Lecture 11: Symmetric Eigen Value Problem

Prof. Krishna R. Pattipati
Dept. of Electrical and Computer Engineering
University of Connecticut
Contact: krishna@engr.uconn.edu (860) 486-2890

ECE 6435

Adv Numerical Methods in Sci Comp

Fall 2008

November 5, 2008

Outline of Lecture 11

- House holder method to convert a *symmetric matrix to tridiagonal form*
- Key Ideas of Symmetric QR method
- Lanczos method for sparse symmetric matrices
  - Relationship with the conjugate gradient (CG) method
- A variety of algorithms exist for finding the Eigen values and Eigen vectors of a symmetric matrix
  - Symmetric QR
  - Jacobi method
  - Bisection method (using Sturm sequence property)
  - Power method
  - Lanczos method (for sparse symmetric matrices)
- However, symmetric QR is the best general purpose algorithm
  - Unless only a few Eigen values/Eigen vectors are desired
  - In the latter case, specialized methods may be useful (see Golub and Van Loan, 1996)

Symmetric QR Algorithm

- Key ideas of symmetric QR algorithm
  - If $Q_0^T A Q_0 = H$, an upper Hessenberg matrix
    - A is symmetric $\Rightarrow H = H^T$
    - **A symmetric upper Hessenberg matrix is a symmetric tridiagonal matrix**
  - Symmetry and tridiagonal band structure are preserved with single shift QR
  - Recall that $\{\lambda_i(A)\}$ are real for a symmetric matrix A

    $\Rightarrow$ **no need for double and complex shifts**

Transformation to Tridiagonal Form - 1

- Transformation to tridiagonal form via Householder
  - Suppose, we have determined $W_1\ W_2\ \ldots\ W_{k-2}$
  - So,

$$A_{k-1} = (W_1 \ldots W_{k-1})^T A W_1 \ldots W_{k-1} = \left[\begin{array}{c|c|c} B & \multicolumn{2}{c}{\underline{0}} \\ & \multicolumn{2}{c}{\underline{b}^T} \\ \hline \underline{0}^T & \underline{b} & D \end{array}\right] \begin{array}{l} k-1 \\ 1 \\ n-k \end{array}$$

$$\qquad\qquad k-1 \qquad 1 \qquad n-k$$

where B is tridiagonal

  - $\widetilde{W}_k$ is an order n-k Householder $\ni$ $W_k = Diag(I_k, \widetilde{W}_k)$

$$A_k = W_k A_{k-1} W_k = \begin{bmatrix} B & 0 \\ & b^T \widetilde{W}_k \\ 0 & \widetilde{W}_k b \quad \widetilde{W}_k D \widetilde{W}_k \end{bmatrix}$$

  - Exploit Symmetry in generating A_k

$$\widetilde{W}_k = I_{n-k} - \frac{2}{\underline{u}^T \underline{u}} . \underline{u}\,\underline{u}^T \ , \ \ \underline{u} \in R^{n-k}$$

Transformation to Tridiagonal Form - 2

$$\underline{p} = \frac{2}{\underline{u}^T \underline{u}} D\underline{u} \quad \text{and} \quad \underline{q} = \underline{p} - \frac{\underline{p}^T \underline{u}}{\underline{u}^T \underline{u}} . \underline{u}$$

$$\widetilde{W}_k D \widetilde{W}_k = \widetilde{W}_k \left[D - \frac{2}{\underline{u}^T \underline{u}} . D\underline{u}\underline{u}^T \right] = \widetilde{W}_k \left[D - \underline{p}\underline{u}^T \right] = \left(I - \frac{2}{\underline{u}^T \underline{u}} . \underline{u}\underline{u}^T \right) \left(D - \underline{p}\underline{u}^T \right)$$

$$= D - \underline{u}\,\underline{p}^T - \underline{p}\underline{u}^T + \frac{2}{\underline{u}^T \underline{u}} . \underline{u}\underline{u}^T \underline{p}\underline{u}^T = D - \underline{u}\underline{q}^T - \underline{q}\underline{u}^T$$

where $\underline{q} = \underline{p} - \frac{\underline{p}\underline{u}}{\underline{u}^T \underline{u}} . \underline{u}$

- Note that only the upper D portion $\widetilde{W}_k D \widetilde{W}_k$ needs to be computed
  $\Rightarrow (n-k)^2$ operations.
- So, the process of going from A_{k-1} to A_k takes $2(n-k)^2$ operations
- Overall, it takes $O(2n^3/3)$ operations to obtain tridiagonal form
- Additional $2n^3/3$ to obtain the transformation matrix $Q_0 = W_1 \; W_2 \ldots \; W_{n-2}$

Rudiments of a Sysmmetric QR

- Starting with $T = A_0 = Q_0^T A Q_0$, where T is tridiagonal, the symmetric QR algorithm employs the following iterations

$$\text{For } k = 1, 2, \ldots$$
$$A_k - \mu I = QR$$
$$A_{k+1} = RQ + \mu I = Q^T (A_k - \mu I) Q + \mu I = Q^T A_k Q$$
$$\text{end DO}$$

- Key: QR decomposition of a tridiagonal matrix requires $O(n)$ operations. The resulting R has bidiagonal structure $\Rightarrow$ diagonal and super diagonal

that is,

$$A = \begin{bmatrix} a_1 & b_2 & 0 & .. & 0 \\ b_2 & a_2 & b_3 & .. & 0 \\ 0 & 0 & 0 & a_{n-1} & b_n \\ 0 & 0 & 0 & b_n & a_n \end{bmatrix} \xrightarrow{Q^T} \begin{bmatrix} x & x & & & 0 \\ & x & x & & \\ & & x & x & \\ & & & x & x \\ 0 & & & & x \end{bmatrix} \longrightarrow \begin{array}{l} RQ = \text{tridiagonal} \\ \text{takes } O(n) \text{ operations} \end{array}$$

Picking the Shift Factor

- Choice of μ:
  - one choice is $\mu = a_n$. Another choice is to set $\mu =$ Eigen value of 2 x 2 block closest to a_n, where the 2 x 2 block is $\begin{pmatrix} a_{n-1} & b_n \\ b_n & a_n \end{pmatrix}$

$$\Rightarrow (\lambda - a_{n-1})(\lambda - a_n) - b_n^2 = \lambda^2 - (a_n + a_{n-1})\lambda + a_n a_{n-1} - b_n^2$$

$$\lambda = \frac{a_n + a_{n-1} \pm \sqrt{(a_n + a_{n-1})^2 - 4a_n a_{n-1} + 4b_n^2}}{2}$$

$$= a_n + \frac{a_{n-1} - a_n}{2} \pm \frac{\sqrt{(a_{n-1} - a_n)^2 + 4b_n^2}}{2}$$

$$\Rightarrow \lambda = a_n + d_n \pm \sqrt{d_n^2 + b_n^2} \quad \text{where } d_n = \frac{a_{n-1} - a_n}{2}$$

$$\Rightarrow \mu = a_n + d_n - \text{sgn}(d_n)\sqrt{d_n^2 + b_n^2}$$

  - This choice of μ is called *Wilkinson shift*
  - Wilkinson shift results in *cubic convergence* of A to diagonal

QR Decomposition of Tridiagonal - 1

- Only question then is: how to get QR form $(A_k - \mu I)$ in $O(n)$ operations ?
  - Use Givens transformations to obtain QR decomposition of a tridiagonal matrix $(A_k - \mu I)$.
  - Consider the initial step $k = 1$
  - The problem is to find

$$c_1, s_1 \ni \begin{bmatrix} c_1 & s_1 \\ -s_1 & c_1 \end{bmatrix} \begin{bmatrix} a_{11} - \mu \\ b_2 \end{bmatrix} = \begin{bmatrix} * \\ 0 \end{bmatrix} = k\underline{e}_1$$

  - Make $a_{21} = b_2 \to 0$ via $J(1,2,\theta) = J_{21}$ and consider $J_{21}^T(A_k - \mu I)J_{21}$

$$\begin{bmatrix} x & x & & 0 \\ x & x & & \\ & & 1 & \\ 0 & & & 1 \end{bmatrix} \begin{bmatrix} a_1 - \mu & b_2 & & & \\ b_2 & a_2 - \mu & b_3 & & \\ & b_3 & a_3 - \mu & b_4 & \\ & & & a_{n-1} - \mu & b_n \\ 0 & & & b_n & a_n - \mu \end{bmatrix} \begin{bmatrix} x & x & & 0 \\ x & x & & \\ & & 1 & \\ 0 & & & 1 \end{bmatrix} = \begin{bmatrix} x & x & + & 0 & .. & 0 \\ x & x & x & 0 & .. & 0 \\ + & x & x & x & .. & 0 \\ & 0 & & . & .. & \\ & & & . & & \\ 0 & & & & .. & 0 \end{bmatrix};$$

$+ \Rightarrow$ unwanted elements

QR Decomposition of Tridiagonal - 2

- This initial step is called implicit Q-step, which creates unwanted elements denoted by +
- **Chase these unwanted elements away via Givens or Householder transformation**:

$$A = J_{31}^T A J_{31} = J_{31}^T J_{21}^T (A_k - \mu I) J_{21} J_{31} = \begin{bmatrix} x & x & & 0 & & 0 \\ x & x & x & + & & \\ 0 & x & x & x & & \\ . & + & x & x & x & \\ & . & . & . & . & \\ 0 & 0 & . & 0 & & \end{bmatrix}$$

$$A = J_{42}^T A J_{42} = \begin{bmatrix} x & x & & & & \\ x & x & x & & & \\ & x & x & x & + & \\ & & & x & x & x \\ & & & + & x & x \end{bmatrix} etc.$$

Illustration of QR → Tridiagonal

- Illustration of the process on a 6 x 6 matrix

$$\begin{bmatrix} x & x & 0 & 0 & 0 & 0 \\ x & x & x & 0 & 0 & 0 \\ 0 & x & x & x & 0 & 0 \\ 0 & 0 & x & x & x & 0 \\ 0 & 0 & 0 & x & x & x \\ 0 & 0 & 0 & 0 & x & x \end{bmatrix} \xrightarrow[\substack{\text{implicit Q step} \\ J_{21}\underline{e}_1 = Q\underline{e}_1 \\ \text{to make it unique}}]{1} \begin{bmatrix} x & x & + & 0 & 0 & 0 \\ x & x & x & 0 & 0 & 0 \\ + & x & x & x & 0 & 0 \\ 0 & 0 & x & x & x & 0 \\ 0 & 0 & 0 & x & x & x \\ 0 & 0 & 0 & 0 & x & x \end{bmatrix} \xrightarrow[J_{31}]{2} \begin{bmatrix} x & x & 0 & 0 & 0 & 0 \\ x & x & x & + & 0 & 0 \\ 0 & x & x & x & 0 & 0 \\ 0 & + & x & x & x & 0 \\ 0 & 0 & 0 & x & x & x \\ 0 & 0 & 0 & 0 & x & x \end{bmatrix}$$

$$\xrightarrow[J_{42}]{3} \begin{bmatrix} x & x & 0 & 0 & 0 & 0 \\ x & x & x & 0 & 0 & 0 \\ 0 & x & x & x & + & 0 \\ 0 & 0 & x & x & x & 0 \\ 0 & 0 & + & x & x & x \\ 0 & 0 & 0 & 0 & x & x \end{bmatrix} \xrightarrow[J_{53}]{4} \begin{bmatrix} x & x & 0 & 0 & 0 & 0 \\ x & x & x & 0 & 0 & 0 \\ 0 & x & x & x & 0 & 0 \\ 0 & 0 & x & x & x & 0 \\ 0 & 0 & 0 & x & x & x \\ 0 & 0 & 0 & + & x & x \end{bmatrix} \xrightarrow[J_{64}]{5} \begin{bmatrix} x & x & 0 & 0 & 0 & 0 \\ x & x & x & 0 & 0 & 0 \\ 0 & x & x & x & 0 & 0 \\ 0 & 0 & x & x & x & 0 \\ 0 & 0 & 0 & x & x & x \\ 0 & 0 & 0 & 0 & x & x \end{bmatrix}$$

(n-1) steps including the implicit Q-step

Wilkinson Shift

- Implicit Symmetric QR – step with Wilkinson shift

$$\mu = a_{nn} + d - \text{sgn}(d)\sqrt{d^2 + a_{n,n-1}^2} = a_{nn} - a_{n,n-1}^2 / (d + \text{sgn}(d)\sqrt{d^2 + a_{n,n-1}^2}$$

$$d = (a_{n-1,n-1} - a_{nn})/2;\ x = a_{11} - \mu;\ z = a_{21}$$

For $k = 1, 2, \ \ldots, \ n\text{-}1$

Determine c_k and s_k ∍

$$\begin{pmatrix} c_k & s_k \\ -s_k & c_k \end{pmatrix}\begin{pmatrix} x \\ z \end{pmatrix} = \begin{pmatrix} * \\ 0 \end{pmatrix}$$

If $k = 1$

form $A \leftarrow J_{k+1,k}^T A J_{k+1,k}$

else

form $J_{k+1,k-1}^T A J_{k+1,k-1}$

end if

If $k < n-1$ then

$x = a_{k+1,k};\ z = a_{k+2,k}$

end if

end DO

- The procedure requires O(14*n*) operations and *n* square roots

Overall Symmetric QR

- To form Q, requires an additional $4n^2$ operations
- The overall Symmetric QR Algorithm
  - Find tridiagonal matrix $A_0 = T = Q_0^T A Q_0$ via Householder transformation
  - Do for ever

$$|a_{i+1,i}| \le \varepsilon\left(|a_{ii}| + |a_{i+1,i+1}|\right)$$

For $i = 1, 2, \ldots, n-1$

find largest q and smallest p ∋ if

$$A = \begin{bmatrix} A_{11} & & 0 \\ & A_{22} & \\ 0 & & A_{33} \end{bmatrix} \begin{matrix} p \\ n-p-q \\ q \end{matrix}$$

where A_{33} is diagonal and A_{22} has no zero subdiagonal elements

if $q = n$ then

quit

else

Apply Wilkinson shift; $A = diag(I_p Q I_q)^T A diag(I_p Q I_q)$

end if

end DO

- The algorithm requires ≈ $2n^3/3$ operations for $\{\lambda_i(A)\}$ and approximately $5n^3$ operations for Eigen vectors also

Lanczos Methods

- Lanczos Methods for sparse symmetric matrices
  - Useful for finding the Eigen values of sparse symmetric matrices
  - Also, related to the conjugate gradient method

- Key fact: if a matrix A is cyclic then
  - $\{\underline{u}\ A\underline{u}\ \ldots\ A^{n-1}\underline{u}\}$ from a basis.
  - The subspaces formed by $\{\underline{u}, A\underline{u}, \ldots A^{k-1}\underline{u}\}$ for $k = 1,2, \ldots, n$ are called Krylov subspaces $K(A, \underline{u}, k)$
  - We know by the power method that $A^k\underline{u}$ goes towards the Eigen vector corresponding to the largest Eigen value.

- Lanczos Idea
  - What if we orthogonalize the vectors associated with Krylov subspaces? This is the basic idea of Lanczos !!
  - It turns out that we can derive a **three term recursion for the orthogonal vectors**

Lanczos Recursion

- Lanczos Recursion: Starting with any unit vector $u = \underline{q}_1$ and any symmetric matrix A, there is an orthogonal sequence $\underline{q}_1\ \underline{q}_2\ \dots\ \underline{q}_n \ni$

$$A\underline{q}_j = b_{j-1}\underline{q}_{j-1} + a_j\underline{q}_j + b_j\underline{q}_{j+1}$$

$$Q^T A Q = T \text{ (tridiagonal)}$$

$$\Rightarrow AQ = QT$$

$$\left[A\underline{q}_1\ A\underline{q}_2\ \dots\ A\underline{q}_n\right] = \left(\underline{q}_1\ \underline{q}_2\ \dots\ \underline{q}_n\right)\begin{bmatrix} a_1 & b_1 & & & & & \\ b_1 & a_2 & b_2 & & & & \\ 0 & b_2 & a_3 & b_3 & & & \\ & & & & .. & b_{n-2} & a_{n-1} & b_{n-1} \\ & & & & & & b_{n-1} & a_n \end{bmatrix}$$

- So, Lanczos can be viewed as a Tridiagonal decomposition of a symmetric matrix A

$$\Rightarrow A\underline{q}_j = b_{j-1}\underline{q}_{j-1} + a_j\underline{q}_j + b_j\underline{q}_{j+1}$$

$$\Rightarrow b_j\underline{q}_{j+1} = (A - a_j I)\underline{q}_j - b_{j-1}\underline{q}_{j-1}$$

$$\Rightarrow b_j = \left\|(A - a_j I)\underline{q}_j - b_{j-1}\underline{q}_{j-1}\right\|$$

- The set of orthogonal vectors $\{\underline{q}_i\}$ are called Lanczos vectors

Lanczos Vectors are Orthogonal

- Note:

1) $\underline{q}_0 = \underline{0}$

2) If $\underline{b}_j = 0$, then $\underline{q}_{j+1}$ is any vector orthogonal to $\underline{q}_1 \dots \underline{q}_j$.

3) If this happens, T splits into two subblocks

4) $A\,\underline{q}_j \perp^r$ to $\underline{q}_1 \dots \underline{q}_{j-2}$

5) Vector $\underline{q}_{j+1}$ is orthogonal to $\{\underline{q}_1 \dots \underline{q}_j\}$

This is because (recall $A=A^T$)

$$\underline{q}_i^T A\underline{q}_j = (A\underline{q}_i)^T \underline{q}_j = (b_{i-1}\underline{q}_{i-1} + a_i\underline{q}_i + b_i\underline{q}_{i+1})^T \underline{q}_j = 0$$

$$\forall\ i = 1, 2,\ \dots,\ j-2$$

For $i \le j-2$, we have

$$\underline{q}_i^T A\underline{q}_j = (A\underline{q}_i)^T \underline{q}_j = (b_{i-1}\underline{q}_{i-1} + A\underline{q}_i + b_i\underline{q}_{i+1})^T \underline{q}_j = 0$$

From $A\underline{q}_j = +b_j\underline{q}_{j+1} + a_j\underline{q}_j + b_{j-1}\underline{q}_{j-1}$

Since $\underline{q}_i^T A\underline{q}_j = 0 \quad \forall\ i \le j-2,$ we have $\underline{q}_i^T \underline{q}_{j+1} = 0$

$\Rightarrow\ \underline{q}_{j+1}$ is $\perp^r$ to all the previous $\{\underline{q}_i\}$

Lanczos Iteration

- So, the Lanczos vectors $\{\underline{q}_j\}$ are such that
  1) Each $\underline{q}_{j+1}$ is $\perp^{r}$ to $\{\underline{q}_1, \underline{q}_2, \ldots, \underline{q}_j\}$
  2) Each $\underline{q}_{j+1}$ is a combination of $\{\underline{q}_1, A\underline{q}_1, \ldots, A^j\underline{q}_1\}$
  3) Each $\underline{q}_{j+1}$ is orthogonal to all combinations of $\{\underline{q}_1\ A\underline{q}_1 \ldots A^{j-1}\underline{q}_1\}$
- Lanczos iteration to find the vectors $\{q_j\}$:

$$j = 0;\ \underline{q}_0 = \underline{0};\ b_0 = 1$$

$$\underline{r}_0 = \underline{q}_1;\ \underline{q}_{j+1} = \underline{r}_j / b_j;\ j = j+1$$

$$a_j = \underline{q}_j A \underline{q}_j;\ \underline{r}_j = (A - a_j I)\underline{q}_j - b_{j-1}\underline{q}_{j-1};\ b_j = \|\underline{r}_j\|$$

  - Requires $O(cn + 4)$ operations where c = # of non-zero elements per row
  - Prone to round off errors … Need to do selective re-orthogonalization of r_j against previous Lanczos vectors.
  - Find Eigen values of the tridiagonal matrix by symmetric QR
- Relationship with the conjugate gradient method
  - Residuals $\{r_j = b - A\,x_j\}$, where x_j is the solution at iteration j of conjugate gradient method, are multiples of the Lanczos vectors $\{q_j\}$

Summary

- House holder method to convert a *symmetric matrix to tridiagonal form*
- Lanczos method for sparse symmetric matrices
  - Relationship with the conjugate gradient (CG) method
- A variety of algorithms exist for finding the Eigen values and Eigen vectors of a symmetric matrix
  - Symmetric QR
  - Jacobi method
  - Bisection method (using Sturm sequence property)
  - Power method
  - Lanczos method (for sparse symmetric matrices)
- However, symmetric QR is the best general purpose algorithm
  - Unless only a few Eigen values/Eigen vectors are desired
  - In the latter case, specialized methods may be useful (see Golub and Van Loan, 1989)