# MATH 612
# Computational methods for equation solving and function minimization – Week # 3

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# Plan for this week

- Discuss any problems you couldn't solve of Lectures 3 to 5 (Lectures are the chapters of the book)
- Read Lectures 6 and 7
- Homework is due Wednesday at class time
- The first coding assignment will be posted at the end of the week
- Friday is a work'n'code day. You'll be given some problems to work on and a small coding assignment.

**Warning**

Typically, I'll keep on updating, correcting, and modifying the slides until the end of each week.

# ORTHOGONAL PROJECTIONS

# Orthogonal decomposition

Consider an orthonormal basis of $\mathbb{C}^m$ (or $\mathbb{R}^m$)

$$\underbrace{q_1, \ldots, q_n}_{\text{basis of } S_1}, \underbrace{q_{n+1}, \ldots, q_m}_{\text{basis of } S_2}. \qquad (S_1 \perp S_2)$$

Given a vector $x$ the vector

$$\sum_{j=1}^{n} (q_j^* x) q_j = \left( \sum_{j=1}^{n} q_j q_j^* \right) x = Px$$

is in $S_1$ and $x - Px$ is in the orthogonal complement of $S_1$. In other words, the decomposition

$$x = Px + (I - P)x$$

is orthogonal.

# The orthogonal projector

Starting again: given orthonormal vectors $q_1, \ldots, q_n$ in $\mathbb{C}^m$, the matrix

$$P = \sum_{j=1}^{n} q_j q_j^*$$

gives the component in $\langle q_1, \ldots, q_n \rangle$ of the decomposition of $x$ as a sum of a vector in this subspace plus a vector orthogonal to it. This matrix is called the **orthogonal projector** onto the subspace $S_1 = \langle q_1, \ldots, q_n \rangle$.

# Easy properties

$$P = \sum_{j=1}^{n} q_j q_j^* \qquad q_1, \ldots, q_n \quad \text{orthonormal}$$

- $P$ is hermitian ($P^* = P$)
- $P^2 = P$
- If $n = m$, then $P = I$
- $Px = x$ for all $x \in \text{range}(P) = \langle q_1, \ldots, q_n \rangle$
- $Px = 0$ if and only if $x \perp \text{range}(P)$
- The eigenvalues of $P$ are 1 (multiplicity $n$) and 0 (multiplicity $n - m$)
- $I - P$ is also an orthogonal projector (what is its range?)

# The SVD of an orthogonal projector

$$P = \sum_{j=1}^{n} q_j q_j^* \qquad q_1, \ldots, q_n \quad \text{orthonormal}$$

If $\widehat{Q}$ is the matrix whose columns are $q_1, \ldots, q_n$, then

$$P = \widehat{Q}\widehat{Q}^*.$$

(Note that $\widehat{Q}^*\widehat{Q} = I_n$ though.) If $Q$ is unitary and contains $q_1, \ldots, q_n$ as its first columns, then

$$P = Q\Sigma Q^*, \qquad \Sigma = \begin{bmatrix} I & O \\ O & O \end{bmatrix}$$

# Orthogonal projectors without orthonormal bases

Let $S_1 = \langle a_1, \ldots, a_n \rangle$ be a subspace of $\mathbb{C}^m$, given as the span of $n$ linearly independent vectors. The orthogonal projector onto $S_1$ is given by the matrix

$$P = A(A^*A)^{-1}A^*.$$

First of all, $P^* = P$ and $P^2 = P$. (This is easy to verify. Do it!) Next, note how

$$\begin{aligned}(Px)^*((I-P)y) &= x^*P(I-P)y = x^*P(I-P)y \\ &= x^*(P-P^2)y = 0.\end{aligned}$$

This means that the decomposition

$$x = Px + (I-P)x$$

is orthogonal and therefore $P$ is an orthogonal projector onto its own range.

# Orthogonal projectors without orthonormal bases (2)

We only need to check that the range of $P$ is the range of $A$, that is, $S_1$. Two things to prove:

- if $x \in \text{range}(P)$, then

$$x = A \underbrace{(A^*A)^{-1}A^*y}_{z} \in \text{range}(A).$$

- if $x \in \text{range}(A)$, then $x = Ay$ and

$$Px = A \underbrace{(A^*A)^{-1}A^*A}_{I} y = Ay = x \in \text{range}(P)$$

# How to compute an orthogonal projection

We will find better ways in the next chapters. Here's the most direct method

You do not construct the matrix $P$. If you only have a basis of the subspace, construct the matrix $A$ whose columns are the elements of the basis. Then

- Multiply $y = A^* x$
- Solve the system $(A^* A)z = y = A^* x$
- Multiply $Az$

The result is the projection of $x$ onto the space spanned by the columns of $A$.

# Oblique projectors

Any square matrix $P$ satisfying $P^2 = P$ is called a projector (an oblique projector).

Two important results on oblique projectors:

1. If $P^2 = P$, then

$$(I - P)^2 = I - 2P + P^2 = I - P,$$

   so $I - P$ is a projector too. It is called the complementary projector

2. If $P$ is a projector, $P$ is an orthogonal projector if and only if $P^* = P$.

And... if $P$ is a projector, $I - 2P$ is invertible. (Why? Show that $(I - 2P)^2 = I$))

# Oblique projectors (2)

Consider an oblique projector $P$. Let $S_1 = \text{range}(P)$. By definition of projector

$$x \in \text{range}(P) \qquad \Longleftrightarrow \qquad Px = x.$$

(Prove this!) Also,

$$x \in \text{range}(I - P) \qquad \Longleftrightarrow \qquad Px = 0,$$

and we denote $S_2 = \text{range}(I - P) = \text{null}(P)$. The projector $P$ projects onto $S_1$ along $S_2$.
We then have a decomposition for every vector

$$x = \underbrace{Px}_{\in S_1} + \underbrace{(I - P)x}_{\in S_2}.$$

Geometrically speaking, to know the projection $P$, you need to know its range $S_1$ and the range of its complementary projection $S_2$. With orthogonal projections, hey are orthogonal to each other and only one of them is needed.

# A particular case

If $S_1 = \langle p \rangle = \langle q \rangle$ where $q = \frac{1}{\|p\|} p$, then the orthogonal projector onto $S_1$ is given by

$$P = qq^* = \frac{1}{\|p\|^2} pp^*,$$

its complementary projection is

$$I - P = I - qq^* = I - \frac{1}{\|p\|^2} pp^*.$$

Finally

$$I - 2P$$

is an operator for symmetry with respect to the hyperplane $S_1^\perp$. Note that $I - 2P$ is a unitary matrix, because $P^2 = P = P^*$.

# Reduced QR decompositions

# Reminder

Let $q_1, \ldots, q_j$ be an orthonormal collection of vectors. The orthogonal projection of $v$ onto $\langle q_1, \ldots, q_j \rangle$ is the vector

$$\sum_{i=1}^{j} (q_j^* v) q_j.$$

# Reduced QR decomposition

For the moment being, let $A$ be an $m \times n$ matrix with full rank by columns. (Therefore $m \geq n$.) A reduced $QR$ decomposition is a factorization

$$A = \widehat{Q}\widehat{R},$$

where:

- $\widehat{Q}$ has orthonormal columns, that is,

$$\widehat{Q}^*\widehat{Q} = I_n$$

- $\widehat{R}$ is upper triangular (with non-zero diagonal elements – why?)
- in some cases, it is also required that $r_{ii} > 0$ for all $i$.

# What does the decomposition mean?

This is the matrix form:

$$\left[\begin{array}{c|c|c} a_1 & \cdots & a_n \end{array}\right] = \left[\begin{array}{c|c|c} q_1 & \cdots & q_n \end{array}\right] \begin{bmatrix} r_{11} & \dots & r_{1n} \\ & \ddots & \vdots \\ & & r_{nn} \end{bmatrix}$$

Now with vectors:

$$\begin{aligned} a_1 &= r_{11} q_1 \\ a_2 &= r_{12} q_1 + r_{22} q_2 \\ &\vdots \\ a_n &= r_{1n} q_1 + \ldots + r_{nn} q_n \end{aligned}$$

# What does the decomposition mean? (2)

With vectors, everything in one expression

$$a_j = r_{1j} q_1 + \ldots + r_{jj} q_j = \sum_{i=1}^{j} r_{ij} q_i, \qquad j = 1, \ldots, n.$$

Something equivalent but written in a funny way (thanks to $r_{jj} \neq 0$ for all $j$)

$$\frac{1}{r_{jj}} \Big( a_j - \sum_{i=1}^{j-1} r_{ij} q_i \Big) = q_j, \qquad j = 1, \ldots, n.$$

Can you see how

$$\langle a_1, \ldots, a_j \rangle = \langle q_1, \ldots, q_j \rangle \qquad j = 1, \ldots, n \quad ?$$

Finding a reduced $QR$ decomposition is equivalent to finding orthonormal bases for the growing column subspaces.

# Existence, uniqueness, computation

We are going to focus our attention in the case of an $m \times 3$ matrix with full rank by columns. We want to find $\{q_1, q_2, q_3\}$ orthonormal, and the elements of an upper triangular matris $r_{ij}$ with positive diagonal[1], satisfying

$$\begin{aligned} a_1 &= r_{11} q_1, \\ a_2 &= r_{12} q_1 + r_{22} q_2, \\ a_3 &= r_{13} q_1 + r_{23} q_2 + r_{33} q_3. \end{aligned}$$

Since $\|q_1\|_2 = 1$ and $r_{11} > 0$, there are no many options for the first equation

$$r_{11} = \|a_1\|_2, \qquad q_1 = \frac{1}{r_{11}} v_1.$$

[1] Otherwise, there's no uniqueness. We'll see how Matlab always computes another $QR$ decomposition

# Existence, uniqueness, computation (2)

What we have so far...

$$\begin{aligned} a_1 &= r_{11} q_1, \\ a_2 &= r_{12} q_1 + r_{22} q_2, \\ a_3 &= r_{13} q_1 + r_{23} q_2 + r_{33} q_3. \end{aligned}$$

Looking at the second equation, we use that $q_1^* q_2 = 0$ and $q_1^* q_1 = 1$ to obtain

$$r_{12} = q_1^* a_2.$$

Then

$$\begin{aligned} r_{22} q_2 &= a_2 - (q_1^* a_2) q_1 \\ &= a_2 - (\text{orth.proj. of } a_2 \text{ onto } \langle q_1 \rangle) = v_2 \end{aligned}$$

leading to

$$r_{22} = \|v_2\|_2, \qquad q_2 = \frac{1}{r_{22}} v_2.$$

# Existence, uniqueness, computation (3)

What we have so far...

$$\begin{aligned} a_1 &= r_{11} q_1, \\ a_2 &= r_{12} q_1 + r_{22} q_2, \\ a_3 &= r_{13} q_1 + r_{23} q_2 + r_{33} q_3. \end{aligned}$$

With the same idea (use that $q_i^* q_j = \delta_{ij}$)

$$r_{13} = q_1^* a_3, \qquad r_{23} = q_2^* a_3,$$

and

$$\begin{aligned} r_{33} q_3 &= a_3 - (q_1^* a_3) q_1 - (q_2^* a_3) q_2 \\ &= a_3 - (\text{orth.proj. of } a_3 \text{ onto } \langle q_1, q_2 \rangle) = v_3, \end{aligned}$$

leading to

$$r_{33} = \|v_3\|_2, \qquad q_3 = \frac{1}{r_{33}} v_3.$$

# Existence, uniqueness, computation (4)

We can continue with as many vectors as we have...

$$a_j = \sum_{i=1}^{j-1} r_{ij} q_i + r_{jj} q_j.$$

We first compute the coefficients

$$r_{ij} = q_i^* a_j \qquad i = 1, \ldots, j-1$$

(upper part of the $j$-th column of $\widehat{R}$), substract the result

$$r_{jj} q_j = v_j = a_j - \sum_{i=1}^{j-1} r_{ij} q_i = a_j - (\text{orth.proj. of } a_j \text{ onto } \langle q_1, \ldots, q_{j-1} \rangle)$$

and finally choose $r_{jj} = \|v_j\|_2$ and $q_j = \frac{1}{r_{jj}} v_j$.

# Sounds familiar?

This is the algorithm in algebraic form: for $j = 1, \ldots, n$, compute

$$r_{ij} = q_i^* a_j \quad (i = 1, \ldots, j-1), \qquad v_j = a_j - \sum_{i=1}^{j-1} r_{ij} q_i,$$

and then

$$r_{jj} = \|v_j\|_2, \qquad q_j = \frac{1}{r_{jj}} v_j.$$

(This is the well-known Gram-Schmidt orthogonalization method.)

# Conclusions from the method

The GS method shows that:

- There is a reduced $QR$ decomposition. The only place where it can fail is if if at a given moment $v_j = 0$. However, this implies that $a_j \in \langle q_1, \ldots, q_{j-1} \rangle = \langle a_1, \ldots, a_{j-1} \rangle$.
- The decomposition is unique if we demand $r_{jj} > 0$ for all $j$ (not true if we don't). When we write

  $$r_{jj} q_j = v_j$$

  with the requirement $\|q_j\|_2 = 1$ we have two choices for $r_{jj}$ (keeping everything real) and infinitely many in the complex case. If we decide a priori to have $r_{jj} > 0$, the algorithm is closed.

# Classical Gram-Schmidt method

Idea. As we compute $r_{ij}$, we subtract the corresponding contribution in $v_j$.

for $j = 1 : n$
  $v_j = a_j$
  for $i = 1 : j - 1$
    $r_{ij} = q_i^* a_j$
    $v_j = v_j - r_{ij} q_i$
  end
  $r_{jj} = \|v_j\|_2$
  $q_j = \frac{1}{r_{jj}} v_j$
end

Warning. This method is unstable. Do not use GS in this form!

# Full QR and rank-deficiency

# Full QR decomposition

Let $A$ be an $m \times n$ matrix with rank equal to $n$. We can then write

$$A = \widehat{Q}\widehat{R}.$$

We then:

- add columns to the right of $\widehat{Q}$ to build a unitary matrix $Q$
- append $m - n$ zero rows under $\widehat{R}$ to have an $m \times n$ upper triangular matrix $R$

(Does this process sound familiar?). This leads to

$$A = Q\,R$$

which is called a full $QR$ decomposition.

The Householder method (first coding assignment) computes a full $QR$ decomposition directly.

# Now, let's see... what are we doing here?

```
l = 1          % counter of orthonormal vectors
for j = 1 : n
    v_j = a_j
    for i = 1 : l - 1
        r_ij = q_i^* a_j
        v_j = v_j - r_ij q_i
    end
    if ||v_j||_2 > 0          % active only for a new indep. column
        r_jl = ||v_j||_2
        q_l = (1/r_jl) v_j
        l = l + 1
    end
end
```