# Outline

# QR Decomposition



Decomposition (or factorization) $\mathbf{A} = \mathbf{QR}$ into two factors, orthogonal $\mathbf{Q}$ and upper-triangular $\mathbf{R}$:

(a) It always exists.
(b) Performing this decomposition is pretty straightforward.
(c) It has a number of properties useful in the solution of the eigenvalue problem.

$$[\mathbf{a}_1 \quad \cdots \quad \mathbf{a}_n] = [\mathbf{q}_1 \quad \cdots \quad \mathbf{q}_n] \begin{bmatrix} r_{11} & \cdots & r_{1n} \\ & \ddots & \vdots \\ & & r_{nn} \end{bmatrix}$$

A simple method based on Gram-Schmidt orthogonalization:
Considering columnwise equality $\mathbf{a}_j = \sum_{i=1}^{j} r_{ij}\mathbf{q}_i$,
for $j = 1, 2, 3, \cdots, n$;

$$r_{ij} = \mathbf{q}_i^T \mathbf{a}_j \quad \forall i < j, \quad \mathbf{a}'_j = \mathbf{a}_j - \sum_{i=1}^{j-1} r_{ij}\mathbf{q}_i, \quad r_{jj} = \|\mathbf{a}'_j\|;$$

$$\mathbf{q}_j = \begin{cases} \mathbf{a}'_j / r_{jj}, & \text{if } r_{jj} \neq 0; \\ \text{any vector satisfying } \mathbf{q}_i^T \mathbf{q}_j = \delta_{ij} \text{ for } 1 \leq i \leq j, & \text{if } r_{jj} = 0. \end{cases}$$

# QR Decomposition



**Practical method:** one-sided Householder transformations, starting with

$$\mathbf{u}_0 = \mathbf{a}_1, \quad \mathbf{v}_0 = \|\mathbf{u}_0\|\mathbf{e}_1 \in R^n \text{ and } \mathbf{w}_0 = \frac{\mathbf{u}_0 - \mathbf{v}_0}{\|\mathbf{u}_0 - \mathbf{v}_0\|}$$

and $\mathbf{P}_0 = \mathbf{H}_n = \mathbf{I}_n - 2\mathbf{w}_0\mathbf{w}_0^T$.

$$\mathbf{P}_{n-2}\mathbf{P}_{n-3}\cdots\mathbf{P}_2\mathbf{P}_1\mathbf{P}_0\mathbf{A} = \mathbf{P}_{n-2}\mathbf{P}_{n-3}\cdots\mathbf{P}_2\mathbf{P}_1\begin{bmatrix} \|\mathbf{a}_1\| & ** \\ \mathbf{0} & \mathbf{A}_0 \end{bmatrix}$$

$$= \mathbf{P}_{n-2}\mathbf{P}_{n-3}\cdots\mathbf{P}_2\begin{bmatrix} r_{11} & * & ** \\ & r_{22} & ** \\ & & \mathbf{A}_1 \end{bmatrix} = \cdots \quad \cdots = \mathbf{R}$$

With

$$\mathbf{Q} = (\mathbf{P}_{n-2}\mathbf{P}_{n-3}\cdots\mathbf{P}_2\mathbf{P}_1\mathbf{P}_0)^T = \mathbf{P}_0\mathbf{P}_1\mathbf{P}_2\cdots\mathbf{P}_{n-3}\mathbf{P}_{n-2},$$

we have $\mathbf{Q}^T\mathbf{A} = \mathbf{R} \Rightarrow \mathbf{A} = \mathbf{QR}$.

# QR Decomposition



**Alternative method useful for tridiagonal and Hessenberg matrices:** One-sided plane rotations

- rotations $\mathbf{P}_{12}$, $\mathbf{P}_{23}$ etc to annihilate $a_{21}$, $a_{32}$ etc in that sequence

Givens rotation matrices!

**Application in solution of a linear system:** $\mathbf{Q}$ and $\mathbf{R}$ factors of a matrix $\mathbf{A}$ come handy in the solution of $\mathbf{Ax} = \mathbf{b}$

$$\mathbf{QRx} = \mathbf{b} \Rightarrow \mathbf{Rx} = \mathbf{Q}^T\mathbf{b}$$

needs only a sequence of back-substitutions.

# QR Iterations



Multiplying **Q** and **R** factors in reverse,

$$\mathbf{A}' = \mathbf{R}\mathbf{Q} = \mathbf{Q}^T\mathbf{A}\mathbf{Q},$$

an orthogonal similarity transformation.

1. If $\mathbf{A}$ is symmetric, then so is $\mathbf{A}'$.
2. If $\mathbf{A}$ is in upper Hessenberg form, then so is $\mathbf{A}'$.
3. If $\mathbf{A}$ is symmetric tridiagonal, then so is $\mathbf{A}'$.

**Complexity of QR iteration:** $\mathcal{O}(n)$ for a symmetric tridiagonal matrix, $\mathcal{O}(n^2)$ operation for an upper Hessenberg matrix and $\mathcal{O}(n^3)$ for the general case.

**Algorithm:** Set $\mathbf{A}_1 = \mathbf{A}$ and for $k = 1, 2, 3, \cdots$,

- decompose $\mathbf{A}_k = \mathbf{Q}_k\mathbf{R}_k$,
- reassemble $\mathbf{A}_{k+1} = \mathbf{R}_k\mathbf{Q}_k$.

As $k \to \infty$, $\mathbf{A}_k$ approaches the *quasi-upper-triangular form*.

# QR Iterations



**Quasi-upper-triangular form:**

$$\begin{bmatrix} \lambda_1 & * & \cdots & * & \star\star & \cdots & * & * \\ & \lambda_2 & \cdots & * & \star\star & \cdots & * & * \\ & & \ddots & * & \star\star & \cdots & * & * \\ & & & \lambda_r & \star\star & \cdots & * & * \\ & & & & \mathbf{B}_k & \cdots & * & * \\ & & & & & \ddots & \vdots & \vdots \\ & & & & & & \multicolumn{2}{c}{\begin{bmatrix} \alpha & -\omega \\ \omega & \beta \end{bmatrix}} \end{bmatrix},$$

with $|\lambda_1| > |\lambda_2| > \cdots$.

- Diagonal blocks $\mathbf{B}_k$ correspond to eigenspaces of equal/close (magnitude) eigenvalues.
- $2 \times 2$ diagonal blocks often correspond to pairs of complex eigenvalues (for non-symmetric matrices).
- For symmetric matrices, the quasi-upper-triangular form reduces to quasi-diagonal form.

# Conceptual Basis of QR Method*



QR decomposition algorithm operates on the basis of the *relative magnitudes* of eigenvalues and segregates subspaces.

With $k \rightarrow \infty$,

$$\mathbf{A}^k Range\{\mathbf{e}_1\} = Range\{\mathbf{q}_1\} \rightarrow Range\{\mathbf{v}_1\}$$

and $(\mathbf{a}_1)_k \rightarrow \mathcal{Q}_k^T \mathbf{A} \mathbf{q}_1 = \lambda_1 \mathcal{Q}_k^T \mathbf{q}_1 = \lambda_1 \mathbf{e}_1$.

Further,

$$\mathbf{A}^k Range\{\mathbf{e}_1, \mathbf{e}_2\} = Range\{\mathbf{q}_1, \mathbf{q}_2\} \rightarrow Range\{\mathbf{v}_1, \mathbf{v}_2\}.$$

and $(\mathbf{a}_2)_k \rightarrow \mathcal{Q}_k^T \mathbf{A} \mathbf{q}_2 = \begin{bmatrix} (\lambda_1 - \lambda_2)\alpha_1 \\ \lambda_2 \\ \mathbf{0} \end{bmatrix}$.

And, so on ...

# QR Algorithm with Shift*



For $\lambda_i < \lambda_j$, entry $a_{ij}$ decays through iterations as $\left(\frac{\lambda_i}{\lambda_j}\right)^k$.

With shift,

$$\begin{aligned}
\bar{\mathbf{A}}_k &= \mathbf{A}_k - \mu_k \mathbf{I};\\
\bar{\mathbf{A}}_k &= \mathbf{Q}_k \mathbf{R}_k, \quad \bar{\mathbf{A}}_{k+1} = \mathbf{R}_k \mathbf{Q}_k;\\
\mathbf{A}_{k+1} &= \bar{\mathbf{A}}_{k+1} + \mu_k \mathbf{I}.
\end{aligned}$$

Resulting transformation is

$$\begin{aligned}
\mathbf{A}_{k+1} &= \mathbf{R}_k \mathbf{Q}_k + \mu_k \mathbf{I} = \mathbf{Q}_k^T \bar{\mathbf{A}}_k \mathbf{Q}_k + \mu_k \mathbf{I}\\
&= \mathbf{Q}_k^T (\mathbf{A}_k - \mu_k \mathbf{I}) \mathbf{Q}_k + \mu_k \mathbf{I} = \mathbf{Q}_k^T \mathbf{A}_k \mathbf{Q}_k.
\end{aligned}$$

For the iteration,

$$\textit{convergence ratio} = \frac{\lambda_i - \mu_k}{\lambda_j - \mu_k}.$$

**Question:** How to find a suitable value for $\mu_k$?

## Points to note



- QR decomposition can be effected on any square matrix.
- Practical methods of QR decomposition use Householder transformations or Givens rotations.
- A QR iteration effects a similarity transformation on a matrix, preserving symmetry, Hessenberg structure and also a symmetric tridiagonal form.
- A sequence of QR iterations converge to an almost upper-triangular form.
- Operations on symmetric tridiagonal and Hessenberg forms are computationally efficient.
- QR iterations tend to order subspaces according to the relative magnitudes of eigenvalues.
- Eigenvalue shifting is useful as an expediting strategy.

Necessary Exercises: **1,3**