# How Orthogonality is Lost in Krylov Methods

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## Overview


Introduction 2

Problem I (eigenvalues) 3

Unified description 5

Convergence and loss of orthogonality 6

Numerical example 8

Reorthogonalization 11

Problem II (linear systems) 12

Conclusions 13

Some more pictures . . . 15

## Introduction

Growing interest in solving

**Problem I**: find $v, \lambda$ so that

$$Av = v\lambda$$

and

**Problem II**: find $x$ so that

$$Ax = b$$

for **huge sparse** matrices $A \in \mathbb{K}^{n \times n}$.

Methods for **dense** systems: $O(n^3)$ operations for solution and verification (Rump, Oishi).

Is verification for sparse matrices possible

- without use of full matrices and
- with less than $O(n^3)$ operations?

## Problem I (eigenvalues)

Three important methods using Krylov spaces:

**symmetric Lanczos**:

$$AQ_k - Q_k T_k = \beta_k q_{k+1} e_k^T + F_k^L$$

$T_k = T_k^T$ tridiagonal, $Q_k^T Q_k = I_k$ if $F_k^L = 0$

**nonsymmetric Lanczos**:

$$\begin{aligned} AQ_k - Q_k T_k &= \beta_k q_{k+1} e_k^T + F_k^Q \\ A^T P_k - P_k T_k^T &= \gamma_k p_{k+1} e_k^T + F_k^P \end{aligned}$$

$T_k$ tridiagonal, $P_k^T Q_k = I_k$ if $F_k^Q = 0 = F_k^P$

**Arnoldi**:

$$AQ_k - Q_k H_k = h_{k,k+1} q_{k+1} e_k^T + F_k^A$$

$H_k$ Hessenberg, $Q_k^T Q_k = I_k$ if $F_k^A = 0$

There exist modifications of symmetric Lanczos for skew-symmetric matrices etc.

In theory ($F_k = 0$) rapid convergence when outer eigenvalues well separated.

**symmetric Lanczos** $\longrightarrow$ Kaniel–Paige–Saad

$$0 \leq \frac{\theta_j - \lambda_j}{\lambda_n - \lambda_j} \leq \left( \frac{\sin \angle \left(q_1, V_j\right)}{\cos \angle \left(q_1, v_j\right)} \cdot \frac{\prod_{\nu=1}^{j-1} (\frac{\theta_\nu - \lambda_n}{\theta_\nu - \lambda_j})}{T_{k-j}(1+2\gamma)} \right)^2.$$

$$V_j = \text{span}\left(v_1, \ldots, v_j\right)$$

Gap ratio:

$$\gamma = \frac{\lambda_j - \lambda_{j+1}}{\lambda_{j+1} - \lambda_n}.$$

Chebyshev polynomials $T_k$ dampen part of the spectrum.

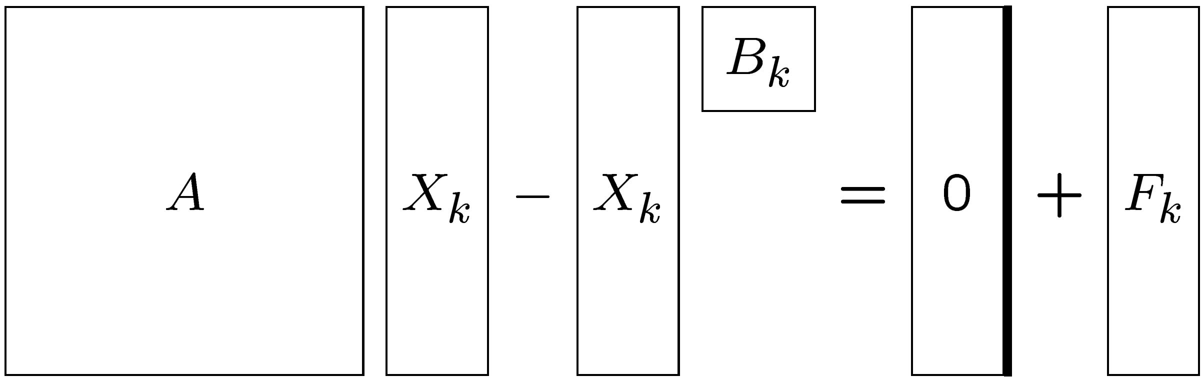
**Arnoldi** $\longrightarrow$ Trefethen

## Unified description

In all cases

$$AX_k - X_kB_k = b_{k,k+1}x_{k+1}e_k^T + F_k \quad (*)$$

holds $\Rightarrow$ Sylvester equation for $X_k$ (linear).




Eigendecomposition of $A$:

$$v_i^T A = \lambda_i v_i^T, \quad Aw_i = w_i \lambda_i.$$

Eigendecomposition of $B_k$:

$$B_k s_j = s_j \theta_j, \quad t_j^T B_k = \theta_j t_j^T.$$

Eigenvectors have unit length.

## Convergence and loss of orthogonality

Ritz pairs (triplets): $\left(\theta_j, y_j = X_k s_j \left[, z_j\right]\right)$

For symmetric Lanczos residual can be estimated ($\|y_j\| = 1$ for $F_k = 0$):

$$Ay_j - y_j\theta_j = b_{k,k+1} s_{kj} x_{k+1} + F_k s_j$$

$$\left|\lambda_i - \theta_j\right| \cdot \|y_j\| \leq b_{k,k+1} \left|s_{kj}\right| + \|F_k s_j\|$$

Diagonalization of $(*)$ yields

$$\left(\lambda_i - \theta_j\right) v_i^T y_j = v_i^T x_{k+1} b_{k,k+1} s_{kj} + v_i^T F_k s_j.$$

Reorder terms:

$$v_i^T x_{k+1} = \frac{\left(\lambda_i - \theta_j\right) v_i^T y_j - v_i^T F_k s_j}{b_{k,k+1} s_{kj}}$$

$\Rightarrow$ formula for local error.

The local error formula shows Paige's result:

| |
|---|
| Loss of orthogonality |
| $\Longleftrightarrow$ |
| $F_k \neq 0$ and convergence |

Relation between convergence and residual for symmetric Lanczos (Temple/Kato):

No eigenvalue in $[\theta_j, \theta_j + \text{gap}]$. Then

$$0 \leq \lambda_i - \theta_j \leq \left(\beta_k s_{kj}\right)^2 \Big/ \text{gap}.$$

Well separated eigenvalues ($\text{gap} = O(1)$)

$\Rightarrow$ convergence quadratic in the residual.

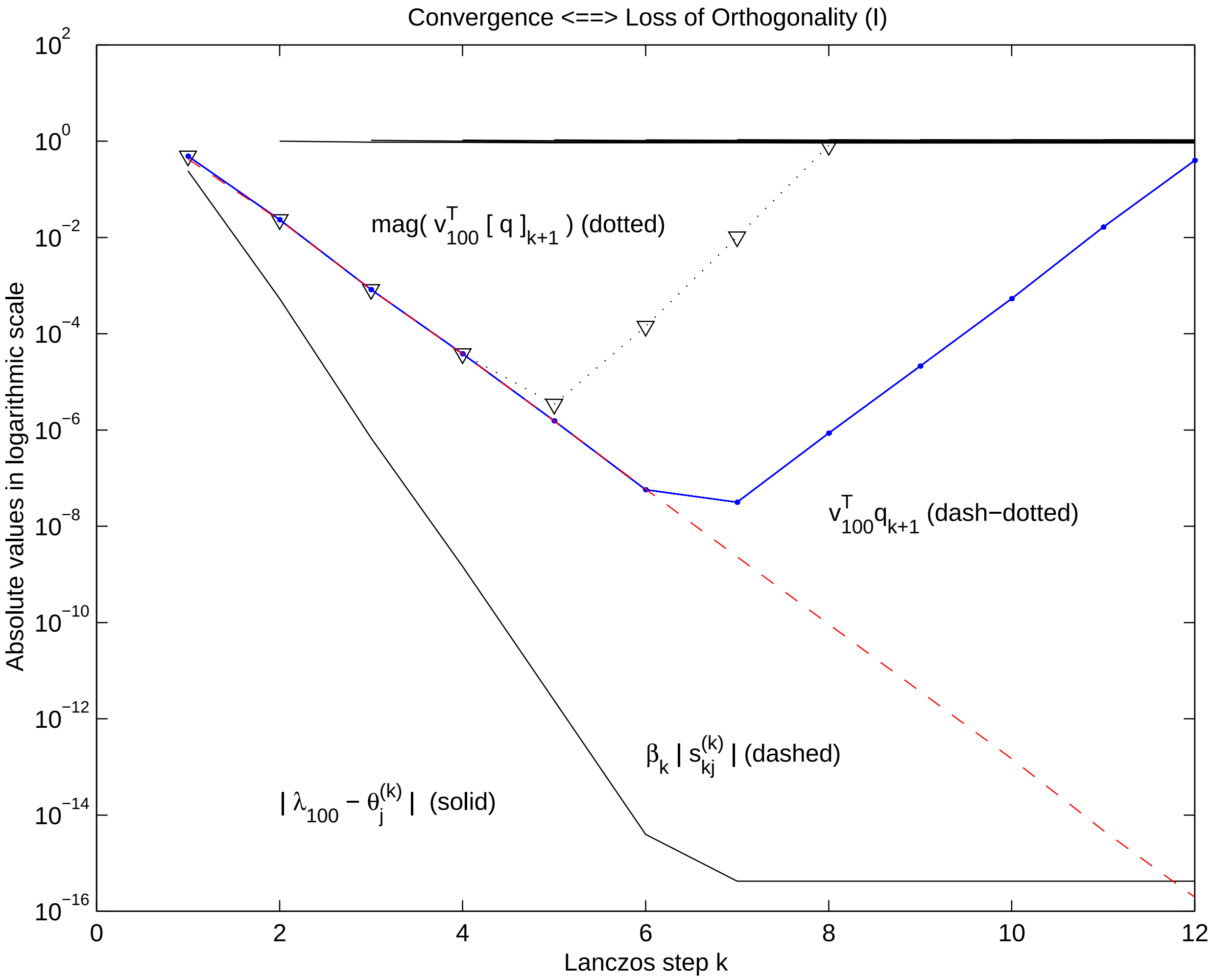
Interval Lanczos (Frommer) can only reach the step where convergence reaches the level of the machine precision $\epsilon$, that means the step where the residual reaches level $\sqrt{\epsilon}$.

## Numerical example

Random $A \in [0,1]^{100\times 100}$ (nonnegative). Plot shows $\lambda_{\max} - \theta_j$, $b_{k,k+1} s_{kj}$ and $v_{\max}^T x_{k+1}$.

Eigenvalues of largest moduli:

$$\lambda_{\max} = \lambda_{100} \approx 50.6, \qquad \lambda_{99} \approx 4.2.$$



Short summary:

Krylov methods in floating point

$$F_k \neq 0$$

without repair (reorthogonalization) will deviate

$$v_i^T x_{k+1} = \frac{\left(\lambda_i - \theta_j\right) v_i^T y_j - v_i^T F_k s_j}{b_{k,k+1} s_{kj}}$$

from exact counterparts when convergence

$$\left(\lambda_i - \theta_j\right) v_i^T y_j = O(v_i^T F_k s_j)$$

occurs.

The Ritz pair (triplet) converges to an eigenpair (eigentriple).

In the unsymmetric cases for some $j$

$$v_i^T y_j$$

converges to

$$v_i^T w_i$$

and thus the condition of $\lambda_i$ comes into play.

One way of dealing with the loss of orthogonality is to understand the behaviour of symmetric Lanczos after first Ritz pair converged.

Stabilization of Ritz values:

$$\forall\ l > 0\ \exists\ i : \left|\theta_i^{(k+l)} - \theta_j^{(k)}\right| \leq \beta_k \left|s_{kj}^{(k)}\right|.$$

Thompson & McEnteggert (1968):

$$\left(s_{kj}^{(k)}\right)^2 = \prod_{i<j} \frac{\theta_j^{(k)} - \theta_i^{(k-1)}}{\theta_j^{(k)} - \theta_i^{(k)}} \cdot \prod_{i>j} \frac{\theta_j^{(k)} - \theta_{i-1}^{(k-1)}}{\theta_j^{(k)} - \theta_i^{(k)}}.$$

For Arnoldi and nonsymmetric Lanczos no similar results exist, but behaviour looks pretty much the same.

Lack of results due to the involved perturbation theory for general matrices.

The other way is **reorthogonalisation**.

- Full reorthogonalization (Wilkinson):

  Computes 'accurate' $Q_k$ in $O(kn)$:

  $$\|Q_k^T Q_k - I_k\| = O\left(\|A\|\varepsilon\right).$$

  Storage amount: full matrices. Arnoldi has to store all vectors and uses reorthogonalization.

- Semiorthogonalization techniques (Parlett, Scott, Bai, Grcar, ...):

  Indicator reaches $O(\|A\|\sqrt{\varepsilon})$

  $\Rightarrow$ Invoke reorthogonalization.

Up to now no way to adopt these techniques for a verification method.

**Problem II (linear systems)**

For every Krylov eigensolver a corresponding linear system solver exists.

| eigensolver | linear system solver |
|---|---|
| symmetric Lanczos | CG ($A$ SPD) |
| Arnoldi | GMRES |
| ... | ... |

Floating point Krylov methods for solution of linear systems correspond to some underlying perturbed Krylov eigensolver.

So it is not possible to use interval arithmetic for Krylov methods in general.

Either the intervals will grow tremendous due to convergence of a Ritz pair or convergence will be delayed to the last step.

## Conclusions

- Krylov methods are **not forward stable**.
- Krylov methods are in some sense **backward stable** (residuals close to bounds).
- Interval evaluation of Krylov methods does not work in the numerically interesting case of rapid convergence.
- Numerically computed results are near the best possible results (as predicted by perturbation theory).
- Krylov methods tend to 'forget' the starting vector (only weak dependence on the starting vector).

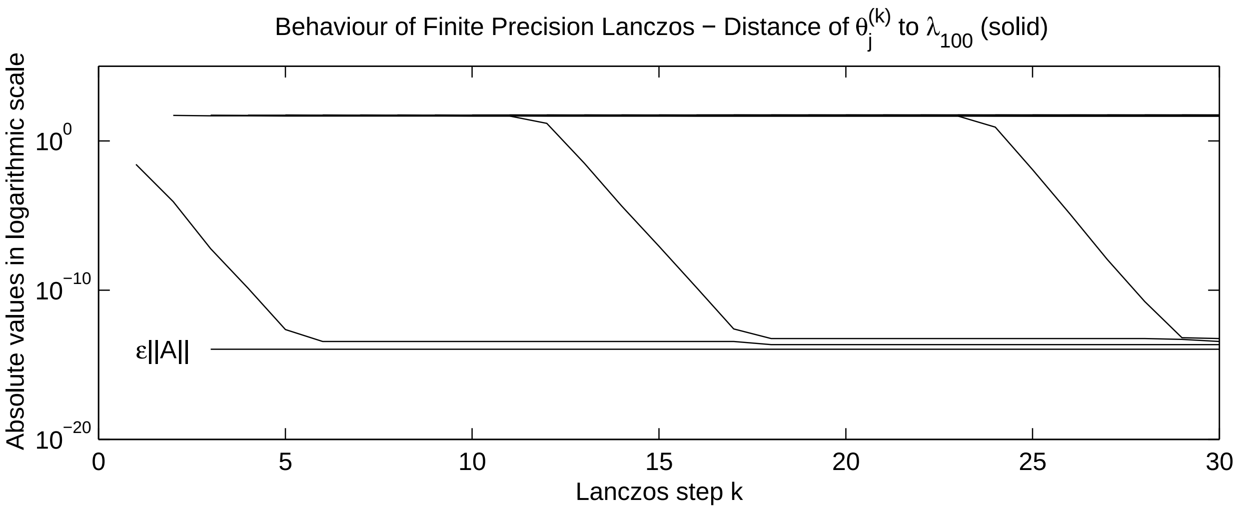
- If no reorthogonalization is used, loss of orthogonality occurs **iff** the residual is small.

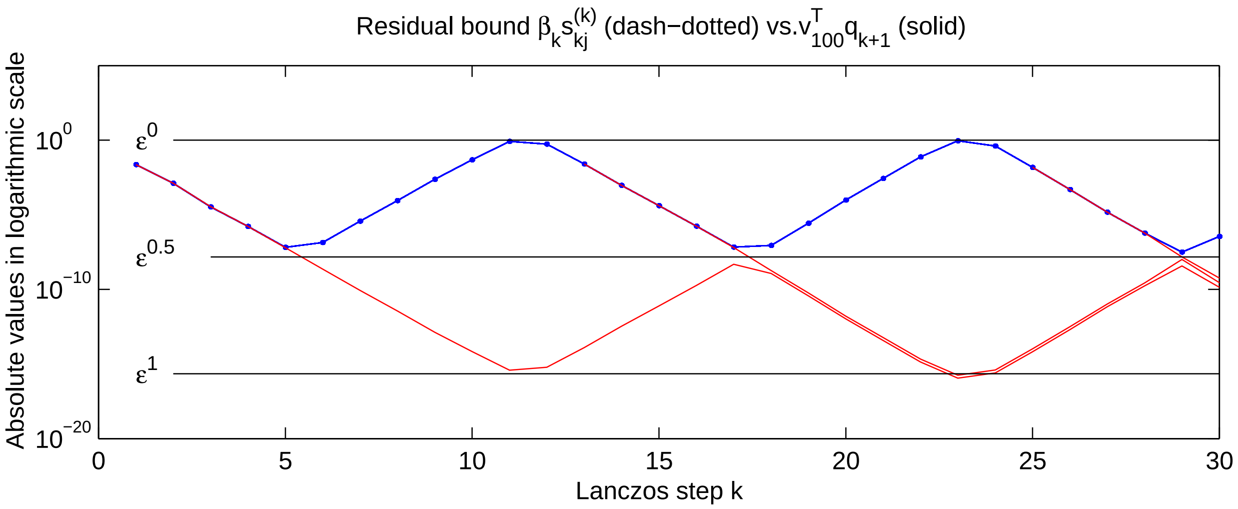
- It is not sufficient to use higher precision in later steps to compute more accurate results. The whole computation has to be done again in higher precision.

## Question

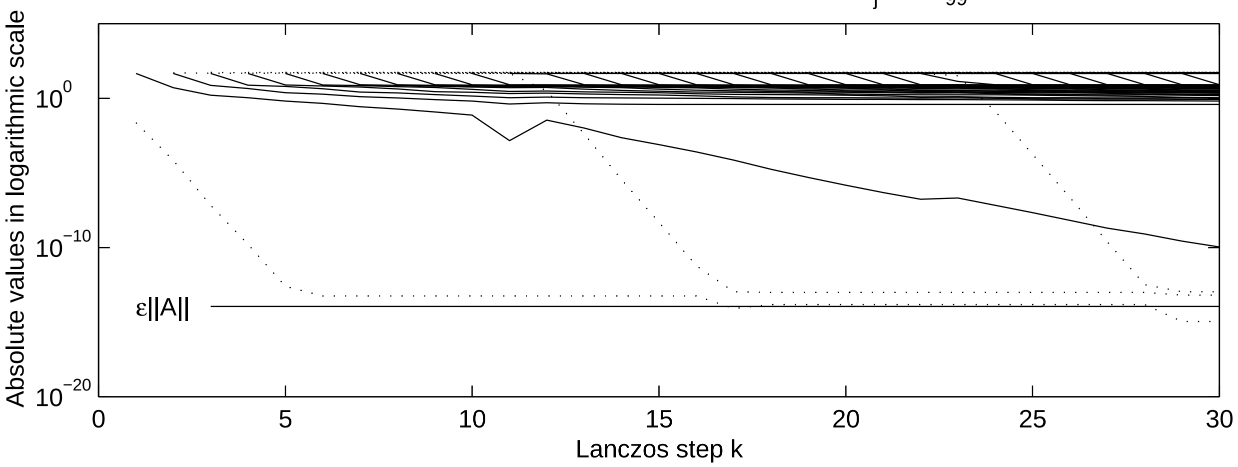
Can there be a Krylov method with fast convergence and huge residual?

# Some more pictures . . .

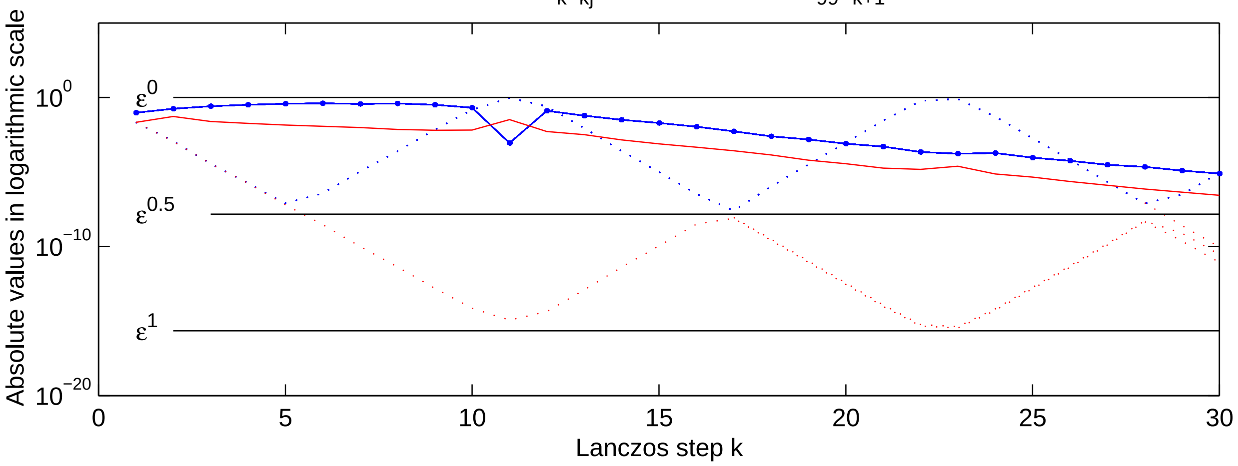


Behaviour of Finite Precision Lanczos − Distance of $\theta_j^{(k)}$ to $\lambda_{99}$ (solid)




Residual bound $\beta_k s_{kj}^{(k)}$ (dash−dotted) vs.$v_{99}^T q_{k+1}$ (solid)



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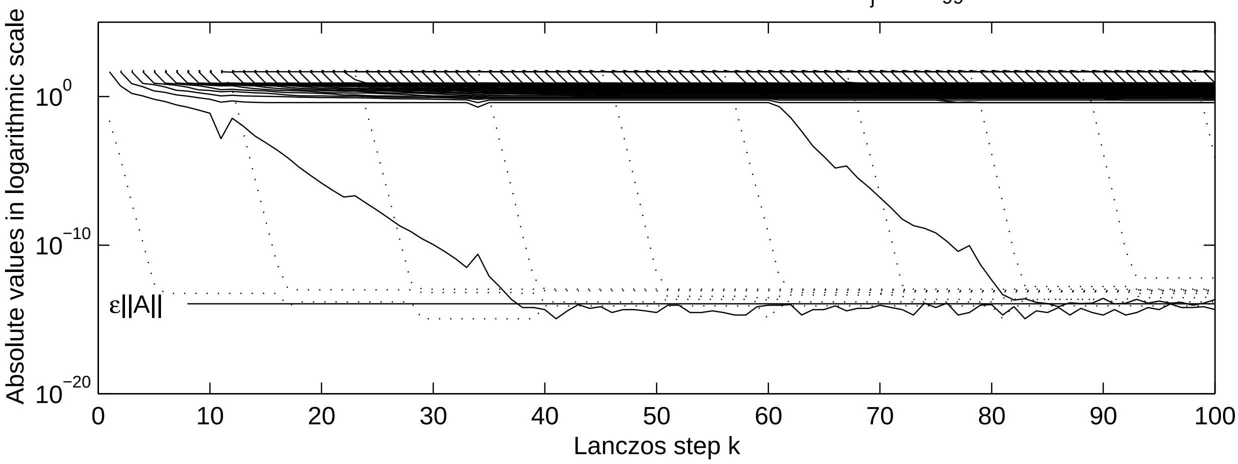


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