

QR factorization of a matrix

QR decomposition

Any real $m \times n$ matrix \mathbf{A} can be decomposed into

$$\mathbf{A} = \mathbf{Q}\mathbf{R}$$

where \mathbf{Q} is an $m \times m$ orthogonal matrix ($\mathbf{Q}^T \mathbf{Q} = \mathbf{I}$) and \mathbf{R} is an $m \times n$ upper triangular matrix.

LOW, a rectangular matrix can be reduced to an upper triangular form by an orthogonal transformation \mathbf{Q}^T

$$\mathbf{Q}^T \mathbf{A} = \mathbf{R}$$

Thin QR factorization

If $m > n$

$$\begin{aligned}\mathbf{A} &= \mathbf{Q} \begin{pmatrix} \mathbf{R}_1 \\ 0 \end{pmatrix} \\ &= (\mathbf{Q}_1 \mathbf{Q}_2) \begin{pmatrix} \mathbf{R}_1 \\ 0 \end{pmatrix} \\ &= \mathbf{Q}_1 \mathbf{R}_1\end{aligned}$$

where \mathbf{R}_1 is $m \times m$ upper triangular, \mathbf{Q}_1 is $m \times n$ and has orthonormal columns.

This is a *thin QR* factorization (or *economic*, or *reduced* factorization).

Thin QR factorization

If \mathbf{A} has full column rank (i.e., columns of \mathbf{A} are all linearly independent), then

- ▶ The thin factorization $\mathbf{A} = \mathbf{Q}_1 \mathbf{R}_1$ is unique
- ▶ Diagonal elements of \mathbf{R}_1 are positive
- ▶ \mathbf{R}_1^T is a lower triangular Cholesky factor of $\mathbf{A}^T \mathbf{A}$

Constructing the QR factorization

- ▶ Householder reflections
- ▶ Givens rotations

Both reduce \mathbf{A} to \mathbf{R} column by column, and construct \mathbf{Q} as a product of orthogonal matrices.

Householder reflections

Householder reflections

Given a vector $\mathbf{x} \in \mathbb{R}^m$, reflect it across a hyperplane with the normal vector \mathbf{u} ($\|\mathbf{u}\|_2 = 1$)

$$\begin{aligned}\mathbf{x} &= \mathbf{x}_{\parallel} + \mathbf{x}_{\perp}, & \mathbf{x}_{\perp} &\perp \mathbf{x}_{\parallel} \\ & & \mathbf{x}_{\perp} &\parallel \mathbf{u}\end{aligned}$$

The perp component is given by $\mathbf{x}_{\perp} = \mathbf{u}\langle \mathbf{u} \cdot \mathbf{x} \rangle$

$$\mathbf{y} = \mathbf{x}_{\parallel} - \mathbf{x}_{\perp} = (\mathbf{x}_{\parallel} + \mathbf{x}_{\perp}) - 2\mathbf{x}_{\perp} = \mathbf{x} - 2\mathbf{u}\langle \mathbf{u} \cdot \mathbf{x} \rangle$$

Householder reflections

In the matrix form, $\langle \mathbf{u} \cdot \mathbf{x} \rangle \equiv \mathbf{u}^T \mathbf{x}$, and the Householder transformation is

$$\mathbf{y} = \mathbf{H}\mathbf{x} = (\mathbf{1} - 2\mathbf{u}\mathbf{u}^T) \mathbf{x}$$

The Householder matrices are

- ▶ Symmetric, $\mathbf{H}^T = \mathbf{H}$
- ▶ Orthogonal, $\mathbf{H}^T \mathbf{H} = \mathbf{1}$

Householder reflections

Given two vectors \mathbf{x} and \mathbf{y} with $\|\mathbf{x}\|_2 = \|\mathbf{y}\|_2$, construct a \mathbf{H} which converts \mathbf{x} to \mathbf{y} .

Reflect \mathbf{x} across the hyperplane which bisects the angle between \mathbf{x} and \mathbf{y} .

The Householder transformation with

$$\mathbf{u} = (\mathbf{x} - \mathbf{y}) / \|\mathbf{x} - \mathbf{y}\|_2$$

Householder reflections

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$$\mathbf{u} = (\mathbf{x} - \mathbf{y}) / \|\mathbf{x} - \mathbf{y}\|_2$$

$$\mathbf{x} = \begin{pmatrix} \times \\ \times \\ \vdots \\ \times \end{pmatrix}$$

$$\mathbf{y} = \begin{pmatrix} \times \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

Householder reflections QR

$$\mathbf{H}_1 \mathbf{A} = \begin{pmatrix} \times & \times & \times & \cdots & \times \\ 0 & \times & \times & \cdots & \times \\ 0 & \times & \times & \cdots & \times \\ & & \cdots & & \\ 0 & \times & \times & \cdots & \times \end{pmatrix}$$

Householder reflections QR

$$\mathbf{H}_1 \mathbf{A} = \begin{pmatrix} \times & \times & \times & \cdots & \times \\ 0 & \times & \times & \cdots & \times \\ 0 & \times & \times & \cdots & \times \\ & & \cdots & & \\ 0 & \times & \times & \cdots & \times \end{pmatrix}$$

$$\mathbf{H}_2 \mathbf{H}_1 \mathbf{A} = \begin{pmatrix} \times & \times & \times & \cdots & \times \\ 0 & \times & \times & \cdots & \times \\ 0 & 0 & \times & \cdots & \times \\ & & \cdots & & \\ 0 & 0 & \times & \cdots & \times \end{pmatrix}$$

Householder reflections QR

After n steps:
so that

$$\mathbf{H}_n \cdots \mathbf{H}_2 \mathbf{H}_1 \mathbf{A} = \mathbf{R}$$

$$\mathbf{A} = \mathbf{Q}\mathbf{R}$$

with

$$\mathbf{Q} = \mathbf{H}_1 \mathbf{H}_2 \cdots \mathbf{H}_n$$

Householder reflections QR

After n steps:
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$$\mathbf{H}_n \cdots \mathbf{H}_2 \mathbf{H}_1 \mathbf{A} = \mathbf{R}$$

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with

$$\mathbf{Q} = \mathbf{H}_1 \mathbf{H}_2 \cdots \mathbf{H}_n$$

Computational complexity strongly depends on the order of calculations.

$$\begin{array}{ll} (\mathbf{u}\mathbf{u}^T) \mathbf{x} & \text{is } O(m^2) \\ \mathbf{u} (\mathbf{u}^T \mathbf{x}) & \text{is } O(m) \end{array}$$

In practice, *never* form the \mathbf{H} matrices explicitly.

Householder reflections: avoiding the roundoff

$$\mathbf{H} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{pmatrix} = \begin{pmatrix} \|\mathbf{x}\|_2 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

involves computing $x_1 - \|\mathbf{x}\|_2$ which is prone to a catastrophic cancellation.

For $x_1 > 0$, write

$$\begin{aligned} x_1 - \|\mathbf{x}\|_2 &= \frac{x_1^2 - \|\mathbf{x}\|_2^2}{x_1 + \|\mathbf{x}\|_2} \\ &= \frac{-x_2^2 - \cdots - x_m^2}{x_1 + \|\mathbf{x}\|_2} \end{aligned}$$

Householder reflections QR

The Householder **QR** algorithm:

- ▶ has excellent stability
- ▶ for square matrices involves only several times more work than **LU**
- ▶ is not easy to parallelize

Givens rotations

Givens rotations

$$\begin{pmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1m} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2m} \\ & & \cdots & & \\ a_{m1} & a_{m2} & a_{m3} & \cdots & a_{mm} \end{pmatrix}$$

Find ϕ such that

$$\begin{pmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{pmatrix} \begin{pmatrix} a_{11} \\ a_{21} \end{pmatrix} = \begin{pmatrix} \times \\ 0 \end{pmatrix}$$

Givens rotations

$$\begin{pmatrix} \cos \phi & 0 & -\sin \phi \\ 0 & 1 & 0 \\ \sin \phi & 0 & \cos \phi \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1m} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2m} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & a_{m3} & \cdots & a_{mm} \end{pmatrix}$$

Find ϕ such that

$$\begin{pmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{pmatrix} \begin{pmatrix} a_{11} \\ a_{31} \end{pmatrix} = \begin{pmatrix} \times \\ 0 \end{pmatrix}$$

QR decomposition via Givens rotations

- ▶ Complexity is $3/2$ of the Householder **QR** algorithm
- ▶ There is flexibility in selecting the order of introducing zeros.