

Numerical Problems in Solving the Normal Equation

LECTURE 07

Note Title

In general, it is not a good idea to solve the normal eqn:

$$A^T A x = A^T b$$

by explicitly forming $A^T A$, and then compute $(A^T A)^{-1}$!

why?

- 1) Forming $A^T A \rightarrow$ loss of info.
- 2) $\kappa(A^T A) = \kappa(A)^2$, i.e.,

the cond. number of $A^T A$ is much worse than that of A in general.

→ This example is a bit extreme... Show previous Julia example
Ex. Forming $A^T A$ is bad.

$$A = \begin{bmatrix} 1 & 1 \\ \varepsilon & 0 \\ 0 & \varepsilon \end{bmatrix}, \text{ say } \varepsilon = 10^{-8} \text{ in double precision floating point sys.}$$

$$\text{Then } A^T A = \begin{bmatrix} 1 + \varepsilon^2 & 1 \\ 1 & 1 + \varepsilon^2 \end{bmatrix}$$

$$\approx \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \text{ because } \varepsilon^2 = 10^{-16}$$

How about the condition numbers?

$$\kappa(A) \approx 1.4142 \times 10^8 \text{ already bad.}$$

$$\kappa(A^T A) \approx +\infty \text{ in double precision.}$$

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If we set $\varepsilon = 10^{-7}$ instead of 10^{-8} ,
then $\kappa(A) \approx 1.4142 \times 10^7$

$$\kappa(A^T A) \approx 1.9903 \times 10^{14}$$

This is still too bad to get any
reliable LS solution for such A .

Often such situations occur
when some of the column vectors
of A are "close to parallel", i.e.,
they become almost linearly dependent.

Def. Let $A \in \mathbb{R}^{m \times n}$. Then

A is called **rank deficient** if
 $\text{rank}(A) < \min(m, n)$.

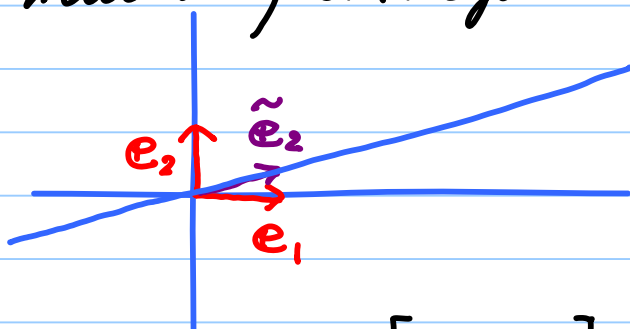
i.e., if A is **not** of full rank.

In general, we should avoid
computing a solution for a given
LS problem by forming $A^T A$ explicitly
and computing $(A^T A)^{-1} A^T b$.

⇒ Better to use the methods
based on **QR decomposition** or
SVD (we'll discuss these later
in this course.)

Orthogonality

The above discussion should convince you that A is quite "good" if its column vectors are mutually orthogonal.



Suppose $A = [e_1 \ e_2]$, $\tilde{A} = [e_1 \ \tilde{e}_2]$ in $\mathbb{R}^2$. You can see that A is much more "well-balanced" and convenient than $\tilde{A}$. For example, suppose we want to represent $x = [1, 1]^T$ in the basis of $\{e_1, e_2\}$ and that of $\{e_1, \tilde{e}_2\}$. Then the coefficient of x w.r.t. $\{e_1, e_2\}$ is the same as x itself since $A^{-1}x = Ax = x$ $A = I$ in $\mathbb{R}^2$

But $\tilde{A}^{-1}x$ behaves badly.

Why? Say $c = \tilde{A}^{-1}x$, $c = [c_1, c_2]^T$

$$\begin{aligned} \text{Then } x &= \tilde{A}c = [e_1 \ \tilde{e}_2] \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} \\ &= c_1 e_1 + c_2 \tilde{e}_2 \end{aligned}$$

$$\begin{aligned} \text{But } x &= e_1 + e_2, \text{ i.e.,} \\ e_1 + e_2 &= c_1 e_1 + c_2 \tilde{e}_2 \end{aligned}$$

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Taking an inner product with $\mathbf{e}_2$ on both sides yields

$$\begin{aligned} \underbrace{\mathbf{e}_2^T (\mathbf{e}_1 + \mathbf{e}_2)}_{\substack{\parallel \\ \mathbf{e}_2^T \mathbf{e}_2 \\ \parallel \\ \|\mathbf{e}_2\|_2^2 = 1}} &= \underbrace{\mathbf{e}_2^T (c_1 \mathbf{e}_1 + c_2 \tilde{\mathbf{e}}_2)}_{\substack{\parallel \\ c_1 \underbrace{\mathbf{e}_2^T \mathbf{e}_1}_{=0} + c_2 \mathbf{e}_2^T \tilde{\mathbf{e}}_2 \\ \parallel \\ c_2 \mathbf{e}_2^T \tilde{\mathbf{e}}_2}} \end{aligned}$$

$$\Rightarrow 1 = c_2 \mathbf{e}_2^T \tilde{\mathbf{e}}_2$$

$$\Rightarrow c_2 = \frac{1}{\mathbf{e}_2^T \tilde{\mathbf{e}}_2}$$

could be huge if $\tilde{\mathbf{e}}_2$ is close to perpendicular to $\mathbf{e}_2$, i.e., close to parallel to $\mathbf{e}_1$!!

★ Orthogonal Vectors

Def. • Two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^m$ are said to be **orthogonal** if $\mathbf{x}^T \mathbf{y} = 0$. So, the zero vector $\mathbf{0}$ is **orthogonal to any vector**.

- Two sets of vectors X, Y are said to be **orthogonal** if $\forall \mathbf{x} \in X, \forall \mathbf{y} \in Y, \mathbf{x}^T \mathbf{y} = 0$.
- A set of vectors S is said to be **orthogonal** if $\forall \mathbf{x} \in S, \forall \mathbf{y} \in S, \mathbf{x} \neq \mathbf{y}, \mathbf{x}^T \mathbf{y} = 0$.

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- A set of vectors S is said to be **orthonormal** if S is orthogonal and $\forall x \in S, \quad \underline{\|x\|_2 = 1}$.

even more balanced!

Thm The vectors in an orthogonal set S are linearly independent.

(Proof) Let $S = \{v_1, \dots, v_n\}$

Suppose they are not lin. indep.

Then $\exists v_k \in S$ s.t. $v_k \neq 0$ and

$$v_k = \sum_{\substack{i=1 \\ i \neq k}}^n c_i v_i \quad \text{with } c \neq 0$$
$$c = [c_1, \dots, c_{k-1}, c_{k+1}, \dots, c_n]^T$$

Since S is an orthogonal set,

$$v_j^T v_i = 0 \quad \text{for } v_j \neq v_i.$$

$$\text{But } v_k^T \left(\sum_{\substack{i=1 \\ i \neq k}}^n c_i v_i \right) = \sum_{\substack{i=1 \\ i \neq k}}^n c_i \underbrace{v_k^T v_i}_{=0} = 0$$

$$\Leftrightarrow v_k^T v_k = 0$$

$$\Leftrightarrow \|v_k\|^2 = 0 \Leftrightarrow v_k = 0 \quad \# \text{ contradiction!}$$

★ Components of a vector

SLOGAN "Inner products can be used to decompose arbitrary vectors into orthogonal components!"

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Suppose $\{ \mathbf{g}_1, \dots, \mathbf{g}_n \} \subset \mathbb{R}^m$ is an orthonormal set. $\mathbf{g}_j \in \mathbb{R}^m, 1 \leq j \leq n$.

Let $\mathbf{v}$ be an arbitrary vector in $\mathbb{R}^m$.

$$\mathbf{r} = \mathbf{v} - (\mathbf{g}_1^T \mathbf{v}) \mathbf{g}_1 - (\mathbf{g}_2^T \mathbf{v}) \mathbf{g}_2 - \dots - (\mathbf{g}_n^T \mathbf{v}) \mathbf{g}_n$$

$\mathbf{r}$ residual vector is $\perp$ to $\{ \mathbf{g}_1, \dots, \mathbf{g}_n \}$
why?

$$\begin{aligned} \mathbf{g}_j^T \mathbf{r} &= \mathbf{g}_j^T \mathbf{v} - (\mathbf{g}_1^T \mathbf{v}) \underbrace{\mathbf{g}_j^T \mathbf{g}_1}_{=0} - \dots - (\mathbf{g}_{j-1}^T \mathbf{v}) \underbrace{\mathbf{g}_j^T \mathbf{g}_{j-1}}_{=0} \\ &\quad - (\mathbf{g}_j^T \mathbf{v}) \underbrace{\mathbf{g}_j^T \mathbf{g}_j}_{=1} - (\mathbf{g}_{j+1}^T \mathbf{v}) \underbrace{\mathbf{g}_j^T \mathbf{g}_{j+1}}_{=0} - \dots - (\mathbf{g}_n^T \mathbf{v}) \underbrace{\mathbf{g}_j^T \mathbf{g}_n}_{=0} \\ &= \mathbf{g}_j^T \mathbf{v} - \mathbf{g}_j^T \mathbf{v} = 0 \end{aligned}$$

This is true for any $j=1, \dots, n$

$$\begin{aligned} \Rightarrow \mathbf{v} &= \mathbf{r} + \sum_{i=1}^n (\mathbf{g}_i^T \mathbf{v}) \mathbf{g}_i \\ \text{any vector in } \mathbb{R}^m &= \mathbf{r} + \sum_{i=1}^n (\mathbf{g}_i \mathbf{g}_i^T) \mathbf{v} \\ &= \mathbf{r} + \mathbf{Q} \mathbf{Q}^T \mathbf{v} \end{aligned}$$

where $\mathbf{Q} := [\mathbf{g}_1 \dots \mathbf{g}_n] \in \mathbb{R}^{m \times n}$

If $\{ \mathbf{g}_1, \dots, \mathbf{g}_n \}$ is a basis of $\mathbb{R}^m$,

then $n=m$ and $\mathbf{r} = \mathbf{0}$

$$\text{i.e., } \mathbf{v} = \sum_{i=1}^m (\mathbf{g}_i^T \mathbf{v}) \mathbf{g}_i = \sum_{i=1}^m (\mathbf{g}_i^T \mathbf{g}_i) \mathbf{v}$$

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In fact, $v = Q Q^T v$, i.e.,

$$\underline{Q Q^T = I}$$

Def. A square matrix $Q \in \mathbb{R}^{m \times m}$ is said to be **orthogonal** if

$$\underline{Q^T = Q^{-1}}$$

↑ should be called orthonormal

$$\text{i.e., } Q^T Q = Q Q^T = I$$

Note: If $Q = [q_1 \dots q_n] \in \mathbb{R}^{m \times n}$ with $\underline{m > n}$ and these vectors are orthonormal, then it is always true that $Q^T Q = I_{n \times n}$ but $Q Q^T \neq I_{m \times m}$ unless $m = n$

e.g.,

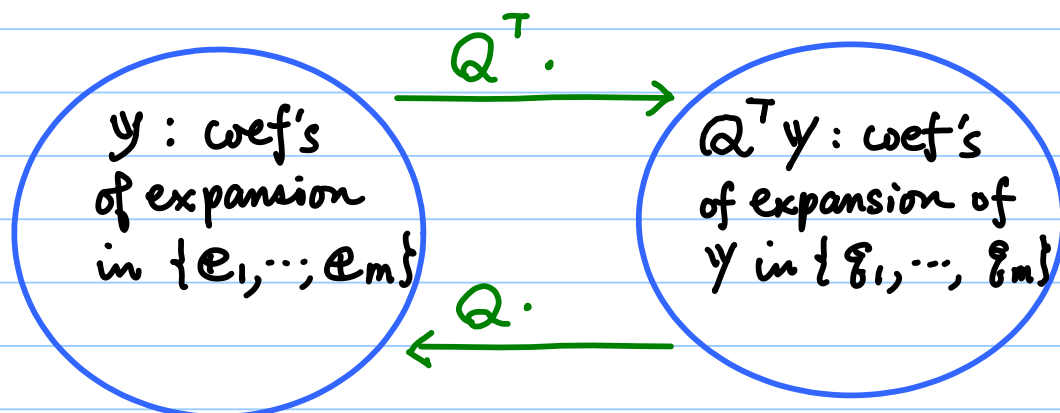
$$Q = \begin{bmatrix} 1/\sqrt{3} & 1/\sqrt{2} \\ 1/\sqrt{3} & 0 \\ 1/\sqrt{3} & -1/\sqrt{2} \end{bmatrix} \text{ then } Q^T Q = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I_{2 \times 2}$$

$$\begin{aligned} \text{But, } Q Q^T &= \begin{bmatrix} 1/\sqrt{3} & 1/\sqrt{2} \\ 1/\sqrt{3} & 0 \\ 1/\sqrt{3} & -1/\sqrt{2} \end{bmatrix} \begin{bmatrix} 1/\sqrt{3} & 1/\sqrt{3} & 1/\sqrt{3} \\ 1/\sqrt{2} & 0 & -1/\sqrt{2} \end{bmatrix} \\ &= \begin{bmatrix} 5/6 & 1/3 & -1/6 \\ 1/3 & 1/3 & 1/3 \\ -1/6 & 1/3 & 5/6 \end{bmatrix} \neq I_{3 \times 3} \end{aligned}$$

Why? $\Rightarrow$ Next lecture on Orthogonal Projector.

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★ Multiplication by an ortho. matrix



Note that $\|y\| = \|Q^T y\|$!
 i.e., **isometry**!

why?

$$\begin{aligned}
 \|Q^T y\|^2 &= (Q^T y)^T (Q^T y) \\
 &= y^T \underbrace{Q Q^T}_{= I} y \\
 &= y^T y = \|y\|^2 !!
 \end{aligned}$$

Compare this with the general situation we discussed before: $A \in \mathbb{R}^{m \times m}$, nonsingular

