Dense linear algebra : QR factorization

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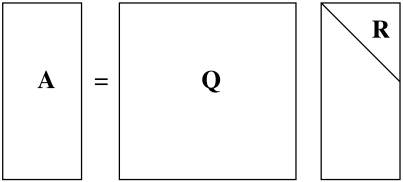
Outline

QR Factorization

QR Factorization

- Definition of an orthonormal set $\{x_1, \ldots, x_k\}$
  - $x_i^T x_j = 0 \quad \forall i \neq j$
  - $x_i^T x_i = 1$
- Orthogonal matrix Q: columns of Q form an orthonormal set $Q^T Q = I$, $Q^{-1} = Q^T$
- QR Factorization:



- Q: orthogonal.
- R: upper trapezoidal.

Example

$$\begin{bmatrix} 1 & -8 \\ 2 & -1 \\ 2 & 14 \end{bmatrix} = \begin{bmatrix} \frac{1}{3} & -\frac{2}{3} & -\frac{2}{3} \\ \frac{2}{3} & -\frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} \end{bmatrix} \begin{bmatrix} 3 & 6 \\ 0 & 15 \\ 0 & 0 \end{bmatrix} = Q \times R$$

QR Factorization

- Factorization built by applying a succession of orthogonal transformations to the data:

  $$Q = Q_1 \dots Q_n$$

  with Q_i orthogonal matrices such that $Q^T A = R$

- Transformations:
  - Householder reflections.
  - Givens rotations.
  - Gram-Schmidt process (in this case $Q \in \mathcal{M}_{m,n}(\mathbb{K})$ and $R \in \mathcal{M}_n(\mathbb{K})$)

QR Factorization - Projections

Exercice 1 (Orthogonal projection)

Let $Q \in \mathcal{M}_{m,n}(\mathbb{R})$, $m \geq n$ *be such that* $Q^T.Q = I_n \in \mathcal{M}_n$. *Let* X *be the n-dimensional span of the orthogonal set made of the columns of* Q.
Show that $P_X = Q.Q^T \in \mathcal{M}_m(\mathbb{R})$ *is the orthogonal projection onto* X.

QR Factorization - Preamble

Definition 1 (Householder matrix)

$\forall \mathbf{u} \in \mathbb{R}^n, \mathbf{u} \neq 0$, the **Householder** *matrix $\mathbf{H}_u \in M_{n,n}(\mathbb{R})$ is defined such that:*
$\mathbf{H}_u = \mathbf{I} - \frac{2}{\mathbf{u}^{\mathrm{T}}\mathbf{u}}\mathbf{u}\mathbf{u}^{\mathrm{T}}$.

Proposition 1

$\mathbf{H}_u$ is orthogonal ($\mathbf{H}_u^{\mathrm{T}}\mathbf{H}_u = \mathbf{I}$) and symmetric.

Proof.

$\mathbf{H}_u$ is obviously symmetric: $\mathbf{H}_u^{\mathrm{T}} = \mathbf{H}_u$.

One has $\mathbf{H}_u^{\mathrm{T}}\mathbf{H}_u = \left(\mathbf{I} - \frac{2}{\mathbf{u}^{\mathrm{T}}\mathbf{u}}\mathbf{u}\mathbf{u}^{\mathrm{T}}\right)^2 = \mathbf{I} + \frac{4}{\left(\mathbf{u}^{\mathrm{T}}\mathbf{u}\right)^2}\mathbf{u}\mathbf{u}^{\mathrm{T}}\mathbf{u}\mathbf{u}^{\mathrm{T}} - \frac{4}{\mathbf{u}^{\mathrm{T}}\mathbf{u}}\mathbf{u}\mathbf{u}^{\mathrm{T}}$.

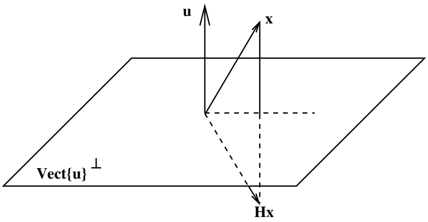
Therefore, $\mathbf{H}_u^{\mathrm{T}}\mathbf{H}_u = \mathbf{I} + \frac{4}{\mathbf{u}^{\mathrm{T}}\mathbf{u}}\mathbf{u}\mathbf{u}^{\mathrm{T}} - \frac{4}{\mathbf{u}^{\mathrm{T}}\mathbf{u}}\mathbf{u}\mathbf{u}^{\mathrm{T}} = \mathbf{I}$. $\square$

Interpretation: $\mathbf{H}_u = \mathbf{I} - \frac{2}{\mathbf{u}^T\mathbf{u}}\mathbf{u}\mathbf{u}^T$.

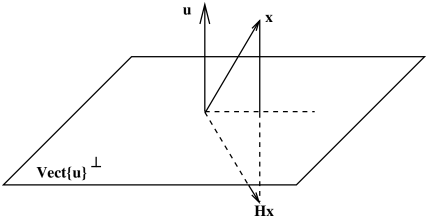
Proposition 2

- $\mathbf{H}_u\mathbf{u} = -\mathbf{u}$
- $\forall \mathbf{x} \in \mathbb{R}^n$, $\mathbf{H}_u\mathbf{x} = \mathbf{x}$ *if* $\mathbf{x}$ *and* $\mathbf{u}$ *orthogonal.*

Geometric interpetation:
$\forall \mathbf{x} \neq 0$, $\mathbf{H}_u\mathbf{x}$ is the symmetric of $\mathbf{x}$ with respect to span$(\mathbf{u})^\perp$
Therefore, $\mathbf{H}_u$ is a reflection.



Another view on: $\mathbf{H}_u = \mathbf{I} - \frac{2}{\mathbf{u}^{\mathrm{T}}\mathbf{u}}\mathbf{u}\mathbf{u}^{\mathrm{T}}$.



Let $\mathbf{Q}_u$ be such that $\mathbf{Q}_u = \frac{\mathbf{u}}{\|u\|_2}$.

From Exercice 1, $\mathbf{Q}_u\mathbf{Q}_u^T$ is a projection onto span($\mathbf{u}$): $\frac{\mathbf{u}\mathbf{u}^{\mathrm{T}}}{\mathbf{u}^{\mathrm{T}}\mathbf{u}}$ is the orthogonal projection onto span($\mathbf{u}$).

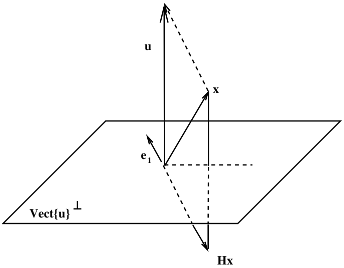
Therefore,

$\mathbf{H}_u = \mathbf{I} - 2\mathbf{Q}_u\mathbf{Q}_u^{\mathrm{T}}$ is a symmetry with respect to span$(\mathbf{u})^{\perp}$.

$\mathbf{H}_u = \mathbf{I} - \frac{2}{\mathbf{u}^T\mathbf{u}}\mathbf{u}\mathbf{u}^T$: towards the QR factorization?

$\forall \mathbf{x} \in \mathbb{R}^n$ ($\mathbf{x} \neq 0$), can we find $\mathbf{u}$ such that $\mathbf{H}_u\mathbf{x}$ and e_1 collinear?

From a given $\mathbf{x}$, $\mathbf{u}$ must be easy to compute.



Defining $\mathbf{u} = \mathbf{x} + \sigma\ \mathbf{e}_1$, we look for σ such that:

$$\mathbf{H}_u\mathbf{x} = \begin{bmatrix} -\sigma \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Computation of σ / $\mathbf{H}_u\mathbf{x} = -\sigma\mathbf{e}_1$

Proposition 3

Let $\mathbf{x} \in \mathbb{R}^n$ be such that $\mathbf{x} \neq 0$, $x = (x_i)_{i=1,n}$ and $\sigma = sign(x_1)\|\mathbf{x}\|$.
Defining $\mathbf{u} = \mathbf{x} + \sigma\ \mathbf{e}_1$, then
$\mathbf{H}_u\mathbf{x} = -\sigma\mathbf{e}_1$, with e_1 the first vector of the standard basis.

Proof.

With $\mathbf{u} = \mathbf{x} + \sigma\ \mathbf{e}_1$ $(u \neq 0)$ we have

$$\mathbf{H}_u\mathbf{x} = \mathbf{H}_u\mathbf{u} - \sigma\mathbf{H}_u\mathbf{e}_1 = -\mathbf{u} - \sigma\left(\mathbf{e}_1 - \frac{2}{\mathbf{u}^{\mathrm{T}}\mathbf{u}}\mathbf{u}\mathbf{u}^{\mathrm{T}}\mathbf{e}_1\right) = -\sigma\mathbf{e}_1 + \frac{2\sigma u_1}{\mathbf{u}^{\mathrm{T}}\mathbf{u}}\mathbf{u} - \mathbf{u}.$$

Furthermore,

$$\mathbf{u}^{\mathrm{T}}\mathbf{u} = \mathbf{x}^{\mathrm{T}}\mathbf{u} + \sigma\mathbf{e}_1^{\mathrm{T}}\mathbf{u} = \mathbf{x}^{\mathrm{T}}(\mathbf{x} + \sigma\ \mathbf{e}_1) + \sigma(\sigma + x_1) = \mathbf{x}^{\mathrm{T}}\mathbf{x} + 2\sigma x_1 + \sigma^2$$

Since $\mathbf{x}^{\mathrm{T}}\mathbf{x} = \sigma^2$ and $u_1 = x_1 + \sigma$,

$$\mathbf{u}^{\mathrm{T}}\mathbf{u} = 2\sigma(x_1 + \sigma) = 2\sigma u_1.$$

Therefore $\mathbf{H}_u\mathbf{x} = -\sigma\mathbf{e}_1$. □

The choice of σ in Proposition 3 is motivated by $\mathbf{u}^{\mathrm{T}}\mathbf{u} \sim 0$ if $\mathbf{x} \sim \mathbf{e}_1$

Householder reflections: an example

$\mathbf{H} = I - 2\mathbf{v}.\mathbf{v}^T$ with $\mathbf{v} \in \mathbb{R}^n$ such that $\|\mathbf{v}\|_2 = 1$.
$\mathbf{H}$ is orthogonal and symmetric.
It provides a way of vanishing all the entries of a vector except for one component.

- Example :

$$x = \begin{bmatrix} 2 \\ -1 \\ 2 \end{bmatrix} \quad u = x + \begin{bmatrix} \|x\|_2 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 5 \\ -1 \\ 2 \end{bmatrix} \text{ and } \mathbf{v} = \frac{u}{\|u\|_2}$$

Then,

$$\mathbf{H}_u = I - 2\mathbf{v} \times \mathbf{v}^T = \frac{1}{15} \times \begin{bmatrix} -10 & 5 & -10 \\ 5 & 14 & 2 \\ -10 & 2 & 11 \end{bmatrix}$$

Therefore,

$$\mathbf{H}_u \times x = \begin{bmatrix} -3 \\ 0 \\ 0 \end{bmatrix}$$

QR Factorization with Householder reflections: existence

Theorem 1

Let $\mathbf{A} \in M_n(\mathbb{R})$ *be a full rank matrix.*
Then, there are $\mathbf{Q} \in M_n(\mathbb{R})$ *orthogonal and* $\mathbf{R} \in M_n(\mathbb{R})$ *upper triangular such that*

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

Proof.

see Exercice 2. □

What about rectangular matrices?

The previous theorem can easily be extended to any matrix $\mathbf{A} \in M_{m,n}(\mathbb{R})$ $m \geq n$, with a rank equal to n. It can be shown that $\exists \mathbf{R} \in \mathbf{M}_n$ upper triangular such that

$$\mathbf{A} = \mathbf{Q} \begin{pmatrix} \mathbf{R} \\ 0 \end{pmatrix}$$

Householder Triangularization

Exercice 2

Let $\mathbf{A} \in M_n(\mathbb{R})$ *be a full rank matrix.*

1. *Show there exists* $\mathbf{H}_1 \in M_n(\mathbb{R})$ *orthogonal and* $\alpha_1 \in \mathbb{R}$ *such that* $\mathbf{H}_1\mathbf{A}(\mathbf{e}_1) = \alpha_1\mathbf{e}_1$
2. *Deduce from 1. that there exists a sequence of orthogonal matrices* $\mathbf{H}_i, 1 \leq i \leq n-1$ *such that* $\mathbf{H}_{n-1} \dots \mathbf{H}_1\mathbf{A} = \mathbf{R}$ *with* $\mathbf{R} \in M_n(\mathbb{R})$ *triangular.*

Definition 2

With $\mathbf{Q}^T = \mathbf{H}_{n-1} \dots \mathbf{H}_1$, *exercice 2 leads to the Householder factorization* $\mathbf{A} = \mathbf{QR}$

Householder Factorization: example

From a Householder vector: $\mathbf{u} = \mathbf{x} \pm \|x\|_2 e_1$, and its normalization $\mathbf{v} = \mathbf{u}/\|\mathbf{u}\|_2$ we can obtain a matrix that reads:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22} & a_{23} \\ 0 & a_{32} & a_{33} \\ 0 & a_{42} & a_{43} \\ 0 & a_{52} & a_{53} \end{bmatrix}$$

Let $\mathbf{H}$ be such that:

$$\mathbf{H} \times \begin{bmatrix} a_{22} \\ a_{32} \\ a_{42} \\ a_{52} \end{bmatrix} = \begin{bmatrix} a'_{22} \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\text{If } \mathbf{H}' = \begin{bmatrix} 1 & 0 \\ 0 & \mathbf{H} \end{bmatrix} \text{ then } \mathbf{H}' \times A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a'_{22} & a'_{23} \\ 0 & 0 & a'_{33} \\ 0 & 0 & a'_{43} \\ 0 & 0 & a'_{53} \end{bmatrix}$$

- Triangularization of a matrix 4×3 : $Q = \mathbf{H}_3 \times \mathbf{H}_2 \times H_1$

```
| x   x   x |      | x   x   x |      | x   x   x |
| x   x   x | H1 | 0   x   x | H2 | 0   x   x |
| x   x   x | -> | 0   x   x | -> | 0   0   x |
| x   x   x |      | 0   x   x |      | 0   0   x |

                   | x   x   x |
               H3 | 0   x   x |
               -> | 0   0   x | = R
                   | 0   0   0 |
```

- QR backward stable, with a lower backward error than LU.

Computational complexity of the **QR** Factorization

Exercice 3 (Memory consumption)

Compute the memory space required to do a QR factorization.

Exercice 4 (Computational complexity)

Estimate the amount of operations that are done during the Householder factorization.

Remark: the most expensive part of the algorithm occurs, at each step, when updating the reduce matrix $\mathbf{A}_k \in M_{n-k,n-k}(\mathbb{R})$.

$$\mathbf{A}_k = \mathbf{A}_k - \beta \mathbf{u}_k (\mathbf{u}_k^{\mathrm{T}} \mathbf{A}_k) \quad \textit{avec} \;\; \beta = \frac{2}{\mathbf{u}_k^{\mathrm{T}} \mathbf{u}_k} \quad \textit{et} \;\; \mathbf{u}_k \in \mathbb{R}^{n-k} \; . \tag{1}$$

Correction

Memory consumption

We do not compute $\mathbf{H}_i$: only the vectors $\mathbf{u}_i$ are required.
The triangular part of $\mathbf{A}$ is used to store these vectors (plus a vector of size n for the diagonal terms).
Therefore, the factorization can be done using the memory space allocated for the initial matrix (and a vector of size n).

Remark 1: $\mathbf{Q}$-matrix product

Matrix product with $\mathbf{Q}$: sequence of Householder transformations.

Remark 2: Computational complexity

We need to specify the **QR** algorithm.

Householder QR factorization algorithm

Function: $[\mathbf{v}, \beta] = house(x)$

Compute $\mathbf{v}$ and β such that $\mathbf{H} = \mathbf{I} - \beta \mathbf{v}.\mathbf{v}^T$ is orthogonal, $v(1) = 1$ and $\mathbf{Hx} = \|\mathbf{x}\|_2 e_1$

$v(1)$ is not stored (known value). We need a vector of size n for β.

Algorithm

Let $\mathbf{A} \in M_{m,n}(\mathbb{R})$ $m \geq n$, be a rectangular matrix.
The step computing the Householder matrices reads

for $k = 1,n$ **do**
  $[\mathbf{v}, \beta] = house(\mathbf{A}(k:m,k))$
  $\mathbf{A}(k:m, k+1:n) = (\mathbf{I}_{m-k+1} - \beta \mathbf{v}.\mathbf{v}^T)\mathbf{A}(k:m; k+1:n)$
  $\mathbf{A}(k,k) = -sign(\mathbf{A}(k,k))\|\mathbf{A}(k:m,k)\|$
  if $k \leq m$ **then**
    $\mathbf{A}(k+1:m, k) = \mathbf{v}(2:m-k+1)$
  end if
end for

Computational complexity of the **QR** factorization

Step factorizing $\mathbf{A} = \mathbf{QR}$ with $\mathbf{A} \in M_{m,n}(\mathbb{R})$

for $k = 1, n$ **do**
(1) Compute β (inner product)
  for $j = 1, n-k$ **do**
   /* Let Col_j be the jth column of $\mathbf{A}_k$ (size $m-k$)*/
(2) $tmp = \mathbf{v}_k^{\mathrm{T}} \times Col_j$ ($\mathbf{v}_k \in M_{m-k}(\mathbb{R})$)
(3) $tmp = \beta \times tmp$
(4) $Col_j = Col_j - tmp \times \mathbf{v}_k$
  end for
end for

$2(m-k)$ flops for step (2) and (4), so $4(m-k)(n-k)$ flops per step k.
It results in

$$4\sum_{k=1}^{n}(m-k)(n-k) \simeq 4\left(n^3/3 + (m-n)n(n-1)/2\right)$$

It leads to a computational complexity of $\frac{4}{3}n^3$ for square matrices of size n

Givens rotations

- 2×2 rotation:

$$G(\theta) = \begin{bmatrix} c & s \\ -s & c \end{bmatrix} \text{ orthogonal}$$

  with $c = cos(\theta)$ and $s = sin(\theta)$.

- Application: $x = \{x_1, x_2\}$

$$c = \frac{x_1}{(x_1^2 + x_2^2)^{\frac{1}{2}}} \text{ et } s = \frac{-x_2}{(x_1^2 + x_2^2)^{\frac{1}{2}}}$$

$$y = (y_1, y_2) = G^T x \text{ then } y_2 = 0$$

- Specify the entries of a matrix that will vanish.

Givens rotations

- Example: QR factorization

$$A = \begin{bmatrix} r_{11} & r_{12} & r_{13} \\ 0 & r_{22} & r_{23} \\ 0 & 0 & r_{33} \\ v_1 & v_2 & v_3 \end{bmatrix}$$

- We find (c, s) such that :

$$\begin{bmatrix} c & s \\ -s & c \end{bmatrix}^T \times \begin{bmatrix} r_{11} \\ v_1 \end{bmatrix} = \begin{bmatrix} r'_{11} \\ 0 \end{bmatrix}$$

Givens rotations

- Rotation in the (1,4) plane:

$$G(1,4) = \begin{bmatrix} c & 0 & 0 & s \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -s & 0 & 0 & c \end{bmatrix}$$

$$G(1,4)^T \times A = \begin{bmatrix} r'_{11} & r'_{12} & r'_{13} \\ 0 & r_{22} & r_{23} \\ 0 & 0 & r_{33} \\ 0 & v'_2 & v'_3 \end{bmatrix}$$

- Computational complexity: $2n^3$ flops for the triangularization of the matrix.