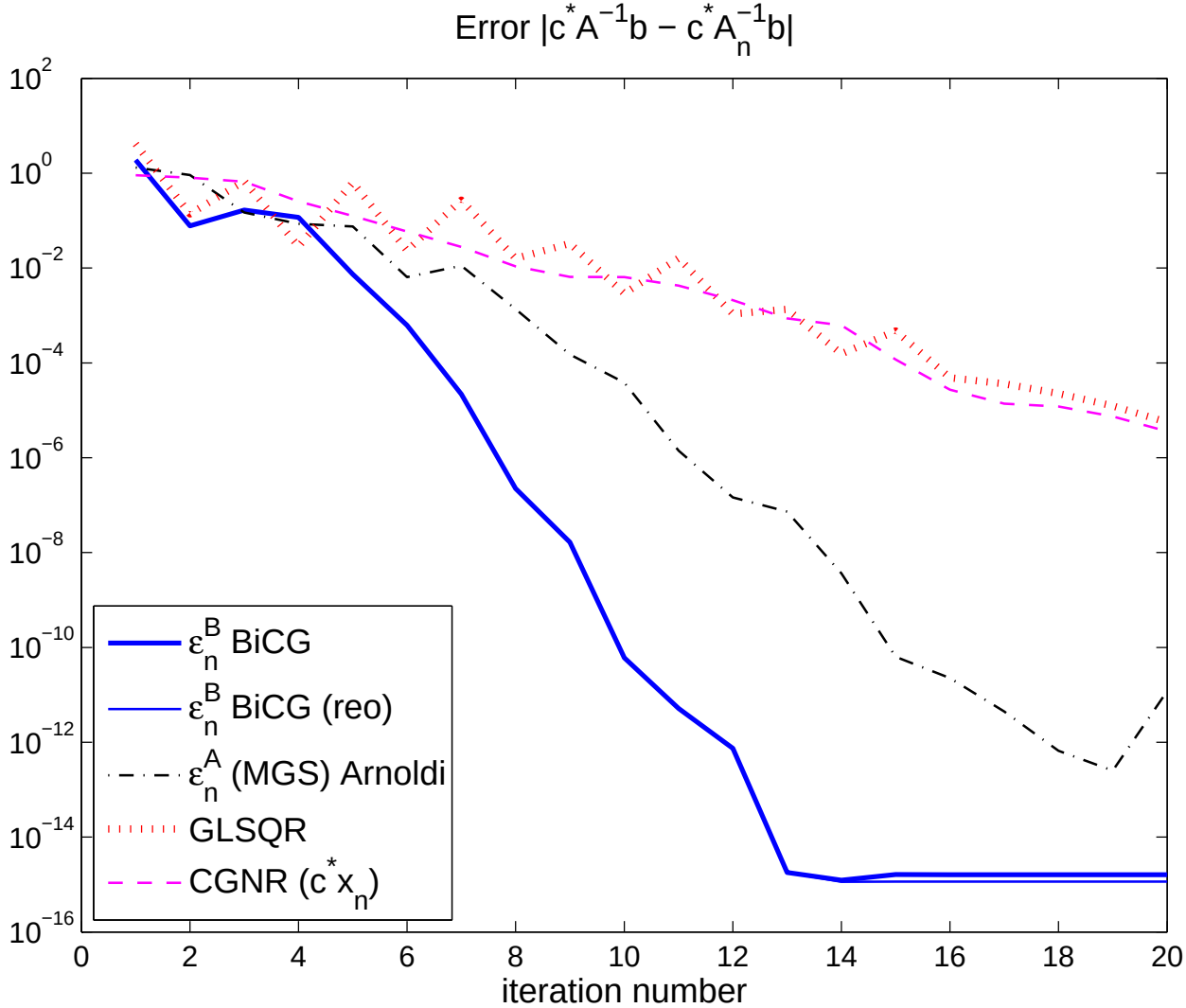
Non-Hermitian Lanczos, Arnoldi, GLSQR



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

Different approaches with preconditioning

Non-Hermitian Lanczos, Arnoldi, GLSQR



Conclusions

- Some Krylov subspace methods can be seen as model reduction via matching moments.
- Generalization of the HPD case:
  - Via Vorobyev moment problem $\longrightarrow$ 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

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

  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 publications

- 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, [Model reduction using the Vorobyev moment problem , Numerical Algorithms, 51, 2009, pp. 363–379].
- 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].

Recent book by G. H. Golub and G. Meurant, [Matrices, Moments and Quadrature With Applications, Princeton University Press, USA, 2010].

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!