

# New Insights into the Equivalence of Thick and Implicit Restarting Lanczos

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# Roadmap

Part 1: Deflating eigenvalues from a small tridiagonal matrix.

$$\begin{bmatrix} Q_m^T \\ \left[ \begin{array}{c} \diagdown \\ \diagup \\ T_m \end{array} \right] \end{bmatrix} \begin{bmatrix} \\ \\ Q_m \end{bmatrix} = \begin{bmatrix} \left[ \begin{array}{c} \diagdown \\ \diagup \\ T_k \end{array} \right] \\ \left[ \begin{array}{c} \diagdown \\ \diagup \\ \ominus_{m-k} \end{array} \right] \end{bmatrix}$$

Part 2: An application: The equivalence of thick and implicit restarting in Lanczos.

# Introduction – Tridiagonal Deflation

Let  $T_m$  be an  $m \times m$  symmetric tridiagonal matrix:  $T_m = \begin{bmatrix} & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{bmatrix}$ .

Compute the eigenpairs  $\{(\theta_i, y_i)\}_{i=1}^m$  of  $T_m$ , and sort into two sets:

$$\underbrace{T_m Y_k = Y_k \Theta_k}_{\text{desired}}$$

$$\underbrace{T_m Y_{m-k} = Y_{m-k} \Theta_{m-k}}_{\text{undesired}}$$

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**Goal:** Find an orthogonal matrix  $Q_m$  such that

$$\begin{bmatrix} Q_m^T & & \\ & \begin{bmatrix} & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{bmatrix} & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{bmatrix} Q_m = \begin{bmatrix} & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{bmatrix}$$

The matrix on the right is a block-diagonal matrix where the top-left block is a green square labeled  $T_k$  and the bottom-right block is a red diagonal line labeled  $\Theta_{m-k}$ .





# Arrowhead Conversion

$$\begin{bmatrix} Q_k^T \\ 1 \end{bmatrix} \begin{bmatrix} \diagdown \\ D_{k+1} \\ \diagup \end{bmatrix} \begin{bmatrix} Q_k \\ 1 \end{bmatrix} = \begin{bmatrix} \diagdown \\ T_{k+1} \\ \diagup \end{bmatrix}$$

Truncate the first  $k$  rows & columns:

$$\begin{bmatrix} Q_k^T \end{bmatrix} \begin{bmatrix} \diagdown \\ \Theta_k \\ \diagup \end{bmatrix} \begin{bmatrix} Q_k \end{bmatrix} = \begin{bmatrix} \diagdown \\ T_k \\ \diagup \end{bmatrix}$$

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Utilizing  $T_m \begin{bmatrix} Y_k & Y_{m-k} \end{bmatrix} = \begin{bmatrix} Y_k & Y_{m-k} \end{bmatrix} \begin{bmatrix} \Theta_k & \\ & \Theta_{m-k} \end{bmatrix}$ :

$$\begin{bmatrix} Y_k & Q_k & Y_{m-k} \end{bmatrix}^T \begin{bmatrix} \diagdown \\ T_m \\ \diagup \end{bmatrix} \begin{bmatrix} Y_k & Q_k & Y_{m-k} \end{bmatrix} = \begin{bmatrix} \diagdown \\ T_k \\ \diagup \\ \Theta_{m-k} \end{bmatrix}$$

## Structure of $Y_k Q_k$

$$\begin{bmatrix} Y_k Q_k & Y_{m-k} \end{bmatrix}^T \begin{bmatrix} \diagdown \\ \diagdown \\ \diagdown \end{bmatrix} T_m \begin{bmatrix} Y_k Q_k & Y_{m-k} \end{bmatrix} = \begin{bmatrix} T_k & \\ & \ominus_{m-k} \end{bmatrix}$$

### Theorem (Baglama, Monette, Perovic 2026)

The  $m \times k$  matrix  $\vec{Y}_k := Y_k Q_k$  has the form

$$\vec{Y}_k = \begin{bmatrix} \left. \begin{array}{c} \phantom{Y_k Q_k} \\ \phantom{Y_k Q_k} \\ \phantom{Y_k Q_k} \end{array} \right\} p+1 \\ \phantom{Y_k Q_k} \end{bmatrix} \quad (\text{where } p = m - k).$$

## Connection to QR Algorithm

Alternatively, use the QR algorithm with  $\{\theta_{k+1}, \dots, \theta_m\}$  as shifts.  
**undesired!**

$$\begin{bmatrix} Q_k^+ & Y_{m-k} \end{bmatrix}^T \begin{bmatrix} \diagdown & & \\ & \diagdown & \\ & & \diagdown \end{bmatrix} \begin{bmatrix} Q_k^+ & Y_{m-k} \end{bmatrix} = \begin{bmatrix} T_k^+ & \\ & \ominus_{m-k} \end{bmatrix}$$

The diagram illustrates the QR algorithm with shifts. It shows the product of the transpose of the QR factorization of  $T_m$  and  $T_m$  itself, resulting in a block diagonal matrix. The left matrix is  $\begin{bmatrix} Q_k^+ & Y_{m-k} \end{bmatrix}^T$ , the middle matrix is  $T_m$  (represented by a tridiagonal matrix with diagonal lines), and the right matrix is  $\begin{bmatrix} Q_k^+ & Y_{m-k} \end{bmatrix}$ . The result is a block diagonal matrix  $\begin{bmatrix} T_k^+ & \\ & \ominus_{m-k} \end{bmatrix}$ , where  $T_k^+$  is a  $k \times k$  upper triangular matrix and  $\ominus_{m-k}$  is a  $(m-k) \times (m-k)$  lower triangular matrix.



# Connection to QR Algorithm

Alternatively, use the QR algorithm with  $\underbrace{\{\theta_{k+1}, \dots, \theta_m\}}_{\text{undesired!}}$  as shifts.

$$\begin{aligned}
 & \begin{bmatrix} Q_k^+ & Y_{m-k} \end{bmatrix}^T \begin{bmatrix} \diagdown & & \\ & \diagdown & \\ & & \diagdown \end{bmatrix} \begin{bmatrix} Q_k^+ & Y_{m-k} \end{bmatrix} = \begin{bmatrix} T_k^+ & \\ & \ominus_{m-k} \end{bmatrix} \\
 & \begin{bmatrix} Y_k Q_k & Y_{m-k} \end{bmatrix}^T \begin{bmatrix} \diagdown & & \\ & \diagdown & \\ & & \diagdown \end{bmatrix} \begin{bmatrix} Y_k Q_k & Y_{m-k} \end{bmatrix} = \begin{bmatrix} T_k & \\ & \ominus_{m-k} \end{bmatrix}
 \end{aligned}$$

## Theorem (Baglama, Monette, Perovic 2026)

Arrowhead method with  $k$  eigenpairs = QR algorithm with  $m - k$  shifts:

$$T_k = S^{-1} T_k^+ S, \quad \vec{Y}_k = Q_k^+ S, \quad S = \text{diag}(\pm 1, \dots, \pm 1).$$

# Examples

Numerical examples for **deflation** of  $p = m - k$  eigenpairs.

**Input:** Tridiagonal  $T$  with eigenpairs  $TX = X\Lambda$ .

**Arrowhead Method** ( $T, k$ )

- Create  $D_{k+1}$  with desired eigenpairs.
- Reduce to  $T_k = Q_k^T D_k Q_k$ .
- $Q = X_k Q_k$ .
- $\tilde{T} = Q^T T Q \in \mathbb{R}^{k \times k}$ .

**Implicit QR Method** ( $T, p$ )

- Apply  $p$  shifts of undesired eigenvalues to  $T$ .
- Accumulate orthogonal matrices in  $Q$ .
- $\tilde{T} = Q^T T Q \in \mathbb{R}^{k \times k}$ .

$$\begin{bmatrix} \color{green} Q \end{bmatrix}^T \begin{bmatrix} \color{black} T \end{bmatrix} \begin{bmatrix} \color{green} Q \end{bmatrix} = \begin{bmatrix} \color{black} \tilde{T} \end{bmatrix}$$

# Examples

- Wilkinson tridiagonal. Eigenvalues are very clustered.
  - Size: 41, shifts:  $p = m - k = 20$  smallest eigenvalues.
- Fann tridiagonal. Applications in computational quantum chemistry; a “difficult” test matrix in LAPACK’s eigensolvers.
  - Size: 120, shifts:  $p = m - k = 60$  smallest eigenvalues.

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	$\ \text{eig}(T(1:k, 1:k)) - \text{eig}(\tilde{T})\ $	$\ \tilde{T} - Q^T T Q\ $
Wilkinson Matrix		
Arrowhead	$2.5 \times 10^{-14}$	$5.7 \times 10^{-14}$
Implicit $QR$	12.4	$2.5 \times 10^{-14}$
Fann Matrix		
Arrowhead	$1.6 \times 10^{-14}$	$4.4 \times 10^{-15}$
Implicit $QR$	1.7	$4 \times 10^{-15}$

## **Restarting the Lanczos Algorithm**





# Restart Methods

$$\begin{bmatrix} A \end{bmatrix} \begin{bmatrix} P_m \end{bmatrix} = \begin{bmatrix} P_m \end{bmatrix} \begin{bmatrix} T_m \end{bmatrix} + \begin{bmatrix} f \end{bmatrix}$$

Eigenpairs  $\{(\theta_i, y_i)\}_{i=1}^m$  of  $T_m$  are used to approximate those of  $A$ :

$$T_m y_i = \theta_i y_i \quad \Rightarrow \quad A(P_m y_i) = \theta_i(P_m y_i) + f e_m^T y_i.$$

We call  $(\theta_i, P_m y_i)$  a **Ritz pair** of  $A$ .

If the residuals  $\|f\| \cdot |y_{m,i}|$  are too large, Lanczos can be restarted:

## Thick Restarts

- MATLAB post-2016
- Krylov-Schur – Stewart 2002
- Thick Restart Lanczos (TRL)–Wu & Simon 2000

## Implicit Restarts

- MATLAB pre-2016 (Octave, ARPACK)
- IRA – Sorensen 1992
- Implicit Restart Lanczos (IRL)

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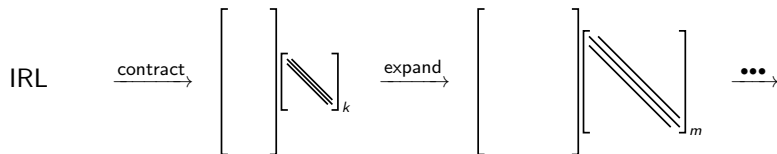
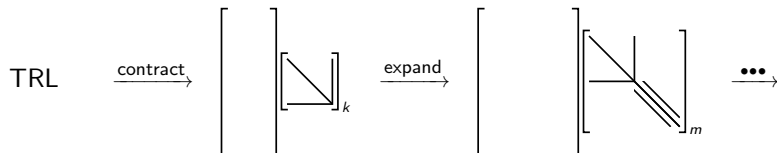
Equivalence has been known: Wu & Simon 2000, Morgan 2004, etc.

**Goal:** A stronger connection using arrowhead matrices.

# Thick Restarts (TRL) and Implicit Restarts (IRL)

Until convergence ...

1. Generate  $m$ -Lanczos factorization:  $AP_m = P_m T_m + fe_m^T$ .
2. Compute Ritz pairs:  $\{(\theta_i, x_i)\}_{i=1}^m$   $x_i = P_m y_i$  and  $T_m y_i = \theta_i y_i$ .
3. **“Restart”** with  $k$  “desired” eigenpairs; build **new**  $m$ -Lanczos.



# Thick Restart Lanczos (TRL)

Initialization:

$$A \begin{bmatrix} | \\ | \\ | \end{bmatrix} P_m = P_m \begin{bmatrix} | \\ | \\ | \end{bmatrix} \begin{matrix} \diagdown \\ \diagdown \\ \diagdown \end{matrix} T_m + \begin{bmatrix} \text{---} \\ \text{---} \\ \text{---} \end{bmatrix} f$$

Repeat:

$$A \begin{bmatrix} | \\ | \\ | \end{bmatrix} = \begin{bmatrix} | \\ | \\ | \end{bmatrix} \begin{bmatrix} \text{---} \\ \text{---} \\ \text{---} \end{bmatrix} + \begin{bmatrix} \text{---} \\ \text{---} \\ \text{---} \end{bmatrix}$$

$$A \begin{bmatrix} | \\ | \\ | \end{bmatrix} = \begin{bmatrix} | \\ | \\ | \end{bmatrix} \begin{bmatrix} \text{---} \\ \text{---} \\ \text{---} \end{bmatrix} \begin{matrix} \diagdown \\ \diagdown \\ \diagdown \end{matrix} + \begin{bmatrix} \text{---} \\ \text{---} \\ \text{---} \end{bmatrix} f$$

## TRL – Contraction Step

“Restart” with desired Ritz vectors  $P_m Y_k$ . Let  $p_{m+1} = f/\beta$ ,  $\beta = \|f\|$ .

$$D_{k+1} := \begin{bmatrix} \theta_1 & & & \beta y_{m,1} \\ & \ddots & & \vdots \\ & & \theta_k & \beta y_{m,k} \\ \beta y_{m,1} & \dots & \beta y_{m,k} & * \end{bmatrix}$$

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... yielding a “not quite”-Lanczos factorization!

$$\begin{bmatrix} A \end{bmatrix} \begin{bmatrix} P_m Y_k & p_{m+1} \end{bmatrix} = \begin{bmatrix} P_m Y_k & p_{m+1} \end{bmatrix} \begin{bmatrix} \diagdown & \\ & D_{k+1} \\ \diagup & \end{bmatrix} + \begin{bmatrix} \text{---} \\ \vec{f} \end{bmatrix}$$

$\vec{f} = \vec{t}_{k+1,k} p_{m+1}$

# Updating Lanczos Factorization

Tridiagonalize the arrowhead matrix  $D_{k+1}$ , with methods from before:

$$\begin{bmatrix} \vec{Q}_k^T \\ \vdots \\ 1 \end{bmatrix} \begin{bmatrix} \diagdown & & \\ & D_{k+1} & \\ \hline & & \diagup \end{bmatrix} \begin{bmatrix} \vec{Q}_k \\ \vdots \\ 1 \end{bmatrix} = \begin{bmatrix} \diagdown & & \\ & \vec{T}_{k+1} & \\ \hline & & \diagup \end{bmatrix}$$

Multiply by  $\vec{Q}_{k+1}$  and truncate, obtaining  $k$ -Lanczos factorization:

$$\begin{bmatrix} A \\ \vdots \\ \vdots \end{bmatrix} \begin{bmatrix} P_m Y_k \vec{Q}_k \\ \vdots \\ \vdots \end{bmatrix} = \begin{bmatrix} P_m Y_k \vec{Q}_k \\ \vdots \\ \vdots \end{bmatrix} \begin{bmatrix} \diagdown & & \\ & \vec{T}_k & \\ \hline & & \diagup \end{bmatrix} + \begin{bmatrix} \text{---} \\ \vdots \\ \vec{f} \end{bmatrix}$$

$\vec{f}$  is not changed!

# TRL + Arrowhead Conversion

$$\begin{bmatrix} A \\ \vdots \end{bmatrix} = \begin{bmatrix} P_m \\ \vdots \end{bmatrix} + \begin{bmatrix} T_m \\ \vdots \end{bmatrix} + \begin{bmatrix} \text{gray block} \\ \vdots \end{bmatrix} + \begin{bmatrix} f \\ \vdots \end{bmatrix}$$

$$\begin{bmatrix} A \\ \vdots \end{bmatrix} = \begin{bmatrix} \text{arrowhead} \\ \vdots \end{bmatrix} + \begin{bmatrix} \text{gray block} \\ \vdots \end{bmatrix}$$

$$\begin{bmatrix} A \\ \vdots \end{bmatrix} = \begin{bmatrix} \text{arrowhead} \\ \vdots \end{bmatrix} + \begin{bmatrix} \text{gray block} \\ \vdots \end{bmatrix}$$

# Implicit Restart Lanczos (IRL) — Exact Shifts

1. Generate  $m$ -Lanczos factorization:  $AP_m = P_m T_m + f e_m^T$ .
2. Apply shifts  $\theta_{k+1}, \dots, \theta_m$  via the QR algorithm to  $T_m$ :

$$T_m^+ = Q_m^{+T} T_m Q_m^+ = \begin{bmatrix} \text{---} & & & \\ \text{---} & T_k^+ & & \\ \text{---} & & \ominus_{m-k} & \\ & & & \text{---} \end{bmatrix}$$

3. Truncate to size  $k$ ; obtain a new [start vector](#).

$$AP_m Q_k^+ = P_m Q_k^+ T_k^+ + q_{m,k}^+ f e_k^T.$$

4. Extend to a new  $m$ -Lanczos factorization.



# Mathematical Equivalence

$$\begin{aligned} \text{TRL} \quad AP_m \vec{Y}_k &= P_m \vec{Y}_k \vec{T}_k + \vec{t}_{k+1,k} P_{m+1} e_k^T \\ \text{IRL} \quad AP_m Q_k^+ &= P_m Q_k^+ T_k^+ + q_{m,k}^+ f e_k^T \end{aligned}$$

## Theorem (Baglama, Monette, Perovic 2026)

$$\begin{array}{ccc} \text{TRL} & = & \text{IRL} \\ \text{with arrowhead reduction} & & \text{with exact shifts} \end{array}$$

That is, there exists  $S = \text{diag}(\pm 1, \dots, \pm 1)$  such that

$$\vec{Y}_k = Q_k^+ S, \quad \vec{T}_k = S^{-1} T_k^+ S, \quad \vec{t}_{k+1,k} = \pm \beta q_{m,k}^+$$

meaning that  $\text{TRL} = \text{IRL} \cdot S$ .

This is a **stronger** result with **no Krylov subspace** arguments!

# Key Takeaways

- The  $QR$  algorithm with multiple shifts can fail to deflate eigenvalues.
- The “arrowhead method” is a significant improvement to this task.
- Thick Restart Lanczos with arrowhead reduction is **equal** to Implicit Restart Lanczos with exact shifts (not just *equivalent!*)
- An Extension: Replace “Lanczos” with “GKLB” and use a half-arrowhead matrix to show equivalence between thick and implicit GKLB for SVD computations.

## A Unified View of Arrowhead Matrix Transformations and Lanczos Restarts

James Baglama, Kyle Monette, Vasilije Perovic

[GitHub codes](#) & [Arxiv paper](#) coming soon on webpage



[kylemonette.github.io](https://kylemonette.github.io)

**Thank you!**