Least Squares

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julia> c=V\temp
4-element Vector{
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When V is invertible this means solve
$$Vc = \text{temp}$$
for c.

What about when V is not invertible?

Minimize $\|Vc - \text{temp}\|_2$

Review Math 330 Solving $Ax = b$, $f(x) = b$

$A \in \mathbb{R}^{m\times n}$: $f(x) = Ax$ $f: \mathbb{R}^n \to \mathbb{R}^m$

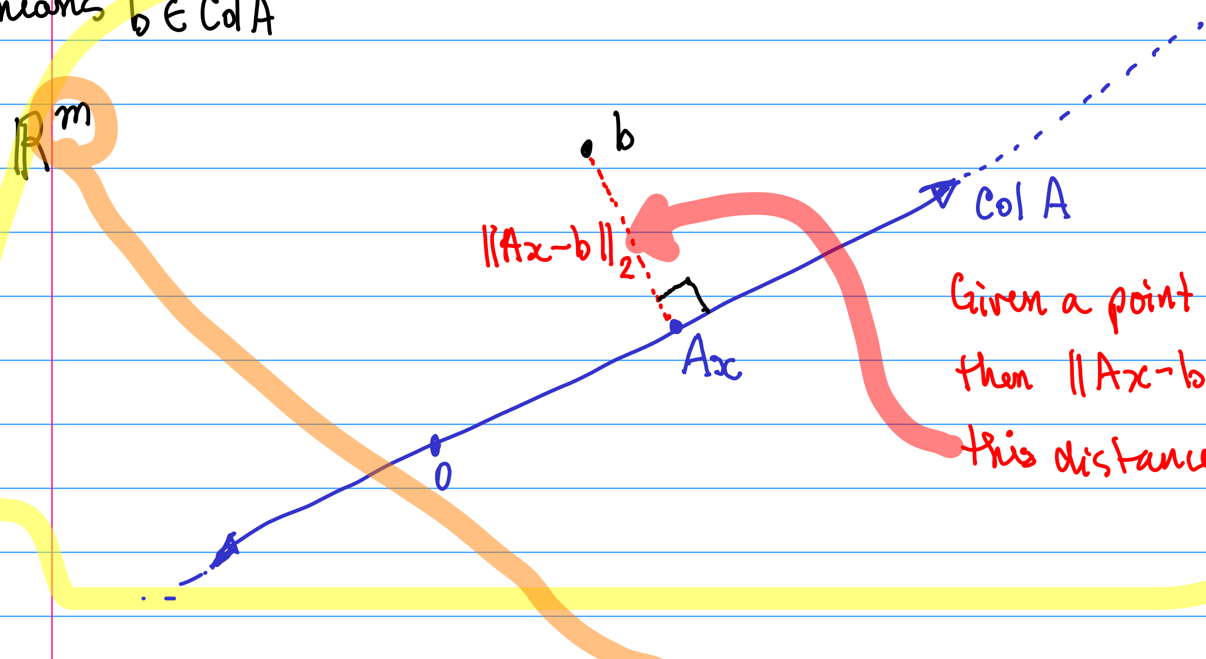
$\text{Col}\, A = \text{range}\, f = \{Ax : x \in \mathbb{R}^n\} \subseteq \mathbb{R}^m$

subspace... means that if $a, b \in \text{Col}\, A$ then $a+b \in \text{Col}\, A$

$m \in \mathbb{R}$ and $a \in \text{Col}\, A$ then $ma \in \text{Col}\, A$

implies $0 \in \text{Col}\, A$.

If I can solve $Ax = b$, that means $b \in \text{Col}\, A$



Given a point $Ax \in \text{Col}\, A$ then $\|Ax - b\|_2$ is this distance

When using Euclidean distance $\|x\| = \sqrt{x \cdot x} = \sqrt{x_1^2 + x_2^2 + \cdots + x_m^2}$ we have a notion of angles and perpendicular.

Need the vector $Ax - b$ to be perpendicular to any other vector Au in $\text{Col} A$.

Thus I want

$$(Ax-b) \cdot Au = 0 \quad \text{for all } u \in \mathbb{R}^n.$$

$$Au \cdot (Ax-b) = 0$$

$$(Au)^T(Ax-b) = 0$$

$$u^T A^T (Ax-b) = 0$$

$$u^T (A^T A x - A^T b) = 0$$

$$u \cdot (A^T A x - A^T b) = 0 \quad \text{for all } u \in \mathbb{R}^n$$

Therefore $\quad A^T A x - A^T b = 0$

Normal equations for solving least squares

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

note $A^T A$ is invertible if the column of A were linearly independent.

$A \in \mathbb{R}^{m \times n}$, $\quad A^T \in \mathbb{R}^{n \times m}$

$$\underset{n \times \cancel{m}}{A^T} \; \underset{\cancel{m} \times n}{A} \in \mathbb{R}^{n \times n}$$

So there are at least as many rows as columns

this condition implies there is a pivot when doing Gaussian elimination in each column of A.

Thus $m \geq n$

Solved in linear algebra $A^TAx = A^Tb$ using augmented Matrix

$$\left[\, A^TA \;\vdots\; A^Tb \,\right]$$ convert to reduced echelon form and read off solution x

Algebraically $$x = \underbrace{(A^TA)^{-1}A^T}_{\text{left pseudo inverse of } A.} b$$

suppose $m >> n$ then $A^TA \in \mathbb{R}^{n \times n}$ is smaller than A was...

Difficulty is A^TA may have a large condition number and even computing A^TA may involve lots of rounding error...

Theorem 3.2.9 : Condition number in the normal equations

If $\mathbf{A}$ is $m \times n$ with $m > n$, then

$$\kappa(\mathbf{A}^T\mathbf{A}) = \kappa(\mathbf{A})^2. \qquad (3.2.4)$$

The condition number is the square of $k(A)$

If you square a large number it gets very large...

$$K(A) = \|A\|_2 \|A^{-1}\|_2 \qquad \|A\|_2 = \max\{\|Ax\|_2 : \|x\|_2 = 1\}$$

Since $I = AA^{-1}$ and $\|I\|_2 = \max\{\|\cancel{I}x\|_2 : \|x\|_2 = 1\} = 1$

also $\|AA^{-1}\| \leq \|A\|\|A^{-1}\|$. Thus $K(A) \geq 1$.

Don't solve the normal equations on a computer because they are not well conditioned...

QR factorization: $A = QR$

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

Two kinds of QR factorizations

has orthonormal columns

upper triangular, and if columns of A were linearly independent then R is invertible...

Reduced QR factorization $\underset{m\times n}{A} = \underset{m\times n}{\tilde{Q}}\ \underset{n\times n}{\tilde{R}}$

$\tilde{Q}$ naturally comes from A using Gram-Schmidt orthogonalization. R is the multipliers in the column operations used.

That's why dimensions of $\tilde{Q}$ are the same as A.

orthogonal columns but also square, so it orthogonal matrix.

Full QR factorization $\underset{m\times n}{A} = \underset{m\times m}{Q}\ \underset{m\times n}{R}$ still upper triangular with lots of zeros in it.

$$Q = \begin{bmatrix} \underset{m\times n}{\tilde{Q}} & \vdots & ? \end{bmatrix} \qquad R = \begin{bmatrix} \tilde{R} \\ \hdashline 0 \end{bmatrix}$$

this could be any way of adding more columns to $\tilde{Q}$ to make it square while preserving the orthonormality of the columns.

$$QR = \begin{bmatrix} \underset{m\times n}{\tilde{Q}} & \vdots & ? \end{bmatrix} \begin{bmatrix} \tilde{R} \\ \hdashline 0 \end{bmatrix} = \begin{bmatrix} \tilde{Q}\tilde{R} + ?\,0 \end{bmatrix} = \tilde{Q}\tilde{R} = A$$

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

$$(\tilde{Q}\tilde{R})^T(\tilde{Q}\tilde{R})x = (\tilde{Q}\tilde{R})^T b$$

$$\tilde{R}^T \cancel{\tilde{Q}^T}\,\cancel{\tilde{Q}}\,\tilde{R}x = \tilde{R}^T\tilde{Q}^T b$$

$$\cancel{\tilde{R}^T}\,\tilde{R}x = \cancel{\tilde{R}^T}\,\tilde{Q}^T b$$

Since $\tilde{R}$ is invertible so is $\tilde{R}^T$.

Cancelling the $\tilde{R}^T$ here algebraically means not so much rounding error

Thus $\tilde{R}x = \tilde{Q}^T b$

Moreover triangular matrices are well conditioned, So no conditioning problem when solving for x.