The QR algorithm

➤ The most common method for solving small (dense) eigenvalue problems. The basic algorithm:

QR without shifts

1. Until Convergence Do:
2. Compute the QR factorization $A = QR$
3. Set $A := RQ$
4. EndDo

➤ "Until Convergence" means "Until A becomes close enough to an upper triangular matrix"

- Note: $A_{new} = RQ = Q^H(QR)Q = Q^H AQ$
- A_{new} is similar to A throughout the algorithm .
- Convergence analysis complicated – but insight: we are implicitly doing a QR factorization of A^k:

	QR-Factorize:	Multiply backward:	
Step 1	$A_0 = Q_0 R_0$	$A_1 = R_0 Q_0$	
Step 2	$A_1 = Q_1 R_1$	$A_2 = R_1 Q_1$	
Step 3:	$A_2 = Q_2 R_2$	$A_3 = R_2 Q_2$	Then:

$$\begin{aligned}[Q_0 Q_1 Q_2][R_2 R_1 R_0] &= Q_0 Q_1 A_2 R_1 R_0 \\ &= Q_0 Q_1 R_1 Q_1 R_1 R_0 \\ &= \underbrace{(Q_0 R_0)}_{A} \underbrace{(Q_0 R_0)}_{A} \underbrace{(Q_0 R_0)}_{A} = A^3\end{aligned}$$

- $[Q_0 Q_1 Q_2][R_2 R_1 R_0] ==$ QR factorization of A^3

➤ Above basic algorithm is never used as is in practice. Two variations:

(1) Use shift of origin and

(2) Start by transforming A into an Hessenberg matrix

Practical QR algorithms: Shifts of origin

Observation: (from theory): Last row converges fastest. Convergence is dictated by $\frac{|\lambda_n|}{|\lambda_{n-1}|}$

$\boxed{\text{➤ We will now consider only the real symmetric case.}}$

➤ Eigenvalues are real.

➤ $A^{(k)}$ remains symmetric throughout process.

➤ As k goes to infinity the last column and row (except $a_{nn}^{(k)}$) converge to zero quickly.,,

➤ and $a_{nn}^{(k)}$ converges to lowest eigenvalue.

$$A^{(k)} = \left(\begin{array}{ccccc|c} . & . & . & . & . & a \\ . & . & . & . & . & a \\ . & . & . & . & . & a \\ . & . & . & . & . & a \\ . & . & . & . & . & a \\ \hline a & a & a & a & a & a \end{array}\right)$$

➤ Idea: Apply QR algorithm to $A^{(k)} - \mu I$ with $\mu = a_{nn}^{(k)}$. Note: eigenvalues of $A^{(k)} - \mu I$ are shifted by μ, and eigenvectors are the same.

QR with shifts

1. Until row $a_{in}, 1 \le i < n$ converges to zero DO:
2. Obtain next shift (e.g. $\mu = a_{nn}$)
3. $A - \mu I = QR$
5. Set $A := RQ + \mu I$
6. EndDo

➤ Convergence (of last row) is cubic at the limit! [for symmetric case]

- Result of algorithm:

$$\boldsymbol{A}^{(k)} = \left(\begin{array}{ccccc|c} . & . & . & . & . & \mathbf{0} \\ . & . & . & . & . & \mathbf{0} \\ . & . & . & . & . & \mathbf{0} \\ . & . & . & . & . & \mathbf{0} \\ . & . & . & . & . & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \boldsymbol{\lambda}_n \end{array}\right)$$

- Next step: deflate, i.e., apply above algorithm to $(\boldsymbol{n}-\mathbf{1}) \times (\boldsymbol{n}-\mathbf{1})$ upper triangular matrix.

Practical algorithm: Use the Hessenberg Form

Recall: Upper Hessenberg matrix is such that

$$a_{ij} = 0 \text{ for } j < i - 1$$

<u>Observation:</u> The QR algorithm preserves Hessenberg form (tridiagonal form in symmetric case). Results in substantial savings.

Transformation to Hessenberg form

$$\begin{pmatrix} \star & \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star & \star \\ \mathbf{0} & \star & \star & \star & \star & \star \\ \mathbf{0} & \star & \star & \star & \star & \star \\ \mathbf{0} & \star & \star & \star & \star & \star \\ \mathbf{0} & \star & \star & \star & \star & \star \end{pmatrix}$$

- Want $H_1 A H_1^T = H_1 A H_1$ to have the form shown on the right

- Consider the first step only on a 6×6 matrix

➤ Choose a w in $H_1 = I - 2ww^T$ to make the first column have zeros from position 3 to n. So $w_1 = 0$.

➤ Apply to left: $B = H_1 A$

➤ Apply to right: $A_1 = BH_1$.

Main observation: the Householder matrix H_1 which transforms the column $A(2:n,1)$ into e_1 works only on rows 2 to n. When applying the transpose H_1 to the right of $B = H_1 A$, we observe that only columns 2 to n will be altered. So the first column will retain the desired pattern (zeros below row 2).

➤ Algorithm continues the same way for columns 2, ...,$n-2$.

QR for Hessenberg matrices

➤ Need the "Implicit Q theorem"

Suppose that Q^TAQ is an unreduced upper Hessenberg matrix. Then columns 2 to n of Q are determined uniquely (up to signs) by the first column of Q.

➤ In other words if $V^TAV = G$ and $Q^TAQ = H$ are both Hessenberg and $V(:,1) = Q(:,1)$ then $V(:,i) = \pm Q(:,i)$ for $i = 2:n$.

Implication: To compute $A_{i+1} = Q_i^TAQ_i$ we can:

➤ Compute 1st column of Q_i [== scalar $\times A(:,1)$]

➤ Choose other columns so Q_i = unitary, and A_{i+1} = Hessenberg.

➤ Wll do this with Givens rotations

$$A = \begin{pmatrix} * & * & * & * & * \\ * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & 0 & * & * & * \\ 0 & 0 & 0 & * & * \end{pmatrix}$$

Example: With $n = 6$:

1. Choose $G_1 = G(1, 2, \theta_1)$ *so that* $(G_1^T A_0)_{21} = 0$

➤ $$A_1 = G_1^T A G_1 = \begin{pmatrix} * & * & * & * & * \\ * & * & * & * & * \\ + & * & * & * & * \\ 0 & 0 & * & * & * \\ 0 & 0 & 0 & * & * \end{pmatrix}$$

2. Choose $G_2 = G(2, 3, \theta_2)$ *so that* $(G_2^T A_1)_{31} = 0$

➤ $A_2 = G_2^T A_1 G_2 = \begin{pmatrix} * & * & * & * & * \\ * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & + & * & * & * \\ 0 & 0 & 0 & * & * \end{pmatrix}$

3. Choose $G_3 = G(3, 4, \theta_3)$ *so that* $(G_3^T A_2)_{42} = 0$

➤ $A_3 = G_3^T A_2 G_3 = \begin{pmatrix} * & * & * & * & * \\ * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & 0 & * & * & * \\ 0 & 0 & + & * & * \end{pmatrix}$

4. Choose $G_4 = G(4, 5, \theta_4)$ *so that* $(G_4^T A_3)_{53} = 0$

- $A_4 = G_4^T A_3 G_4 = \begin{pmatrix} * & * & * & * & * \\ * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & 0 & * & * & * \\ 0 & 0 & 0 & * & * \end{pmatrix}$

- Process known as “Bulge chasing”
- Similar idea for the symmetric (tridiagonal) case

The symmetric eigenvalue problem: Basic facts

➤ Consider the Schur form of a real symmetric matrix $\boldsymbol{A}$:

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

Since $\boldsymbol{A}^H = \boldsymbol{A}$ then $\boldsymbol{R} = \boldsymbol{R}^H$ ➤

Eigenvalues of $\boldsymbol{A}$ are real

and

There is an orthonormal basis of eigenvectors of $\boldsymbol{A}$

In addition, $\boldsymbol{Q}$ can be taken to be real when $\boldsymbol{A}$ is real.

$$(\boldsymbol{A} - \boldsymbol{\lambda}\boldsymbol{I})(\boldsymbol{u} + i\boldsymbol{v}) = 0 \rightarrow (\boldsymbol{A} - \boldsymbol{\lambda}\boldsymbol{I})\boldsymbol{u} = 0 \;\&\; (\boldsymbol{A} - \boldsymbol{\lambda}\boldsymbol{I})\boldsymbol{v} = 0$$

➤ Can select eigenvector to be either $\boldsymbol{u}$ or $\boldsymbol{v}$

The min-max theorem (Courant-Fischer)

Label eigenvalues decreasingly:

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$$

The eigenvalues of a Hermitian matrix A are characterized by the relation

$$\lambda_k = \max_{S,\ \dim(S)=k} \quad \min_{x \in S, x \neq 0} \frac{(Ax, x)}{(x, x)}$$

Proof: Preparation: Since A is symmetric real (or Hermitian complex) there is an orthonormal basis of eigenvectors $u_1, u_2, \cdots, u_n$. Express any vector x in this basis as $x = \sum_{i=1}^{n} \alpha_i u_i$. Then : $(Ax, x)/(x, x) = [\sum \lambda_i |\alpha_i|^2]/[\sum |\alpha_i|^2]$.

(a) Let S be any subspace of dimension k and let $\mathcal{W} = \mathrm{span}\{u_k, u_{k+1}, \cdots, u_n\}$. A dimension argument (used before) shows that $S \cap \mathcal{W} \neq \{0\}$. So there is a non-zero x_w in $S \cap \mathcal{W}$. Express this x_w in the eigenbasis as $x_w = \sum_{i=k}^{n} \alpha_i u_i$. Then since $\lambda_i \le \lambda_k$ for $i \ge k$ we have:

$$\frac{(Ax_w, x_w)}{(x_w, x_w)} = \frac{\sum_{i=k}^{n} \lambda_i |\alpha_i|^2}{\sum_{i=k}^{n} |\alpha_i|^2} \le \lambda_k$$

So for any subspace S of dim. k we have $\min_{x \in S, x \ne 0} (Ax, x)/(x, x) \le \lambda_k$.

(b) We now take $S_* = \mathrm{span}\{u_1, u_2, \cdots, u_k\}$. Since $\lambda_i \ge \lambda_k$ for $i \le k$, for this particular subspace we have:

$$\min_{x\,\in\,S_*,\ x \ne 0} \frac{(Ax, x)}{(x, x)} = \min_{x\,\in\,S_*,\ x \ne 0} \frac{\sum_{i=1}^{k} \lambda_i |\alpha_i|^2}{\sum_{i=k}^{n} |\alpha_i|^2} = \lambda_k.$$

(c) The results of (a) and (b) imply that the max over all subspaces S of dim. k of $\min_{x \in S, x \ne 0} (Ax, x)/(x, x)$ is equal to λ_k $\blacksquare$

➤ Consequences:

$$\lambda_1 = \max_{x \neq 0} \frac{(Ax, x)}{(x, x)} \qquad \lambda_n = \min_{x \neq 0} \frac{(Ax, x)}{(x, x)}$$

➤ Actually 4 versions of the same theorem. 2nd version:

$$\lambda_k = \min_{S,\ \dim(S)=n-k+1} \quad \max_{x \in S, x \neq 0} \frac{(Ax, x)}{(x, x)}$$

➤ Other 2 versions come from ordering eigenvalues increasingly instead of decreasingly.

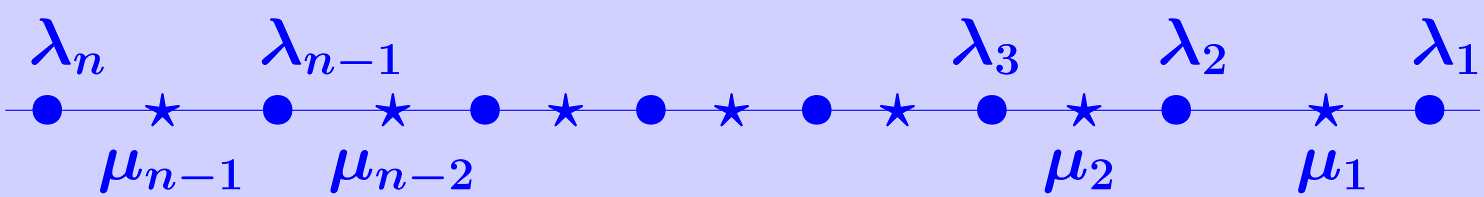
✍ Write down all 4 versions of the theorem

✍ Use the min-max theorem to show that $\|A\|_2 = \sigma_1(A)$ - the largest singular value of A.

➤ Interlacing Theorem: Denote the $k \times k$ principal submatrix of A as A_k, with eigenvalues $\{\lambda_i^{[k]}\}_{i=1}^{k}$. Then

$$\lambda_1^{[k]} \geq \lambda_1^{[k-1]} \geq \lambda_2^{[k]} \geq \lambda_2^{[k-1]} \geq \cdots \lambda_{k-1}^{[k-1]} \geq \lambda_k^{[k]}$$

Example: λ_i's = eigenvalues of A, μ_i's = eigenvalues of A_{n-1}:



➤ Many uses.

➤ For example: interlacing theorem for roots of orthogonal polynomials

The Law of inertia

➤ Inertia of a matrix = [m, z, p] with m = number of < 0 eigenvalues, z = number of zero eigenvalues, and p = number of > 0 eigenvalues.

Sylvester's Law of inertia: If $X \in \mathbb{R}^{n\times n}$ is nonsingular, then A and X^TAX have the same inertia.

✍ Suppose that $A = LDL^T$ where L is unit lower triangular, and D diagonal. How many negative eigenvalues does A have?

✍ Assume that A is tridiagonal. How many operations are required to determine the number of negative eigenvalues of A?

✍ Devise an algorithm based on the inertia theorem to compute the $\boldsymbol{i}$-th eigenvalue of a tridiagonal matrix.

✍ What is the inertia of the matrix

$$\begin{pmatrix} \boldsymbol{I} & \boldsymbol{F} \\ \boldsymbol{F}^T & \boldsymbol{0} \end{pmatrix}$$

where $\boldsymbol{F}$ is $\boldsymbol{m} \times \boldsymbol{n}$, with $\boldsymbol{n} < \boldsymbol{m}$, and of full rank?

[Hint: use a block LU factorization]

Bisection algorithm for tridiagonal matrices:

➤ Goal: to compute i-th eigenvalue of A (tridiagonal)

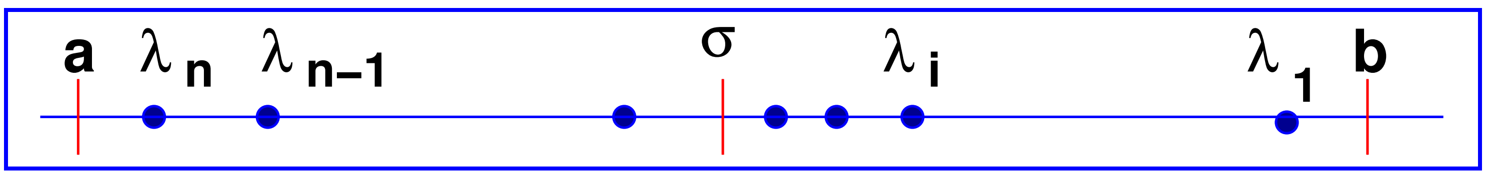
➤ Get interval $[a, b]$ containing spectrum [Gershgorin]:

$$a \le \lambda_n \le \cdots \le \lambda_1 \le b$$

➤ Let $\sigma = (a + b)/2$ = middle of interval

➤ Calculate p = number of positive eigenvalues of $A - \sigma I$

- If $p \ge i$ then $\lambda_i \in (\sigma, b] \rightarrow$ set $a := \sigma$



- Else then $\lambda_i \in [a, \sigma] \rightarrow$ set $b := \sigma$

➤ Repeat until $b - a$ is small enough.

The QR algorithm for symmetric matrices

➤ Most important method used : reduce to tridiagonal form and apply the QR algorithm with shifts.

➤ Householder transformation to Hessenberg form yields a tridiagonal matrix because

$$\boldsymbol{HAH^T = A_1}$$

is symmetric and also of Hessenberg form ➤ it is tridiagonal symmetric.

> Tridiagonal form preserved by QR similarity transformation

Practical method

- How to implement the QR algorithm with shifts?
- It is best to use Givens rotations – can do a shifted QR step without explicitly shifting the matrix..
- Two most popular shifts:

$s = a_{nn}$ and $s =$ smallest e.v. of $A(n-1:n, n-1:n)$

Jacobi iteration - Symmetric matrices

➤ Main idea: Rotation matrices of the form

$$J(p,q,\theta) = \begin{array}{cc} \begin{pmatrix} 1 & \dots & 0 & & \dots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & c & \cdots & s & \cdots & 0 \\ \vdots & \cdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & \cdots & -s & \cdots & c & \cdots & 0 \\ \vdots & \cdots & \vdots & \cdots & \vdots & \cdots & \vdots \\ 0 & \dots & 0 & & \dots & & 1 \end{pmatrix} & \begin{array}{c} \\ \\ p \\ \\ q \\ \\ \\ \end{array} \end{array}$$

$c = \cos\theta$ and $s = \sin\theta$ are so that $J(p,q,\theta)^T A J(p,q,\theta)$ has a zero in position (p,q) (and also (q,p))

➤ Frobenius norm of matrix is preserved – but diagonal elements become larger ➤ convergence to a diagonal.

- Let $B = J^T A J$ (where $J \equiv J_{p,q,\theta}$).
- Look at 2×2 matrix $B([p,q],[p,q])$ (matlab notation)
- Keep in mind that $a_{pq} = a_{qp}$ and $b_{pq} = b_{qp}$

$$\begin{pmatrix} b_{pp} & b_{pq} \\ b_{qp} & b_{qq} \end{pmatrix} = \begin{pmatrix} c & -s \\ s & c \end{pmatrix} \begin{pmatrix} a_{pp} & a_{pq} \\ a_{qp} & a_{qq} \end{pmatrix} \begin{pmatrix} c & s \\ -s & c \end{pmatrix}$$

$$= \begin{pmatrix} c & -s \\ s & c \end{pmatrix} \left[\begin{array}{c|c} ca_{pp} - sa_{pq} & sa_{pp} + ca_{pq} \\ \hline ca_{qp} - sa_{qq} & sa_{pq} + ca_{qq} \end{array} \right]$$

$$= \left[\begin{array}{c|c} c^2 a_{pp} + s^2 a_{qq} - 2sc\, a_{pq} & (c^2 - s^2) a_{pq} - sc(a_{qq} - a_{pp}) \\ \hline * & c^2 a_{qq} + s^2 a_{pp} + 2sc\, a_{pq} \end{array} \right]$$

- Want: $$(c^2 - s^2) a_{pq} - sc(a_{qq} - a_{pp}) = 0$$

$$\frac{c^2 - s^2}{2sc} = \frac{a_{qq} - a_{pp}}{2a_{pq}} \equiv \tau$$

- Letting $t = s/c \; (= \tan\theta)$ $\quad \rightarrow$ quad. equation

$$\boxed{t^2 + 2\tau t - 1 = 0}$$

- $t = -\tau \pm \sqrt{1+\tau^2} = \frac{1}{\tau \pm \sqrt{1+\tau^2}}$
- Select sign to get a smaller t so $\theta \le \pi/4$.
- Then : $\qquad c = \dfrac{1}{\sqrt{1+t^2}}; \qquad s = c * t$
- Implemented in matlab script `jacrot(A,p,q)` – See HW6.

- Define: $\boxed{A_O = A - \text{Diag}(A)}$ $\equiv$ A 'with its diagonal entries replaced by zeros'

- Observations: (1) Unitary transformations preserve $\|.\|_F$. (2) Only changes are in rows and columns p and q.

- Let $B = J^T A J$ (where $J \equiv J_{p,q,\theta}$). Then,

$$\boxed{a_{pp}^2 + a_{qq}^2 + 2a_{pq}^2 = b_{pp}^2 + b_{qq}^2 + 2b_{pq}^2 = b_{pp}^2 + b_{qq}^2}$$

because $b_{pq} = 0$. Then, a little calculation leads to:

$$\begin{aligned}
\|B_O\|_F^2 &= \|B\|_F^2 - \sum b_{ii}^2 = \|A\|_F^2 - \sum b_{ii}^2 \\
&= \|A\|_F^2 - \sum a_{ii}^2 + \sum a_{ii}^2 - \sum b_{ii}^2 \\
&= \|A_O\|_F^2 + (a_{pp}^2 + a_{qq}^2 - b_{pp}^2 - b_{qq}^2) \\
&= \|A_O\|_F^2 - 2a_{pq}^2
\end{aligned}$$

➤ $\|A_O\|_F$ will decrease from one step to the next.

✍ Let $\|A_O\|_I = \max_{i \neq j} |a_{ij}|$. Show that

$$\|A_O\|_F \leq \sqrt{n(n-1)}\|A_O\|_I$$

✍ Use this to show convergence in the case when largest entry is zeroed at each step.