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

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joint work with

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Given a nonsingular matrix $A$ and vectors $b$ and $c$.

We want to approximate

$$c^* A^{-1} b.$$ 

Equivalently, we look for an approximation to

$$c^* x \quad \text{such that} \quad A x = b.$$
Motivation

- **Approximation of the $j$th component of the solution**
  - i.e., we want to approximate $e_j^T A^{-1} b$.

- **Signal processing (the scattering amplitude)**
  - $b$ and $c$ represent incoming and outgoing waves, respectively, and the operator $A$ relates the incoming and scattered fields on the surface of an object,
  - $Ax = b$ 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

\[ \mathcal{K}_n(A, b) = \text{span}\{b, Ab, \ldots A^{n-1}b\} . \]
Krylov subspace methods approach

Projection of the original problem onto Krylov subspaces

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

\[ c^* A^{-1} b = c^* x \approx c^* x_n . \]
Krylov subspace methods approach

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- The approximation \( c^* x_n \) can be highly inefficient!

How to approximate \( c^* x \) without looking for \( x_n \)?
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  How to approximate \( c^* x \) without looking for \( x_n \)?

- We need a theoretical background
  (find the best possible approximation in some sense).
Krylov subspace methods approach
Projection of the original problem onto Krylov subspaces

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- 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 bilinear form $c^* A^{-1} b$
4. Numerical experiments
Outline

1 Symmetric, positive definite case

2 Matching moments

3 Approximation of the bilinear form $c^*A^{-1}b$

4 Numerical experiments
The CG method
Let $A$ be symmetric, positive definite

Solve $Ax = b$.

**input** $A$, $b$

$x_0 = 0$

$r_0 = p_0 = b$

**for** $k = 0, 1, \ldots$

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

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

$$r_{k+1} = r_k - \alpha_k Ap_k,$$

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

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

**end**
The Lanczos algorithm

Let $A$ be symmetric

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

**input** $A$, $b$

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

**for** $k = 1, 2, \ldots$

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

**end**
The Lanczos algorithm
Let \( \mathbf{A} \) be symmetric

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

**input** \( \mathbf{A}, b \)

\[
v_1 = b/\|b\|, \quad \delta_1 = 0,
\]

**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 $A$ be symmetric, positive definite

Let

$$
T_n = \begin{bmatrix}
\gamma_1 & \delta_2 \\
\delta_2 & \ddots & \ddots \\
\delta_n & \ddots & \ddots & \ddots \\
\delta_n & \gamma_n
\end{bmatrix} = L_n L_n^T
$$

where

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

The CG approximation is the given by

$$
T_n y_n = \|b\| e_1, \quad x_n = x_0 + V_n y_n.
$$
Distribution function $\omega(\lambda)$

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

\[
(\lambda_i, u_i) \ldots \text{eigenpair of } A, \quad \omega_i = (b^T u_i)^2.
\]
Distribution function $\omega(\lambda)$

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

$(\lambda_i, u_i)$ \ldots eigenpair of $A$, \hfill \omega_i = (b^T u_i)^2$. 

\[
\int_{\zeta}^{\xi} f(\lambda) \, d\omega(\lambda) = \sum_{i=1}^{N} \omega_i \, f(\lambda_i) .
\]
At any iteration step \( n \), CG (implicitly) determines weights and nodes of the \( n \)-point Gauss quadrature

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

\( T_n \) ... the corresponding Jacobi matrices,
\( \theta_i^{(n)} \) ... eigenvalues of \( T_n \), \( \omega_i^{(n)} \) ... scaled and squared first components of the normalized eigenvectors of \( T_n \).
At any iteration step $n$, CG (implicitly) determines weights and nodes of the $n$-point Gauss quadrature

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

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

CG matches the first $2n$ moments, $f(\lambda) = \lambda^k$, $k = 0, \ldots, 2n - 1$

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

Moment problem:

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

$$\frac{\|x\|_A^2}{\|b\|_2^2} = n\text{-th Gauss quadrature} + \frac{\|x - x_n\|_A^2}{\|b\|_2^2}.$$
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],

\[
\frac{\|x\|_{A}^{2}}{\|b\|^{2}} = n\text{-th Gauss quadrature} + \frac{\|x - x_{n}\|_{A}^{2}}{\|b\|^{2}}.
\]

We can approximate

\[
\|x\|_{A}^{2} = x^{T}Ax = b^{T}x = b^{T}A^{-1}b
\]

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

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

Gauss Quadrature based formula:

$$\|x\|_A^2 = \|b\|^2 C_n + \|x - x_n\|_A^2,$$

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


Formulas based on algebraic manipulations

$$\|x\|_A^2 = b^T x_n + \|x - x_n\|_A^2$$

$$\|x\|_A^2 = \sum_{i=0}^{n-1} \alpha_i \|r_i\|^2 + \|x - x_j\|_A^2.$$

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

\[ \|x\|_A^2 = \|b\|^2 \text{ } n\text{-th Gauss quadrature} + \|x - x_n\|_A^2. \]

If \(\|x - x_n\|_A^2\) is small then

\[ b^T A^{-1} b \approx \|b\|^2 \text{ } n\text{-th Gauss quadrature} \]
CG and the approximation of $b^T A^{-1} b$

Mathematically equivalent approximations

Approximation based on the formula

$$\|x\|_A^2 = \|b\|^2 \text{ n-th Gauss quadrature} + \|x - x_n\|_A^2.$$ 

If $\|x - x_n\|_A^2$ is small then

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

Mathematically equivalent approximations:

$$\|b\|^2 C_n, \quad b^T x_n \quad \text{and} \quad \sum_{i=0}^{n-1} \alpha_i \|r_i\|^2.$$
Orthogonality is lost, convergence is delayed!

Relations need not hold in finite precision arithmetic!
Do the relations hold for computed quantities?

\[ \|x\|_A^2 = b^T x_n + \|x - x_n\|_A^2 \]

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

1

\[ \| x \|_A^2 = b^T x_n + \| x - x_n \|_A^2 \]

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

2

\[ \| x \|_A^2 = \sum_{i=0}^{n-1} \alpha_i \| r_i \|^2 + \| x - x_n \|_A^2. \]

holds also for computed quantities - it is based on preserving local orthogonality between \( r_{n+1} \) and \( p_n \).
Behavior in finite precision arithmetic

\[ b^T x_n \quad \text{versus} \quad \sum_{i=0}^{n-1} \alpha_i \| r_i \|^2 \]
Symmetric, positive definite case

Summary

Theoretical background: Gauss quadrature

\[
\frac{b^T A^{-1} b}{\|b\|^2} = n\text{-th Gauss quadrature} + \frac{\|x - x_n\|^2_A}{\|b\|^2}.
\]
Symmetric, positive definite case

Summary

Theoretical background: Gauss quadrature

\[
\frac{b^T A^{-1} b}{\|b\|^2} = n\text{-th Gauss quadrature} + \frac{\|x - x_n\|^2_A}{\|b\|^2}.
\]

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

\[
b^T A^{-1} b \approx \sum_{i=0}^{n-1} \alpha_i \|r_i\|^2.
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Symmetric, positive definite case

Summary

Theoretical background: Gauss quadrature

\[
\frac{b^T A^{-1} b}{\|b\|^2} = \text{n-th Gauss quadrature} + \frac{\|x - x_n\|^2_A}{\|b\|^2}.
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\]

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

- How to generalize ideas from the SPD case to a general case?
Outline

1 Symmetric, positive definite case
2 Matching moments
3 Approximation of the bilinear form $c^* A^{-1} b$
4 Numerical experiments
CG, Gauss Quadrature and Matching Moments

Overview

CG, Lanczos, Jacobi matrices

Moment problem
matching moments

Gauss Quadrature
nodes, weights
CG, Gauss Quadrature and Matching Moments

Overview

- CG, Lanczos, Jacobi matrices
- Moment problem matching moments
- Gauss Quadrature nodes, weights
How to express moments in terms of $A$, $b$ and $T_n$?

\[
\int_0^\infty \lambda^k d\omega(\lambda) = \sum_{i=1}^N \omega_j (\lambda_j)^k = b^* A^k b, \\
\int_0^\infty \lambda^k d\omega^{(n)}(\lambda) = \sum_{i=1}^n \omega_i^{(n)} (\theta_i^{(n)})^k = e_1^T T_n^k e_1.
\]
Matching moments

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

How to express moments in terms of $A$, $b$ and $T_n$?

$$\int_{0}^{\infty} \lambda^k d\omega(\lambda) = \sum_{i=1}^{N} \omega_j (\lambda_j)^k = b^* A^k b,$$

$$\int_{0}^{\infty} \lambda^k d\omega^{(n)}(\lambda) = \sum_{i=1}^{n} \omega_i^{(n)} (\theta_i^{(n)})^k = e_1^T T_n^k e_1.$$

Matching the first $2n$ moments therefore means

$$b^* A^k b \equiv e_1^T T_n^k e_1, \quad k = 0, 1, \ldots, 2n - 1.$$
Let $\|b\| = 1$.

CG (Lanczos) reduces for $A$ HPD at the step $n$ the original model

$$Ax = b \quad \text{to} \quad T_n y_n = e_1$$
Let $\|b\| = 1$.

CG (Lanczos) reduces for $A$ HPD at the step $n$ the original model

$$Ax = b \quad \text{to} \quad T_n y_n = e_1$$

such that $2n$ moments are matched,

$$b^* A^k b = e_1^T T_n^k e_1, \quad k = 0, 1, \ldots, 2n - 1.$$
Find a linear HPD operator $A_n$ on $\mathcal{K}_n(A, v)$ such that

\[
A_n v = A v, \\
A^2_n v = A^2 v, \\
\vdots \\
A^{n-1}_n v = A^{n-1} v, \\
A^n_n v = Q_n A^n v,
\]

where $Q_n$ projects onto $\mathcal{K}_n(A, b)$ orthogonally to $\mathcal{K}_n(A, b)$. 
The Vorobyev moment problem
Vorobyev ’58, ’65, popularized by Brezinski ’97, Strakoš ’08

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

\[
\begin{align*}
A_n v &= A v, \\
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&\vdots \\
A^{n-1}_n v &= A^{n-1} v, \\
A^n_n v &= Q_n A^n v,
\end{align*}
\]

where \( Q_n \) projects onto \( \mathcal{K}_n(A, b) \) orthogonally to \( \mathcal{K}_n(A, b) \).

Moment problem:

\[
\omega(\lambda) \rightarrow \omega^{(n)}(\lambda).
\]

Vorobyev moment problem:

\[
A, v \rightarrow A_n, v.
\]
Let $V_n$ and $T_n$ are matrices from the Lanczos algorithm. Then

$$Q_n = V_n V_n^*, \quad A_n = V_n T_n V_n^*.$$ 

We can identify Lanczos with the Vorobyev moment problem.
Lanczos and the Vorobyev moment problem
Model reduction via matching moments

Let $V_n$ and $T_n$ are matrices from the Lanczos algorithm. Then

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

$$b^* A^k b = b^* A_n^k b = e_1^* T_n^k e_1, \quad k = 0, \ldots, 2n - 1.$$  

The matching moment property of Lanczos (CG) can be shown without using Gauss Quadrature!
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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 $A_n$ on $\mathcal{K}_n(A, v)$ such that

\[
A_n v = Av,
\]
\[
A^2_n v = A^2 v,
\]
\[
\vdots
\]
\[
A^{n-1}_n v = A^{n-1} v,
\]
\[
A^n_n v = Q_n A^n v,
\]

where $Q_n$ is a given linear projection operator.
Vorobyev moment problem

General case

Find a linear operator $A_n$ on $K_n(A, v)$ such that

\[
\begin{align*}
A_n v &= A v, \\
A^2_n v &= A^2 v, \\
&\vdots \\
A^{n-1}_n v &= A^{n-1} v, \\
A^n_n v &= Q_n A^n v,
\end{align*}
\]

where $Q_n$ 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 $A$, $v$ and $w$.

Non-Hermitian Lanczos algorithm is represented by

$$\begin{align*}
AV_n &= V_n T_n + \delta_{n+1} v_{n+1} e_n^T, \\
A^* W_n &= W_n T_n^* + \eta_{n+1}^* w_{n+1} e_n^T,
\end{align*}$$

where $W_n^* V_n = I$ and $T_n = W_n^* A V_n$ is tridiagonal,

$$T_n = \begin{bmatrix}
\gamma_1 & \eta_2 \\
\delta_2 & \gamma_2 & \ddots \\
& \ddots & \ddots & \eta_n \\
& & \delta_n & \gamma_n
\end{bmatrix}.$$
Arnoldi algorithm

Given a nonsingular $A$ and $v$, Arnoldi algorithm is represented by

$$AV_n = V_n H_n + h_{n+1,n}v_{n+1}e_n^T,$$

where $V_n^* V_n = I$, and $H_n = V_n^* A V_n$ is upper Hessenberg,

$$H_n = \begin{bmatrix}
h_{1,1} & h_{1,2} & \cdots & h_{1,n} \\
h_{2,1} & h_{2,2} & \ddots & \vdots \\
\vdots & \ddots & \ddots & h_{n-n,n} \\
h_{n,n-1} & h_{n,n-1} & \cdots & h_{n,n}
\end{bmatrix}.$$
Define $Q_n$: it projects onto $\mathcal{K}_n(A, v)$ orthogonally to $\mathcal{K}_n(A^*, w)$. 
Define $Q_n$: it projects onto $\mathcal{K}_n(A, \nu)$ orthogonally to $\mathcal{K}_n(A^*, \omega)$.

Then

$$Q_n = V_n W_n^*, \quad A_n = V_n T_n W_n^*.$$
Define $Q_n$: it projects onto $\mathcal{K}_n(A, v)$ orthogonally to $\mathcal{K}_n(A^*, w)$.

Then

$$Q_n = V_n W_n^*, \quad A_n = V_n T_n W_n^*.$$ 

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]

$$w^* A^k v = w^* A_n^k v = e_1^* T_n^k e_1, \quad k = 0, \ldots, 2n - 1.$$
Define $Q_n$: it projects onto $\mathcal{K}_n(A, v)$ orthogonally to $\mathcal{K}_n(A^*, w)$.

- Then

\[
Q_n = V_n W_n^*, \\
A_n = V_n T_n W_n^*.
\]

- 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]

\[
w^* A^k v = w^* A_n^k v = e_1^* T_n^k e_1, \quad k = 0, \ldots, 2n - 1.
\]

- Model reduction

\[
A, v, w \rightarrow T_n, e_1, e_1.
\]
Arnoldi algorithm
Vorobyev moment problem, matching moments, model reduction

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

- Then

$$Q_n = V_n V_n^*, \quad A_n = V_n H_n V_n^*.$$

- Matching moments property of Arnoldi:

$$w^* A^k v = w^* A_n^k v = t_n^* H_n^k e_1, \quad k = 0, \ldots, n - 1,$$

$w$ is given, $t_n = V_n^* w$.

- Model reduction

$$A, v, w \rightarrow H_n, e_1, t_n.$$
1 Symmetric, positive definite case

2 Matching moments

3 Approximation of the bilinear form $c^*A^{-1}b$

4 Numerical experiments
Approximation of $c^* A^{-1} b$

Theoretical background - general framework, Strakoš & T. ’09

Vorobyev moment problem: $A \rightarrow A_n$

Define approximation:

$$c^* A^{-1} b \approx c^* A_n^{-1} b$$

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

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Vorobyev moment problem: \( A \rightarrow A_n \)

Define approximation:

\[
 c^* A^{-1} b \approx c^* A_n^{-1} b
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\( A_n^{-1} \) is the matrix representation of the inverse of the reduced order operator \( A_n \) which is restricted onto \( \mathcal{K}_n(A, b) \),

- \( A_n^{-1} = V_n T_n^{-1} W_n^* \) in Non-Hermitian Lanczos,
- \( A_n^{-1} = V_n H_n^{-1} V_n^* \) in Arnoldi.
Approximation of $c^* A^{-1} b$

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Questions:

- How to compute $c^* A_n^{-1} b$ efficiently?
- Relationship to the existing approximations?
Approximation of $c^* A^{-1} b$

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Define approximation:

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Questions:

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We concentrate only to non-Hermitian Lanczos approach.
Define

\[ v_1 = \frac{b}{\|b\|}, \quad w_1 = \frac{c}{c^*v_1}, \quad \text{i.e.} \quad w_1^*v_1 = 1. \]

Then

\[ c^*A_n^{-1}b = c^*V_nT_n^{-1}W_n^*b = (c^*v_1) \|b\| (T_n^{-1})_{1,1}. \]
Non-Hermitian Lanczos approach

Define

\[ v_1 = \frac{b}{\|b\|}, \quad w_1 = \frac{c}{c^*v_1}, \quad \text{i.e.} \quad w_1^*v_1 = 1. \]

Then

\[ c^*A_n^{-1}b = c^*V_nT_n^{-1}W_n^*b = (c^*v_1)\|b\|(T_n^{-1})_{1,1}. \]

Let \( x_0 = 0 \). We also know that \( x_n = \|b\|V_nT_n^{-1}e_1 \) is the approximate solution computed via BiCG. Therefore,

\[ c^*A_n^{-1}b = c^*\|b\|V_nT_n^{-1}W_n^*V_n e_1 = c^*x_n. \]
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We used the global biorthogonality!
The BiCG method

Simultaneous solving of

\[ A x = b , \quad A^* y = c . \]

**input** \( A, b, c \)

\[ x_0 = y_0 = 0 \]
\[ r_0 = p_0 = b, \quad s_0 = q_0 = c \]

**for** \( n = 0, 1, \ldots \)

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

**end**
An efficient approximation based on the BiCG method

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

Using local biorthogonality we can show that

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

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

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

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Approximations based on the BiCG method
and possible troubles in finite precision arithmetic

It holds that

\[ c^* A^{-1} b = \sum_{j=0}^{n-1} \alpha_j s_j^* r_j + s_n^* A^{-1} r_n + \text{error} \sim \|y_n\|\|r_n\| \]

It can be shown that

\[ c^* A^{-1} b = c^* x_n + y_n^* r_n + s_n^* A^{-1} r_n + \text{error} \sim \|y_n\|\|r_n\| \]

In exact arithmetic \(y_n^* r_n = 0\).

If the global biorthogonality is lost, one can expect that

\[ |y_n^* r_n| \sim \|y_n\|\|r_n\|. \]
Approximations based on the BiCG method

Mathematically equivalent approximations $\xi_B^n$ and $c^*x_n$, $\zeta \equiv c^*A^{-1}b$

\[
|c^*A^{-1}b - c^*x_n| \approx |y_n^*r_n + s_n^*A^{-1}r_n|, \\
|c^*A^{-1}b - \xi_B^n| \approx |s_n^*A^{-1}r_n|.
\]
Yet another approach
Hybrid BiCG methods

We know that

\[ c^* A_n^{-1} b = \sum_{j=0}^{n-1} \alpha_j s_j^* r_j \quad \text{and} \quad s_j^* r_j = (c^* b) \prod_{k=0}^{j-1} \beta_k. \]
Yet another approach

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In hybrid BiCG methods like CGS, BiCGStab, BiCGStab(\(\ell\)), the BiCG coefficients are available, i.e. we can compute the approximation \( c^* A_n^{-1} b \) during the run of these methods.
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**Question:** Hybrid BiCG methods produce approximations \( x_n \), better than \( x_n \) produced by BiCG.

Is \( c^* x_n \) a better approximation of \( c^* A^{-1} b \) than \( c^* x_n \)?
We know that

\[ c^* A_{n}^{-1} b = \sum_{j=0}^{n-1} \alpha_j s_j^* r_j \quad \text{and} \quad s_j^* r_j = (c^* b) \prod_{k=0}^{j-1} \beta_k. \]

In hybrid BiCG methods like CGS, BiCGStab, BiCGStab(\(\ell\)), the BiCG coefficients are available, i.e. we can compute the approximation \(c^* A_{n}^{-1} b\) during the run of these methods.

**Question:** Hybrid BiCG methods produce approximations \(x_n\), better than \(x_n\) produced by BiCG.

Is \(c^* x_n\) a better approximation of \(c^* A_{n}^{-1} b\) than \(c^* x_n\)?

**No.** We showed that mathematically [Strakoš & T. '09],

\[ c^* x_n = c^* x_n. \]
Summary (non-Hermitian Lanczos approach)

How to compute $c^* A_n^{-1} b$?

**Algorithm of choice:**

- non-Hermitian Lanczos
- BiCG
- hybrid BiCG methods

**Way of computing the approximation:**

- $c^* x_n$
- $(c^* v_1) \| b \| (T_n^{-1})_{1,1}$
- From the BiCG coefficients, or, in BiCG using

$$\xi_n^B \equiv \sum_{j=0}^{n-1} \alpha_j s_j^* r_j.$$
Let $P_L$ and $P_R$ be a left and a right preconditioner. Then

$$c^* A^{-1} b = \left( \frac{P^* R c}{\hat{c}} \right)^* \left( \frac{P_L A P_R^{-1}}{\hat{A}^{-1}} \right)^{-1} \left( \frac{P_L^{-1} b}{\hat{b}} \right).$$

The approximation techniques can be applied to the problem

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

It is obvious that $\hat{A}$ need not be formed explicitly.
Let $P_L$ and $P_R$ be a left and a right preconditioner. Then

$$c^* A^{-1} b = ( P_R^{-*} c)^* \left( P_L^{-1} A P_R^{-1} \right)^{-1} ( P_L^{-1} b ).$$

The approximation techniques can be applied to the problem

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

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

It is easier to derive the preconditioned algorithm for approximating the bilinear form $c^* A^{-1} b$ than the preconditioned algorithm for solving linear systems.
Theoretical background: Model reduction via matching moments.

Several Krylov subspace methods (Lanczos, Arnoldi) can be identified with the Vorobyev moment problem $A \rightarrow A_n$.

Approximation:

$$c^* A^{-1} b \approx c^* A_n^{-1} b.$$
General case

Summary

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Several Krylov subspace methods (Lanczos, Arnoldi) can be identified with the Vorobyev moment problem $A \rightarrow A_n$.

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Promising approaches:

BiCG and

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

Arnoldi and

$$c^* A^{-1} b \approx \|b\| t_n^* H_n^{-1} e_1,$$

where $t_n = V_n^* c$. 
Outline

1. Symmetric, positive definite case
2. Matching moments
3. Approximation of the bilinear form $c^* A^{-1} b$
4. Numerical experiments
Numerical experiments
Diffraction of light on periodic structures, RCWA method

[Hench & Strakoš '08]

\[
A \mathbf{x} \equiv \begin{bmatrix}
-\mathbf{I} & \mathbf{I} & e^{i\sqrt{C}\varrho} & 0 \\
\mathbf{Y}_I & \sqrt{C} & -\sqrt{C}e^{i\sqrt{C}\varrho} & 0 \\
0 & e^{i\sqrt{C}\varrho} & I & -\mathbf{I} \\
0 & \sqrt{C}e^{i\sqrt{C}\varrho} & -\sqrt{C} & -\mathbf{Y}_II
\end{bmatrix} \mathbf{x} = \mathbf{b},
\]

\[\mathbf{Y}_I, \mathbf{Y}_II, \mathbf{C} \in \mathbb{C}^{(2M+1) \times (2M+1)}, \varrho > 0, \ M \text{ is the discretization parameter representing the number of Fourier modes used for approximation of the electric and magnetic fields as well as the material properties.}\]
Numerical experiments
Diffraction of light on periodic structures, RCWA method

[Hench & Strakoš '08]

\[
A x \equiv \begin{bmatrix}
-I & I & e^{i\sqrt{C}q} & 0 \\
Y_I & \sqrt{C} & -\sqrt{C}e^{i\sqrt{C}q} & 0 \\
0 & e^{i\sqrt{C}q} & I & -I \\
0 & \sqrt{C}e^{i\sqrt{C}q} & -\sqrt{C} & -Y_{II}
\end{bmatrix} x = b,
\]

\(Y_I, Y_{II}, C \in \mathbb{C}^{(2M+1) \times (2M+1)}, \varrho > 0, M\) 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

\[e_{M+1}^* A^{-1} b.\]

In our experiments \(M = 20\), i.e. \(A \in \mathbb{C}^{164 \times 164}\). [Strakoš & T. '10]
Approximations based on the BiCG method

\[ b^T x_n \quad \text{versus} \quad \sum_{j=0}^{n-1} \alpha_j s_j^* r_j \]

![Graph showing approximations](image-url)
The BiCGStab and CGS approximations are significantly more affected by rounding errors than the BiCG approximations.
Hybrid BiCG methods can be more efficient than BiCG when approximating the solution of $A x = b$. 
Non-Hermitian Lanczos approach
Mathematically equivalent approximations based on hybrid BiCG methods

BiCG is usually more efficient than hybrid BiCG methods when approximation the bilinear form $c^* A^{-1} b$. 
Different approaches with preconditioning

TE polarization, 20 slabs, $A \in \mathbb{C}^{1722 \times 1722}$
Different approaches with preconditioning

AF23560: from set AIRFOIL, from the NEP Collection
Some Krylov subspace methods can be seen as model reduction via matching moments.
Conclusions

- Some Krylov subspace methods can be seen as model reduction via matching moments.
- Generalization of the HPD case: Via Vorobyev moment problem → very natural and general.
  - no assumptions on $A$, based on approximation properties
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- We proved **mathematical equivalence** of the existing approximations based on Non-Hermitian Lanczos.
Conclusions

- Some Krylov subspace methods can be seen as model reduction via matching moments.
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  - no assumptions on $A$, based on approximation properties
- 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.
Some Krylov subspace methods can be seen as model reduction via matching moments.

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Preferable approximation

\[
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\]

It is simple and numerically better justified.

In finite precision arithmetic, the relations need not hold. A justification is necessary (e.g. local biorthogonality).
Related papers


More details can be found at

http://www.karlin.mff.cuni.cz/~strakos/
http://www.cs.cas.cz/tichy
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Thank you for your attention!