Symmetric Eigenvalue Problems

Kyle Monette

Department of Mathematics and Applied Mathematical Sciences
University of Rhode Island

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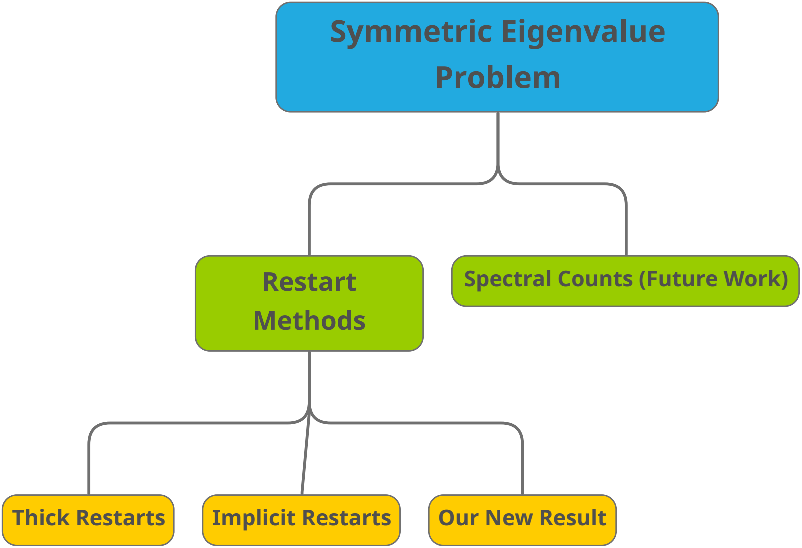

Symmetric Eigenvalue Problem
Restart Methods
Spectral Counts (Future Work)
Thick Restarts
Implicit Restarts
Our New Result

Symmetric Eigenvalue Problem

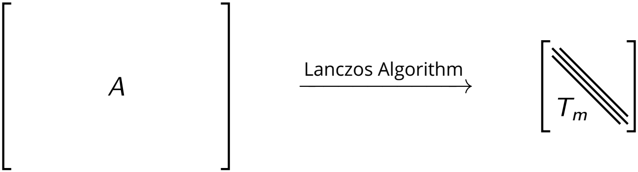
Given: Large, sparse, symmetric $A \in \mathbb{R}^{n\times n}$.
Compute some approximate eigenpairs (λ, x). That is, $Ax = \lambda x$.

If n is small, then A can be "tridiagonalized" to T. An $\mathcal{O}(n^3)$ process.

$$A = \begin{bmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \end{bmatrix} \longrightarrow T = Q^T A Q = \begin{bmatrix} * & * & & \\ * & * & * & \\ & * & * & * \\ & & * & * \end{bmatrix} \longrightarrow \text{Eigenpairs of } T$$

We assume n is too large for this to be done.

Instead, we'll "reduce" A to a **smaller** tridiagonal matrix T_m.



Lanczos Algorithm

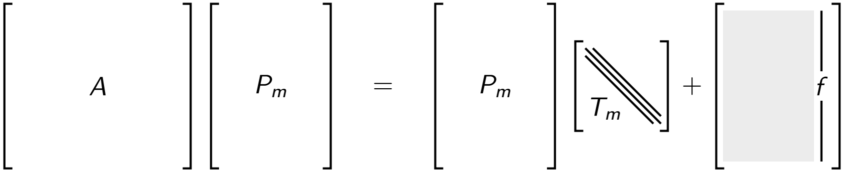
Given symmetric $A \in \mathbb{R}^{n\times n}$, $m \ll n$, and unit vector $p_1 \in \mathbb{R}^n$, generate

$$AP_m = P_m T_m + f e_m^T.$$

$[P, T, f] = \texttt{Lanczos}(A, p_1, m)$

for $j = 1, 2, \ldots, m$ **do**
    $f = Ap_j$
    if $j > 1$ **then** $f = f - p_{j-1}\beta_{j-1}$
    $\alpha_j = f^T p_j$
    $f = f - p_j \alpha_j$ $f = f - P_j(P_j^T f)$
    if $j < m$ **then** $\beta_j = \|f\|$ $p_{j+1} = f/\beta_j$
end for

$$T_m = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \beta_2 & \ddots & \ddots & \\ & & \ddots & \alpha_{m-1} & \beta_{m-1} \\ & & & \beta_{m-1} & \alpha_m \end{bmatrix}$$



Ritz Pairs of A

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

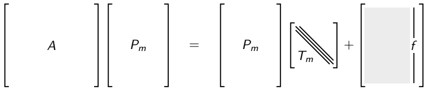
If (θ_j, y_j) is an eigenpair of T_m $\quad (T_m y_j = \theta_j y_j)$ $\quad$ then Ritz pairs of A are

$$(\theta_j, x_j), \quad \text{where} \quad x_j = P_m y_j.$$

The residual is

$$\|Ax_j - \theta_j x_j\| \quad = \quad \|AP_m y_j - \theta_j P_m y_j\| \quad = \quad \left\|f e_m^T y_j\right\| \quad = \quad \|f\| \cdot \left|e_m^T y_j\right|$$

What if residual is large? *Restart* Lanczos, “keeping” desired Ritz vectors.



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What if residual is large? *Restart* Lanczos, “keeping” desired Ritz vectors.

Thick Restarts

- MATLAB post-2016
- Krylov-Schur [Ste02], [Wu&Sim00]

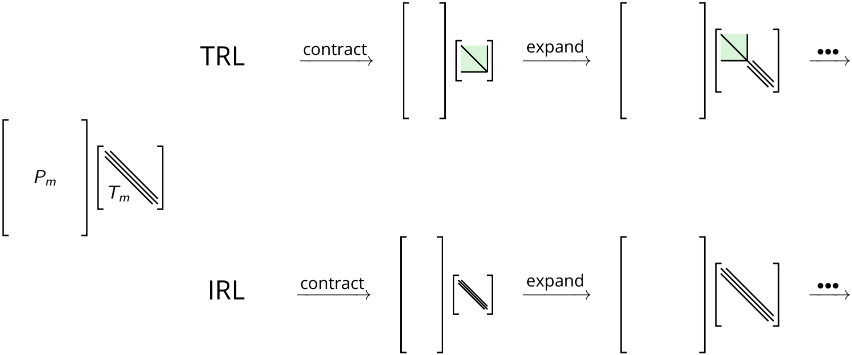
Implicit Restarts

- MATLAB pre-2016
  (Octave, ARPACK)
- IRA / IRL [Sor92] / [Cal&Sor94]

TRL and IRL

Until convergence . . .

1. Generate m-Lanczos factorization: $AP_m = P_m T_m + f e_m^T$.
2. Compute Ritz pairs: (θ_j, x_j) $\quad x_j = P_m y_j$ and $T_m y_j = \theta_j y_j$.
3. Choose $k < m$ "desired" Ritz pairs.
4. "Restart" with these pairs; build a new m-Lanczos factorization.



Thick Restarting Lanczos

$$Ax_j - \theta_j x_j \;=\; f e_m^T y_j \quad \Rightarrow \quad Ax_j \;=\; \underbrace{\beta_m p_{m+1}}_{f} e_m^T y_j + \theta_j x_j \;=\; \underbrace{\overline{\beta}_j}_{\beta_m e_m^T y_j} p_{m+1} + \theta_j x_j$$

Let $\overline{P}_k = \begin{bmatrix} x_1 & \ldots & x_k \end{bmatrix}$ and $\overline{P}_{k+1} = \begin{bmatrix} x_1 & \ldots & x_k & p_{m+1} \end{bmatrix}$.

One can show that

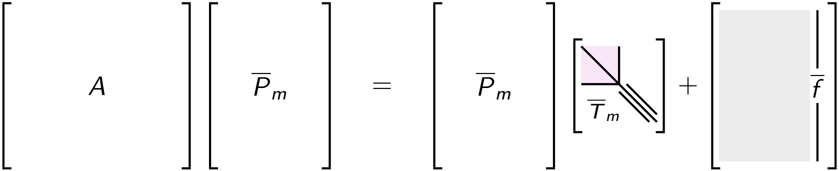
$$\overline{P}_{k+1}^T A \overline{P}_{k+1} \;:=\; \overline{T}_{k+1} \;=\; \begin{bmatrix} \theta_1 & & & & \overline{\beta}_1 \\ & \theta_2 & & & \overline{\beta}_2 \\ & & \ddots & & \vdots \\ & & & \theta_k & \overline{\beta}_k \\ \overline{\beta}_1 & \overline{\beta}_2 & \ldots & \overline{\beta}_k & \alpha_{k+1} \end{bmatrix}$$

where $\alpha_{k+1} = p_{m+1}^T A p_{m+1}$.

Now the “restart” makes sense:

Start Lanczos with vector p_{m+1}, and do $m-(k+1)$ steps.

The first $k+1$ chunk is $A\overline{P}_{k+1} = \overline{P}_{k+1}\,\overline{T}_{k+1} + \beta_{k+1} p_{k+2} e_{k+1}^T$.



Thick Restarting Lanczos

Now the "restart" makes sense:

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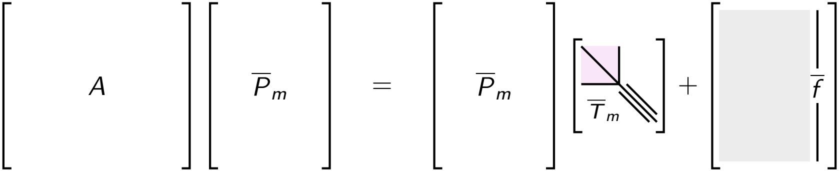
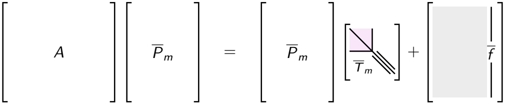


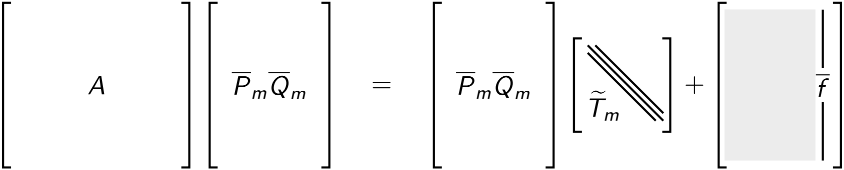
Question: Can the "arrowhead" $\overline{T}_{k+1}$ be "tridiagonalized" efficiently?

Is there a benefit?



We showed [Bag,Mon,Per25+] that we can tridiagonalize $\overline{T}_{k+1}$ via

$$\widetilde{T}_{k+1} = \overline{Q}_{k+1}^T \, \overline{T}_{k+1} \, \overline{Q}_{k+1} \qquad \overline{Q}_{k+1} = \begin{bmatrix} & \overline{Q}_k & & \begin{matrix} 0 \\ \vdots \\ 0 \end{matrix} \\ 0 & \dots & 0 & 1 \end{bmatrix}$$



Equating the first k columns: $A\overline{P}_k\overline{Q}_k = \overline{P}_k\overline{Q}_k\widetilde{T}_k + \widetilde{t}_{k+1,k}\, p_{m+1} e_k^T$

Another Restart Method — IRL

TRL Summary: Restart with k Ritz vectors.

Another Variation: Can we choose a new (better) initial vector $\widehat{p}_1$?

Goal: $$\widehat{p}_1 \approx \underbrace{c_1 x_1 + \cdots + c_k x_k}_{\text{large } c_i} + \underbrace{c_{k+1} x_{k+1} + \cdots + c_n x_n}_{\text{small } c_i}$$

IRL applies a polynomial filter to update the starting vector.

$$\widehat{p}_1 = q(A) p_1 = c_1 q(\lambda_1) x_1 + \cdots + c_k q(\lambda_k) x_k + c_{k+1} q(\lambda_{k+1}) x_{k+1} + \cdots + c_n q(\lambda_n) x_n$$

Which polynomial q?

Applying Shifts

Say (μ, x) is an approximate eigenpair of A. Then

$$x^T(A - \mu I)p_1 \quad \approx \quad 0.$$

So $(A - \mu I)p_1$ has (approx.) no components in direction of x.

Choose μ to be a "shift" from the undesired part of the spectrum.

Result: A vector $(A - \mu I)p_1$ *enriched* in direction of desired eigenvectors.

However, notice that

$$(A - \mu I)P_m \quad = \quad P_m(T_m - \mu I) + fe_m^T.$$

So, we shift T_m instead of A.

Applying Shifts

Given the undesired eigenvalues $\theta_{k+1}, \ldots, \theta_m$ of T_m, we consider

$$q(T_m) \quad = \quad (T_m - \theta_{k+1} I) \ldots (T_m - \theta_m I)$$

(*which is not formed explicitly!*).

Use the implicit *QR* algorithm with shifts $\theta_{k+1}, \ldots, \theta_m$ to obtain

$$T_m^+ \quad := \quad {Q_m^+}^T T_m Q_m^+, \qquad q(T_m) = Q_m^+ R_m^+.$$

Implicit QR Algorithm

Choose a shift μ.

Create a rotation matrix $\widetilde{G}_1 = \begin{bmatrix} c & -s \\ s & c \end{bmatrix}$ such that $\widetilde{G}_1^T \begin{bmatrix} t_{11} - \mu \\ t_{21} \end{bmatrix} = \begin{bmatrix} \star \\ 0 \end{bmatrix}$.

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$$T_m = \begin{bmatrix} * & * & & & \\ * & * & * & & \\ & * & * & * & \\ & & * & * & * \\ & & & * & * \end{bmatrix} \quad \to \quad G_1^T T_m G_1 = \begin{bmatrix} \times & \times & \bullet & & \\ \times & \times & \times & & \\ \bullet & \times & * & * & \\ & & * & * & * \\ & & & * & * \end{bmatrix}.$$

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$$\underbrace{\begin{bmatrix} * & \times & & & \\ \times & \times & \times & \bullet & \\ & \times & \times & \times & \\ & \bullet & * & * & * \\ & & & * & * \end{bmatrix}}_{\text{Action of } G_2}$$

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$$\underbrace{\begin{bmatrix} * & \times & & & \\ \times & \times & \times & \bullet & \\ & \times & \times & \times & \\ & \bullet & * & * & * \\ & & & * & * \end{bmatrix}}_{\text{Action of } G_2} \quad \underbrace{\begin{bmatrix} * & * & & & \\ * & * & \times & & \\ & \times & \times & \times & \bullet \\ & & \times & \times & \times \\ & & \bullet & \times & * \end{bmatrix}}_{\text{Action of } G_3} \quad \underbrace{\begin{bmatrix} * & * & & & \\ * & * & * & & \\ & * & * & \times & \\ & & \times & \times & \times \\ & & & \times & \times \end{bmatrix}}_{\text{Action of } G_4}$$

Implicit QR Algorithm

So after one shift μ, we obtain

$$T_m^+ \quad := \quad {Q_m^+}^T T_m Q_m^+, \qquad Q_m^+ = G_1 \dots G_{m-1}.$$

If μ is an (undesired) eigenvalue of T_m (an "exact shift"):

Then $\quad t_{m,m}^+ = \mu \quad$ and $\quad t_{m,m-1}^+ = t_{m-1,m}^+ = 0.$

Implicit QR Algorithm

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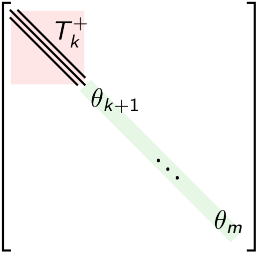
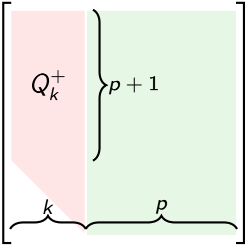
Repeat for $p := m - k$ exact shifts:

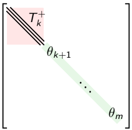
$T_m^+ =$

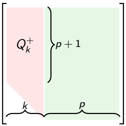


$Q_m^+ =$



$$
\begin{aligned}
AP_mQ_m^+ &= P_mQ_m^+T_m^+ + fe_m^TQ_m^+ \\
A\underbrace{P_k^+}_{P_mQ_k^+} &= P_k^+T_k^+ + \underbrace{q_{m,k}^+ f}_{f^+} e_k^T
\end{aligned}
$$

$T_m^+ =$ 

$Q_m^+ =$ 

Now, restart Lanczos with f^+ and build to size m.

Revisiting the initial vector:

From $AP_m = P_mT_m + fe_m^T$ one can show $q(A)P_me_1 = P_m\underbrace{q(T_m)}_{Q_m^+R_m^+}e_1$.

Then $q(A)p_1 = P_mQ_m^+r_{11}^+e_1 \quad \Rightarrow \quad q(A)p_1 = r_{11}^+\widehat{p}_1$.

Therefore, $\widehat{p}_1 \propto q(A)p_1$ is a “polynomial filter” update to p_1.

Which has stronger components in desired Ritz vectors.

Equivalence

TRL and IRL (exact shifts) are “mathematically equivalent”.

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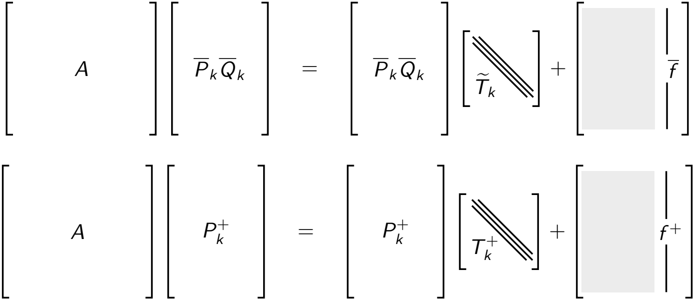
By considering the k-Lanczos factorizations …

$$
\begin{array}{lrcl}
\text{TRL} & A\overline{P}_k\overline{Q}_k & = & \overline{P}_k\overline{Q}_k\widetilde{T}_k + \widetilde{t}_{k+1,k}\,p_{m+1}e_k^T \\
\text{IRL} & AP_k^+ & = & P_k^+T_k^+ + q_{m,k}^+\,p_{m+1}e_k^T
\end{array}
$$

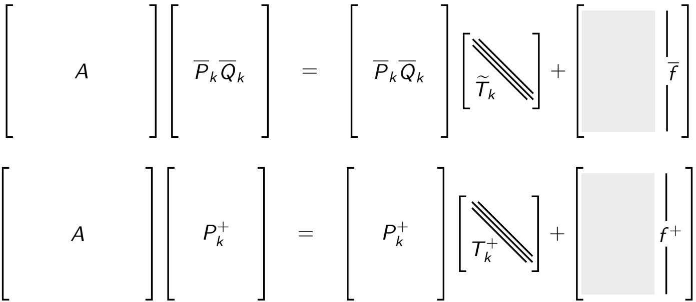


TRL and IRL (exact shifts) are "mathematically equivalent".

By considering the k-Lanczos factorizations . . .

$$\text{TRL} \qquad A\overline{P}_k\overline{Q}_k = \overline{P}_k\overline{Q}_k\widetilde{T}_k + \widetilde{t}_{k+1,k}p_{m+1}e_k^T$$

$$\text{IRL} \qquad AP_k^+ = P_k^+T_k^+ + q_{m,k}^+p_{m+1}e_k^T$$



Our New Result: $\overline{P}_k\overline{Q}_k = \pm P_k^+, \qquad \widetilde{T}_k = \pm T_k^+, \qquad \overline{f} = \pm f^+.$

In Summary . . .

Our new method [Bag,Mon,Per25+] (arrowhead to tridiagonal) . . .

- **Maintains** tridiagonal structure.
- **Not** sensitive to numerical round-off.
- **Equivalent** to a new method [Mas&Dor18].
- Provides new, **stronger** insight: TRL $=$ IRL (not just equivalent!)
- Adapts to the bidiagonal case & singular value problem.
  A seminar presentation (and another paper!) to come . . .

New Topic — Spectral Counts

Let $A \in \mathbb{R}^{n \times n}$ be a (large!) symmetric matrix and $[a, b] \subset \mathbb{R}$.

Question: How many eigenvalues of A are in $[a, b]$? c.f. [Nap16]

Our (Future) Interest: Accelerating algorithms with this count.

Potential Insight: Form the projection matrix P

$$P \quad := \quad \sum_{\substack{i \\ \lambda_i \in [a,b]}} u_i u_i^T$$

which satisfies $P^2 = P$, so eigenvalues of P are 0 and 1.

Key Result: $\mathrm{trace}(P)$ is the number of eigenvalues of A in $[a, b]$.

Approximate trace(P)

Let $h(t)$ be the indicator function

$$h(t) \quad = \quad \begin{cases} 1 & t \in [a, b] \\ 0 & \text{otherwise} \end{cases}$$

and consider its representation in the Chebyshev basis

$$h(t) \quad \approx \quad \sum_{j=0}^{p} \gamma_j T_j(t).$$

Linearly map eigenvalues of A and $[a, b]$ into $[-1, 1]$. Then

$$P \quad \approx \quad h(A) \quad \approx \quad \sum_{j=0}^{p} \gamma_j T_j(A)$$

has eigenvalues of 1 if $\lambda_i \in [a, b]$ and eigenvalues of 0 otherwise.

Therefore: $\quad \text{trace}(P) \; = \; \#\,\text{eigenvalues of } A \text{ in } [a, b] \; \approx \; \text{trace}(h(A)).$

Hutchinson's Theorem
Suppose each component of $v \in \mathbb{R}^n$ is drawn independently from a distribution with mean 0 and variance 1; that is, $\mathbb{E}[v] = 0$ and $\mathbb{E}[vv^T] = I_n$.

Then for any symmetric matrix A and matrix function f defined on A,

$$\mathbb{E}\left[v^T f(A) v\right] \quad = \quad \text{trace}\, f(A).$$

In particular, we'll use $v \sim \mathrm{unif}\{-1, 1\}^n$, called Rademacher vectors (for the least variance estimator).

Therefore, $$\text{trace}(P) \approx \text{trace}(h(A)) = \mathbb{E}\left[v^T h(A) v\right].$$

Computing $\mathrm{trace}(P) \approx \mathbb{E}\left[v^T h(A) v\right]$

From before ...

$$
\begin{aligned}
\#\text{ eigenvalues of } A \text{ in } [a, b] \quad &= \quad \mathrm{trace}(P) \\
&\approx \quad \mathrm{trace}(h(A)) \\
&= \quad \mathbb{E}\left[v^T h(A) v\right] \\
&= \quad \mathbb{E}\left[\sum_{j=0}^{p} \gamma_j v^T T_j(A) v\right] \\
&= \quad n \cdot \mathbb{E}\left[\sum_{j=0}^{p} \gamma_j v^T T_j(A) v\right] \qquad \text{(normalize } v\text{)} \\
&\approx \quad \frac{n}{n_v} \sum_{k=1}^{n_v} \sum_{j=0}^{p} \gamma_j v_k^T T_j(A) v_k
\end{aligned}
$$

Future Work

$T_p(A)v$ is a (modest size) polynomial of A times $v \dots$

Then $w = T_p(A)v$ has components in the eigenvectors of A from $[a, b]$.

Future work: Optimizing existing algorithms by using w.

- Solving $A(x + w) = b + Aw$ instead of $Ax = b$.
- Symmetric eigenvalue problems.
- Singular value thresholding (since $\sigma(A) = \sqrt{\lambda(A^T A)}$).
- $\dots$

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Thank you!

Questions?

Lanczos Recurrence

Three term recurrence: Arnoldi gives $T_{ij} = p_i^T A p_j$, for $1 \leq i \leq j$.

If A is symmetric, then $T_{ij} = (Ap_i)^T p_j$.

For $i < j - 1$, then $Ap_i \in \text{span}\{p_1, \ldots, p_{j-1}\}$ and p_j is perpendicular to this span, so it must be that $(Ap_i)^T p_j = 0$.

Therefore, T has zero 2nd off-diagonals.

Ritz Extraction

Let $\mathcal{K}_m$ be an m-dimensional subspace of $\mathbb{R}^n$.

We say (θ, x), where $x \in \mathcal{K}_m$, is a *Ritz pair* of A if $Ax - \theta x \perp \mathcal{K}_m$.

Let $P_m \in \mathbb{R}^{n \times m}$ be an ONB for $\mathcal{K}_m$.

Then $\exists\, y \in \mathbb{R}^m$ such that $x = P_m y$.

Let $T_m = P_m^T A P_m \in \mathbb{R}^{m \times m}$.

Then (θ, x) is a Ritz pair iff (θ, y) is an eigenpair of T_m.

TRL Step

Let $\Theta_k = \text{diag}(\theta_1, \ldots, \theta_k)$ and $Y_k = Y_{:,1:k}$. Then $A\overline{P}_k = \overline{P}_k \Theta_k + \beta_m p_{m+1} e_m^T Y_k$, or equivalently $A\overline{P}_k = \overline{P}_{k+1} \overline{T}_{k+1,k}$. Orthogonalize Ap_{m+1} against $\overline{P}_{k+1}$:

$$
\begin{aligned}
r &= (I - \overline{P}_{k+1}\overline{P}_{k+1}^T)Ap_{m+1} = Ap_{m+1} - \begin{bmatrix} \overline{P}_k & p_{m+1} \end{bmatrix} \begin{bmatrix} \overline{P}_k^T \\ p_{m+1}^T \end{bmatrix} Ap_{m+1} \\
&= Ap_{m+1} - \overline{P}_k \overline{P}_k^T Ap_{m+1} - p_{m+1}p_{m+1}^T Ap_{m+1} \\
&= Ap_{m+1} - \overline{P}_k (A\overline{P}_k)^T p_{m+1} - p_{m+1}p_{m+1}^T Ap_{m+1} \\
&= Ap_{m+1} - \overline{P}_k(\Theta_k \overline{P}_k^T p_{m+1}) - \overline{P}_k \beta_m Y_k^T e_m p_{m+1}^T p_{m+1} - p_{m+1}p_{m+1}^T Ap_{m+1} \\
&= Ap_{m+1} - p_{m+1}p_{m+1}^T Ap_{m+1} - \overline{P}_k \beta_m Y_k^T e_m.
\end{aligned}
$$

Let $p_{k+2} = r/\|r\| = r/\beta_{k+1}$, and $\alpha_{k+1} = p_{m+1}^T Ap_{m+1}$. Then

$$
Ap_{m+1} = \beta_{k+1} p_{k+2} + \alpha_{k+1} p_{m+1} + \overline{P}_k \overline{\beta}
$$

where $\overline{\beta}$ is a vector of $(\overline{\beta}_1, \ldots, \overline{\beta}_k)$ and $\overline{\beta}_i = \beta_m y_i^T e_m$.

TRL Step

$$
\begin{aligned}
A\overline{P}_{k+1} &= \left[\overline{P}_{k+1}\overline{T}_{k+1,k} \mid Ap_{m+1}\right] \\
&= \left[\ \overline{P}_{k+1}\overline{T}_{k+1,k} \ \middle|\ \beta_{k+1}p_{k+2} + \alpha_{k+1}p_{m+1} + \overline{P}_k\overline{\beta}\ \right] \\
&= \left[\ \overline{P}_{k+1}\overline{T}_{k+1,k} \ \middle|\ \overline{P}_{k+1}\begin{bmatrix} \overline{\beta} \\ \alpha_{k+1} \end{bmatrix}\ \right] + \beta_{k+1}p_{k+2}e_{k+1}^T \\
&= \overline{P}_{k+1}\overline{T}_{k+1} + \beta_{k+1}p_{k+2}e_{k+1}^T
\end{aligned}
$$

which also shows that $\overline{P}_{k+1}^T A\overline{P}_{k+1} = \overline{T}_{k+1}$ by orthogonality.

TRL Truncation

From $A\overline{P}_{k+1} = \overline{P}_{k+1}\overline{T}_{k+1} + \beta_{k+1}p_{k+2}e_{k+1}^T$, then

$$A\overline{P}_{k+1}\overline{Q}_{k+1} = \overline{P}_{k+1}\overline{Q}_{k+1}\widetilde{T}_{k+1} + \beta_{k+1}p_{k+2}e_{k+1}^T\overline{Q}_{k+1}.$$

Note that $e_{k+1}^T\overline{Q}_{k+1} = e_{k+1}^T$ and the first k columns of $p_{k+2}e_{k+1}^T$ are zeros. Therefore,

$$A\begin{bmatrix} \overline{P}_k & p_{m+1} \end{bmatrix}\begin{bmatrix} \overline{Q}_k & 0 \\ 0 & 1 \end{bmatrix} = \underbrace{\begin{bmatrix} \overline{P}_k & p_{m+1} \end{bmatrix}\begin{bmatrix} \overline{Q}_k & 0 \\ 0 & 1 \end{bmatrix}}_{=\begin{bmatrix} \overline{P}_k\overline{Q}_k & p_{m+1} \\ 0 & 0 \end{bmatrix}}\begin{bmatrix} \widetilde{T}_k & \widetilde{t}_{k+1,k}e_k \\ \widetilde{t}_{k+1,k}e_k^T & \widetilde{t}_{k,k} \end{bmatrix} + \beta_{k+1}p_{k+2}e_{k+1}^T$$

which gives us

$$A\overline{P}_k\overline{Q}_k = \overline{P}_k\overline{Q}_k\widetilde{T}_k + \widetilde{t}_{k+1,k}p_{m+1}e_k^T.$$

IRL Truncation

From $AP_m = P_m T_m + f e_m^T$, then $AP_m Q_m^+ = P_m Q_m^+ T_m^+ + f e_m^T Q_m^+$.

$$AP_m \left[\begin{array}{c|c} Q_k^+ & Q^+ \end{array}\right] = P_m \left[\begin{array}{c|c} Q_k^+ & Q^+ \end{array}\right] \left[\begin{array}{cc} T_k^+ & t_{k,k+1}^+ e_k e_1^T \\ t_{k+1,k}^+ e_1 e_k^T & \Theta \end{array}\right] + f e_m^T \left[\begin{array}{c|c} Q_k^+ & Q^+ \end{array}\right]$$

Then $AP_m Q_k^+ = P_m Q_k^+ T_k^+ + P_m Q^+ t_{k+1,k}^+ e_1 e_k^T + f \underbrace{e_m^T Q_k^+}_{= q_{m,k}^+ e_k^T}$.

Mathematically, $t_{k+1,k}^+ = 0$. But we need to include this term, so

$$AP_m Q_k^+ = P_m Q_k^+ T_k^+ + \left(P_m Q_m^+ e_{k+1} t_{k+1,k}^+ + q_{m,k}^+ f\right) e_k^T$$

since $Q^+ e_1 \coloneqq Q_m^+ e_{k+1}$.

Example

200×200 symmetric matrix $\mu^* = 15$ (exact)

(Left) Varying p, $n_v = 80$ fixed

(Right) Varying n_v, $p = 20$ fixed