

Numerical Matrix Analysis

Notes #19 — Eigenvalues Hessenberg Form, Rayleigh Quotient

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 - Phase#1 – Upper Hessenberg Form
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Last Time: Introduction to Eigenvalue Problems

Three factorizations which expose the eigenvalues of a matrix.

Type	Form	Restrictions on A	Vectors	↓ less restrictions ↓
Unitary Diagonalization	$A = Q\Lambda Q^*$	Normal, $A^*A = AA^*$	✓	
Diagonalization	$A = X\Lambda X^{-1}$	Non-defective	✓	
Schur Triangularization	$A = QTQ^*$	None	—	

Eigenvalue problems are fundamentally more difficult than solution of linear systems and/or least squares problems. We cannot guarantee, **even in exact arithmetic**, a solution in a finite number of steps.

Therefore —

Fact

Any eigenvalue solver must be iterative.



Schur Factorization and Diagonalization

1 of 2

Modern general-purpose eigenvalue algorithms tend to be based on the Schur factorization. We get $A = QTQ^*$ by finding a sequence of unitary similarity transformations

$$\underbrace{Q_k^* \cdots Q_3^* Q_2^* Q_1^*}_{Q^*} A \underbrace{Q_1 Q_2 Q_3 \cdots Q_k}_Q = T, \quad k \rightarrow \infty,$$

where T is upper triangular.

If $A \in \mathbb{R}^{m \times m}$, but not symmetric ($A^T \neq A$), then T may have **complex eigenvalues**. — We either must implement complex arithmetic, or we can allow T to have (2×2) -blocks along the diagonal.

$$\begin{bmatrix} \ddots & & & \\ & \lambda_r & -\lambda_i & \\ & \lambda_i & \lambda_r & \\ & & & \ddots \end{bmatrix}, \quad \lambda = \lambda_r \pm \sqrt{-1} \lambda_i$$



Schur Factorization and Diagonalization

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Allowing (2×2) -blocks along the diagonal saves the overhead of complex arithmetic, and is known as the **real Schur factorization**.

Special Case

When A is Hermitian ($A = A^*$), then

$$Q_k^* \cdots Q_3^* Q_2^* Q_1^* A Q_1 Q_2 Q_3 \cdots Q_k = T, \quad k \rightarrow \infty$$

is also Hermitian, *i.e.* $T = T^*$, and upper triangular \rightsquigarrow T is **diagonal**.

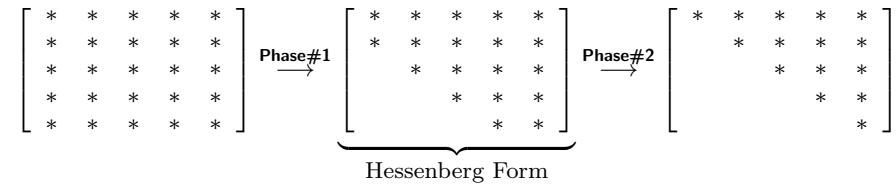
The eigenvalue computation is usually split into **2 phases** — (PHASE#1) completes in a finite number of steps and transforms the matrix into **upper Hessenberg** form; (PHASE#2) is iterative and converges ($k \rightarrow \infty$) to upper triangular form.



Two-Phase Eigenvalue Computation

1 of 2

When $A \neq A^*$: $A \mapsto H_A \mapsto T_A$



When $A = A^*$: $A \mapsto T_A \mapsto D_A$



In this case, the Hessenberg Form is Tri-Diagonal.



Two-Phase Eigenvalue Computation

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Phase#1 Requires $\mathcal{O}(m^3)$ operations.

Phase#2 May (in theory) require infinitely many iterations, each of which requires $\mathcal{O}(m^2)$ operations. In practice, convergence to $\mathcal{O}(\epsilon_{\text{mach}})$ can usually be achieved in $\mathcal{O}(m)$ iterations, *i.e.* the total work requirement is $\mathcal{O}(m^3)$.

When A is Hermitian, **Phase#2** can be executed with only $\mathcal{O}(m)$ operations/iteration; thus the total work estimate for the second phase is only $\mathcal{O}(m^2)$ in this case. Hence, the “infinite” part of the algorithm is an order of magnitude faster than the “finite” part.



Why Hessenberg Form?

1 of 2

We are looking to compute the Schur factorization $A = QTQ^*$.

Why not go straight for T ???

Ponder... the first standard Householder reflector Q_1^*



Whoops!!! The multiplication from the right will fill in \otimes the first column again... The sub-diagonal elements are typically reduced in magnitude, but at this point this does not get us closer to the goal...



Why Hessenberg Form?

2 of 2

Let's instead use a Householder reflector Q_1^* which ignores the first row (the \otimes s are completely untouched), and introduces zeros as shown below

$$\begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix} \xrightarrow{Q_1^* A} \begin{bmatrix} \otimes & \otimes & \otimes & \otimes & \otimes \\ + & + & + & + & + \\ 0 & + & + & + & + \\ 0 & + & + & + & + \\ 0 & + & + & + & + \end{bmatrix} \xrightarrow{Q_1^* A Q_1} \begin{bmatrix} \otimes & + & + & + & + \\ \otimes & + & + & + & + \\ 0 & + & + & + & + \\ 0 & + & + & + & + \\ 0 & + & + & + & + \end{bmatrix}$$

When we multiply by Q_1 from the right, the first column is completely untouched, and the other columns are replaced by linear combinations of the columns in $Q_1^* A$.

Note that when $A = A^*$, the Q -multiplication from the right leads to the analogous row combinations, so the that top row turns into $[\otimes + \mathbf{0} \mathbf{0} \mathbf{0}]$

We now repeat the same strategy...



To Hessenberg Form

$$\begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & * & * & * & * \\ 0 & * & * & * & * \end{bmatrix} \xrightarrow{Q_2^* []} \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ 0 & + & + & + & + \\ 0 & \mathbf{0} & + & + & + \\ 0 & \mathbf{0} & + & + & + \end{bmatrix} \xrightarrow{Q_2^* [] Q_2} \begin{bmatrix} * & * & + & + & + \\ * & * & + & + & + \\ 0 & * & + & + & + \\ 0 & 0 & + & + & + \\ 0 & 0 & + & + & + \end{bmatrix}$$

$$\begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & 0 & * & * & * \\ 0 & 0 & * & * & * \end{bmatrix} \xrightarrow{Q_3^* []} \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & 0 & + & + & + \\ 0 & 0 & \mathbf{0} & + & + \end{bmatrix} \xrightarrow{Q_3^* [] Q_3} \begin{bmatrix} * & * & * & + & + \\ * & * & * & + & + \\ 0 & * & * & + & + \\ 0 & 0 & * & + & + \\ 0 & 0 & 0 & + & + \end{bmatrix}$$

Elements marked with $*$ are not changed/touched and elements marked with $+$ are changed/touched. In the practical code, we can skip “touching” the known zeros to save some work.



Householder Reduction to Hessenberg Form

Algorithm (Householder Reduction to Hessenberg Form)

Transform $A \in \mathbb{R}^{m \times m}$ to Hessenberg Form

```
for k = 1:(m-2)
    x = A((k+1):m, k)
    v_k = sign(x_1) * ||x|| * e_1 + x
    v_k = v_k / ||v_k||_2
    A((k+1):m, k:m) = A((k+1):m, k:m) - 2*v_k*(v_k'*A((k+1):m, k:m)) [*]
    A(1:m, (k+1):m) = A(1:m, (k+1):m) - 2*(A(1:m, (k+1):m)*v_k)*v_k'
endfor
```

[*] Only operates on the non-zero columns.

Just as when we compute the QR-factorization using Householder reflections, the matrix Q is never formed explicitly. If we save the vectors \vec{v}_k , then we can reconstruct Q , or the action of Q as needed.

The work needed for Hessenberg reduction is $\sim \left(\frac{10}{3}m^3\right)$ operations.



Backward Stability of Hessenberg Reduction

1 of 2

Since Hessenberg reduction contains operations of the forms

- “Householder reflection from the left,” and
- “Householder reflection from the right,”

it should not come as a big surprise that the stability result looks very much like the one for QR-factorization (which is built on “Householder reflection from the left”-operations).



Backward Stability of Hessenberg Reduction

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Theorem (Backward Stability of Hessenberg Reduction)

Let the Hessenberg reduction $A = QHQ^*$ of a matrix $A \in \mathbb{C}^{m \times m}$ be computed by the algorithm described above, in a floating point environment satisfying the axioms. Let \tilde{H} be computed Hessenberg matrix and \tilde{Q} be the exactly unitary matrix corresponding to the computed reflection vectors \tilde{v}_k , then

$$\tilde{Q}\tilde{H}\tilde{Q}^* = A + \delta A, \quad \frac{\|\delta A\|}{\|A\|} = \mathcal{O}(\varepsilon_{mach})$$

for some $\delta A \in \mathbb{C}^{m \times m}$.



Phase#1 — ✓

Phase#2 — ?

We take a small detour and discuss some classical eigenvalue algorithms*; they are useful in their own right under certain circumstances, and will form the foundation for **“Phase#2-algorithms.”**

* The Rayleigh quotient, Power iteration, Inverse Iteration, and Rayleigh quotient iteration.



Restriction to $A \in \mathbb{R}^{m \times m}$, $A = A^*$

For simplicity, we briefly restrict our study to real symmetric matrices, and note that when we are ready to apply these methods (in Phase#2), A will be real, symmetric, and tri-diagonal.

The discussion is simplified since

- ① we can guarantee that all eigenvalues $\lambda_k(A) \in \mathbb{R}$ are real, and
- ② A has a complete set of orthonormal eigenvectors, \vec{q}_k .

For real quantities $\vec{x}^* = \vec{x}^T$, and $A^* = A^T$.



The Rayleigh Quotient

The **Rayleigh quotient** — after Lord Rayleigh (John William Strutt), Nobel Prize in Physics 1904, “for his investigations of the densities of the most important gases and for his discovery of argon in connection with these studies.”



Figure: Lord Rayleigh.

— of a vector $\vec{x} \in \mathbb{R}^m$ — is the scalar quantity

$$r(\vec{x}) = \frac{\vec{x}^* A \vec{x}}{\vec{x}^* \vec{x}}.$$

We note that if $\vec{x} = \vec{q}_k$ is an eigenvector, then $r(\vec{q}_k) = \lambda_k$.

(Copyright — Figure of Lord Rayleigh) — This file comes from Wellcome Images, a website operated by Wellcome Trust, a global charitable foundation based in the United Kingdom. Licensed under the Creative Commons Attribution 4.0 International license. File Located at https://commons.wikimedia.org/wiki/File:John.William.Strutt,_3rd_Baron_Rayleigh._Photogravure_after_Wellcome.V0006603.jpg



The Rayleigh Quotient

Interpretation

For a general \vec{x} , $r(\vec{x})$ is the value which “acts most like an eigenvalue” in the least squares sense, i.e.

$$r(\vec{x}) = \min_{r \in \mathbb{R}} \|A\vec{x} - r\vec{x}\|_2$$

The corresponding normal equation

$$[\vec{x}^* \vec{x}] r = \vec{x}^* A \vec{x}$$

gives r as the Rayleigh quotient.



The Rayleigh Quotient...

Quadratic Accuracy

Let's view the Rayleigh quotient as a function $r(\vec{x}) : \mathbb{R}^m \mapsto \mathbb{R}$.

We are interested in the local behavior of $r(\vec{x})$ when \vec{x} is close to an eigenvector... We compute the gradient of $r(\vec{x})$

$$\begin{aligned} \frac{\partial}{\partial x_j} r(\vec{x}) &= \frac{1}{\vec{x}^* \vec{x}} \left[\frac{\partial}{\partial x_j} (\vec{x}^* A \vec{x}) \right] - \frac{(\vec{x}^* A \vec{x})}{(\vec{x}^* \vec{x})^2} \left[\frac{\partial}{\partial x_j} (\vec{x}^* \vec{x}) \right] \\ &= \frac{2(A\vec{x})_j}{\vec{x}^* \vec{x}} - \frac{(\vec{x}^* A \vec{x}) 2x_j}{(\vec{x}^* \vec{x})^2} = \frac{2}{\vec{x}^* \vec{x}} \left[A\vec{x} - r(\vec{x})\vec{x} \right]_j, \end{aligned}$$

i.e.

$$\nabla_{\vec{x}} r(\vec{x}) = \frac{2}{\vec{x}^* \vec{x}} \left[A\vec{x} - r(\vec{x})\vec{x} \right].$$

Bottom line: $\nabla_{\vec{x}} r(\vec{x}) = 0$, $\vec{x} \neq 0$ if and only if $(\vec{x}, r(\vec{x}))$ is an eigenvector-eigenvalue pair.



The Rayleigh Quotient...

Quadratic Accuracy

Now, let \vec{q}_k be one of the eigenvectors of A , and let $\vec{x} = (\vec{q}_k + \vec{\epsilon})$, with $\|\vec{\epsilon}\|_2 \ll 1$. By Taylor's theorem

$$r(\vec{x}) - r(\vec{q}_k) = \underbrace{\vec{\epsilon}^* \nabla(r(\vec{q}_k))}_0 + \frac{1}{2} \vec{\epsilon}^* \underbrace{\nabla^2(r(\vec{q}_k + t\vec{\epsilon}))}_{\text{The Hessian}} \vec{\epsilon}, \quad t \in [0, 1].$$

This shows that

$$|r(\vec{x}) - r(\vec{q}_k)| = \mathcal{O}(\|\vec{\epsilon}\|^2), \quad \vec{x} = \vec{q}_k + \vec{\epsilon}.$$

Thus,

Theorem

The Rayleigh quotient is a quadratically accurate estimate of an eigenvalue.



Power Iteration

We have already written this idea off once... but it turns out that it can be made useful.

Algorithm (Power Iteration)

$\vec{v}_{(0)}$ = some vector, so that $\|\vec{v}_{(0)}\|_2 = 1$

$k = 0$

while(*termination criteria (details swept under the rug)*)

$k = k + 1$

$\vec{w} = A\vec{v}_{(k-1)}$

$\vec{v}_{(k)} = \vec{w} / \|\vec{w}\|$

$\lambda_{(k)} = \vec{v}_{(k)}^* A \vec{v}_{(k)}$

endwhile

This algorithm produces a sequence of approximate eigenvalue-vector pairs $(\lambda_{(k)}, \vec{v}_{(k)})$ which converge to $(\lambda_{\max}, \vec{q}_{\max})$



Power Iteration

Convergence

Theorem

Suppose $|\lambda_1| > |\lambda_2| \geq \dots \geq |\lambda_m| \geq 0$ and $\vec{q}_1^* \vec{v}_{(0)} \neq 0$. Then the iterates of the power iteration satisfy

$$\|\vec{v}_{(k)} - \vec{q}_1\| = \mathcal{O}\left(\left|\frac{\lambda_2}{\lambda_1}\right|^k\right), \quad |\lambda_{(k)} - \lambda_1| = \mathcal{O}\left(\left|\frac{\lambda_2}{\lambda_1}\right|^{2k}\right)$$

As it stands this is not very useful —

- (1) We can only find the eigenvector corresponding to the largest eigenvalue;
- (2) convergence for the eigenvector is only linear;
- (3) the convergence factor $|\lambda_2/\lambda_1|$ can be very close to 1.

It turns out we can use this basic idea (power iteration) to build scheme where we can guarantee that $|\lambda_2/\lambda_1|$ is small, and further we can find any eigenvector...



Inverse Iteration

The Algorithm

Algorithm (Inverse Iteration)

$\vec{v}_{(0)}$ = some vector, so that $\|\vec{v}_{(0)}\|_2 = 1$

$k = 0$

while(*termination criteria (details swept under the rug)*)

$k = k + 1$

 Solve^[1] $(A - \mu I)\vec{w} = \vec{v}_{(k-1)}$ for \vec{w}

$\vec{v}_{(k)} = \vec{w}/\|\vec{w}\|$

$\lambda_{(k)} = \vec{v}_{(k)}^* A \vec{v}_{(k)}$

endwhile

Even though $(A - \mu I)$ becomes singular as $\mu \rightarrow \lambda_k$, the solution $\vec{w} = (A - \mu I)^{-1} \vec{v}_{(k-1)}$ still gives a good **rescaled** $\vec{v}_{(k)} = \vec{w}/\|\vec{w}\|$.

[1] Solve by QR-, or Cholesky-factorization.



Inverse Iteration

Motivation: For any $\mu \in \mathbb{R}$ that is **not** an eigenvalue of A , the eigenvectors of

$$A \quad \text{and} \quad (A - \mu I)^{-1},$$

are the same, and the corresponding eigenvalues are

$$\lambda_j \quad \text{and} \quad \frac{1}{\lambda_j - \mu}.$$

Suppose μ is close to λ_k for some k , then since $\lim_{\mu \rightarrow \lambda_k} \frac{1}{\lambda_k - \mu} = \infty$, this suggests that

$$\frac{1}{|\lambda_k - \mu|} \gg \frac{1}{|\lambda_j - \mu|}, \quad j \neq k.$$

Thus applying power iteration to $(A - \mu I)^{-1}$ should give rapid convergence to \vec{q}_k .



Inverse Iteration

Discussion

Like power iteration, inverse iteration only exhibits linear convergence.

However, the positive features are

- We can **choose** what eigenvector to compute by supplying and estimate μ of the corresponding eigenvalue.
- We can control the rate of linear convergence since for $\mu \approx \lambda_k$

$$\left| \frac{\lambda_2([A - \mu I]^{-1})}{\lambda_1([A - \mu I]^{-1})} \right| = \max_{j \neq k} \left| \frac{\lambda_k - \mu}{\lambda_j - \mu} \right| \ll 1.$$

We make this precise in a theorem...



Inverse Iteration

Convergence Theorem

Theorem

Suppose that λ_J is the closest eigenvalue to μ , and λ_K is the second closest, i.e. $|\mu - \lambda_J| < |\mu - \lambda_K| \leq |\mu - \lambda_j|, \forall j \notin \{J, K\}$. Furthermore, assume $\vec{q}_J^* \vec{v}_{(0)} \neq 0$. Then the iterates of the inverse iteration satisfy

$$\|\vec{v}_{(k)} \mp \vec{q}_J\| = \mathcal{O} \left(\left| \frac{\mu - \lambda_J}{\mu - \lambda_K} \right|^k \right), \quad |\lambda_{(k)} - \lambda_J| = \mathcal{O} \left(\left| \frac{\mu - \lambda_J}{\mu - \lambda_K} \right|^{2k} \right)$$

Inverse iteration is the **standard method** for calculating the eigenvectors of a matrix if the eigenvalues are already known. In this setting, the algorithm is applied as described, but the calculation of the Rayleigh quotient $\lambda_{(k)} = \vec{v}_{(k)}^* A \vec{v}_{(k)}$ is skipped.



Rayleigh Quotient + Inverse Iteration = Rayleigh Quotient Iteration

Rayleigh Quotient Get an eigenvalue estimate from a eigenvector estimate.

Inverse Iteration Get an eigenvector estimate from an eigenvalue estimate.



Mix them together, and **BAM!!!**

Algorithm (Rayleigh Quotient Iteration)

```

vec{v}_{(0)} = some vector, so that ||vec{v}_{(0)}||_2 = 1
lambda_{(0)} = vec{v}_{(0)}^* A vec{v}_{(0)}, k = 0
while( termination criteria (details swept under the rug) )
    k = k + 1
    Solve (A - lambda_{(k-1)} I) wvec = vec{v}_{(k-1)} for wvec
    vec{v}_{(k)} = wvec / ||wvec||
    lambda_{(k)} = vec{v}_{(k)}^* A vec{v}_{(k)}
endwhile
    
```



Rayleigh Quotient Iteration

Cubic Convergence

Theorem (Convergence of the Rayleigh Quotient Iteration)

Rayleigh Quotient Iteration converges to an eigenvalue-eigenvector pair for all, except a set of measure zero, starting vectors $\vec{v}_{(0)}$. When it converges, the convergence is ultimately **cubic** in the sense that if λ_J is an eigenvalue of A and $\vec{v}_{(0)}$ is sufficiently close to the eigenvector \vec{q}_J , then

$$\|\vec{v}_{(k+1)} \mp \vec{q}_J\| = \mathcal{O} \left(\|\vec{v}_{(k)} \mp \vec{q}_J\|^3 \right)$$

and

$$|\lambda_{(k+1)} - \lambda_J| = \mathcal{O} \left(|\lambda_{(k)} - \lambda_J|^3 \right)$$

as $k \rightarrow \infty$. The \mp signs are not necessarily the same on the two sides of the equalities.



Rayleigh Quotient Iteration

Convergence

Informal Pattern

$\ \vec{v}_{(k)} \mp \vec{q}_J\ $	$ \lambda_{(k)} - \lambda_J $
$\mathcal{O}(\epsilon)$	$\mathcal{O}(\epsilon^2)$
$\downarrow \checkmark$	$\downarrow \checkmark$
$\mathcal{O}(\epsilon^3)$	$\mathcal{O}(\epsilon^6)$
$\downarrow \checkmark$	$\downarrow \checkmark$
$\mathcal{O}(\epsilon^9)$	$\mathcal{O}(\epsilon^{18})$
\vdots	\vdots

$\mathcal{O}(\epsilon^k) \rightarrow \mathcal{O}(\epsilon^{2k})$ comes from quadratic accuracy of the Rayleigh quotient. $\{\mathcal{O}(\epsilon^k), \mathcal{O}(\epsilon^{2k})\} \rightarrow \mathcal{O}(\epsilon^{3k})$, since for the inverse iteration

$$\|\vec{v}_{(k)} \mp \vec{q}_J\| = \mathcal{O} \left(\left| \frac{\lambda_{(k)} - \lambda_J}{\lambda_{(k)} - \lambda_K} \right| \cdot \|\vec{v}_{(k-1)} \mp \vec{q}_J\| \right) = \mathcal{O}(\epsilon^{2k}) \cdot \mathcal{O}(\epsilon^k) = \mathcal{O}(\epsilon^{3k})$$



Work per Iteration...

$A \in \mathbb{R}^{m \times m}$, Full, $A^* = A$

Power Iteration	$\mathcal{O}(m^2)$	
Inverse Iteration	$\mathcal{O}(m^2)$	LU, QR, or Cholesky
Inverse Iteration	$\mathcal{O}(m^3)$	Unfactored
Rayleigh Quotient Iteration	$\mathcal{O}(m^3)$	$(A - \lambda_{(k)}I)$ changes ^[1]

$A \in \mathbb{R}^{m \times m}$, Tri-Diagonal, $A^* = A$ **Hessenberg**, $A^* \neq A$

Power Iteration	$\mathcal{O}(m)$	$\mathcal{O}(m^2)$
Inverse Iteration	$\mathcal{O}(m)$	$\mathcal{O}(m^2)$
Rayleigh Quotient Iteration	$\mathcal{O}(m)$	$\mathcal{O}(m^2)$

^[1] Unless we can find an update formula for the factorization of $(A - \lambda_{(k)}I)$, beating $\mathcal{O}(m^3)$ operations per iteration is hard...



Homework #7

Due Date in Canvas/Gradescope

[SUBMIT] Trefethen-&-Bau 24.3

Hints: 1: Use `expm` or `scipy.linalg.expm` (not the `exp` versions) for matrix exponentiation e^{tA} . 2: Make sure you have many points in the interval of interest, e.g. use `linspace/np.linspace` with at least 100 points. 3: It is useful to (additionally) plot $\|e^{tA}\|_2 / e^{t\alpha(A)}$.

[SUBMIT] Implement-and-Test — Householder Reduction to Hessenberg form.

- Submit: Code + Validation, show working (5×5) and (7×7) examples.
- Compare with a library call (e.g. `hess/scipy.linalg.hessenberg`) — for validation use a (9×9) example. *Comment on similarities and differences.*

[SUBMIT] Implement-and-Test — Rayleigh Quotient Iteration.

- Submit: Code + Validation
- Minimum Validation: (11×11) matrix; (explicitly) show that at least one eigenvalue–eigenvector pair matches library (matlab/python) call.

Trefethen-&-Bau 26.1, 26.3, 27.3 — Read and think.

[OPTIONAL] Trefethen-&-Bau 26.2 (bonus fun) —

Use `eigtool` (<http://http://www.cs.ox.ac.uk/projects/pseudospectra/eigtool/>) or `pseudopy` (<https://github.com/andrenarchy/pseudopy>) to compute the pseudospectra

