Relating computed and exact entities in Krylov subspace methods based on short recurrences

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Content of the talk

1. Krylov subspace methods
2. Overview of FP behavior
3. Comparison by pairing
4. Conclusions and Outlook
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Krylov subspace methods

Krylov subspace methods for

\[ Ax = b, \quad A \in \mathbb{R}^{n \times n}, \ b \in \mathbb{R}^n, \ x_0 \in \mathbb{R}^n \]

often rely mathematically on the computation of an orthonormal basis

\[ V_k = [v_1, \ldots, v_k] \]

of the Krylov subspace

\[ \mathcal{K}_k(A, r_0) \equiv \text{span}\{r_0, Ar_0, \ldots, A^{k-1}r_0\}, \quad r_0 = b - Ax_0. \]

Symmetric and positive definite matrix \( A \):

⇒ Short recurrences, Lanczos tridiagonalization

We consider here

- Conjugate gradient method via the Lanczos process (CGL);
- Minimal Residual method (MINRES).
**CGL and MINRES**

**Input:** matrix $A$ symmetric and positive definite, vector $b$

CGL: $\|x - x_k^L\|_A = \min_{y \in \mathcal{K}_k(A, r_0)} \|x - y\|_A$, $r_k^L \perp \mathcal{K}_k(A, r_0)$;

MINRES: $\|r_k^M\| = \min_{y \in \mathcal{K}_k(A, r_0)} \|b - Ay\|.$

<table>
<thead>
<tr>
<th>method/quantity</th>
<th>$|x_k - x|$</th>
<th>$|x_k - x|_A$</th>
<th>$|r_k|$</th>
<th>$|r_k|_A$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CGL</td>
<td>monotone</td>
<td>minimized</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>MINRES</td>
<td>monotone</td>
<td>monotone</td>
<td>minimized</td>
<td>–</td>
</tr>
</tbody>
</table>

Peak-plateau relationship; see, e.g., [Cullum, Greenbaum (1996)]:

$$\|r_k^L\| = \frac{\|r_k^M\|}{\sqrt{1 - (\|r_k^M\|/\|r_{k-1}\|)^2}}.$$
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Situation in finite precision arithmetic

We will focus on situation
- serious loss of orthogonality present;
- after finite number of iterations;
- no reorthogonalization, no restarts.

In general, the structure of Krylov subspace methods seems to be lost:
- Computed Lanczos vectors generally do not span Krylov subspaces defined by the input data or their small perturbations.
- Computed residuals generally do not satisfy Galerkin orthogonality or norm minimization property.
Analysis in FP arithmetic

Results for Lanczos algorithm reveal that important structure is preserved:

- Loss of orthogonality may appear only in the directions of eigenvectors of $A$ (Ritz vectors associated with converged Ritz values).
  [Paige (1971, 1980)]

- Finite precision Lanczos process can be described via the exact Lanczos process applied on augmented system containing both the matrix $A$ and the currently computed tridiagonal Jacobi matrix.
  [Paige (2010)]

Related question of sensitivity and perturbation analysis
[Carproux, Godunov, Kuznetsov (1997); Paige, Van Dooren (1998)]
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  Relates FP computations with exact computations with larger matrix.

- Related question of sensitivity and perturbation analysis [Carproux, Godunov, Kuznetsov (1997); Paige, Van Dooren (1998)]

  Assumption of full rank of the computed subspace.
Backward-like analysis associates the sequence of computed Jacobi matrices with a larger matrix $\hat{A}$ with clustered eigenvalues. [Greenbaum (1989); Greenbaum, Strakoš (1992)]
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Relates FP computations with exact computations with larger matrix.
Questions to be asked

- How do the computed subspaces differ from exact Krylov subspaces?
- How do the computed approximation or residual vectors resemble their exact arithmetic counterparts?
- Which phenomena and results present in exact arithmetic can be restored in or adopted to finite-precision computation? How and to which extent?

Study the mutual relationship of computed quantities and their exact arithmetic counterparts for the same $A$ and $b$.

Short recurrences $\rightarrow$ rank deficiency!
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Idea of pairings

We investigate whether, in which sense, and how accurately, we can relate $k$ steps of the FP computation $\times l$ steps of the exact computation.

- $k - l \approx$ delay of convergence
- $k - l \approx$ rank-deficiency of generated subspace

This enables to compare:

$$\|x - x_k^L\|_A \times \|x - x_l^L\|_A,$$

$$x_k, r_k \times x_l, r_l,$$

$$\bar{K}_k(A, r_0) \times \bar{K}_l(A, r_0),$$

$$\ldots \times \ldots$$
Pairing approaches

- Using **numerical rank** of the matrix of the computed Lanczos vectors $\tilde{V}_k$:
  
  $$k_l \equiv \max\{k \mid \text{num\_rank}(\tilde{V}_k) = l\}.$$

- Explicit **fitting of the convergence curves**:
  - **CGL**:
    $$k_l \equiv \arg\min_k \left|\left| x^L_k - x \right|_A - \left|\left| \tilde{x}^L_k - x \right|_A \right| \right|$$
  - **MINRES**:
    $$k_l \equiv \arg\min_k \left|\left| r^M_l - \tilde{r}^M_k \right| \right|$$

The plots illustrate $\{k_l\}$ and the singular values $\sigma^{(k)}_l$ of $\tilde{V}_k$.
Convergence curves

Since the computed $\bar{V}_{k_l}$ and the exact $V_l$ have for considered pairing approaches approximately the same rank, it may be reasonable to expect:

$$\|x^L_l - x\|_A \approx \|\bar{x}^L_{k_l} - x\|_A, \quad \|r^M_l\| \approx \|\bar{r}^M_{k_l}\|.$$
Moreover, in practice we even observe:

\[ x_l^L - x \approx x_k^L - x, \]

\[ r_l^M \approx r_k^M. \]
Question: What can we say about other quantities?

\[ \| r_L^l \| \approx \| \bar{r}_k^L \| \]

CGL residual norms

**Question:** What can we say about other quantities?

\[ \| r^L \| \approx \| \bar{r}^L \| \]

**Answer:** NO!!!

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Question: What can we say about other quantities?

\[ \| r_l^L \| \approx \| \tilde{r}_{k_l}^L \| \]

Answer: NO!!!

But assuming \( \| r_l^M \| \approx \| \tilde{r}_{k_l}^M \| \), the relations

\[
\| r_l^L \| = \frac{\| r_l^M \|}{\sqrt{1 - (\| r_l^M \|/\| r_{l-1}^M \|)^2}}, \quad \| \tilde{r}_{k_l}^L \| \approx \frac{\| \tilde{r}_{k_l}^M \|}{\sqrt{1 - (\| \tilde{r}_{k_l}^M \|/\| \tilde{r}_{k_{l-1}}^M \|)^2}}
\]

(see [Cullum, Greenbaum (1996)]) give for \( \| r_l^M \|/\| r_{l-1}^M \| \approx 1 \) that

\[
\| r_l^L \| \approx \frac{1}{\sqrt{\sum_{j=k_l-1+1}^{k_l} 1/\| \tilde{r}_j^L \|^2}}.
\]

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Conclusion: CGL residual norms cannot be compared directly but must be aggregated over the intermediate iterations.

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CGL residual vectors

**Question:** What can we say about other quantities?

\[ r_l^L \approx \bar{r}_{k_l}^L \]

**Answer:** Similarly, for \( \| r_l^M \| / \| r_{l-1}^M \| \not\approx 1 \),

\[
\frac{1}{\| r_l^L \|^2} r_l^L \approx \sum_{j=k_l-1+1}^{k_l} \frac{1}{\| \bar{r}_j^L \|^2} \bar{r}_j^L.
\]
Stagnation: \( \| r^{M}_l \| \approx \| r^{M}_{l-1} \| \)

**CGL residual norms:**

We proceed \( p \) iterations forward to achieve \( \| r^{M}_{l+p} \| / \| r^{M}_{l-1} \| \ll 1 \). Then,

\[
\frac{1}{\sqrt{\sum_{j=l}^{l+p} 1/\| r^L_j \|^2}} \approx \frac{1}{\sqrt{\sum_{j=k_{l-1}+1}^{k_{l+p}} 1/\| \bar{r}^L_j \|^2}}.
\]
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Conclusions and Outlook

- Proposed pairings allow us to compare simultaneously the quantities of interest (convergence curves, approximation vectors, residuals) for two methods – CGL and MINRES.
- Computed CGL residuals cannot be related directly to their exact counterparts, but need to be aggregated over the intermediate iterations.
- When post-processed accordingly, finite-precision computations resemble exact computations.
- Nearness of computed subspace to exact Krylov subspace
- Stagnation of exact MINRES convergence curve.


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