The Symmetric QR Iteration – in brief

FACT: (Symmetric Schur Decomp): If $A \in \mathbb{R}^{n\times n}$ is symmetric then $\exists$ a real orthogonal Q s.t.

$$Q^T A Q = \begin{bmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{bmatrix}$$

Moreover, for $k=1:n$, $AQ(:,k) = \lambda_k Q(:,k)$

Orthogonal Iteration:

$$\left|\begin{array}{l} \text{for } k=1,2\dots \\ \quad Z_k = AQ_{k-1} \\ \quad Q_k R_k = Z_k \\ \text{end} \end{array}\right| \quad Q_0 \in \mathbb{R}^{n\times r}$$

$Q^T A Q = D = \mathrm{diag}(\lambda_i)$

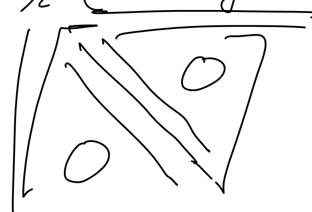
Assume $|\lambda_1| \geq |\lambda_2| \geq \dots \geq |\lambda_n|$, $Q = [\underset{r}{Q_\alpha} \mid \underset{n-r}{Q_\beta}]$, $D = \left[\begin{array}{c|c} D_1 & 0 \\ \hline 0 & D_2 \end{array}\right]$

FACT: If $|\lambda_r| > |\lambda_{r+1}|$,
and if $d_k := \mathrm{dist}(D_r(A), \mathcal{R}(Q_k))$ $k>0$
& if $d_0 < 1$, then the Q_k's satisfy:

$$d_k \leq \left|\frac{\lambda_{r+1}}{\lambda_r}\right|^k \frac{d_0}{\sqrt{1-d_0^2}}$$

Symmetric QR Iteration

If $A = A^T$ then $\exists Q$ s.t. $Q^T A Q = T_r$ (tri-diagonal)



$$A = \begin{bmatrix} a_{11} & b^T \\ b & \hat{A} \end{bmatrix} \quad Q_1 = \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & \hat{Q}_1 \end{array}\right]$$

$$A_1 = Q_1 A Q_1 = \left[\begin{array}{c|c} a_{11} & \tau_1\ 0 \cdots 0 \\ \hline \tau_1 & \\ 0 & \hat{Q}_1 \hat{A} \hat{Q}_1 \\ \vdots & \\ 0 & \end{array}\right]$$

s.t. $\hat{Q}_1 b = \begin{bmatrix} \tau_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$ (Householder reflection)

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Implicit Q Theorem is clearly valid. ("Upper Hessenberg" replaced by "tri-diagonal")

Preservation of Form: If $T = QR$
Hence $T^+ = RQ = Q^TQRQ = Q^TTQ$ is also symmetric $\Rightarrow$ tri-diagonal

Shifts: If $s \in \mathbb{R}$, $T - sI = QR$ (factorization)
then $T_+ = RQ + sI = Q^TTQ$ is symmetric → hence tri-diagonal

Cost: The QR fact. costs $O(n)$ flops (from $n-1$ Given rotation)

Implicit Shift QR works more efficiently: $\frac{4n^3}{3}$ flops without Q & $9n^3$ with Q.
(Recall the Unsymmetric QR took $10n^3$ without Q & $25n^3$ with Q)

Special Real Shift: (Wilkinson Shift)

If $T = \begin{bmatrix} a_1 & b_1 & & 0 \\ b_1 & a_2 & \ddots & \\ & \ddots & \ddots & b_{n-1} \\ 0 & & b_{n-1} & a_n \end{bmatrix}$ usual choice of shift $\stackrel{?}{=} \mu = a_n$

Instead consider $\begin{bmatrix} a_{n-1} & b_{n-1} \\ b_{n-1} & a_n \end{bmatrix} \xrightarrow{\text{eigenvalues}} (\lambda - a_{n-1})(\lambda - a_n) - b_{n-1}^2$

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

$$\lambda_{1,2} = a_n + \underbrace{\frac{(a_{n-1} - a_n)}{2}}_{d} \pm \sqrt{\left(\frac{a_{n-1} - a_n}{2}\right)^2 + b_{n-1}^2}$$

Choose the eig. value closer to a_n

$\Rightarrow$ shift $\mu = a_n + d - \text{sign}(d)\sqrt{d^2 + b_{n-1}^2}$

<u>Implicit shift</u>: We can implement the QR iteration steps with shift implicitly:

\# Normally: $QR = T - \mu I$; $T_+ = RQ + \mu I = Q^T T Q$

\# Instead compute c, s s.t.

$$\begin{bmatrix} c & s \\ -s & c \end{bmatrix}^T \begin{bmatrix} a_1 - \mu \\ b_1 \end{bmatrix} = \begin{bmatrix} * \\ 0 \end{bmatrix}$$

Let $G_1 = \left[\begin{array}{cc|ccc} c & s & & 0 & \\ -s & c & & & \\ \hline & & 1 & & \\ & 0 & & \ddots & \\ & & & & 1 \end{array}\right]$. Then as before, $G_1 e_1 = Q e_1$

and $G_1^T T G_1 = \begin{bmatrix} \times & \times & + & 0 & 0 & \cdots \\ \times & \times & \times & 0 & 0 & \\ + & \times & \times & \times & 0 & \cdots \\ 0 & 0 & \times & \times & \times & \cdots \\ 0 & 0 & 0 & \times & \times & \times \\ & & & \times & \times & \times \\ - & - & - & & \times & \times \end{bmatrix}$ bulge

Tri-diagonal

\# Chase the bulge out with Givens rotations $G_2 \cdots G_{n-1}$

Then $Z = G_1 G_2 \cdots G_{n-1}$ will satisfy

i) $Ze_1 = G_1 e_1 = Q e_1$

and $Z^T T Z$ is tri-diagonal

<u>Symmetric QR Algo</u>: Given $A \in \mathbb{R}^{n \times n}$ symmetric we compute the Schur decomposition

$$D = Q^T A Q$$

Step 1: Tri-diagonalize A i.e. compute reflections $P_1 \cdots P_{n-2}$ s.t.

$$D = (P_1 \cdots P_{n-2})^T A (P_1 \cdots P_{n-2}) \text{ is}$$

tri-diagonal.

while $q \leq n$

$i = 1 : n-1$, set $d_{i+1,i}$ & $d_{i,i+1}$ to zero

if $|d_{i+1,i}| = |d_{i,i+1}| \leq tol.(|d_{ii}| + |d_{i+1,i+1}|)$

Find largest q & smallest p s.t.

$$D = \begin{array}{cc} \begin{bmatrix} D_{11} & 0 & 0 \\ 0 & D_{22} & 0 \\ 0 & 0 & D_{33} \end{bmatrix} & \begin{array}{l} \} p \\ \} n-p-q \\ \} q \end{array} \\ \begin{array}{ccc} \underbrace{\quad}_{p} & \underbrace{\quad}_{n-p-q} & \underbrace{\quad}_{q} \end{array} & \end{array}$$

where D_{33} is diagonal

D_{22} is unreduced

if $q < n$

apply Wilkinson shift implicitly on D_{22}.

end

end

Computing the SVD : $A \in \mathbb{R}^{m \times n}$ $(m \geq n)$

Let $S_1 = A^T A$, $S_2 = AA^T$, $S_3 = \begin{bmatrix} 0 & A^T \\ A & 0 \end{bmatrix}$

If $U^T A V = \underbrace{\mathrm{diag}(\sigma_1, \cdots, \sigma_n)}_{\Sigma} = \begin{bmatrix} \sigma_1 \cdots \sigma_n \\ \hline 0 \end{bmatrix}_{m \times n}$, then

$A = U \Sigma V^T$

1) $V^T(A^T A) V = V^T \left[(V \Sigma^T U^T)(U \Sigma V^T) \right] V = \Sigma^T \Sigma = \begin{bmatrix} \sigma_1^2 & & 0 \\ & \ddots & \\ 0 & & \sigma_n^2 \end{bmatrix}_{n \times n}$

2) $U^T(AA^T)U = \begin{array}{cc} \left[\begin{array}{c|c} \begin{matrix} \sigma_1^2 & & 0 \\ & \ddots & \\ 0 & & \sigma_n^2 \end{matrix} & 0 \\ \hline 0 & \begin{matrix} 0 & & \\ & \ddots & \\ & & 0 \end{matrix} \end{array} \right] & \begin{array}{l} n \\ m-n \end{array} \end{array} \in \mathbb{R}^{m \times m}$

3) If $U = [\underbrace{U_1}_{n} \mid \underbrace{U_2}_{m-n}]$, and $Q := \frac{1}{\sqrt{2}}\begin{bmatrix} V & V & 0 \\ U_1 & -U_1 & \sqrt{2}U_2 \end{bmatrix}$

then $$Q^T \begin{bmatrix} 0 & A^T \\ A & 0 \end{bmatrix} Q = \frac{1}{\sqrt{2}} \underbrace{\begin{bmatrix} V^T & U_1^T \\ V^T & -U_1^T \\ 0 & \sqrt{2}U_2^T \end{bmatrix}}_{[2n+(m-n)] \times [n+m]} \underbrace{\begin{array}{c|cc} & n & m \\ \hline n & 0 & A^T \\ m & A & 0 \end{array}}_{(m+n) \times (m+n)} \underbrace{\begin{bmatrix} V & V & 0 \\ U_1 & -U_1 & \sqrt{2}U_2 \end{bmatrix}}_{(n+m) \times (n+m)} \frac{1}{\sqrt{2}}$$

$$= \begin{array}{c|l} \left[\begin{array}{c|c|c} \begin{matrix} \sigma_1 & & 0 \\ & \ddots & \\ 0 & & \sigma_n \end{matrix} & 0 & 0 \\ \hline 0 & \begin{matrix} -\sigma_1 & & 0 \\ & \ddots & \\ 0 & & -\sigma_n \end{matrix} & \\ \hline 0 & 0 & \underbrace{0}_{m-n} \end{array}\right] & \begin{matrix} \}\, n \\ \\ \}\, n \\ \\ \}\, m-n \end{matrix} \end{array}$$

InDirect Method (not used in Practice):

Compute the eigenvalues + eigenvectors of AA^T & A^TA OR $\begin{bmatrix} 0 & A^T \\ A & 0 \end{bmatrix}$

Loss of Information through squaring

Say $A = U\begin{bmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & \underbrace{10^{-3}}_{\text{should be computable}} \end{bmatrix}V^T$ $\quad A^TA = V\begin{bmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & \underbrace{10^{-6}}_{\text{might be too low} \approx \text{errors.}} \end{bmatrix}V^T$

Hence indirect computation through explicit A^TA / AA^T computation is avoided.

Direct Comp of SVD

<u>Orthogonally Equivalent</u>: If $\exists$ orthogonal $P \in \mathbb{R}^{m\times m}$ & $Q \in \mathbb{R}^{n\times n}$ s.t.

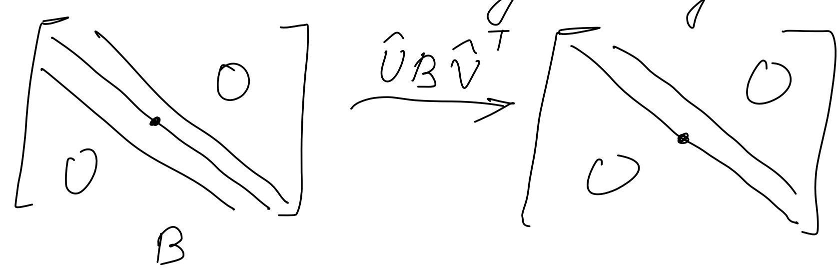
$$\underset{m\times n}{B} = \underset{m\times m}{P}\,\underset{m\times n}{A}\,\underset{n\times n}{Q}$$

then A and B are orthogonally equivalent.

$\Rightarrow$ If $A = U\Sigma V^T$ then

$$\left.\begin{aligned} B &= PU\Sigma V^T Q \\ &= \hat{U}\Sigma\hat{V}^T \end{aligned}\right\} \Rightarrow A \text{ \& } B \text{ have same singular values.}$$

<u>Step 1</u>: Reduction to Bi-diagonal form



<u>Thm</u>: Let $A \in \mathbb{R}^{m\times n}$ with $m \geq n$. Then $\exists$ orthogonal $\hat{U} \in \mathbb{R}^{m\times m}$ & $\hat{V} \in \mathbb{R}^{n\times n}$ s.t.

$$B = \hat{U}^T A \hat{V} \quad \text{is bi-diagonal}$$

Moreover $\hat{U}$ & $\hat{V}$ are products of <u>finite</u> no of reflectors.

<u>Proof</u>: (Golub-Kahan Algo - Step 1)

1) $$\underset{m\times m \text{ reflector}}{\hat{U}_1} \overbrace{\begin{bmatrix} a_{11} & \\ \vdots & \\ a_{m1} & \end{bmatrix}}^{A} = \left[\begin{array}{c|c} \hat{a}_{11} & \hat{a}_{12} \cdots \hat{a}_{1n} \\ \hline 0 & \\ \vdots & * \\ 0 & \end{array}\right]$$

2) Consider $\bar{V}_1$ be a reflector s.t.

$$[\hat{a}_{12} \cdots \hat{a}_{1n}]\,\underset{(n-1)\times(n-1)}{\bar{V}_1} = [\ast\ 0 \cdots 0]$$

& create $\hat{V}_1 = \left[\begin{array}{c|c} 1 & 0 \cdots 0 \cdots 0 \\ \hline 0 & \\ 0 & \bar{V}_1 \\ 0 & \end{array}\right] \in \mathbb{R}^{n\times n}$

3) Then $\hat{U}_1 A \hat{V}_1 = \left[\begin{array}{c|c} \ast & \ast\ 0 \cdots 0 \\ \hline 0 & \\ \vdots & \hat{A} \\ 0 & \end{array}\right]$

$$\left. n \right\{ \left[\begin{array}{c|c} \ast & \overbrace{\ast \cdots \ast}^{n-1} \\ \hline 0 & \\ \vdots & \\ 0 & \end{array}\right] \left[\begin{array}{c|c} 1 & 0 \cdots 0 \\ \hline 0 & \\ \vdots & \underbrace{\bar{V}_1}_{n-1} \\ 0 & \end{array}\right]\Big\}{n-1} = \left[\begin{array}{c|c} \ast & \ast\ 0 \cdots 0 \\ \hline 0 & \\ 0 & \ast \\ \vdots & \\ 0 & \end{array}\right]$$

Recursing similarly:

$$\hat{U}_n \cdots \hat{U}_1 A \hat{V}_1 \hat{V}_2 \cdots \hat{V}_{n-2} = \begin{bmatrix} \boxed{\ast} & \ast & 0 & 0 & 0 \\ 0 & \ast & \ast & 0 & 0 \\ & 0 & \ast & \ast & 0 \\ & & 0 & \ast & \ast \\ & 0 & & 0 & \ast \\ & & & & 0 \end{bmatrix} \to \text{Upper Bi-diagonal} = B$$

<u>Result of Step 1:</u>

$$\hat{U} A \hat{V} = \begin{bmatrix} B \\ 0 \end{bmatrix} = \left[\begin{array}{cccc} d_1 & f_1 & & 0 \\ & \ddots & \ddots & \\ & 0 & \ddots & f_{n-1} \\ & & & d_n \\ \hline & & 0 & \end{array}\right] \quad B \in \mathbb{R}^{n\times n}$$

$\hookrightarrow$ upper bi-diagonal

<u>Step 2</u>: Apply the implicit-shift QR to the tri-diagonal matrix $T = B^T B$

[check $B^T B$ is tri-diagonal — Exercise)

Naive way (not done in practice)

1) Compute $T = B^T B$

$$T(n-1:n, n-1:n) = \begin{bmatrix} d_{n-1}^2 + f_{n-2}^2 & d_{n-1} f_{n-1} \\ d_{n-1} f_{n-1} & d_n^2 + f_{n-1}^2 \end{bmatrix}$$

Compute Wilkinson shift. $\to \mu$ (eig. value closer to $d_n^2 + f_{n-1}^2$)

2) Compute c_1, s_1 s.t

$$\begin{bmatrix} c_1 & s_1 \\ -s_1 & c_1 \end{bmatrix}^T \begin{bmatrix} d_1^2 - \lambda \\ d_1 f_1 \end{bmatrix} = \begin{bmatrix} x \\ 0 \end{bmatrix}$$

Set $G_1 = \left[\begin{array}{cc|ccc} c_1 & s_1 & & 0 & \\ -s_1 & c_1 & & & \\ \hline & & 1 & & 0 \\ & 0 & & \ddots & \\ & & 0 & & 1 \end{array}\right]$

If $QR = T - \lambda I$
$T^+ = RQ + \lambda I$
Then $T^+ = Q^T T Q$

$\Downarrow$ then

$G_1 e_1 = Q e_1$

3) Compute Givens rotation to chase the (tri-diagonal bulge) in $G_1^T T G_1$

Result:

$[G_1 \cdots G_{n-1}]^T B^T B [G_1 \cdots G_{n-1}]$ is tri-diagonal

Step 3: $\to$ Repeat step 2 until convergence
$\to$ then deflate
$\to$ then repeat on smaller matrices

To prevent loss of information through squaring we do not explicitly compute $T = B^T B$

<u>Instead</u> (Practical Method - Golub-Kahan step 2)

1) Apply G_1 to B directly

$$BG_1 = \begin{bmatrix} d_1 & f_1 & 0 & & \\ 0 & d_2 & f_2 & 0 & \\ 0 & & \ddots & \ddots & \\ \vdots & & & \ddots & f_{n-1} \\ 0 & & 0 & & d_n \end{bmatrix} \left[\begin{array}{cc|ccc} c_1 & s_1 & & 0 & \\ -s_1 & c_1 & & & \\ \hline & & 1 & & \\ & 0 & & \ddots & \\ & & & & 1 \end{array}\right]$$

bulge

$$= \begin{bmatrix} \times & \times & 0 & & 0 \\ + & \times & \times & 0 & \\ & & \times & \times & \\ & & & \times & \ddots \\ & 0 & & & \ddots \end{bmatrix}$$

bi-diagonal

2) Compute Givens rotations $U_1, V_2, U_2, \dots, V_{n-1}$ & U_{n-1} to chase the bulge down the diagonal

$$\underbrace{\left[\begin{array}{cc|c} c_2 & s_2 & \\ -s_2 & c_2 & \\ \hline & & \\ \end{array}\right]}_{U_1^T} \underbrace{\begin{bmatrix} \times & \times & 0 & \\ + & \times & \times & \\ & & \times & \ddots \\ & & & \ddots \end{bmatrix}}_{BG_1} = \begin{bmatrix} \times & \times & + & \\ 0 & \times & \times & \\ & & \times & \ddots \\ & & & \ddots \end{bmatrix}$$

$$\begin{bmatrix} \times & \times & + & \\ 0 & \times & \times & \\ 0 & & \times & \ddots \\ & & & \ddots \end{bmatrix} \left[\begin{array}{c|cc|c} 1 & 0 & 0 & 0 \\ \hline 0 & c_3 & s_3 & \\ 0 & -s_3 & c_3 & 0 \\ \hline 0 & 0 & & 1 \quad \ddots \quad 1 \end{array}\right] = \begin{bmatrix} \times & \times & 0 & \\ 0 & \times & \times & \\ & + & \times & \ddots \\ & & 0 & \ddots \end{bmatrix}$$

$$\tilde{B} = [U_{n-1}^T \cdots U_1^T]\, B\, [G_1, V_2 \cdots V_{n-1}]$$

$$= \tilde{U}^T B \tilde{V}$$

If $QR = \overset{(B^TB)}{T} - \lambda I$

$T^+ = RQ + \lambda I$

Then $T^+ = Q^T T Q$

$\Downarrow$ then

$G_1 e_1 = Q e_1$

$$\Rightarrow \quad \tilde{V} e_1 = G_1 e_1 = Q e_1$$

Also, $\quad \tilde{B}^T \tilde{B} = \tilde{V}^T B^T \tilde{U}\, \tilde{U}^T B \tilde{V} = \tilde{V}^T (B^T B) \tilde{V}$

Hence by implicit Q-theorem, $\tilde{V}$ & Q are essentially same

If $f_i = 0$, $\left[\begin{array}{ccc|cc} \times & \times & & & \\ & \times & \times & 0 & \\ & & \times & 0 & \\ \hline & 0 & & \times & \times \\ & & & & \times \end{array}\right] \to \tilde{B}$ decouples into two smaller subproblems

If $d_i = 0$, use a series of Givens rotations to zero out the entire row

$$\begin{bmatrix} \times & \times & & & & \\ & \times & \times & & 0 & \\ & & 0 & \times & & \\ & 0 & & \times & \times & \\ & & & & \times & \times \\ & & & & & \times \end{bmatrix} \xrightarrow{(3,4)} \begin{bmatrix} \times & \times & & & & \\ & \times & \times & & & \\ 0 & 0 & 0 & 0 & + & 0 \\ & & & \times & \times & 0 \\ & & & & \times & \times \\ & & & & & \times \end{bmatrix}$$

$$\Big\downarrow (3,5)$$

$$\begin{bmatrix} \times & \times & & & & \\ & \times & \times & & & \\ 0 & 0 & 0 & 0 & 0 & 0 \\ & & & \times & \times & 0 \\ & & & & \times & \times \\ & & & & & \times \end{bmatrix} \xleftarrow{(3,6)} \begin{bmatrix} \times & \times & & & & \\ & \times & \times & & & \\ 0 & 0 & 0 & 0 & 0 & + \\ & & & \times & \times & 0 \\ & & & & \times & \times \\ & & & & & \times \end{bmatrix}$$

SVD Algo: Given $A \in \mathbb{R}^{m \times n}$

Step 1: Compute the bi-diagonalization:

$$\begin{bmatrix} B \\ 0 \end{bmatrix} = (U_1 \cdots U_n)^T A (V_1 \cdots V_{n-2})$$

while $q < n$

For $i = 1:n-1$ set $b_{i,i+1} = 0$

if $|b_{i,i+1}| < tol(|b_{ii}| + |b_{i+1,i+1}|)$

Find largest q and smallest p s.t.

$$B = \begin{array}{cc} \begin{bmatrix} B_{11} & 0 & 0 \\ 0 & B_{22} & 0 \\ 0 & 0 & B_{33} \end{bmatrix} & \begin{array}{c} p \\ n-p-q \\ q \end{array} \\ \begin{array}{ccc} p & n-p-q & q \end{array} & \end{array}$$

then B_{33} is diagonal & B_{22} is bi-diagonal with a non-zero super-diagonal

if $q < n$

if ~~if~~ any diagonal entry is zero in B_{22} then zero the super-diagonal entry in same row

else

apply the Golub-Kahan step 2 to B_{22}

$$\overline{B_{22}} = U^T B_{22} V$$

end

end

End