5374 Fall '22

Numerical Linear Algebra — Lecture 15

Today: Least squares and QR

Warmup: 2nd order polynomials in $\mathbb{R}^n$

Ex $q(x) = x_1^2 + x_2^2 + \cdots + x_n^2 + x_1x_2 + x_3x_5 + x_2x_n + 7x_2 - 3x_1 + 8x_{23} + 8$

$$x = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$$

Every such polynomial can be written in the form

$$q(x) = \tfrac{1}{2}(Mx, x) + (p, x) + c$$

for some symmetric matrix M, vector p, and constant c.

(compare with Problem Set 3, question #2)

How can we think about the gradient of p?

Fix $x \in \mathbb{R}^n$, and let $h \in \mathbb{R}^n$

$$q(x+h) = \tfrac{1}{2}(M(x+h), x+h) + (p, x+h) + c$$

$$= \tfrac{1}{2}\big((Mx,x) + (Mx,h) + (Mh,x) + (Mh,h)\big) + (p,x) + (p,h) + c$$

so, $$q(x+h) = \frac{1}{2}\left((Mx,x) + 2(Mx,h) + (Mh,h)\right) + (P,x) + (P,h) + C$$

$$\Rightarrow \quad q(x+h) = \overbrace{\frac{1}{2}(Mx,x) + (P,x) + C}^{q(x)} + (Mx,h) + \frac{1}{2}(Mh,h) + (P,h)$$

In conclusion,

$$q(x+h) = q(x) + (Mx+P, h) + \frac{1}{2}(Mh,h)$$

if h is now fixed, and $t \in \mathbb{R}$ $(t \neq 0)$

(compare with the Taylor expansion of a scalar function in $\mathbb{R}^n$)

$$q(x+th) = q(x) + (Mx+P, th) + \frac{1}{2}(Mth, th)$$

$$(*) \quad \frac{q(x+th) - q(x)}{t} = (Mx+P, h) + t\,\frac{1}{2}(Mh,h)$$

$$\lim_{t \to 0} \frac{q(x+th) - q(x)}{t} = (\nabla q(x), h)$$

so, this shows that

$$(\nabla q(x), h) = (Mx+P, h)$$

for any $h \in \mathbb{R}^n$, i.e. $\nabla q(x) = Mx + P$

By the same token, what if we take

$$\lim_{t \to 0} \frac{q(x+th) + q(x-th) - 2q(x)}{t} = (D^2 q(x) h, h) \,?$$

Using $(*)$ at th and $-th$, we have

$$(D^2 q(x) h, h) = (M h, h)$$

so, $\qquad D^2 q(x) = M \qquad$ for all x.

In summary, given a quadratic function $q(x)$ defined by

$$q(x) = \frac{1}{2}(Mx, x) + (P, x) + C$$

then $\quad \nabla q(x) = Mx + P, \quad D^2 q(x) = M$

(Compare with $n=1$ case and problem set 3 Q#2

$$q(x) = \frac{1}{2} m x^2 + px + c$$

$$q'(x) = mx + p, \quad q''(x) = m$$

)

Least squares continued

The normal equations and orthogonality

Last time we introduced the problem:

"Given a $m \times n$ matrix A, a vector b in $\mathbb{R}^m$, minimize

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

over all $x \in \mathbb{R}^n$"

i.e. minimize $f(x) := \frac{1}{2}\|Ax-b\|_2^2$.

Let's rewrite $f(x)$

$$\begin{aligned} f(x) &= \tfrac{1}{2}(Ax-b, Ax-b) \\ &= \tfrac{1}{2}\big((Ax-b, Ax) - (b, Ax-b)\big) \\ &= \tfrac{1}{2}\big((Ax, Ax) - 2(b, Ax) + (b, b)\big) \end{aligned}$$

$$f(x) = \tfrac{1}{2}(A^tAx, x) - (A^tb, x) + \tfrac{1}{2}(b, b)$$

This is a special case of the quadratic

polynomial discussed in the warmup discussion where

$$M = A^t A, \quad p = -A^t b, \quad c = \tfrac{1}{2}\|b\|_2^2$$

It follows then

$$\nabla f(x) = \overbrace{A^t A x - A^t b}^{(Mx+p)}, \quad D^2 f(x) = \overbrace{A^t A}^{(M)}$$

First, $(A^t A n, n) \geq 0 \;\; \forall\, n \in \mathbb{R}^n$ so the function $f(x)$ is convex in x. In particular, if $x_* \in \mathbb{R}^n$ is any point such that $\nabla f(x_*) = 0$, then f achieves its global minimum at x_*; conversely, if x_* is a minimum of f, then $\nabla f(x_*) = 0$

These observations prove the following

Theorem : Solving the least squares problem is equivalent to solving the $n \times n$ system of equation

$$A^t A x = A^t b$$

and this is called the Normal equation.

Remark: If A is a $m \times n$ matrix of rank n, with $m \geq n$, then A is injective as a linear transformation and we know in that case (problem set 2) that $A^t A$ is invertible.

Therefore, in such cases the normal equations have exactly one solution for any $b \in \mathbb{R}^m$.

Remark: (About the numerical difficulty of the normal equations)

Consider

$$A^t A x = A^t b$$

and suppose for a moment that A is a square matrix, and suppose A has eigenvalues

$$\lambda_1, \ldots, \lambda_n \qquad (A \text{ is } n \times n)$$

where

$$|\lambda_n| \geq |\lambda_{n-1}| \geq \cdots \geq |\lambda_1| > 0$$

Then $$\operatorname{cond}(A) = \frac{|\lambda_n|}{|\lambda_1|}$$

On the other hand (check this!)

$$\operatorname{cond}(A^t A) = \left(\frac{|\lambda_n|}{|\lambda_1|}\right)^2 = \left(\operatorname{cond}(A)\right)^2$$

For example, if $\mathrm{cond}(A) = 1000$, then

$$\mathrm{cond}(A^t A) = 10^6.$$

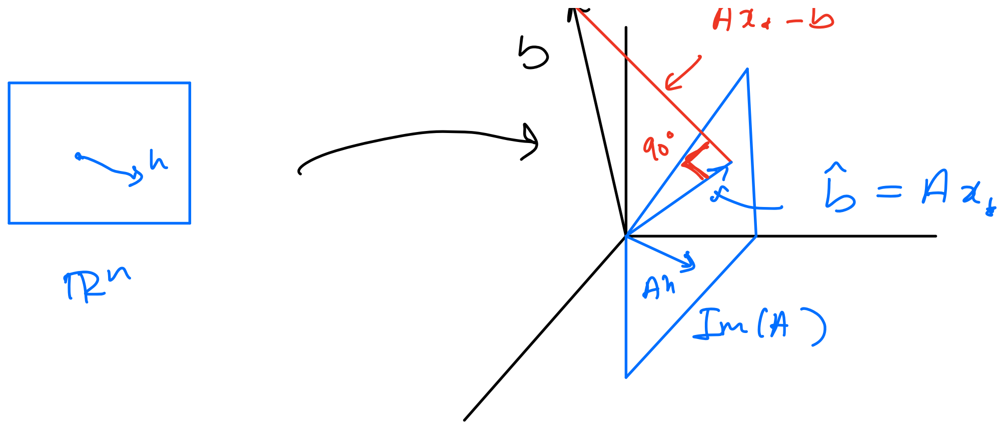
What this shows is that solving the normal equations can become quite ill-conditioned if A is not a reasonable matrix.

(↓ i.e. $\mathrm{cond}(A)$ is not too large, and this depends on how much accuracy we need)

For this reason the normal equations are not the only tool used to solve a least squares problem. If you can afford the longer computation time and require higher precision then it is best to solve the least squares problem using the QR decomposition (which we are about to explain).

First, a bit more about orthogonality

Proposition : x_* solves the normal equations ($A^t A x = A^t b$) if and only if $Ax_* - b \perp \mathrm{Im}(A)$.



Proof: If $A^t A x_* = A^t b$, then

$$A^t(Ax_* - b) = 0$$

so, given any $h \in \mathbb{R}^n$, we have

$$(A^t(Ax_* - b), h) = 0$$

using the definition of the transpose,

$$(Ax_* - b, Ah) = 0 \quad \forall h \in \mathbb{R}^n$$

i.e. $Ax_* - b \perp$ to any vector in $\mathrm{Im}(A)$ ∎

We see then that for x_* the solution to the least squares problem, the vector

$$\hat{b} := Ax_*$$

must be the orthogonal projection of b into the $\mathrm{Im}(A)$. This is how the QR decomposition arises naturally.

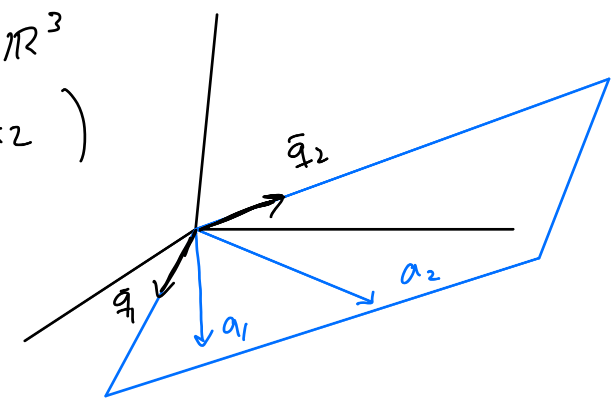
Recall that we saw how given a $m \times n$ matrix A of rank n $(m \geq n)$ we can find a matrix Q $(m \times n)$ whose columns are orthonormal and a $n \times n$ upper triangular matrix R s.t.

$$A = QR$$

We also learned that the columns of Q form an orthonormal basis for the subspace $\mathrm{Im}(A)$.

$\mathbb{R}^3$

(This is A 3×2)



$A = (a_1 \ a_2)$

$Q = (q_1, q_2)$

In terms of Q, $\hat{b}$ is simply

$$\hat{b} = QQ^t b$$

(we saw QQ^t is the projection of $\mathbb{R}^m$ into $\mathrm{Im}(A)$)

so, the normal equation become

$$A^t A x = A^t b$$

since $A = QR$,

$$A^t A = R^t Q^t Q R$$

$$R^t Q^t Q R x = R^t Q^t b$$

Now, R is $n \times n$ and invertible

$$\cancel{R^t} Q^t Q R x = \cancel{R^t} Q^t b$$

and the normal equation become equivalent to

$$Q^t Q R x = Q^t b$$

Multiply both sides by Q, ...

$$Q \underbrace{Q^t}_{= I} Q R x = Q Q^t b$$

or

$QQ^t (Ax)$

$\parallel$

Ax

$\parallel$

QR

$$QRx = (QQ^t) b$$

Now, the matrix Q is $m \times n$ and has rank n, so it is injective ... means

$$Q(Rx) = Q(Q^t b)$$

$$\Leftrightarrow \quad Rx = Q^t b$$

The normal equation (for A of rank n, $m \geq n$) reduce to

$$Rx = Q^t b$$

when R is upper triangular and $n \times n$.