QR factorization of a matrix

QR decomposition

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

$$\mathbf{A} = \mathbf{QR}$$

where $\mathbf{Q}$ is an $m \times m$ orthogonal matrix ($\mathbf{Q}^T\mathbf{Q} = 1$) and $\mathbf{R}$ is an $m \times n$ upper triangular matrix.

IOW, 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 $m > n$

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

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

This is a *thin* $\mathbf{QR}$ 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 $\mathbf{u}$ ($\|\mathbf{u}\|_2 = 1$)

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

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

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

Householder reflections

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

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

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

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

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

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

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

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

Householder reflections QR

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

$$\mathbf{A} = \mathbf{QR}$$

with

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

Householder reflections QR

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Computational complexity strongly depends on the order of calculations.

$$\left(\mathbf{u}\mathbf{u}^T\right)\mathbf{x} \quad \text{is} \quad O(m^2)$$
$$\mathbf{u}\left(\mathbf{u}^T\mathbf{x}\right) \quad \text{is} \quad O(m)$$

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 $\mathbf{QR}$

The Householder $\mathbf{QR}$ algorithm:

- has excellent stability
- for square matrices involves only several times more work than $\mathbf{LU}$
- 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

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

Find ϕ such that

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

$\mathbf{QR}$ decomposition via Givens rotations

- Complexity is $3/2$ of the Householder $\mathbf{QR}$ algorithm
- There is flexibility in selecting the order of introducing zeros.