CS 450: Numerical Anlaysis[1]

Eigenvalue Problems

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[1] *These slides have been drafted by Edgar Solomonik as lecture templates and supplementary material for the book "Scientific Computing: An Introductory Survey" by Michael T. Heath (slides).*

Eigenvalues and Eigenvectors

- A matrix $\boldsymbol{A}$ has eigenvector-eigenvalue pair (eigenpair) $(\lambda, \boldsymbol{x})$ if

$$\boldsymbol{A}\boldsymbol{x} = \lambda\boldsymbol{x}$$

  - *For any scalar α, $\alpha\boldsymbol{x}$ is also an eigenvector of $\boldsymbol{A}$ with eigenvalue λ*
  - *Generally, an eigenvalue λ is associated with an eigenspace $\mathcal{X} \subseteq \mathbb{C}^n$ such that each $\boldsymbol{x} \in \mathcal{X}$ is an eigenvector of $\boldsymbol{A}$ with eigenvalue λ.*
  - *The dimensionality of an eigenspace is at most the multiplicity of an eigenvalue (when less, matrix is defective, otherwise matrix is diagonalizable).*
- Each $n \times n$ matrix has up to n eigenvalues, which are either real or complex
  - *The conjugate of any complex eigenvalue of a real matrix is also an eigenvalue.*
  - *The dimensionalities of all the eigenspaces (multiplicity associated with each eigenvalue) sum up to n for a diagonalizable matrix.*
  - *If the matrix is real, real eigenvalues are associated with real eigenvectors, but complex eigenvalues may not be.*

Eigenvalue Decomposition

- If a matrix $\boldsymbol{A}$ is diagonalizable, it has an *eigenvalue decomposition*

$$\boldsymbol{A} = \boldsymbol{X}\boldsymbol{D}\boldsymbol{X}^{-1}$$

where $\boldsymbol{X}$ are the right eigenvectors, $\boldsymbol{X}^{-1}$ are the left eigenvectors and $\boldsymbol{D}$ are eigenvalues

$$\boldsymbol{A}\boldsymbol{X} = \begin{bmatrix}\boldsymbol{A}\boldsymbol{x}_1 & \cdots \boldsymbol{A}\boldsymbol{x}_n\end{bmatrix} = \boldsymbol{X}\boldsymbol{D} = \begin{bmatrix}d_{11}\boldsymbol{x}_1 & \cdots & d_{nn}\boldsymbol{x}_n\end{bmatrix}.$$

  - *If $\boldsymbol{A}$ is Hermitian, its right and left singular vectors are the same by symmetry, hence in this case $\boldsymbol{X}^{-1} = \boldsymbol{X}^H$.*
  - *More generally, any normal matrix, $\boldsymbol{A}^H\boldsymbol{A} = \boldsymbol{A}\boldsymbol{A}^H$, has unitary eigenvectors.*
- $\boldsymbol{A}$ and $\boldsymbol{B}$ are *similar*, if there exist $\boldsymbol{Z}$ such that $\boldsymbol{A} = \boldsymbol{Z}\boldsymbol{B}\boldsymbol{Z}^{-1}$
  - *Normal matrices are unitarily similar ($\boldsymbol{Z}^{-1} = \boldsymbol{Z}^H$) to diagonal matrices*
  - *Symmetric real matrices are orthogonally similar ($\boldsymbol{Z}^{-1} = \boldsymbol{Z}^T$) to real diagonal matrices*
  - *Hermitian matrices are unitarily similar to real diagonal matrices*

Similarity of Matrices

Invertible similarity transformations $\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{A}\boldsymbol{X}^{-1}$

matrix ($\boldsymbol{A}$)	*similarity* ($\boldsymbol{X}$)	*reduced form* ($\boldsymbol{Y}$)
arbitrary	invertible	bidiagonal
diagonalizable	invertible	diagonal

Unitary similarity transformations $\boldsymbol{Y} = \boldsymbol{U}\boldsymbol{A}\boldsymbol{U}^{H}$

matrix ($\boldsymbol{A}$)	*similarity* ($\boldsymbol{U}$)	*reduced form* ($\boldsymbol{Y}$)
arbitrary	unitary	triangular
normal	unitary	diagonal
Hermitian	unitary	real diagonal

Orthogonal similarity transformations $\boldsymbol{Y} = \boldsymbol{Q}\boldsymbol{A}\boldsymbol{Q}^{T}$

matrix ($\boldsymbol{A}$)	*similarity* ($\boldsymbol{Q}$)	*reduced form* ($\boldsymbol{Y}$)
real	orthogonal	real Hessenberg
real symmetric	orthogonal	real diagonal
SPD	orthogonal	real positive diagonal

Canonical Forms

- Any matrix is *similar* to a bidiagonal matrix, giving its *Jordan form*:

$$\boldsymbol{A} = \boldsymbol{X} \begin{bmatrix} \boldsymbol{J}_1 & & \\ & \ddots & \\ & & \boldsymbol{J}_k \end{bmatrix} \boldsymbol{X}^{-1}, \quad \forall i, \quad \boldsymbol{J}_i = \begin{bmatrix} \lambda_i & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_i \end{bmatrix}$$

the Jordan form is unique modulo ordering of the diagonal Jordan blocks.

- Any diagonalizable matrix is *unitarily similar* to a triangular matrix, giving its *Schur form*:

$$\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{T}\boldsymbol{Q}^H$$

where $\boldsymbol{T}$ is upper-triangular, so the eigenvalues of $\boldsymbol{A}$ is the diagonal of $\boldsymbol{T}$. Columns of $\boldsymbol{Q}$ are the Schur vectors.

Eigenvectors from Schur Form

- Given the eigenvectors of one matrix, we seek those of a similar matrix:
  Suppose that $\boldsymbol{A} = \boldsymbol{S}\boldsymbol{B}\boldsymbol{S}^{-1}$ *and* $\boldsymbol{B} = \boldsymbol{X}\boldsymbol{D}\boldsymbol{X}^{-1}$ *where* $\boldsymbol{D}$ *is diagonal,*
  - *The eigenvalues of* $\boldsymbol{A}$ *are* $\{d_{11}, \ldots, d_{nn}\}$
  - $\boldsymbol{A} = \boldsymbol{S}\boldsymbol{B}\boldsymbol{S}^{-1} = \boldsymbol{S}\boldsymbol{X}\boldsymbol{D}\boldsymbol{X}^{-1}\boldsymbol{S}^{-1}$ *so* $\boldsymbol{S}\boldsymbol{X}$ *are the eigenvectors of* $\boldsymbol{A}$
- Its easy to obtain eigenvectors of triangular matrix $\boldsymbol{T}$:
  - *One eigenvector is simply the first elementary vector.*
  - *The eigenvector associated with any diagonal entry (eigenvalue* λ*) may be obtaining by observing that*

$$\mathbf{0} = (\boldsymbol{T} - \lambda \boldsymbol{I})\boldsymbol{x} = \begin{bmatrix} \boldsymbol{U}_{11} & \boldsymbol{u} & \boldsymbol{T}_{13} \\ & 0 & \boldsymbol{v}^T \\ & & \boldsymbol{U}_{33} \end{bmatrix} \begin{bmatrix} -\boldsymbol{U}_{11}^{-1}\boldsymbol{u} \\ 1 \\ \mathbf{0} \end{bmatrix},$$

so it suffices to solve $\boldsymbol{U}_{11}\boldsymbol{y} = -\boldsymbol{u}$ *to obtain eigenvector* $\boldsymbol{x}$*.*

Rayleigh Quotient

- For any vector $\boldsymbol{x}$, the *Rayleigh quotient* provides an estimate for some eigenvalue of $\boldsymbol{A}$:

$$\rho_{\boldsymbol{A}}(\boldsymbol{x}) = \frac{\boldsymbol{x}^H \boldsymbol{A}\boldsymbol{x}}{\boldsymbol{x}^H \boldsymbol{x}}.$$

  - *If $\boldsymbol{x}$ is an eigenvector of $\boldsymbol{A}$, then $\rho_{\boldsymbol{A}}(\boldsymbol{x})$ is the associated eigenvalue.*
  - *Moreover, for $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$, the Rayleigh quotient is the best possible eigenvalue estimate given $\boldsymbol{x}$ and $\boldsymbol{y}$, as it is the solution to $\boldsymbol{x}\alpha \cong \boldsymbol{y}$.*
  - *The normal equations for this scalar-output least squares problem are*

$$\boldsymbol{x}^T \boldsymbol{x}\alpha = \boldsymbol{x}^T \boldsymbol{y} \quad \Rightarrow \quad \alpha = \frac{\boldsymbol{x}^T \boldsymbol{y}}{\boldsymbol{x}^T \boldsymbol{x}} = \frac{\boldsymbol{x}^T \boldsymbol{A}\boldsymbol{x}}{\boldsymbol{x}^T \boldsymbol{x}}.$$

Perturbation Analysis of Eigenvalue Problems

- Suppose we seek eigenvalues $\boldsymbol{D} = \boldsymbol{X}^{-1}\boldsymbol{A}\boldsymbol{X}$, but find those of a slightly perturbed matrix $\boldsymbol{D} + \boldsymbol{\delta D} = \hat{\boldsymbol{X}}^{-1}(\boldsymbol{A} + \boldsymbol{\delta A})\hat{\boldsymbol{X}}$:

  Note that the eigenvalues of $\boldsymbol{X}^{-1}(\boldsymbol{A} + \boldsymbol{\delta A})\boldsymbol{X} = \boldsymbol{D} + \boldsymbol{X}^{-1}\boldsymbol{\delta A}\boldsymbol{X}$ are also $\boldsymbol{D} + \boldsymbol{\delta D}$. So if we have perturbation to the matrix $||\boldsymbol{\delta A}||_F$, its effect on the eigenvalues corresponds to a (non-diagonal/arbitrary) perturbation $\boldsymbol{\delta \hat{A}} = \boldsymbol{X}^{-1}\boldsymbol{\delta A}\boldsymbol{X}$ of a diagonal matrix of eigenvalues $\boldsymbol{D}$, with norm

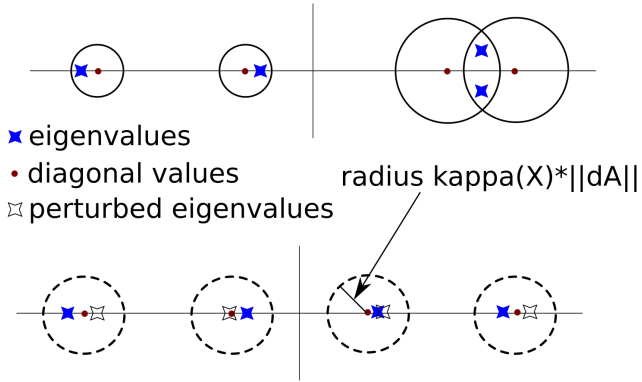
$$||\boldsymbol{\delta \hat{A}}||_F \leq ||\boldsymbol{X}^{-1}||_2||\boldsymbol{\delta A}||_F||\boldsymbol{X}||_2 = \kappa(\boldsymbol{X})||\boldsymbol{\delta A}||_F.$$

- Gershgorin's theorem allows us to bound the effect of the perturbation on the eigenvalues of a (diagonal) matrix:
  Given a matrix $\boldsymbol{A} \in \mathbb{R}^{n\times n}$, let $r_i = \sum_{j\neq i} |a_{ij}|$, define the Gershgorin disks as

$$D_i = \{z \in \mathbb{C} : |z - a_{ii}| \leq r_i\}.$$

  The eigenvalues $\lambda_1, \ldots, \lambda_n$ of any matrix $\boldsymbol{A} \in \mathbb{R}^{n\times n}$ are contained in the union of the Gershgorin disks, $\forall i \in \{1, \ldots, n\}, \lambda_i \in \bigcup_{j=1}^{n} D_j$.

Gershgorin Theorem Perturbation Visualization



- Top corresponds to Gershgorin disks on complex plane of 4-by-4 real matrix.
- Bottom part corresponds to bounds on Gershgorin disks of $\boldsymbol{X}^{-1}(\boldsymbol{A}+\boldsymbol{\delta A})\boldsymbol{X}$, which contain the eigenvalues $\boldsymbol{D}$ of $\boldsymbol{A}$ and the perturbed eigenvalues $\boldsymbol{D}+\boldsymbol{\delta D}$ of $\boldsymbol{A}+\boldsymbol{\delta A}$ provided that $||\boldsymbol{\delta A}||$ is sufficiently small.

Conditioning of Particular Eigenpairs

- Consider the effect of a matrix perturbation on an eigenvalue λ associated with a right eigenvector $\boldsymbol{x}$ and a left eigenvector $\boldsymbol{y}$, $\lambda = \boldsymbol{y}^H \boldsymbol{A}\boldsymbol{x}/\boldsymbol{y}^H\boldsymbol{x}$

  For a sufficiently small perturbation $\boldsymbol{\delta A}$, the eigenvalue λ is perturbed to an eigenvalue $\hat{\lambda}$ of $\hat{\boldsymbol{A}} = \boldsymbol{A} + \boldsymbol{\delta A}$. The eigenvalue perturbation, ignoring error due to the change in eigenvectors, is

$$|\hat{\lambda} - \lambda| \approx |\boldsymbol{y}^H \boldsymbol{\delta A}\boldsymbol{x}/\boldsymbol{y}^H\boldsymbol{x}| \leq \frac{||\boldsymbol{\delta A}||}{|\boldsymbol{y}^H\boldsymbol{x}|}.$$

  This is small if $\boldsymbol{x}$ is near-parallel to $\boldsymbol{y}$ and large if they are near-perpendicular.

- A more accurate eigenvalue approximation than Rayleigh quotient for a normalized perturbed eigenvector (e.g., iterative guess) $\hat{\boldsymbol{x}} = \boldsymbol{x} + \boldsymbol{\delta x}$, can be obtained with an estimate of both eigenvectors (also $\hat{\boldsymbol{y}} = \boldsymbol{y} + \boldsymbol{\delta y}$),

$$|\hat{\lambda}_{xAx} - \lambda| \approx |\boldsymbol{\delta x}^H \boldsymbol{A}\boldsymbol{x} + \boldsymbol{x}^H \boldsymbol{A}\boldsymbol{\delta x}| \leq |\lambda|||\boldsymbol{\delta x}|| + \Big(|\lambda||\boldsymbol{y}^H\boldsymbol{x}| + |1 - \boldsymbol{y}^H\boldsymbol{x}| \cdot ||\boldsymbol{A}||\Big)||\boldsymbol{\delta x}||$$

$$|\hat{\lambda}_{yAx} - \lambda| \approx \left|\frac{\boldsymbol{\delta y}^H \boldsymbol{A}\boldsymbol{x} + \boldsymbol{y}^H \boldsymbol{A}\boldsymbol{\delta x}}{\boldsymbol{y}^H\boldsymbol{x}}\right| \leq |\lambda|\frac{||\boldsymbol{\delta x}|| + ||\boldsymbol{\delta y}||}{|\boldsymbol{y}^H\boldsymbol{x}|}$$

Google's PageRank

A well-known application of eigenproblems is the problem of ranking n web-pages

- *Based on web-data, we compute transition probability from webpage i to webpage j at a_{ij}*
- *We seek a measure of webpage popularity, which we can take to be the probability x_i of a web-surfer being on webpage i as opposed to the other $n-1$ webpages*
- *These probability $\boldsymbol{x}$ must be consistent with the probability of transitions among states, and so are eigenvectors of $\boldsymbol{A}$ with eigenvalue 1,*

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{x}$$

- *$\boldsymbol{A}$ is a transition probability (stochastic) matrix and generally has a single eigenvalue of 1 with all remaining eigenvalues being less than 1*

Power Iteration

- *Power iteration* can be used to compute the largest eigenvalue of a real symmetric matrix $\boldsymbol{A}$:

  $$\boldsymbol{x}^{(i)} = \boldsymbol{A}\boldsymbol{x}^{(i-1)} \quad \textit{(typically with normalization of } \boldsymbol{x}^{(i)} \textit{ at each step)}.$$

  For a random $\boldsymbol{x}^{(0)}$, power iteration converges eigenvalue of $\boldsymbol{A}$ with largest modulus, $\lim_{i\to\infty} \rho_{\boldsymbol{A}}(\boldsymbol{x}^{(i)}) = \lambda_{max}(\boldsymbol{A})$. If this eigenvalue has multiplicity one, power iteration converges to dominant eigenvector.

- The error of power iteration decreases at each step by the ratio of the largest eigenvalues:

  Assuming $\boldsymbol{A}$ is diagonalizable with eigenvectors $\boldsymbol{U}$ and $\boldsymbol{V}^H = \boldsymbol{U}^{-1}$,

  $$\boldsymbol{x}^{(k)} = \boldsymbol{A}^k\boldsymbol{x}^{(0)} = (\boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^H)^k\boldsymbol{x}^{(0)} = \boldsymbol{U}\boldsymbol{D}^k\boldsymbol{V}^H\boldsymbol{x}^{(0)} = \sum_{i=1}^{n} \boldsymbol{u}_i \underbrace{\lambda_i^k \boldsymbol{v}_i^H \boldsymbol{x}^{(0)}}_{\alpha^{(i,k)}}.$$

  The coefficient $\alpha^{(i,k)}$ associated with the maximum λ_i and dominant eigenvector $\boldsymbol{u}_i$ grows relatively, since $|\alpha^{(i,k)}/\alpha^{(j,k)}| = (|\lambda_i|/|\lambda_j|)^k \underbrace{|\alpha^{(i,0)}/\alpha^{(j,0)}|}_{\textit{constant}}$.

Rates of Convergence

- If the error at the kth step with respect to the desired solution is $\boldsymbol{e}_k$, rth order convergence implies that $\lim_{k\to\infty} \|\boldsymbol{e}_k\|/\|\boldsymbol{e}_{k-1}\|^r \leq C$
  - *Power iteration achieves linear convergence with $C = |\lambda_1|/|\lambda_2|$.*
  - *Convergence of order $r > 1$ (superlinear) implies that the number of digits of correctness increases by a factor of r at each step.*
  - *For $r > 1$, error $e_k \leq \epsilon$ is achieved after $O(\log_r(\log(1/\epsilon)))$ steps.*
  - *Having achieved superlinear convergence ($r > 1$), methods differ only by constant factors in complexity.*

Inverse and Rayleigh Quotient Iteration

- *Inverse iteration* uses LU/QR/SVD of $\boldsymbol{A}$ to run power iteration on $\boldsymbol{A}^{-1}$
  - *For a randomly chosen $\boldsymbol{x}^{(0)}$, solving*

$$\boldsymbol{A}\boldsymbol{x}^{(i)} = \boldsymbol{x}^{(i-1)} \quad \textit{(typically with normalization of } \boldsymbol{x}^{(i)} \textit{ at each step).}$$

    converges to $\lim_{i\to\infty} \rho_{\boldsymbol{A}}(\boldsymbol{x}^{(i)}) = \lambda_{min}(\boldsymbol{A})$ provided there is a unique eigenvalue with minimum magnitude.
  - *Inverse iteration on $\boldsymbol{A} - \sigma\boldsymbol{I}$ converges to the eigenvalue closes to σ, since all eigenvalues are shifted by σ.*
- *Rayleigh quotient iteration* provides rapid convergence to an eigenpair

$$(\boldsymbol{A} - \rho_{\boldsymbol{A}}(\boldsymbol{x}^{(i-1)})\boldsymbol{I})\boldsymbol{x}^{(i)} = \boldsymbol{x}^{(i-1)},$$

since at each step the relative magnitude largest eigenvalue of $(\boldsymbol{A} - \rho_{\boldsymbol{A}}(\boldsymbol{x}^{(i-1)})\boldsymbol{I})^{-1}$ grows. Formally, it achieves cubic convergence, but requires matrix refactorization at each step.

Deflation

- Power, inverse, and Rayleigh-quotient iteration compute a single eigenpair, to obtain further eigenpairs, can perform *deflation*
  - *Given eigenvalue λ_1 and right eigenvector $\boldsymbol{x}_1$, seek $\boldsymbol{v}$ so that $\boldsymbol{B} = \boldsymbol{A} - \lambda_1 \boldsymbol{u}\boldsymbol{v}^T$ has eigenvalues $0, \lambda_2, \ldots, \lambda_n$, where*

$$\boldsymbol{A} = \boldsymbol{X}\boldsymbol{D}\underbrace{\boldsymbol{Y}^T}_{\boldsymbol{X}^{-1}} = \sum_{i=1}^{n} \lambda_i \boldsymbol{x}_i \boldsymbol{y}_i^T.$$

  - *Ideal choice would be $\boldsymbol{v} = \boldsymbol{y}_1^T$, i.e., the left eigenvector associated with λ_1, as then the $n-1$ other eigenvectors of $\boldsymbol{B}$ would be the same as those of $\boldsymbol{A}$.*
  - *For symmetric matrices $\boldsymbol{y}_1 = \boldsymbol{x}_1$, but for nonsymmetric, obtaining $\boldsymbol{y}_1$ may require more work.*
  - *Good alternative choice for nonsymmetric is to select $\boldsymbol{v} = \boldsymbol{x}_1$, as then the Schur vectors are unmodified, since for $\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{T}\boldsymbol{Q}^T$, with $t_{11} = \lambda_1$, $\boldsymbol{q}_1 = \boldsymbol{x}_1$, we get*

$$\boldsymbol{B} = \boldsymbol{Q}\boldsymbol{T}\boldsymbol{Q}^T - \lambda_1 \boldsymbol{q}_1 \boldsymbol{q}_1^T = \boldsymbol{Q}(\boldsymbol{T} - \lambda_1 \boldsymbol{Q}^T \boldsymbol{q}_1 \boldsymbol{q}_1^T \boldsymbol{Q})\boldsymbol{Q}^T = \boldsymbol{Q}(\boldsymbol{T} - \lambda_1 \boldsymbol{e}_1 \boldsymbol{e}_1^T)\boldsymbol{Q}^T.$$

Direct Matrix Reductions

Demo: *Householder Similarity Transforms*

- We can always compute an orthogonal similarity transformation to reduce a general matrix to *upper-Hessenberg* (upper-triangular plus the first subdiagonal) matrix $\boldsymbol{H}$, i.e. $\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{H}\boldsymbol{Q}^T$:

  We can perform successive two-sided application of Householder reflectors

$$\boldsymbol{A} = \begin{bmatrix} h_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \\ \vdots & & \ddots \end{bmatrix} = \boldsymbol{Q}_1 \begin{bmatrix} h_{11} & a_{12} & \cdots \\ h_{21} & t_{22} & \cdots \\ \mathbf{0} & \vdots & \ddots \end{bmatrix} = \boldsymbol{Q}_1 \begin{bmatrix} h_{11} & h_{12} & \cdots \\ h_{21} & h_{22} & \cdots \\ \mathbf{0} & \vdots & \ddots \end{bmatrix} \boldsymbol{Q}_1^T = \cdots$$

  subsequent columns can be reduced by induction, so we can always stably reduce to upper-Hessenberg with roughly the same cost as QR.

- In the symmetric case, Hessenberg form implies tridiagonal:

  If $\boldsymbol{A} = \boldsymbol{A}^T$ then $\boldsymbol{H} = \boldsymbol{Q}\boldsymbol{A}\boldsymbol{Q}^T = \boldsymbol{H}^T$, and a symmetric upper-Hessenberg matrix must be tridiagonal.

Simultaneous and Orthogonal Iteration

Demo: *Orthogonal Iteration*

- *Simultaneous iteration* provides the main idea for computing many eigenvectors at once:
  - *Initialize* $\boldsymbol{X}_0 \in \mathbb{R}^{n \times k}$ *to be random and perform*

$$\boldsymbol{X}_{i+1} = \boldsymbol{A}\boldsymbol{X}_i.$$

  - *Observe that* $\lim_{i \to \infty} \text{span}(\boldsymbol{X}_i) = \mathbb{S}$ *where* $\mathbb{S}$ *is the subspace spanned by the* k *eigenvectors of* $\boldsymbol{A}$ *with the largest eigenvalues in magnitude.*
- Orthogonal iteration performs QR at each step to ensure stability

$$\boldsymbol{Q}_{i+1}\boldsymbol{R}_{i+1} = \boldsymbol{A}\boldsymbol{Q}_i$$

  - $\boldsymbol{Q}_i$ *has the same span as* $\boldsymbol{X}_i$ *in orthogonal iteration.*
  - *QR has cost* $O(nk^2)$ *while product has cost* $O(n^2k)$ *per iteration.*
  - *Can use this to compute the right singular vectors of matrix* $\boldsymbol{M}$ *by using* $\boldsymbol{A} = \boldsymbol{M}^T\boldsymbol{M}$ *(no need to form* $\boldsymbol{A}$*, just multiply* $\boldsymbol{Q}_i$ *by* $\boldsymbol{M}^T$ *then* $\boldsymbol{M}$*).*
  - *Small number of iterations suffice to obtain reasonable low-rank approximation of* $\boldsymbol{M}$*, and ultimately* $\boldsymbol{Q}$ *converges to singular vectors in its truncated SVD.*

QR Iteration

- QR iteration reformulates orthogonal iteration for $n = k$ to reduce cost/step,
  - *Orthogonal iteration computes* $\hat{\boldsymbol{Q}}_{i+1}\hat{\boldsymbol{R}}_{i+1} = \boldsymbol{A}\hat{\boldsymbol{Q}}_i$
  - *QR iteration computes* $\boldsymbol{A}_{i+1} = \boldsymbol{R}_i\boldsymbol{Q}_i$ *at iteration* i
- Using induction, we assume $\boldsymbol{A}_i = \hat{\boldsymbol{Q}}_i^T\boldsymbol{A}\hat{\boldsymbol{Q}}_i$ and show that QR iteration obtains $\boldsymbol{A}_{i+1} = \hat{\boldsymbol{Q}}_{i+1}^T\boldsymbol{A}\hat{\boldsymbol{Q}}_{i+1}$
  - *QR iteration performs QR to obtain* $\boldsymbol{Q}_i\boldsymbol{R}_i = \boldsymbol{A}_i$
  - *Orthogonal iteration performs QR*

$$\hat{\boldsymbol{Q}}_{i+1}\hat{\boldsymbol{R}}_{i+1} = \boldsymbol{A}\hat{\boldsymbol{Q}}_i \underbrace{=}_{\text{inductive assumption}} \hat{\boldsymbol{Q}}_i\boldsymbol{A}_i = \underbrace{\hat{\boldsymbol{Q}}_i\boldsymbol{Q}_i}_{\hat{\boldsymbol{Q}}_{i+1}}\underbrace{\boldsymbol{R}_i}_{\hat{\boldsymbol{R}}_{i+1}}$$

consequently, we can observe that $\boldsymbol{R}_i = \underbrace{\boldsymbol{Q}_i^T\hat{\boldsymbol{Q}}_i^T}_{\hat{\boldsymbol{Q}}_{i+1}^T}\boldsymbol{A}\hat{\boldsymbol{Q}}_i$

  - *QR iteration performs product* $\boldsymbol{A}_{i+1} = \boldsymbol{R}_i\boldsymbol{Q}_i = \hat{\boldsymbol{Q}}_{i+1}^T\boldsymbol{A}\hat{\boldsymbol{Q}}_{i+1}$

QR Iteration with Shift

- QR iteration can be accelerated using shifting:

$$\boldsymbol{Q}_i \boldsymbol{R}_i = \boldsymbol{A}_i - \sigma_i \boldsymbol{I}$$
$$\boldsymbol{A}_{i+1} = \boldsymbol{R}_i \boldsymbol{Q}_i + \sigma_i \boldsymbol{I}$$

note that $\boldsymbol{A}_{i+1}$ is similar to $\boldsymbol{A}_i$, since we can reorganize the above as

$$\boldsymbol{R}_i \boldsymbol{Q}_i = \boldsymbol{Q}_i^T (\boldsymbol{A}_i - \sigma_i \boldsymbol{I}) \boldsymbol{Q}_i,$$
$$\boldsymbol{Q}_i (\boldsymbol{A}_{i+1} - \sigma_i \boldsymbol{I}) \boldsymbol{Q}_i^T = \boldsymbol{Q}_i \boldsymbol{R}_i,$$

and observe that $\boldsymbol{R}_i \boldsymbol{Q}_i$ is similar to $\boldsymbol{Q}_i \boldsymbol{R}_i$.

- The shift is typically selected to accelerate convergence with respect to a particular eigenvalue:

  We can select the shift as the bottom right element of $\boldsymbol{A}_i$, which would be the smallest eigenvalue if $\boldsymbol{A}_i$ is triangular (we have converged). Such shifting should accelerate convergence of the last column of $\boldsymbol{A}_i$, once finished we should operate only on the first $n-1$ columns, and so on.

QR Iteration Complexity

- QR iteration is accelerated by first reducing to upper-Hessenberg or tridiagonal form:

  Reduction to upper-Hessenberg or tridiagonal in the symmetric case, costs $O(n^3)$ operations and can be done in a similar style to Householder QR.

  Given an upper-Hessenberg matrix, $\boldsymbol{H}_i = \boldsymbol{A}_i$

  - *reduction to upper-triangular requires $n-1$ Givens rotations, if $\boldsymbol{G}_i$ rotates the $(i+1)$th row into the ith to eliminate the ith element on the first subdiagonal, $\boldsymbol{R}_i = \boldsymbol{G}_1^T \cdots \boldsymbol{G}_{n-1}^T \boldsymbol{H}_i$*
  - *computation of $\boldsymbol{H}_{i+1} = \boldsymbol{R}\boldsymbol{Q}$ can be done by application of the $n-1$ Givens rotations to $\boldsymbol{R}$ from the right $\boldsymbol{H}_{i+1} = \boldsymbol{R}_i \boldsymbol{G}_{n-1} \cdots \boldsymbol{G}_1$.*

  Both cost $O(n^2)$, for $O(n^3)$ overall if QR iteration converges in $O(n)$ steps.

  Given a tridiagonal matrix, the same two general steps are required, but now each step costs $O(n)$, so overall the eigenvalues and eigenvectors of a tridiagonal matrix can be computed with $O(n^2)$ work.

Solving Tridiagonal Symmetric Eigenproblems

A variety of methods exists for the tridiagonal eigenproblem:

- QR iteration *requires $O(1)$ QR factorizations per eigenvalue, $O(n^2)$ cost to get eigenvalues, $O(n^3)$ for eigenvectors. The last cost is not optimal.*
- Divide and conquer *reduces tridiagonal $\boldsymbol{T}$ by a similarity transformation to a rank-1 perturbation of identity, then computes its eigenvalues using roots of secular equation*

$$
\begin{aligned}
\boldsymbol{T} &= \begin{bmatrix} \boldsymbol{T}_1 & t_{n/2+1,n/2}\boldsymbol{e}_{n/2}\boldsymbol{e}_1^T \\ t_{n/2+1,n/2}\boldsymbol{e}_1\boldsymbol{e}_{n/2}^T & \boldsymbol{T}_2 \end{bmatrix} \\
&= \begin{bmatrix} \hat{\boldsymbol{T}}_1 & \\ & \hat{\boldsymbol{T}}_2 \end{bmatrix} + t_{n/2+1,n/2} \begin{bmatrix} \boldsymbol{e}_{n/2} \\ \boldsymbol{e}_1 \end{bmatrix} \begin{bmatrix} \boldsymbol{e}_{n/2}^T & \boldsymbol{e}_1^T \end{bmatrix} = \begin{bmatrix} \boldsymbol{Q}_1\boldsymbol{D}_1\boldsymbol{Q}_1^T & \\ & \boldsymbol{Q}_2\boldsymbol{D}_2\boldsymbol{Q}_2^T \end{bmatrix} + \cdots \\
&= \begin{bmatrix} \boldsymbol{Q}_1 & \\ & \boldsymbol{Q}_2 \end{bmatrix} \Bigg(\underbrace{\begin{bmatrix} \boldsymbol{D}_1 & \\ & \boldsymbol{D}_2 \end{bmatrix} + t_{n/2+1,n/2} \begin{bmatrix} \boldsymbol{Q}_1^T\boldsymbol{e}_{n/2} \\ \boldsymbol{Q}_2^T\boldsymbol{e}_1 \end{bmatrix} \begin{bmatrix} \boldsymbol{e}_{n/2}^T\boldsymbol{Q}_1 & \boldsymbol{e}_1^T\boldsymbol{Q}_2 \end{bmatrix}}_{\boldsymbol{D}+\alpha\boldsymbol{u}\boldsymbol{u}^T} \Bigg) \begin{bmatrix} \boldsymbol{Q}_1^T & \\ & \boldsymbol{Q}_2^T \end{bmatrix}
\end{aligned}
$$

Solving the Secular Equation for Divide and Conquer

To solve the eigenproblem at each step, the divide and conquer method needs to diagonalize a rank-1 perturbation of a diagonal matrix

$$\boldsymbol{A} = \boldsymbol{D} + \alpha \boldsymbol{u}\boldsymbol{u}^T.$$

- *The zeros of the characteristic polynomial define the eigenvalues,*

$$f(\lambda) = \det(\boldsymbol{D} + \alpha \boldsymbol{u}\boldsymbol{u}^T - \lambda \boldsymbol{I}) = 1 + \alpha \boldsymbol{u}^T (\boldsymbol{D} - \lambda \boldsymbol{I})^{-1} \boldsymbol{u} = 1 + \alpha \sum_{i=1}^{n} \frac{u_i^2}{d_{ii} - \lambda} = 0.$$

- *This nonlinear equation can be solved efficiently by a variant of Newton's method (covered in the next chapter) that uses hyperbolic rather than linear extrapolations at each step.*
- *Major alternatives to divide and conquer include spectral bisection and the MRRR algorithm.*

Introduction to Krylov Subspace Methods

- *Krylov subspace methods* work with information contained in the $n \times k$ matrix

$$\boldsymbol{K}_k = \begin{bmatrix} \boldsymbol{x_0} & \boldsymbol{A x_0} & \cdots & \boldsymbol{A}^{k-1}\boldsymbol{x_0} \end{bmatrix}$$

We seek to best use the information from the matrix vector product results (columns of $\boldsymbol{K}_k$) to solve eigenvalue problems.

- Assuming $\boldsymbol{K}_n$ is invertible, the matrix $\boldsymbol{K}_n^{-1}\boldsymbol{A}\boldsymbol{K}_n$ is a *companion matrix* $\boldsymbol{C}$:

Letting $\boldsymbol{k}_n^{(i)} = \boldsymbol{A}^{i-1}\boldsymbol{x}$, we observe that

$$\boldsymbol{A}\boldsymbol{K}_n = \begin{bmatrix} \boldsymbol{A}\boldsymbol{k}_n^{(1)} & \cdots & \boldsymbol{A}\boldsymbol{k}_n^{(n-1)} & \boldsymbol{A}\boldsymbol{k}_n^{(n)} \end{bmatrix} = \begin{bmatrix} \boldsymbol{k}_n^{(2)} & \cdots & \boldsymbol{k}_n^{(n)} & \boldsymbol{A}\boldsymbol{k}_n^{(n)} \end{bmatrix},$$

therefore premultiplying by $\boldsymbol{K}_m^{-1}$ transforms the first $n-1$ columns of $\boldsymbol{A}\boldsymbol{K}_n$ into the last $n-1$ columns of $\boldsymbol{I}$,

$$\begin{aligned} \boldsymbol{K}_n^{-1}\boldsymbol{A}\boldsymbol{K}_n &= \begin{bmatrix} \boldsymbol{K}_n^{-1}\boldsymbol{k}_n^{(2)} & \cdots & \boldsymbol{K}_n^{-1}\boldsymbol{k}_n^{(n)} & \boldsymbol{K}_n^{-1}\boldsymbol{A}\boldsymbol{k}_n^{(n)} \end{bmatrix} \\ &= \begin{bmatrix} \boldsymbol{e}_2 & \cdots & \boldsymbol{e}_n & \boldsymbol{K}_n^{-1}\boldsymbol{A}\boldsymbol{k}_n^{(n)} \end{bmatrix} \end{aligned}$$

Krylov Subspaces

- Given $\boldsymbol{Q}_k\boldsymbol{R}_k = \boldsymbol{K}_k$, we obtain an orthonormal basis for the Krylov subspace,

$$\mathcal{K}_k(\boldsymbol{A}, \boldsymbol{x}_0) = span(\boldsymbol{Q}_k) = \{p(\boldsymbol{A})\boldsymbol{x}_0 : deg(p) < k\},$$

  where p is any polynomial of degree less than k.

- The Krylov subspace includes the $k-1$ approximate dominant eigenvectors generated by $k-1$ steps of power iteration:
  - *The approximation obtained from $k-1$ steps of power iteration starting from $\boldsymbol{x}_0$ is given by the Rayleigh-quotient of $\boldsymbol{y} = \boldsymbol{A}^k\boldsymbol{x}_0$.*
  - *This vector is within the Krylov subspace, $\boldsymbol{y} \in \mathcal{K}_k(\boldsymbol{A}, \boldsymbol{x}_0)$.*
  - *Consequently, Krylov subspace methods will generally obtain strictly better approximations of the dominant eigenpair than power iteration.*

Krylov Subspace Methods

- The $k \times k$ matrix $\boldsymbol{H}_k = \boldsymbol{Q}_k^T \boldsymbol{A} \boldsymbol{Q}_k$ minimizes $\|\boldsymbol{A}\boldsymbol{Q}_k - \boldsymbol{Q}_k \boldsymbol{H}_k\|_2$:

  We can prove this as follows,

  $$\|\boldsymbol{A}\boldsymbol{Q}_k - \boldsymbol{Q}_k \boldsymbol{H}_k\|_2 = \|(\boldsymbol{I} - \boldsymbol{Q}_k \boldsymbol{Q}_k^T)(\boldsymbol{A}\boldsymbol{Q}_k - \boldsymbol{Q}_k \boldsymbol{H}_k)\|_2 + \|\boldsymbol{Q}_k \boldsymbol{Q}_k^T (\boldsymbol{A}\boldsymbol{Q}_k - \boldsymbol{Q}_k \boldsymbol{H}_k)\|_2$$

  since $\|\boldsymbol{M}\boldsymbol{x}\|_2 = \|(\boldsymbol{I} - \boldsymbol{Q}_k \boldsymbol{Q}_k^T)\boldsymbol{M}\boldsymbol{x} + \boldsymbol{Q}_k \boldsymbol{Q}_k^T \boldsymbol{M}\boldsymbol{x}\|_2$ *is the norm of a sum of two orthogonal components of* $\boldsymbol{M}\boldsymbol{x}$*. Then it suffices to observe that* $(\boldsymbol{I} - \boldsymbol{Q}_k \boldsymbol{Q}_k^T)(\boldsymbol{A}\boldsymbol{Q}_k - \boldsymbol{Q}_k \boldsymbol{H}_k) = (\boldsymbol{I} - \boldsymbol{Q}_k \boldsymbol{Q}_k^T)\boldsymbol{A}\boldsymbol{Q}_k$*, so the first term is independent of* $\boldsymbol{H}_k$*. The second term is minimized (zero) with the choice* $\boldsymbol{H}_k = \boldsymbol{Q}_k^T \boldsymbol{A} \boldsymbol{Q}_k$*.*

- $\boldsymbol{H}_k$ is Hessenberg, because the companion matrix $\boldsymbol{C}_k$ is Hessenberg:

  $$\boldsymbol{H}_k = \boldsymbol{Q}_k^T \boldsymbol{A} \boldsymbol{Q}_k = \boldsymbol{R}_k \boldsymbol{K}_k^{-1} \boldsymbol{A} \boldsymbol{K}_k \boldsymbol{R}_k^{-1} = \boldsymbol{R}_k \boldsymbol{C}_k \boldsymbol{R}_k^{-1}$$

  is a product of three matrices: upper-triangular $\boldsymbol{R}_k$*, upper-Hessenberg* $\boldsymbol{C}_k$ *, and upper-triangular* $\boldsymbol{R}_k^{-1}$*, which results in upper-Hessenberg* $\boldsymbol{H}_k$*.*

Rayleigh-Ritz Procedure

Demo: *Arnoldi vs Power Iteration*
Activity: *Computing the Maximum Ritz Value*

- The eigenvalues/eigenvectors of $\boldsymbol{H}_k$ are the *Ritz values/vectors*:

$$\boldsymbol{H}_k = \boldsymbol{X}\boldsymbol{D}\boldsymbol{X}^{-1}$$

eigenvalue approximations based on Ritz vectors $\boldsymbol{X}$ are given by $\boldsymbol{Q}_k\boldsymbol{X}$.

- The Ritz vectors and values are the *ideal approximations* of the actual eigenvalues and eigenvectors based on only $\boldsymbol{H}_k$ and $\boldsymbol{Q}_k$:

Assuming $\boldsymbol{A}$ is a symmetric matrix with positive eigenvalues, the largest Ritz value $\lambda_{max}(\boldsymbol{H}_k)$ will be the maximum Rayleigh quotient of any vector in $\mathcal{K}_k = span(\boldsymbol{Q}_k)$,

$$\max_{\boldsymbol{x}\in span(\boldsymbol{Q}_k)} \frac{\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x}}{\boldsymbol{x}^T\boldsymbol{x}} = \max_{\boldsymbol{y}\neq 0} \frac{\boldsymbol{y}^T\boldsymbol{Q}_k^T\boldsymbol{A}\boldsymbol{Q}_k\boldsymbol{y}}{\boldsymbol{y}^T\boldsymbol{y}} = \max_{\boldsymbol{y}\neq 0} \frac{\boldsymbol{y}^T\boldsymbol{H}_k\boldsymbol{y}}{\boldsymbol{y}^T\boldsymbol{y}} = \lambda_{max}(\boldsymbol{H}_k),$$

which is the best approximation to $\lambda_{max}(\boldsymbol{A}) = \max_{\boldsymbol{x}\neq 0} \frac{\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x}}{\boldsymbol{x}^T\boldsymbol{x}}$ available in $\mathcal{K}_k$. The quality of the approximation can also be shown to be optimal for other eigenvalues/eigenvectors.

Arnoldi Iteration

Demo: *Arnoldi Iteration*
Demo: *Arnoldi Iteration with Complex Eigenvalues*

- Arnoldi iteration computes $\boldsymbol{H}_k$ and $\boldsymbol{Q}_k$ directly using the recurrence $\boldsymbol{A}\boldsymbol{q}_i = \boldsymbol{Q}_n \boldsymbol{h}_i = \sum_{j=1}^{i+1} h_{ji}\boldsymbol{q}_j$
  - *We have that $\boldsymbol{A}\boldsymbol{Q}_n = \boldsymbol{Q}_n \boldsymbol{H}_n$, from which the recurrence follows by considering respective columns of the two sides.*
  - *Thus, the Arnoldi algorithm computes $\boldsymbol{q}_{i+1}$ from $\boldsymbol{q}_1, \ldots, \boldsymbol{q}_i$ via orthogonalization, first obtaining,*

$$h_{ji}\boldsymbol{q}_{i+1} = \boldsymbol{A}\boldsymbol{q}_i - \sum_{j=1}^{i} h_{ji}\boldsymbol{q}_j$$

  then computing the norm of the vector to obtain h_{ji}.
  - *Further, note that,*

$$\boldsymbol{q}_i^T \boldsymbol{A}\boldsymbol{q}_j = \boldsymbol{q}_i^T (\boldsymbol{Q}_n \boldsymbol{H}_n \boldsymbol{Q}_n^T)\boldsymbol{q}_j = \boldsymbol{e}_i^T \boldsymbol{H}_n \boldsymbol{e}_j = h_{ij}.$$

- After each matrix-vector product, orthogonalization is done with respect to each previous vector:

  Given $\boldsymbol{u}_j = \boldsymbol{A}\boldsymbol{q}_j$, compute $h_{ij} = \boldsymbol{q}_i^T \boldsymbol{u}_j$ for each $i \leq j$, forming a column of the $\boldsymbol{H}_n$ matrix at a time.

Lanczos Iteration

- Lanczos iteration provides a method to reduce a symmetric matrix to a tridiagonal matrix:

  Arnoldi iteration on a symmetric matrix will result in an upper-Hessenberg matrix $\boldsymbol{H}_n$ as before, except that it must also be symmetric, since

  $$\boldsymbol{H}_n^T = (\boldsymbol{Q}_n^T \boldsymbol{A} \boldsymbol{Q}_n)^T = \boldsymbol{Q}_n^T \boldsymbol{A}^T \boldsymbol{Q}_n = \boldsymbol{Q}_n^T \boldsymbol{A} \boldsymbol{Q}_n = \boldsymbol{H}_n,$$

  which implies that $\boldsymbol{H}_n$ must be tridiagonal.

- After each matrix-vector product, it suffices to orthogonalize with respect to two previous vectors:

  Since $h_{ij} = 0$ if $|i - j| > 1$, given $\boldsymbol{u}_j = \boldsymbol{A}\boldsymbol{q}_j$, it suffices to compute only $h_{jj} = \boldsymbol{q}_j^T \boldsymbol{u}_j$ and $h_{j-1,j} = h_{j,j-1} = \boldsymbol{q}_{j-1}^T \boldsymbol{u}_j$.

Cost Krylov Subspace Methods

- The cost of matrix-vector multiplication when the matrix has m nonzeros *is m multiplications and at most m additions, so roughly $2m$ in total.*
- The cost of orthogonalization at the kth iteration of a Krylov subspace method is
  - $O(nk)$ *for k inner products in Arnoldi,*
  - $O(n)$ *in Lanczos, since only 2 orthogonalizations needed.*
  - *For Arnoldi with k-dimensional subspace, in total, orthogonalization costs $O(nk^2)$, matrix-vector products cost $O(mk)$, so generally desire $nk < m$.*

Restarting Krylov Subspace Methods

- In finite precision, Lanczos generally loses orthogonality, while orthogonalization in Arnoldi can become prohibitively expensive:
  - *Arnoldi cost of orthogonalization dominates if $k > m/n$.*
  - *In Lanczos, reorthogonalizing iterate to previous guesses can ensure orthogonality in the presence of round-off error.*
  - *Selective orthogonalization strategies control when and with respect to what previous columns of $\boldsymbol{Q}$, each new iterate $\boldsymbol{u}_j = \boldsymbol{A}\boldsymbol{q}_j$ should be orthogonalized.*

- Consequently, in practice, low-dimensional Krylov subspace methods are constructed repeatedly using carefully selected new starting vectors:

  If we wish to find a particular eigenvector isolate some eigenspaces, restarting is beneficial
  - *can orthogonalize to previous eigenvector estimates to perform deflation,*
  - *can pick starting vector as Ritz vector estimate associated with desired eigenpair,*
  - *given new starting vector, can discard previous Krylov subspace, which helps make storing the needed parts of $\boldsymbol{Q}$ possible.*

Generalized Eigenvalue Problem

- A generalized eigenvalue problem has the form $\boldsymbol{A}\boldsymbol{x} = \lambda \boldsymbol{B}\boldsymbol{x}$,

$$\boldsymbol{A}\boldsymbol{X} = \boldsymbol{B}\boldsymbol{X}\boldsymbol{D}$$
$$\boldsymbol{B}^{-1}\boldsymbol{A} = \boldsymbol{X}\boldsymbol{D}\boldsymbol{X}^{-1}$$

  Generalized eigenvalue problems arise frequently, especially in solving partial differential equations.

- When $\boldsymbol{A}$ and $\boldsymbol{B}$ are symmetric and $\boldsymbol{B}$ is SPD, we can perform Cholesky on $\boldsymbol{B}$, multiply $\boldsymbol{A}$ by the inverted factors, and diagonalize it:

$$\boldsymbol{A}\boldsymbol{X} = \boldsymbol{L}\boldsymbol{L}^T\boldsymbol{X}\boldsymbol{D}$$
$$\underbrace{\boldsymbol{L}^{-1}\boldsymbol{A}\boldsymbol{L}^{-T}}_{\tilde{\boldsymbol{A}}}\underbrace{\boldsymbol{L}^T\boldsymbol{X}}_{\tilde{\boldsymbol{X}}} = \underbrace{\boldsymbol{L}^T\boldsymbol{X}}_{\tilde{\boldsymbol{X}}}\boldsymbol{D}$$

- Alternative canonical forms and methods exist that are specialized to the generalized eigenproblem.