VII. Matrix Eigenvalue Problems

2008. 10

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VII. Matrix Eigenvalue Problems

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1.1 Basic Formulation (1/4)

□ Basics of Matrix Eigenvalue Problems

- **Form:** $Ax = \lambda x$ or $Mx = \lambda Fx \longrightarrow F^{-1}Mx = \lambda x$ or $\frac{1}{\lambda}x = M^{-1}Fx$
- **Eigenvalue**

$$(A - \lambda I)x = 0\,;\ \text{Non trivial solution} \rightarrow Det(A - \lambda I) = 0$$

  - Characteristic polynomial (n-th order) having n roots (can be repeated)
- **Eigenvector**

$$\text{Solve } (A - \lambda_i I)x = 0 \text{ for nontririvial solution} \qquad x = (\chi_1, \chi_2, \cdots \chi_n)^T$$

  - Gauss elimination would lead the last to be a null equation $0 \cdot \chi_n = 0$
  - The last entry is free to choose → magnitude of eigenvector not unique
  - Eigenvectors are linearly independent each other

□ Power Method

- **In most cases, finding only the largest eigenvalue and corresponding eigenvector is sufficient. E.g. Spectral radius**
- **Find those by repeating only matrix vector multiplication**

$$x^{(k)} = Ax^{(k-1)} \text{ and } \qquad \lambda^{(k)} = \frac{< x^{(k)}, x^{(k)} >}{< x^{(k)}, x^{(k-1)} >}$$

1.1 Basic Formulation (2/4)

□ Convergence

$$x^{(k)} = Ax^{(k-1)} \rightarrow \quad x^{(k)} = AAx^{(k-2)} = A^k x^{(0)}$$

- **Expansion of the initial (guess) vector in terms of eigenvectors which are mutually linearly independent**

$$x^{(0)} = c_1 u_1 + c_2 u_2 + \cdots + c_n u_n \quad ; \text{ eigenvectors numbered such that } |\lambda_1| > |\lambda_2| > \cdots > |\lambda_n|$$

$$x^{(k)} = A^k (c_1 u_1 + c_2 u_2 + \cdots + c_n u_n) = c_1 A^k u_1 + c_2 A^k u_2 + \cdots + c_n A^k u_n$$

$$= c_1 \lambda_1^k u_1 + c_2 \lambda_2^k u_2 + \cdots + c_n \lambda_n^k u_n = \lambda_1^k \left(c_1 u_1 + c_2 \left[\frac{\lambda_2}{\lambda_1} \right]^k u_2 + \cdots + c_n \left[\frac{\lambda_n}{\lambda_1} \right]^k u_n \right)$$

$$\approx c_1 \lambda_1^k u_1 \text{ as } k \rightarrow \infty \quad \because \quad \left| \frac{\lambda_i}{\lambda_1} \right|^k < 1 \quad \forall i$$

- **Convergence Rate**

$$\text{determined by dominance ratio } \sigma = \left| \frac{\lambda_2}{\lambda_1} \right|$$

How much the fundamental (largest) eigenvalue dominates over other eigenvalues

1.1 Basic Formulation (3/4)

□Determination of Eigenvalue

For a large k, $x^{(k)} = Ax^{(k-1)} \cong \lambda_1 x^{(k-1)} \quad \because x^{(k)} \to u_1$

Inner Product with $x^{(k)} \to < x^{(k)}, x^{(k)} > \cong \lambda_1 < x^{(k)}, x^{(k-1)} >$

$$\lambda_1 \cong \frac{< x^{(k)}, x^{(k)} >}{< x^{(k)}, x^{(k-1)} >} = \lambda^{(k)}$$

□Eigenvector Scaling

- **The iteration scheme above will result in continuously increasing (eig. val. > 1.0) infinitely or decreasing (eig. val <1.0)**
  - Truncation error would ruin the iteration scheme
- **Scale the eigenvector at each step by dividing the current estimate of the eigenvalue**

$$\hat{x}^{(k-1)} = \frac{x^{(k-1)}}{\lambda^{(k-1)}} \rightarrow x^{(k)} = A\hat{x}^{(k-1)} = \frac{1}{\lambda^{(k-1)}} Ax^{(k-1)}; \ \lambda^{(k)} = \frac{< x^{(k)}, x^{(k)} >}{< x^{(k)}, \hat{x}^{(k-1)} >} = \lambda^{(k-1)} \frac{< x^{(k)}, x^{(k)} >}{< x^{(k)}, x^{(k-1)} >}$$

$$\cong \lambda_1 \hat{x}^{(k-1)}$$

1.1 Basic Formulation (4/4)

Convergence After Scaling

$$x^{(k)} = \frac{1}{\lambda^{(k-1)}} A x^{(k-1)} = \frac{1}{\lambda^{(k-1)}\lambda^{(k-2)}} A^2 x^{(k-2)} = \frac{1}{\prod_{i=0}^{k-1} \lambda^{(i)}} A^k x^{(0)} \cong \frac{\lambda_1^k}{\prod_{i=0}^{k-1} \lambda^{(i)}} c_1 u_1$$

Scaling by Normalization

- **Divide the eigenvector by the maximum entry (*l*$_{\circledcirc}$ *norm*)**
- **The resulting eigenvector will always have 1.0 as the max. val**
- **The max. entry after the matrix-vector multiplication is the new eigenvalue** $\because \left(x^{(k)} = A[\cdots 1 \cdots]^T = \lambda [\cdots 1 \cdots]^T = [\cdots \lambda \cdots]^T \right)$

Power Iteration Sequence

0) **Make an initial guess of eigenvector, e.g. all entries of 1.0, and eigenvalue, e.g. 1.0.**
1) **Scale the eigenvector with the eigenvalue**
2) **Perform matrix-vector multiplication to determine new vector**
3) **Obtain the inner products and take the ratio as eigenvalue**
4) **Repeat Steps 1-3 until the change in eigenvalue is less than ♏**

1.2 Inverse Power Method

- **Objective: Find the minimum eigenvalue**
- **Method: Apply the power method to the inverse**
  - **Eigenvalue of the Inverse**

$$\det(A^{-1}-\tilde{\lambda}I)=0 \rightarrow \det\left(A^{-1}(I-\tilde{\lambda}A)\right)=0 \rightarrow \det(A^{-1})\det\left((I-\tilde{\lambda}A)\right)=0 \rightarrow \det\left(\tilde{\lambda}(\frac{I}{\tilde{\lambda}}-A)\right)=0$$

$$\rightarrow \tilde{\lambda}^n \det\left((\frac{1}{\tilde{\lambda}}I-A)\right)=0 \rightarrow \det(A-\lambda I)=0 \quad \leftarrow \frac{1}{\tilde{\lambda}}=\lambda;\text{ inverse of original eigevalue}$$

    - Minimum eigenvalue of original matrix = maximum eigenvalue of inverse
  - **Application**

$$x^{(k)}=A^{-1}\hat{x}^{(k-1)};\ \lambda^{(k)}=\frac{<x^{(k)},x^{(k)}>}{<x^{(k)},\hat{x}^{(k-1)}>}$$

    - Since finding the inverse is difficult, solve the following instead

$$Ax^{(k)}=\hat{x}^{(k-1)}$$

    - If A is LU factored, the repeated solution of the linear system with changed RHS will be easy.

1.3 Method of Deflation and Decontamination

- **Objective: Find the second eigenvalue**
- **Method: Apply the power method to a deflated matrix**
  - **Deflation : Remove the components contributing to the first eigenvector**
  - **After finding the first eigenvector,**

$$\text{Let } \hat{u}_1 = \frac{u_1}{\|u_1\|} \text{ be normalized eigenvector} \longrightarrow \;<\hat{u}_1, \hat{u}_1> = \hat{u}_1^T \hat{u}_1 = 1$$

  - **Construct a new matrix**

$$B = A - \lambda_1 \hat{u}_1 \hat{u}_1^T \longrightarrow B\hat{u}_1 = A\hat{u}_1 - \lambda_1 \hat{u}_1 \hat{u}_1^T \hat{u}_1 = \lambda_1 \hat{u}_1 - \lambda_1 \hat{u}_1 \left(\hat{u}_1^T \hat{u}_1\right) = o$$

  - **Power method applied to B**

$$x^{(k)} = B^k x^{(0)} = \sum_{i=1}^{n} c_i B^k u_i = o + \sum_{i=2}^{n} c_i \lambda_i^k u_i = \lambda_2^k \sum_{i=2}^{n} c_i \left(\frac{\lambda_i}{\lambda_2}\right)^k u_i \cong c_2 \lambda_2^k u_2$$

- **Successive Deflation→ Lower eigenvalues**
- **Drawback: B becomes full → Flops increases for Bx even though A is sparse**

1.3 Method of Deflation and Decontamination

- **Decontamination: Remove the first eigenvector component from the k-th vector**
- **For Symmetric matrices**
  - **Eigenvectors are orthogonal**

$$x^{(k-1)} = c_1^{(k-1)}u_1 + c_2^{(k-1)}u_2 + \cdots c_n^{(k-1)}u_n \longrightarrow c_1^{(k-1)} = \frac{< x^{(k-1)}, u_1 >}{< u_1, u_1 >}$$

  - **Decontaminated vector**

$$\tilde{x}^{(k-1)} = c_2^{(k-1)}u_2 + \cdots c_n^{(k-1)}u_n = x^{(k-1)} - c_1^{(k-1)}u_1 = x^{(k-1)} - \frac{u_1^T x^{(k-1)}}{u_1^T u_1}u_1$$

  - **Power method with decontaminated vector**

scaling

$$\hat{x}^{(k-1)} = \frac{1}{\lambda_2^{(k-1)}}\tilde{x}^{(k-1)}; \longrightarrow x^{(k)} = A\hat{x}^{(k-1)} \cong c_2\lambda_2^k u_2$$

- **Successive Decontamination→ Lower eigenvalues**
- **Can work for non-symmetric matrices**

2.1 Chebyshev Acceleration Method (1/2)

☐ Example of Large Dominance Ratio Cases (Causing Slow Convergence of Power Method)

- **Consider an eigenvalue problem in one-d particle diffusion**

$$-D\frac{d^2\phi}{dx^2}+\sigma_A\phi=\lambda\sigma_S\phi\,,\quad x\in[0,a],\quad \phi(0)=0,\quad \phi(a)=0$$

$$A\phi^{(n)}=\lambda^{(n-1)}S\phi^{(n-1)}$$

- Discretization would lead to $A\phi=\lambda S\phi$ $\quad min\ Eig.\frac{1}{\lambda}\phi=A^{-1}S\phi \qquad \frac{1}{\lambda}\phi^{(n)}=A^{-1}S\phi^{(n-1)}$
- Rearrange after dividing by D, $\frac{d^2\phi}{dx^2}+\frac{\lambda\sigma_S-\sigma}{D}\phi=0$
- Let $B^2=\frac{\lambda\sigma_S-\sigma_A}{D}\rightarrow\frac{d^2\phi}{dx^2}+B^2\phi=0$

0 Flux Boundary Condition $\rightarrow\ B_n=\frac{n\pi}{a}$

- Eigenvalue $\lambda_n=\frac{\sigma_A+DB_n^2}{\sigma_S}=\frac{\sigma_A+\frac{n^2\pi^2}{a^2}}{\sigma_S}$
- Dominance Ratio $\sigma=\frac{\frac{1}{\lambda_2}}{\frac{1}{\lambda_1}}=\frac{\sigma_A+D\frac{\pi^2}{a^2}}{\sigma_A+D\frac{4\pi^2}{a^2}}$

Need minimum Eigenvalue for least adjusment

- $\sigma_A\rightarrow 0,\ \sigma\rightarrow 0.25.$

Conversely, as $a\rightarrow\infty$ or $D\downarrow$ or $\sigma_A\uparrow,\ \sigma\rightarrow 1.0$

- **Diffusion problems for large domain or weak diffusivity have large dominance ratio → Slow convergence of power method**

Chebyshev Acceleration Method

- Single Parameter Method
  - Extrapolation of eigenvector using the current estimate by power method and the previous iterate

$$x^{(k)} = \omega^{(k)} x_{Pow}^{(k)} + \left(1-\omega^{(k)}\right) x^{(k-1)} = \omega^{(k)} \frac{1}{\lambda^{(k-1)}} A x^{(k-1)} + \left(1-\omega^{(k)}\right) x^{(k-1)}$$

  - The extrapolation parameter is the single parameter and it is iteration dependent

- Two Parameter Method
  - Extrapolation using two previous iterates

$$x^{(k)} = \alpha^{(k)} x_{Pow}^{(k)} + \left(1-\alpha^{(k)} + \beta^{(k)}\right) x^{(k-1)} - \beta^{(k)} x^{(k-2)}$$

Single Parameter Chebyshev Acceleration (1/6)

- Eigenvector Extrapolation

$$x^{(k)} = \omega^{(k)} x_{Pow}^{(k)} + (1-\omega^{(k)}) x^{(k-1)} = \omega^{(k)} \frac{1}{\lambda^{(k-1)}} A x^{(k-1)} + (1-\omega^{(k)}) x^{(k-1)}$$

$$= \left(\omega^{(k)} \frac{1}{\lambda^{(k-1)}} A + (1-\omega^{(k)}) I \right) x^{(k-1)} \quad \rightarrow x^{(k)} = \prod_{p=1}^{k} \left(\omega^{(p)} \frac{1}{\lambda^{(p-1)}} A + (1-\omega^{(p)}) I \right) x^{(0)}$$

– For $x^{(0)} = c_1 u_1 + c_2 u_2 + \cdots + c_n u_n$

$$x^{(k)} = \sum_{i=1}^{n} \left[c_i \left\{ \prod_{p=1}^{k} \left(\omega^{(p)} \frac{1}{\lambda^{(p-1)}} A + \left(1-\omega^{(p)}\right) I \right) \right\} u_i \right] = \sum_{i=1}^{n} \left[c_i \left\{ \prod_{p=1}^{k} \left(\omega^{(p)} \frac{\lambda_i}{\lambda^{(p-1)}} + \left(1-\omega^{(p)}\right) \right) \right\} u_i \right]$$

– Note that $\prod_{p=1}^{k} \left(\omega^{(p)} \frac{\lambda_i}{\lambda^{(p-1)}} + \left(1-\omega^{(p)}\right) \right)$ is a k-th order polynomial of λ_i

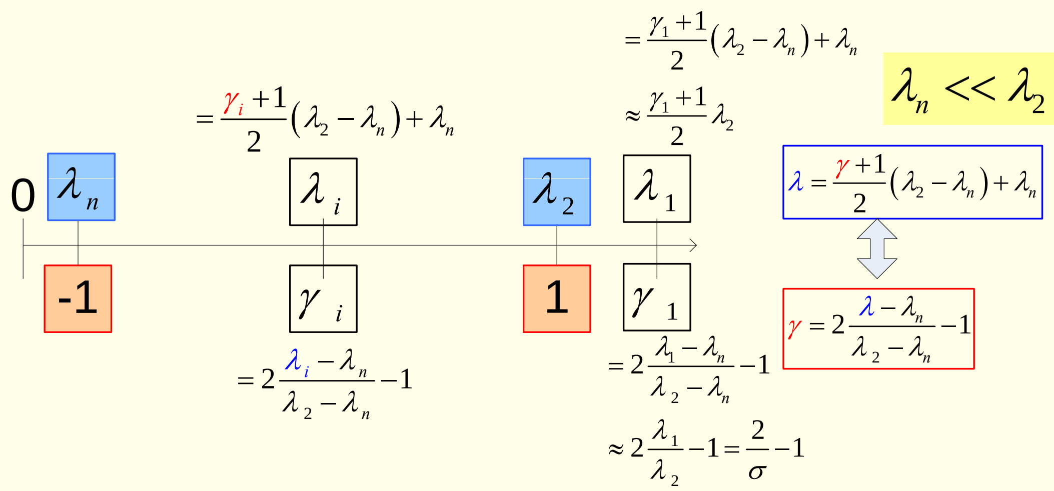
and $\lambda^{(p-1)} \cong \lambda^*$, the largest eigenvalue we seek to find so that $\frac{\lambda_i}{\lambda^{(p-1)}} \leq 1.0$

Single Parameter Chebyshev Acceleration (2/6)

- Change of Variable

$$\gamma = 2\frac{\lambda-\lambda_n}{\lambda_2-\lambda_n}-1 \;\leftarrow\; \begin{pmatrix} \lambda_i : \lambda_n \to \lambda_2 \\ \gamma_i : -1 \to 1 \end{pmatrix}$$

$$\lambda_1 > \lambda_2 \to \gamma_1 = 2\frac{\lambda_1}{\lambda_2} - 1 = \frac{2}{\sigma} - 1 > 1$$



- Passage to Chebyshev Polynomial

Assume the minimum eigenvalue $\lambda_n << 1$, $\gamma_i \cong 2\frac{\lambda_i}{\lambda_2} - 1 \;\to\; \lambda_i = \frac{\gamma_i + 1}{2}\lambda_2$

Then, $\prod_{p=1}^{k}\left(\omega^{(p)}\frac{\lambda_i}{\lambda^{(p-1)}} + \left(1-\omega^{(p)}\right)\right) = \prod_{p=1}^{k}\left(\omega^{(p)}\frac{\lambda_2}{\lambda^{(p-1)}}\frac{\gamma_i+1}{2} + \left(1-\omega^{(p)}\right)\right) \equiv \eta(\gamma_i)$

$\to$ a k-th order polynomial of $\gamma_i, -1 < \gamma_i \le 1, \;\; \forall i > 1$

Since $\lambda^{(p-1)} \cong \lambda_1$, $\eta(\gamma_i) \cong \prod_{p=1}^{k}\left(\omega^{(p)}\frac{\lambda_2}{\lambda_1}\frac{\gamma_i+1}{2} + \left(1-\omega^{(p)}\right)\right) = \prod_{p=1}^{k}\left(\omega^{(p)}\sigma\frac{\gamma_i+1}{2} + \left(1-\omega^{(p)}\right)\right)$

Single Parameter Chebyshev Acceleration (3/6)

- New Form Extrapolation Expression

Error Term

$$x^{(k)} = \sum_{i=1}^{n}\left[c_i\left\{\prod_{p=1}^{k}\left(\omega^{(p)}\frac{1}{\lambda^{(p-1)}}A + \left(1-\omega^{(p)}\right)I\right)\right\}u_i\right] = \sum_{i=1}^{n}[c_i\eta(\gamma_i)u_i] = c_1\eta(\gamma_1)u_1 + \sum_{i=2}^{n}c_i\eta(\gamma_i)u_i$$

$$= \eta(\gamma_1)\left(c_1u_1 + \sum_{i=2}^{n}c_i\frac{\eta(\gamma_i)}{\eta(\gamma_1)}u_i\right) \qquad \eta(\gamma_i) = \prod_{p=1}^{k}\left(\omega^{(p)}\sigma\frac{\gamma_i+1}{2} + \left(1-\omega^{(p)}\right)\right)$$

- Minimax Problem
  - For the maximum convergence in K iterations, try to minimize the error

    $\rightarrow$ Minimize the maximum value of $\frac{\eta(\gamma_i)}{\eta(\gamma_1)}$ for all possible values of $|\gamma_i| \le 1$

  - Make $\eta(\gamma)$ be the Chebyshev polynomial of Order K by properly choosing $\omega^{(p)}$

- How to Choose the extrapolation parameter?

At each step p, make $\omega^{(p)}\sigma\frac{\xi_p+1}{2} + (1-\omega^{(p)}) = 0$ with ξ_p be the $p-$th root of the Chebyshev Polynomial!

Single Parameter Chebyshev Acceleration (4/6)

- Roots of Chebyshev Polynomial of Order K

$$T_K(x) = \cos(K\cos^{-1}x) = \cos(K\theta); x = \cos\theta$$

$$K\theta = p\pi - \frac{1}{2}\pi \rightarrow \xi_p = \cos\theta = \cos^{-1}\frac{2p-1}{2K}\pi$$

- Optimum Extrapolation Parameter

$$\omega^{(p)}\sigma\frac{\xi_p+1}{2} + (1-\omega^{(p)}) = 0$$

$$\omega^{(p)} = \frac{1}{1-\sigma\frac{\xi_p+1}{2}} = \frac{1}{1-\frac{\sigma}{2}\left(\cos(\frac{2p-1}{2K}\pi)\right)}$$

– By choosing the extrapolation parameter this way,
  the K-th order chebyshev polynomial will be obtained after the K-th iteration

– But this requires the dominance ratio to be known.

– Dominance ratio can be estimated during the iteration by using the pseudo error vectors

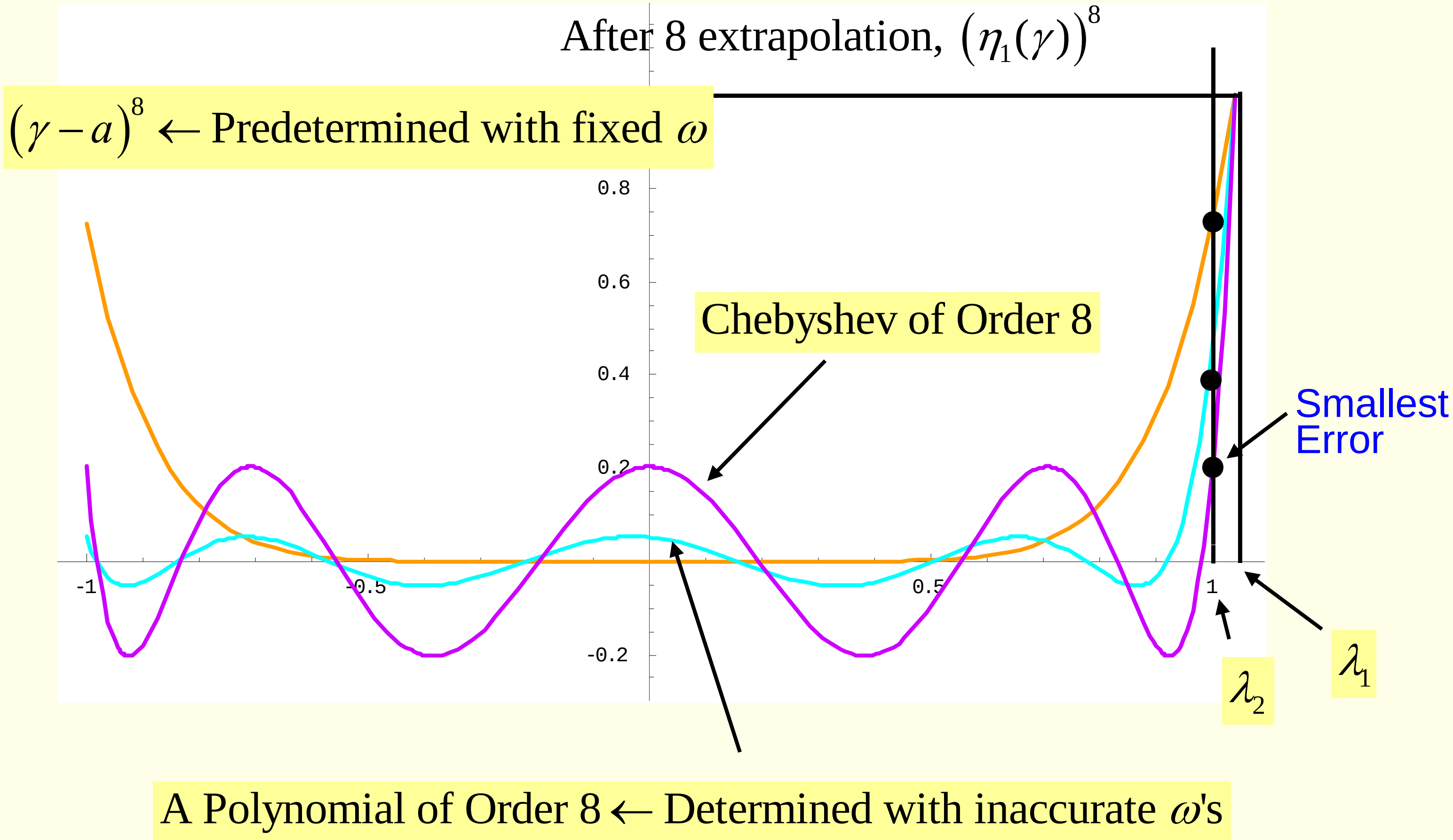
$$\tilde{e}^{(p)} = x^{(p)} - x^{(p-1)}$$

Single Parameter Chebyshev Acceleration (5/6)

- Examples for a system $\quad \sigma = 0.98 \rightarrow \gamma_1 = \frac{2}{\sigma} - 1 = 1.0408$
  - $K = 1 \rightarrow \xi_1 = 0,\ \theta_1 = \frac{1}{1 - \frac{\sigma}{2}} = 1.9608;$ Predetermined Fixed Parameter Extrapolation
  - $K = 8 \rightarrow \theta^{(p)} = 1.009, \cdots, 33.996;$ Extrapolation with Cheby
  - $K = 8,$ but with $\sigma = 0.95 \rightarrow \theta^{(p)} = 1.009, \cdots, 16.912;$ Extrapolation with Not Quite Cheby

Single Parameter Chebyshev Acceleration (6/6)

- Examples for a system $\eta_1(\gamma) = \omega^{(1)}\sigma\frac{\gamma+1}{2} + \left(1-\omega^{(1)}\right) = c(\gamma - a)$



2.2 Wielandt Shift Method

□Eigenvalue Shift

- **Consider an Eigenvalue Problem with Shifted Matrix**

$$A' = A - \alpha I$$

- If x is an eigenvector of A, it is also an eigenvector of A'.

$$A'x = (A - \alpha I)x = Ax - \alpha x = (\lambda - \alpha)x$$

$$A'x = \lambda' x$$

- Eigenvaue is shifted by α.

□Convergence of Power Method with Shifted Matrix

$$\sigma' = \frac{\lambda_2 - \alpha}{\lambda_1 - \alpha} < \frac{\lambda_2}{\lambda_1} = \sigma'$$

$$\text{Ex)}\ \sigma = \frac{\lambda_2}{\lambda_1} = \frac{0.99}{1.00} \rightarrow \sigma' = \frac{0.99 - 0.9}{1.00 - 0.9} = \frac{0.09}{0.10} = 0.9 < 0.99$$

- **Dominance ratio can be made significantly smaller if ♋ is chosen to be close to ●$_1$**

2.2 Wielandt Shift Method

☐ Inverse Power Method with Eigenvalue Shift

$$(A-\alpha I)x^{(k)} = x^{(k-1)} \Leftrightarrow x^{(k)} = (A-\alpha I)^{-1}x^{(k-1)} \quad \rightarrow x^{(k)} = (A-\alpha I)^{-k}x^{(0)}$$

$x^{(0)} = c_1u_1 + c_2u_2 + \cdots + c_nu_n$ with eigenvectors numbered such that $|\lambda_1| > |\lambda_2| > \cdots > |\lambda_n|$

$$(A-\alpha I)^{-1}u_i = \frac{u_i}{\lambda_1 - \alpha} \quad \rightarrow x^{(k)} = \frac{c_1u_1}{(\lambda_1-\alpha)^k} + \cdots + \frac{c_{n-1}u_{n-1}}{(\lambda_{n-1}-\alpha)^k} + \frac{c_nu_n}{(\lambda_n-\alpha)^k}$$

- If α is chosen close to λ_n, the last term dominates largely.

☐ Application Sequence

- Solve $(A-\alpha I)x^{(k)} = \hat{x}^{(k-1)}$
- Obtain $\lambda'^{(k)} = \dfrac{< x^{(k)}, \hat{x}^{(k-1)} >}{< x^{(k)}, x^{(k)} >} \rightarrow \lambda^{(k)} = \lambda'^{(k)} + \alpha$
- Scale $\hat{x}^{(k)} = \lambda'^{(k)}x^{(k)}$, then repeat iteration until convergence.
- Then repeat iteration until convergence ($|\Delta\lambda| < \varepsilon$)

3. Q-R Method

QR Factor of a Matrix

$$A = QR = \begin{bmatrix} q_{11} & q_{12} & \cdots & q_{1n} \\ q_{21} & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ q_{n1} & \cdots & & q_{nn} \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & & \\ & & \ddots & \\ & & & r_{nn} \end{bmatrix}$$

- Q is orthogonal (unitary):

$$Q = [q_1, q_2, \cdots, q_n]$$

$$Q^T Q = I \rightarrow Q^T = Q^{-1}$$

$$\because < q_i, q_j >= \delta_{ij}$$

Similarity Transform

$A' = S^{-1}AS$ which is *similar* to A in that the eigenvalues are unchanged

- For two eigenvalue problems, $Ax = \lambda x$ and $A'x' = \lambda' x'$

$$Det(A' - \lambda' I) = Det(S^{-1}AS - \lambda' I) = Det\left(S^{-1}(AS - \lambda' S)\right) = Det\left(S^{-1}(A - \lambda' I)S\right)$$

$$= Det(S^{-1})Det(A - \lambda' I)Det(S) = Det(A - \lambda' I) = 0 \rightarrow \text{Same Chracteristic Eqn.} \rightarrow \lambda' = \lambda$$

$$A'x' = \lambda' x' \rightarrow S^{-1}ASx' = \lambda' x' \rightarrow ASx' = \lambda' Sx' \rightarrow Ax = \lambda x \rightarrow x = Sx' \text{ or } x' = S^{-1}x$$

- Eigenvalue unchanged, but eigvector changes to $x' = S^{-1}x$
- Diagonalization: $S = [u_1 \cdots u_n] \rightarrow S^{-1}AS = D$

3. Q-R Method

- **Similarity Transform Using Q (Orthogonal Transform)**

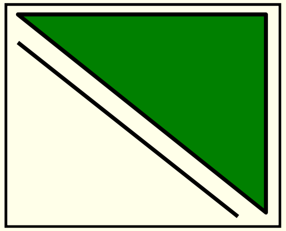
  $A' = Q^{-1}AQ = Q^{-1}QRQ = RQ$ $\leftarrow QR$ factors reversed!
  with smaller entries in lower diagonal

- **Q-R Algorithm with Repeated Orthogonal Transform**

  0. Let $A_1 = A$
  1. For A_k, determine Q_k and R_k such that $A_k = Q_k R_k$
  2. Set $A_{k+1} = R_k Q_k$ (Orthogonal transform)
  3. Repeat Steps 1 and 2 until lower-diagonal entries of A_k vanish

  $\rightarrow$ Eigenvalues are diagonal entries of A_k

Hessenberg Matrix



- **Can be applicable to any matrix to find all the eigenvalues and eigenvectors**
- **For efficient application, need to transform the matrix first into Hessenberg form (Upper triangular+one band below the diagonal) by Householder Transform**

3.1 QR Factorization

□ Objective and Results

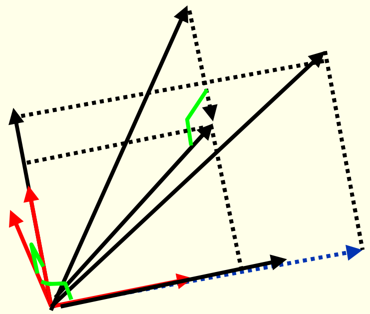
For $A = (v_1, v_2, \cdots, v_n)$,

Generate a set of orthonormal vectors $\{q_1, q_2, \cdots, q_n\}$ from $\{v_1, v_2, \cdots, v_n\}$

Let r_i be a vector consisting of the components of v_i with repect to $q_1, \cdots, q_n$
and $R = (r_1, \cdots, r_n)$, $Q = (q_1, \cdots, q_n)$

Then $A = QR$ and R is an upper triangular matrix.

□ Gram-Schmidt Orthogonalization Process



- Suppose that $q_1, \cdots, q_{k-1}$ are known at the k-th step.
- Determine the components of v_k w.r.t $q_1, \cdots, q_{k-1}$ by

$$r_{ik} = q_i^T v_k = < q_i, v_k >, \quad i = 1, \cdots, k-1$$

- Determine the new orthonormal vector q_k by

$$\tilde{q}_k = v_k - \sum_{i=1}^{k-1} r_{ik} q_i \qquad \rightarrow q_k = \frac{\tilde{q}_k}{\|\tilde{q}_k\|} \qquad \rightarrow r_{kk} = q_k^T v_k \quad \rightarrow r_k \text{ has only k elements}$$

3.1 QR Factorization

- After all orthogonalization

$$v_j = r_{1j}q_1 + r_{2j}q_2 + \cdots + r_{jj}q_j$$

$$\rightarrow v_j = [q_1, q_2, \cdots, q_n] \begin{bmatrix} r_{1j} \\ \vdots \\ r_{jj} \\ 0 \\ 0 \end{bmatrix}$$

$$Note : Bc = [u_1, u_2, \cdots, u_n] \begin{bmatrix} c_1 \\ \vdots \\ c_n \end{bmatrix} \leftarrow \text{Matrix - vector Product}$$

$\rightarrow$ Linear combination of column vector u_j's

with coefficients c_j

$$A = [v_1, v_2, \cdots, v_n] = [q_1, q_2, \cdots, q_n] \begin{bmatrix} r_{11} & r_{12} & r_{13} & \cdots & \cdots & r_{11} \\ 0 & r_{22} & r_{23} & & & \\ 0 & 0 & r_{33} & & & \\ \vdots & \vdots & 0 & \ddots & & \\ 0 & 0 & 0 & 0 & & \\ 0 & 0 & 0 & 0 & 0 & r_{nn} \end{bmatrix} = QR$$

3.2 Householder Transformation

□ Objective: Transform a Matrix into Hessenberg Form

- **Make the lower diagonal entries zero except the one right below the diagonal entry**

□ Householder Matrix

- For a normalize vector, $\hat{v} = \dfrac{v}{\|v\|}$ and $\hat{v}^T\hat{v} = 1$, define $H = I - 2\hat{v}\hat{v}^T$

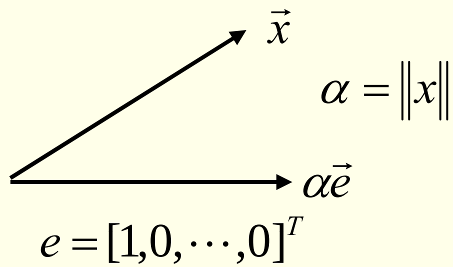
- **Properties**

$$H^T = \left(I - 2\hat{v}\hat{v}^T\right)^T = I - 2\hat{v}\hat{v}^T = H \rightarrow \text{Symmetric}$$

$$H^T H = \left(I - 2\hat{v}\hat{v}^T\right)\left(I - 2\hat{v}\hat{v}^T\right) = I - 4\hat{v}\hat{v}^T + 4\hat{v}\hat{v}^T\hat{v}\hat{v}^T = I - 4\hat{v}\hat{v}^T + 4\hat{v}\hat{v}^T = I$$
$$\rightarrow H^{-1} = H \rightarrow \text{Orthonormal}$$

□ Rotation of Vector

- **Which matrix rotates a vector x onto a vector on x axis with the same length?**

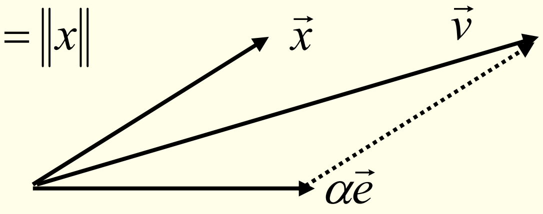


3.2 Householder Transformation

□Rotation of Vector

- Let $v = x + \alpha e$
- Then $H = I - 2\hat{v}\hat{v}^T$ rotates x to $-\alpha e$.
- Proof

$\alpha = \|x\|$



$$\alpha e = [\alpha, 0, \cdots, 0]^T$$

$$\alpha^2 = x^T x \qquad e^T x = x^T e, \; e^T e = 1$$

$$\|v\|^2 = (x+\alpha e)^T (x+\alpha e) = x^T x + \alpha e^T x + \alpha e x^T + \alpha^2 e^T e = 2\alpha^2 + 2\alpha e^T x = 2\alpha(\alpha + e^T x)$$

$$Hx = \left(I - 2\hat{v}\hat{v}^T\right) x = x - 2\frac{vv^T}{\|v\|^2} x = x - \frac{1}{\alpha(\alpha + e^T x)} vv^T x$$

$$vv^T x = (x+\alpha e)(x+\alpha e)^T x = (xx^T + \alpha e x^T + \alpha x e^T + \alpha^2 e e^T) x$$

$$= xx^T x + \alpha e x^T x + \alpha x e^T x + \alpha^2 e e^T x = \alpha^2 x + \alpha^3 e + \alpha(e^T x) x + \alpha^2 (e^T x) e$$

$$= \alpha(\alpha + e^T x) x + \alpha^2 (\alpha + e^T x) e = \alpha(\alpha + e^T x)(x + \alpha e)$$

$$\therefore Hx = x - \frac{1}{\alpha(\alpha + e^T x)} \alpha(\alpha + e^T x)(x + \alpha e) = -\alpha e \longrightarrow x = \begin{bmatrix} \chi_1 \\ \chi_2 \\ \vdots \\ \chi_n \end{bmatrix} \rightarrow Hx \rightarrow \begin{bmatrix} -\alpha \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

3.2 Householder Transformation

□ Similarity Transform with Householder Matrix

- For Householder Matrix of Order n -1
  - Construct H out of the first column n-1 entries below diagonal of $A_1 = A$

$$U_1 = \begin{bmatrix} 1 & \begin{bmatrix} & o^T & \end{bmatrix} \\ \begin{bmatrix} \\ o \\ \\ \end{bmatrix} & \begin{bmatrix} & & \\ & H & \\ & & \end{bmatrix} \end{bmatrix} \quad A_1 = \begin{bmatrix} a_{11} & \begin{bmatrix} & y^T & \end{bmatrix} \\ \begin{bmatrix} \\ x \\ \\ \end{bmatrix} & \begin{bmatrix} & & \\ & B & \\ & & \end{bmatrix} \end{bmatrix} \qquad U_1 = U_1^{-1}$$

$$U_1^{-1}A = \begin{bmatrix} a_{11} & * & * & & * \\ -\alpha & * & & & * \\ 0 & * & & & \\ \vdots & \vdots & & & \\ 0 & * & * & & * \end{bmatrix} \qquad U_1^{-1}A = \begin{bmatrix} a_{11} + o^T x & y^T + o^T B \\ a_{11} o + Hx & oy^T + HB \end{bmatrix} = \begin{bmatrix} a_{11} & y^T \\ Hx & HB \end{bmatrix}$$

$$A_2 = U_1^{-1} A U_1 = \begin{bmatrix} a_{11} & * & * & & * \\ -\alpha & * & & & * \\ 0 & * & & & \\ \vdots & \vdots & & & \\ 0 & * & * & & * \end{bmatrix} \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & H & \\ 0 & & & \end{bmatrix} = \begin{bmatrix} a_{11} & * & * & & * \\ -\alpha & * & & & * \\ 0 & * & & & \\ \vdots & \vdots & & & \\ 0 & * & * & & * \end{bmatrix}$$

U_1 multiplied additionally for similarity transform

3.2 Householder Transformation

□ Subsequent Householder Transformation with Reduced Order

– Construct H out of the second column n-2 entries below diagonal of A_2

$$U_2 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & & & \\ 0 & 0 & & H & \\ 0 & 0 & & & \end{bmatrix} \qquad U_2^{-1}\left(U_1^{-1} A U_1\right)U_2 = \begin{bmatrix} a_{11} & * & * & & * \\ * & * & & & * \\ 0 & * & * & & \\ \vdots & 0 & * & * & \\ 0 & 0 & * & * & * \end{bmatrix}$$

– Continue n-2 steps of Householder Transformation

$$U^{-1} = U_{n-2}^{-1} U_{n-3}^{-1} \cdots U_1^{-1} \rightarrow U = U_1 U_2 \cdots U_{n-2}$$

$A' = U^{-1} A U$ is a similarity transform of A which appears as Hessenberg form.

3.2 Householder Transformation

□Householder Transformation for Symmetric Matrix

$$U_1 = \begin{bmatrix} 1 & \begin{bmatrix} o^T \end{bmatrix} \\ \begin{bmatrix} o \end{bmatrix} & \begin{bmatrix} H \end{bmatrix} \end{bmatrix} \qquad A_1 = \begin{bmatrix} a_{11} & \begin{bmatrix} x^T \end{bmatrix} \\ \begin{bmatrix} x \end{bmatrix} & \begin{bmatrix} B \end{bmatrix} \end{bmatrix}$$

$$U_1 A_1 = \begin{bmatrix} a_{11} + o^T x & \begin{bmatrix} x^T + o^T B \end{bmatrix} \\ \begin{bmatrix} a_{11} o + Hx \end{bmatrix} & \begin{bmatrix} o x^T + HB \end{bmatrix} \end{bmatrix} = \begin{bmatrix} a_{11} & \begin{bmatrix} x^T \end{bmatrix} \\ \begin{bmatrix} Hx \end{bmatrix} & \begin{bmatrix} HB \end{bmatrix} \end{bmatrix}$$

$$U_1 A_1 U_1 = \begin{bmatrix} a_{11} & \begin{bmatrix} x^T \end{bmatrix} \\ \begin{bmatrix} Hx \end{bmatrix} & \begin{bmatrix} HB \end{bmatrix} \end{bmatrix} \begin{bmatrix} 1 & \begin{bmatrix} o^T \end{bmatrix} \\ \begin{bmatrix} o \end{bmatrix} & \begin{bmatrix} H \end{bmatrix} \end{bmatrix} = \begin{bmatrix} a_{11} & \begin{bmatrix} x^T H \end{bmatrix} \\ \begin{bmatrix} Hx \end{bmatrix} & \begin{bmatrix} HBH \end{bmatrix} \end{bmatrix}$$

3.2 Householder Transformation

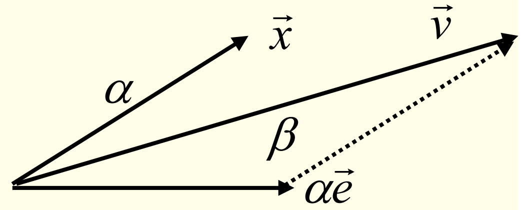
□Householder Transformation for Symmetric Matrix

$$Hx = \begin{bmatrix} 1 \\ -\alpha \\ 0 \\ \vdots \\ 0 \end{bmatrix} \longrightarrow \begin{bmatrix} a_{11} & \begin{bmatrix} -\alpha & 0 & \cdots & 0 \end{bmatrix} \\ \begin{bmatrix} -\alpha \\ 0 \\ \vdots \\ 0 \end{bmatrix} & \begin{bmatrix} \\ HBH \\ \\ \end{bmatrix} \end{bmatrix}$$

- **Elements on the right of the diagonal were also eliminated except the one right next to the diagonal.**
- **Continued Householder transformation with lower dimensions yields tridiagonal matrix**

Practical Householder Algorithm

$$x^{(k)} = \begin{bmatrix} a_{k+1,k} \\ a_{k+2,k} \\ \vdots \\ a_{n,k} \end{bmatrix},\ e^{(k)} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \alpha = \left\| x^{(k)} \right\| = \sqrt{\sum_{i=k+1}^{n} a_{ik}^2},\ v = x^{(k)} + \alpha e^{(k)}$$



$$\beta = \|v\| = \sqrt{(a_{k+1,k} + \alpha)^2 + \sum_{i=k+2}^{n} a_{ik}^2} = \sqrt{a_{k+1,k}^2 + 2\alpha a_{k+1,k} + \alpha^2 + \sum_{i=k+2}^{n} a_{ik}^2} \quad = \sqrt{2(\alpha a_{k+1,k} + \alpha^2)}$$

$$\hat{v} = \frac{1}{\beta} \begin{bmatrix} a_{k+1,k} + \alpha \\ a_{k+2,k} \\ \vdots \\ a_{n,k} \end{bmatrix} \qquad H_k = I - 2\hat{v}\hat{v}^T \qquad U_k = \begin{bmatrix} I_k & O_k^T \\ O_k & H_k \end{bmatrix} \longrightarrow A_{k+1} = U_k A_k U_k$$

$$\dim(I_k) = k$$

$$\dim(H_k) = n - k$$

- What if $\beta = 0$? $\leftarrow \alpha = -a_{k+1,k} \rightarrow a_{k+1,k} < 0$ and $a_{i,k} = 0 \quad \forall i \geq k+2$

Algorithm breaks down. $\longrightarrow$ Remedy: Choose $\alpha = -\left\| x^{(k)} \right\|$ if $a_{k+1,k} < 0$.

3.2 Householder Transform

MATLAB Script

```
%function H=householder(A)
%
% dimension of input matrix
n=length(A);
%
% matrix to contain householder transform matrix at each step
U=zeros(n);
H=A;
In=eye(n); %identity matrix of dimension n
for k=1:n-2
   nmk=n-k;
   kp1=k+1;
   x=H(k+1:n,k);
   alpha=norm(x);
   if(x(1)<0) alpha=-alpha; end %make sure the same direction
   v=x;
   v(1)=v(1)+alpha;
   beta=norm(v);
   vhat=v/beta;
   Hk=eye(nmk)-2*vhat*vhat'; %householder matrix of order n-k
%    U=In;
%    U(kp1:n,kp1:n)=Hk;
%    H2=U*H*U;
   H(kp1,k)=-alpha;
   H(kp1+1:n,k)=0; %zero out the lower diagonal entries
   H(kp1:n,kp1:n)=Hk*H(kp1:n,kp1:n)*Hk; %update the remainder
   H(k,kp1:n)=H(k,kp1:n)*Hk; %update the row vector
%    H2-H
   pause
end
```

Q-R Factorization of a Hessenberg Matrix

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & \ddots & & \vdots \\ 0 & \ddots & \ddots & \vdots \\ 0 & 0 & a_{nn-1} & a_{nn} \end{bmatrix} = QR = \begin{bmatrix} q_{11} & q_{12} & \cdots & q_{1n} \\ q_{21} & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ q_{n1} & \cdots & & q_{nn} \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & & \\ & & \ddots & \\ & & & r_{nn} \end{bmatrix}$$

$$\longrightarrow Q^{-1}A = R$$

$$\begin{bmatrix} a_{12} \\ a_{22} \\ a_{32} \\ 0 \\ 0 \end{bmatrix} \rightarrow \begin{bmatrix} a'_{12} \\ 0 \\ a'_{32} \\ 0 \\ 0 \end{bmatrix}$$

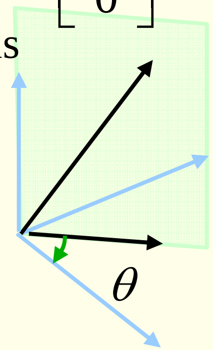
- Which operation on A can make A to upper triagonal matrix?

  $\rightarrow$ Eliminate the subdiagonal entry one-by-one.

- Plane Rotation

  - Rotate the plane normal to the xy-plane by θ so that it is aligned with the x-axis to remove $y-$component in the rotated vector

$$\text{First Rotation Matrix, } P_1 = \begin{bmatrix} \cos\theta & -\sin\theta & & \\ \sin\theta & \cos\theta & & \\ & & 1 & \\ & & & 1 \end{bmatrix}$$



3.3 Q-R Method

Determination of Rotation Angle

$$\begin{bmatrix} \cos\theta & -\sin\theta & & \\ \sin\theta & \cos\theta & & \\ & & 1 & \\ & & & 1 \end{bmatrix} \begin{bmatrix} a_{11} \\ a_{21} \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} a'_{11} \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$a_{11}\sin\theta + a_{21}\cos\theta = 0$$

$$\sin\theta = -\frac{a_{12}}{\sqrt{a_{11}^2 + a_{21}^2}}$$

$$a_{11}^2(1-\mu^2) = a_{21}^2\mu^2 \rightarrow \mu = \frac{a_{11}}{\sqrt{a_{11}^2 + a_{21}^2}} = \cos\theta$$

$$a'_{11} = a_{11}\frac{a_{11}}{\sqrt{a_{11}^2 + a_{21}^2}} + a_2\frac{a_{21}}{\sqrt{a_{11}^2 + a_{21}^2}}$$

Repeated Plane Rotation

$$P_k = \begin{bmatrix} I_k & & & \\ & \cos\theta & -\sin\theta & \\ & \sin\theta & \cos\theta & \\ & & & I_{n-k-2} \end{bmatrix}$$

← k - th row

Properties of Rotation Matrix P_k

- P is an orthonormal matrix $\rightarrow P^{-1} = P^T$

Final Form

$$P_{n-1}P_{n-2}\cdots P_1 A = R$$

$$A = P_1^{-1}P_2^{-1}\cdots P_{n-1}^{-1}R = P_1^T P_2^T \cdots P_{n-1}^T R$$

$$Q = P_1^T P_2^T \cdots P_{n-1}^T$$

3.3 Q-R Method

□ Eigenvalue Shift

- Consider QR factorization of $H_k - \lambda^{(k)} I = Q_k R_k$
- Similarity Transform : $Q_k^{-1}\left(H_k - \lambda^{(k)} I\right) Q_k = R_k Q_k$

  $Q_k^{-1} H_k Q_k = R_k Q_k + \lambda^{(k)} I \equiv H_{k+1} \rightarrow$ Similar to H_k
- Shifted Factorization with the last diagonal entry of H as a guess of eigenvalue can accelerate convergence

□ Summary of QR Factorization

1. Obtain a Hessenberg from by a Series of Householder Transformation : $H_1 = U^{-1} A U$
2. Shift Eigenvalue : $\tilde{H}_k = H_k - \lambda^{(k)} I; \lambda^{(k)} = H_k(n,n)$
3. Perform Q - R Factorization by Successvie Plane Rotation : $\tilde{H}_k = Q_k R_k$
4. Determine New Matrix by $H_{k+1} = R_k Q_k + \lambda^{(k)} I$
5. Repeat Steps 2 - 4 until subdiagonal entries are small enough.

3.3 Q-R Method

□Determination of Eigenvector after Getting Eigenvalues

- Inverse Power Method for $A-\tilde{\lambda}_k I$ with $\tilde{\lambda}_k \approx \lambda_k$

$$\left(A-\tilde{\lambda}_k I\right)x^{(1)} = \hat{x}^{(0)} \rightarrow x^{(1)} = \left(A-\tilde{\lambda}_k I\right)^{-1}\hat{x}^{(0)} = \sum_{i=1}^{n}\frac{c_i u_i}{\lambda_i - \tilde{\lambda}_k} \cong \frac{c_i u_i}{\lambda_k - \tilde{\lambda}_k}$$

$\rightarrow$ Single step of inverse power method is sufficient to obtain eigenvector!

3.3 Q-R Method

MATLAB Script

```
%function lam=qralgo(H);
% assume hessenberg form for H
n=length(H);
% identity matrix of dimension n
In=eye(n);
while (1>0)
    %factorize by plane rotation
    lam=H(n,n); %guess of eigenvector
    Hk=H-lam*In; %shift eigenvalue
    Q=In; %reset Q to identity matrix before factorization
    for i=1:n-1
      ip1=i+1;
      d=Hk(i,i); %diagonnal entry
      s=Hk(i+1,i); %subdiagonal entry to eliminate
      afac=1/sqrt(d*d+s*s);
      cosv=d*afac; %cosine value
      sinv=-s/d*cosv; %sine value, this way ensures s*sinv+d*cosv=0
      Hk(i,i)=d*cosv-s*sinv; %new diagonal value after rotation
      Hk(i+1,i)=0; %subdiagonal entry now being 0
      P=In; %rotation matrix initially identity
      P(i,i)=cosv;P(i,ip1)=-sinv; %fill rotation matrix
      P(ip1,i)=sinv;P(ip1,i+1)=cosv;
      Hk(i:ip1,i+1:n)=P(i:ip1,i:ip1)*Hk(i:ip1,i+1:n); %update entries on
        plane
      Pt=P'; %transpose of rotation matrix
      Q=Q*Pt; %Q matrix being constructed stepwise
    end
    R=Hk; %upper trianglular matrix
    H=R*Q+lam*In; %new matrix
    diag(H) %current guess of eigenvalues
    pause
end
```