MATH 3795
Lecture 8. Linear Least Squares. Using QR Decomposition.

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Goals

- Orthogonal matrices.
- QR-decomposition.
- Solving LLS with QR-decomposition.

Orthogonal matrices.

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  i.e. the angle between Qx and Qy is equal to the angle between x and y
- As a result

  $$\|Qx\|_2 = \|x\|_2$$

  i.e. orthogonal matrices preserve the 2-norm.

Matrix Norms

Example

In two dimensions a rotation matrix

$$Q = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

is orthogonal matrix. This fact can easily be checked

$$\begin{aligned} Q^T Q &= \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \\ &= \begin{pmatrix} \cos^2\theta + \sin^2\theta & 0 \\ 0 & \cos^2\theta + \sin^2\theta \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \end{aligned}$$

QR-Decomposition.

- Let $m \geq n$. For each $A \in \mathbb{R}^{m \times n}$ there exists a permutation matrix $P \in \mathbb{R}^{mn \times n}$, an orthogonal matrix $Q \in \mathbb{R}^{m \times m}$, and an upper triangular matrix $R \in \mathbb{R}^{n \times n}$ such that

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- The QR decomposition of A can be computed using the Matlab command $[Q, R, P] = qr(A)$.
- We will not go into the details of how Q, P, R are computed. If you interested check Chapter 5 of the book

  Gene Golub and Charles Van Loan, *Matrix Computations*

Solving LLS using QR-Decomposition: Rank(A)=n

Assume that $A \in \mathbb{R}^{m \times n}$, has full rank n. (Rank deficient case will be considered later.)

- Let

$$AP = Q \begin{pmatrix} R \\ 0 \end{pmatrix} \begin{array}{ll} \} & n \\ \} & m-n \end{array} \quad \Leftrightarrow \quad Q^T AP = \begin{pmatrix} R \\ 0 \end{pmatrix} \begin{array}{ll} \} & n \\ \} & m-n \end{array}$$

  where $R \in \mathbb{R}^{n \times n}$ is upper triangular matrix.

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  where $R \in \mathbb{R}^{n \times n}$ is upper triangular matrix.

- Since A has full rank n the matrix R also has rank n and, therefore, is nonsingular.
- Moreover, since Q is orthogonal it obeys $QQ^T = I$. Hence

$$\|Q^T y\|_2 = \|y\|_2 \quad \forall y \in \mathbb{R}^m.$$

  In addition, the permutation matrix satisfies $PP^T = I$.

Solving LLS using QR-Decomposition: Rank(A)=n

Using these properties of Q we get Let

$$\begin{aligned}
\|Ax - b\|_2^2 &= \|Q^T(Ax - b)\|_2^2 \\
&= \|Q^T(APP^Tx - b)\|_2^2 \\
&= \|(Q^TAP)P^Tx - Q^Tb\|_2^2 \\
&= \| \begin{pmatrix} R \\ 0 \end{pmatrix} P^Tx - Q^Tb\|_2^2
\end{aligned}$$

Solving LLS using QR-Decomposition: Rank(A)=n

Partitioning $Q^T b$ as

$$Q^T b = \left(\begin{array}{c} c \\ d \end{array} \right) \begin{array}{ll} \} & n \\ \} & m-n \end{array}$$

and putting $y = P^T x$ we get

$$\begin{aligned} \|Ax - b\|_2^2 &= \left\| \left(\begin{array}{c} R \\ 0 \end{array} \right) y - \left(\begin{array}{c} c \\ d \end{array} \right) \right\|_2^2 = \left\| \left(\begin{array}{c} Ry - c \\ -d \end{array} \right) \right\|_2^2 \\ &= \|Ry - c\|_2^2 + \|d\|_2^2. \end{aligned}$$

Thus,

$$\min_x \|Ax - b\|_2^2 \quad \Leftrightarrow \quad \min_y \|Ry - c\|_2^2 + \|d\|_2^2$$

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Recall

$$y = P^T x, \quad PP^T = I, \quad \Rightarrow \quad x = Py.$$

Hence the solution is $x = Py = PR^{-1}c$.

Solving LLS using QR-Decomposition. Summary.

To solve a Linear Least Squares Problem using the QR-Decomposition with matrix $A \in \mathbb{R}^{m\times n}$, of rank n and $b \in \mathbb{R}^m$:

1. Compute an orthogonal matrix $Q \in \mathbb{R}^{m\times m}$, an upper triangular matrix $R \in \mathbb{R}^{n\times n}$, and a permutation matrix $P \in \mathbb{R}^{n\times n}$ such that

$$Q^T A P = \begin{pmatrix} R \\ 0 \end{pmatrix}.$$

2. Compute

$$Q^T b = \begin{pmatrix} c \\ d \end{pmatrix}.$$

3. Solve

$$Ry = c.$$

4. Set

$$x = Py.$$

Solving LLS using QR-Decomposition. MATLAB Implementation.

```
[m,n] = size(A);
[Q,R,P] = qr(A);
c = Q'*b;
y = R(1:n,1:n) \ c(1:n);
x = P*y;
```

If you type

$$x = A\backslash b;$$

in Matlab, then Matlab computes the solution of the linear least squares problem

$$\min_x \|Ax - b\|_2^2$$

using the QR decomposition as described above.

Solving LLS using QR-Decomposition: Rank(A)<n

The Rank Deficient Case: Assume that $A \in \mathbb{R}^{m \times n}$, $m \geq n$ has rank $r < n$. (The case $m < n$ can be handled analogously.)
Suppose that

$$AP = QR,$$

where $Q \in \mathbb{R}^{m \times m}$ is orthogonal, $P \in \mathbb{R}^{n \times n}$ is a permutation matrix, and $R \in \mathbb{R}^{n \times n}$ is an upper triangular matrix of the form

$$R = \begin{pmatrix} R_1 & R_2 \\ 0 & 0 \end{pmatrix}$$

with nonsingular upper triangle $R_1 \in \mathbb{R}^{r \times r}$ and $R_2 \in \mathbb{R}^{r \times (n-r)}$
We can write

$$\begin{aligned} \|Ax - b\|_2^2 &= \|Q^T(APP^Tx - b)\|_2^2 \\ &= \left\| \begin{pmatrix} R_1 R_2 \\ 0 \end{pmatrix} P^T x - Q^T b \right\|_2^2. \end{aligned}$$

Solving LLS using QR-Decomposition: Rank(A)<n

Partition $Q^T b$ as

$$Q^T b = \begin{pmatrix} c_1 \\ c_2 \\ d \end{pmatrix} \begin{array}{l} \} \quad r \\ \} \quad n-r \\ \} \quad m-n \end{array}$$

and put $y = P^T x$.
Partition

$$y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \begin{array}{l} \} \quad r \\ \} \quad n-r \end{array}$$

This give us

$$\begin{aligned} \|Ax - b\|_2^2 &= \left\| \begin{pmatrix} R_1 y_1 + R_2 y_2 - c_1 \\ c_2 \\ d \end{pmatrix} \right\|_2^2 \\ &= \|R_1 y_1 + R_2 y_2 - c_1\|_2^2 + \|c_2\|_2^2 + \|d\|_2^2. \end{aligned}$$

Solving LLS using QR-Decomposition: Rank(A)<n

Linear least squares problem $\min_x \|Ax - b\|_2^2$ is equivalent to

$$\|R_1 y_1 + R_2 y_2 - c_1\|_2^2 + \|c_2\|_2^2 + \|d\|_2^2,$$

where $R_1 \in \mathbb{R}^{r \times r}$ is nonsingular.

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Solution is

$$y_1 = R_1^{-1}(c_1 - R_2 y_2)$$

for any $y_2 \in \mathbb{R}^{n-r}$.
Since $y = P^T x$ and $P^T P = I$,

$$x = Py = P \begin{pmatrix} R_1^{-1}(c_1 - R_2 y_2) \\ y_2 \end{pmatrix}$$

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We have infinitely many solutions since y_2 is arbitrary. Which one to choose?
If we use Matlab $x = A \backslash b$, then Matlab computes the one with $y_2 = 0$

$$x = P \begin{pmatrix} R_1^{-1} c_1 \\ 0 \end{pmatrix}.$$

Solving LLS using QR-Decomposition. MATLAB Implementation.

```
[m,n] = size(A);
[Q,R,P] = qr(A);
c = Q'*b;
% Determine rank of A.
% The diagonal entries of R satisfy
%|R(1,1)| >= |R(2,2)| >= |R(3,3)| >= ..
% Find the smallest integer r such that
%|R(r+1,r+1)| < max(size(A))*eps*|R(1,1)|
tol = max(size(A))*eps*abs(R(1,1));
r = 1;
while ( abs(R(r+1,r+1)) >= tol & r < n ); r = r+1; end
y1 = R(1:r,1:r) \ c(1:r);
y2 = zeros(n-r,1);
x = P*[y1;y2];
```

Solving LLS using QR-Decomposition: Rank(A)<n

All solutions of

$$\min_x \|Ax - b\|_2^2$$

are given by

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where $y_2 \in \mathbb{R}^{n-r}$ is arbitrary.

Minimum norm solution:

Of all solutions, pick the one with the smallest 2-norm. This leads to

$$\min_{y_2} \left\| P \begin{pmatrix} R_1^{-1}(c_1 - R_2 y_2) \\ y_2 \end{pmatrix} \right\|_2^2$$

Solving LLS using QR-Decomposition: Rank(A)<n

Since permutation matrix P is orthogonal

$$\left\| P \begin{pmatrix} R_1^{-1}(c_1 - R_2 y_2) \\ y_2 \end{pmatrix} \right\|_2^2 =$$

$$\left\| \begin{matrix} R_1^{-1}(c_1 - R_2 y_2) \\ y_2 \end{matrix} \right\|_2^2 =$$

$$\left\| \begin{matrix} R_1^{-1}(c_1 - R_2 y_2) \\ -y_2 \end{matrix} \right\|_2^2 =$$

$$\left\| \begin{pmatrix} R_1^{-1} R_2 \\ I \end{pmatrix} y_2 - \begin{pmatrix} R_1^{-1} c_1 \\ 0 \end{pmatrix} \right\|_2^2$$

which is another linear least squares problem with unknown y_2. This problem is $n \times (n-r)$ and it has full rank. It can be solved using the techniques discussed earlier.

Solving LLS using QR-Decomposition. MATLAB Implementation.

```
[m,n] = size(A);
[Q,R,P] = qr(A);
c = Q'*b;
% Determine rank of A (as before).
tol = max(size(A))*eps*abs(R(1,1));
r = 1;
while ( abs(R(r+1,r+1)) >= tol & r < n ); r = r+1; end
% Solve least squares problem to get y2
S = [ R(1:r,1:r) \ R(1:r,r+1:n);
eye(n-r) ];
t = [ R(1:r,1:r) \ c(1:r);
zeros(n-r,1) ];
y2 = S \ t; % solve least squares problem using backslash
% Compute x
y1 = R(1:r,1:r) \ ( c(1:r) - R(1:r,r+1:n) * y2 );
x = P*[y1;y2];
```

Solving LLS using QR-Decomposition: Rank(A)<n

- Determination of the effective rank of $A \in \mathbb{R}^{n\times n}$ using the QR decomposition
$$AP = QR,$$
where the diagonal entries of R satisfy $|R_{11}| \geq |R_{22}| \geq \ldots$.
- The effective rank r of $A \in \mathbb{R}^{n\times n}$ is the smallest integer r such that
$$|R_{r+1,r+1}| < \varepsilon \max\{m,n\} |R_{11}|$$
-
```
tol = max(size(A))*eps*abs(R(1,1));
r = 0;
while ( abs(R(r+1,r+1)) >= tol & r < n )
r = r+1;
end
```