Arrowhead Matrix Transformations and Lanczos Restarts

SIAM NE Annual Meeting 2026

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Joint Work With: James Baglama & Vasilije Perovic

THE UNIVERSITY OF RHODE ISLAND

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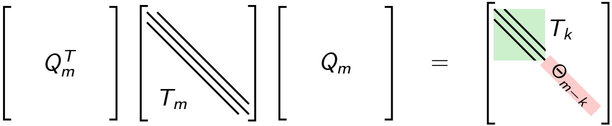
Roadmap

Part 1: Deflating eigenvalues from a small tridiagonal matrix.



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: $T_m = \begin{bmatrix} \diagdown\!\!\diagdown\!\!\diagdown \end{bmatrix}$.

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

$$\underbrace{T_m Y_k = Y_k \Theta_k}_{\text{desired}} \qquad \underbrace{T_m Y_{m-k} = Y_{m-k} \Theta_{m-k}}_{\text{undesired}}$$

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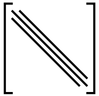
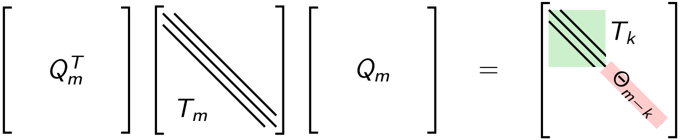
Let T_m be an $m \times m$ symmetric tridiagonal matrix: $T_m =$  .

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

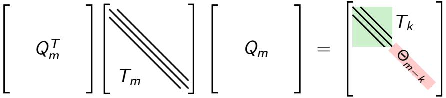
$$\underbrace{T_m Y_k = Y_k \Theta_k}_{\text{desired}} \qquad \underbrace{T_m Y_{m-k} = Y_{m-k} \Theta_{m-k}}_{\text{undesired}}$$

Goal: Find an orthogonal matrix Q_m such that



Arrowhead Matrices

Goal:



Our insight is a special *arrowhead matrix* created from the k desired eigenpairs (θ_i, y_i):

$$D_{k+1} \quad = \quad \begin{bmatrix} \theta_1 & & & \beta y_{m,1} \\ & \ddots & & \vdots \\ & & \theta_k & \beta y_{m,k} \\ \beta y_{m,1} & \dots & \beta y_{m,k} & \star \end{bmatrix} \qquad (\beta \neq 0, \;\; \star \in \mathbb{R}).$$

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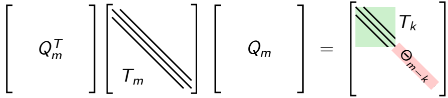

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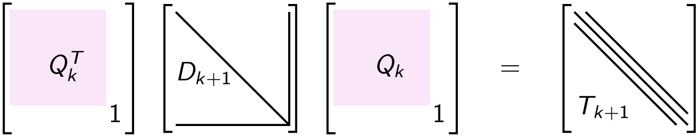
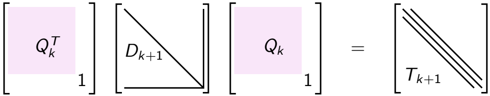
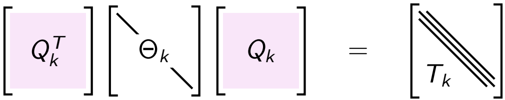
Various methods (Householder, Givens, etc.) can *tridiagonalize* D_{k+1}:



Arrowhead Conversion



Truncate the first k rows & columns:



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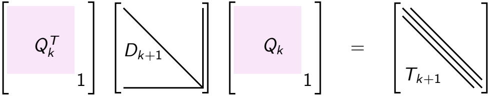

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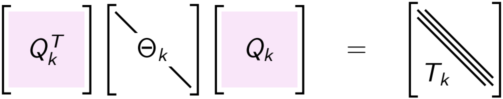
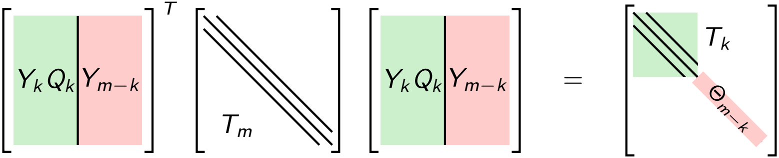
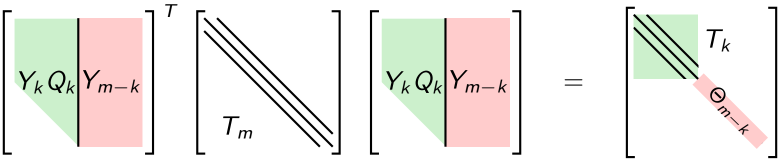


Utilizing $T_m \begin{bmatrix} Y_k & Y_{m-k} \end{bmatrix} = \begin{bmatrix} Y_k & Y_{m-k} \end{bmatrix} \begin{bmatrix} \Theta_k & \\ & \Theta_{m-k} \end{bmatrix}$:

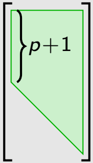


Structure of $Y_k Q_k$



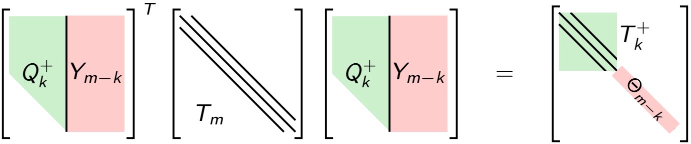
Theorem 2.4 (Baglama, Monette, Perovic 2026)

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

$\vec{Y}_k \quad =$  (where $p = m - k$).

Connection to QR Algorithm

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



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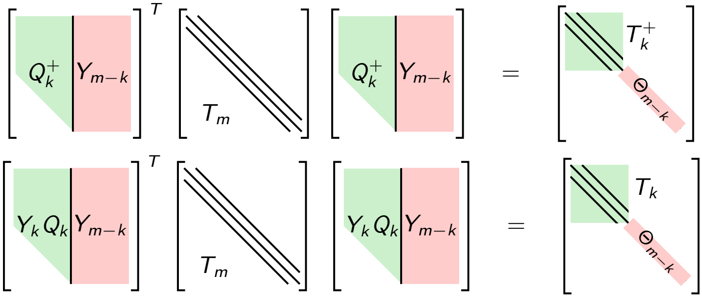

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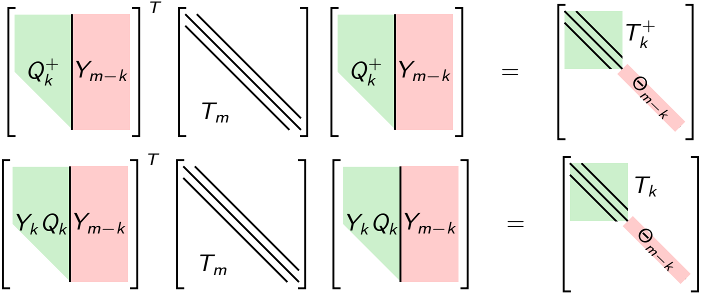


Theorem 2.6 (Baglama, Monette, Perovic 2026)

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

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

Examples

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

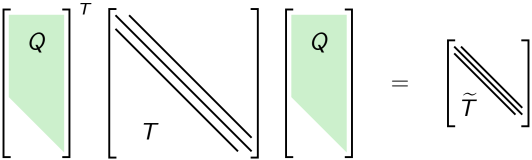
Input: Tridiagonal T with eigenpairs $TX = X\Lambda$.

Arrowhead Method (T, k)

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

Implicit QR Method (T, p)

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



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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	$\left\lVert \mathrm{eig}(T(1:k,1:k)) - \mathrm{eig}(\widetilde{T}) \right\rVert$	$\left\lVert \widetilde{T} - Q^T T Q \right\rVert$
	Wilkinson Matrix	
Arrowhead	2.5×10^{-14}	5.7×10^{-14}
Implicit QR	12.4	2.5×10^{-14}
	Fann Matrix	
Arrowhead	1.6×10^{-14}	4.4×10^{-15}
Implicit QR	1.7	4×10^{-15}

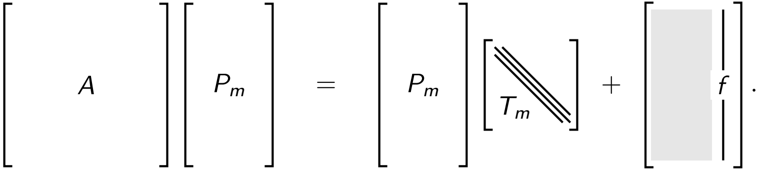
Restarting the Lanczos Algorithm

Introduction

Goal: Compute a few (k) *eigenpairs* $\{(\lambda_i, x_i)\}_{i=1}^{k}$ of a large, sparse, symmetric $A \in \mathbb{R}^{n \times n}$.

Utilize the Lanczos Algorithm — project A onto an $m \ll n$ dimensional subspace:

$$AP_m \quad = \quad P_m T_m + f e_m^T$$



Restart Methods

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

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.

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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

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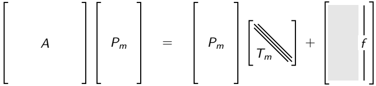

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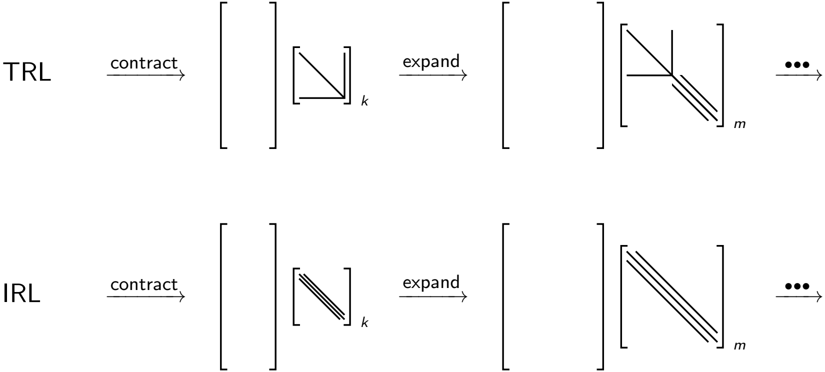
Equivalence has been known: Wu & Simon 2000, Morgan 2004, etc.
Goal: A stronger connection using arrowhead matrices.

Thick Restarts (TRL) and Implicit Restarts (IRL)

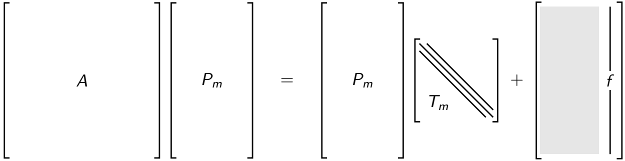
Until convergence ...

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

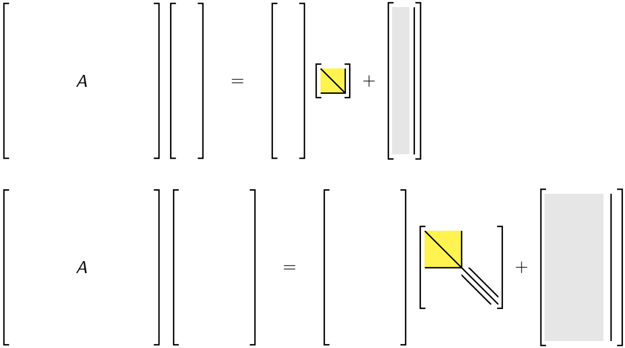


Thick Restart Lanczos (TRL)

Initialization:



Repeat:



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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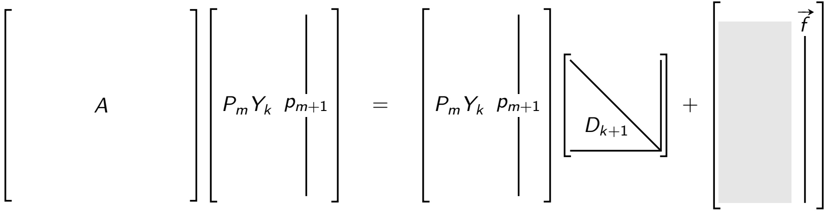
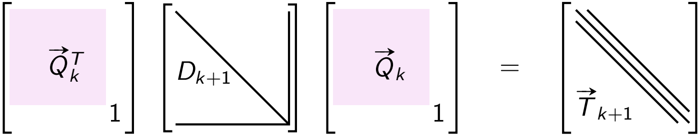
... yielding a "not quite"-Lanczos factorization!



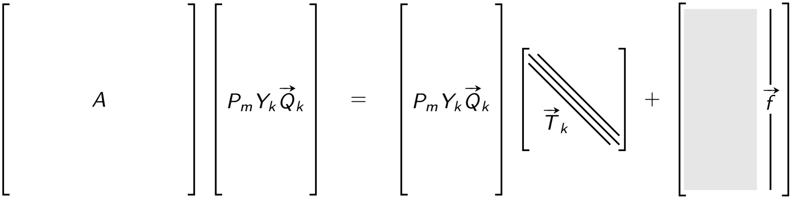
$\vec{f} = \vec{t}_{k+1,k}\, p_{m+1}$

Updating Lanczos Factorization

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

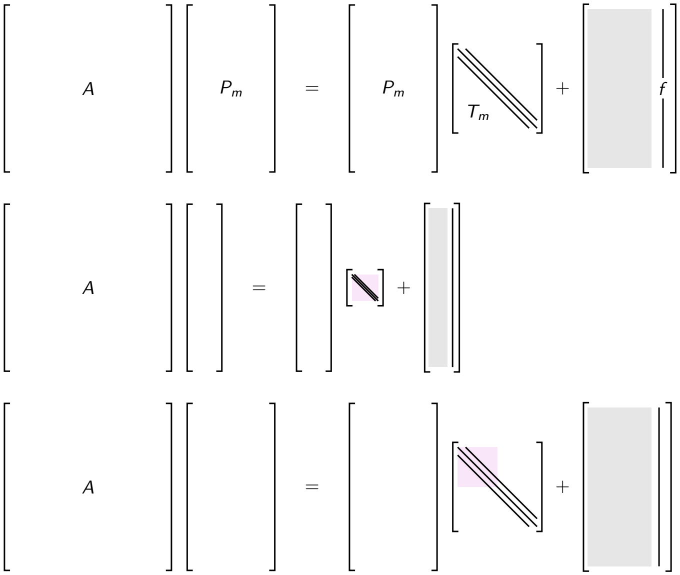


Multiply by $\vec{Q}_{k+1}$ and truncate, obtaining k-Lanczos factorization:



$\vec{f}$ is not changed!

TRL + Arrowhead Conversion

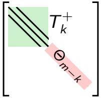


Implicit Restart Lanczos (IRL) — Exact Shifts

1. Generate m-Lanczos factorization: $\quad AP_m = P_m T_m + f e_m^T.$

2. Apply shifts $\theta_{k+1}, \ldots, \theta_m$ via the QR algorithm to T_m:

$$T_m^+ \quad = \quad {Q_m^+}^T T_m Q_m^+ \quad =$$



3. Truncate to size k; obtain a new start vector.

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

4. Extend to a new m-Lanczos factorization.

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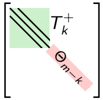

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$$AP_m Q_k^+ \quad = \quad P_m Q_k^+ T_k^+ + q_{m,k}^+ f e_k^T .$$

4. Extend to a new m-Lanczos factorization.

... sound familiar?

Mathematical Equivalence

$$\begin{array}{lrcl} \text{TRL} & AP_m\vec{Y}_k & = & P_m\vec{Y}_k\vec{T}_k + \vec{t}_{k+1,k}p_{m+1}e_k^T \\ \text{IRL} & AP_mQ_k^+ & = & P_mQ_k^+T_k^+ + q_{m,k}^+fe_k^T \end{array}$$

Theorem (Baglama, Monette, Perovic 2026)

TRL	=	IRL
with arrowhead reduction		with exact shifts

That is, there exists $S = \text{diag}(\pm1, \dots, \pm1)$ such that

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

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

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.

In Press — Coming Soon!

A Unified View of Arrowhead Matrix Transformations and Lanczos Restarts

James Baglama, Kyle Monette, Vasilije Perovic

GitHub Code

Website

Thank you!