$$\underbrace{\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & a_{m3} & \cdots & a_{mn} \end{bmatrix}_{m\times n}}_{A} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix}_{n\times 1}}_{x} = \underbrace{\begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}_{m\times 1}}_{b}$$

CX1104: **Linear Algebra for Computing**

Chap. No : **7.1.3A**

Lecture : **Least Squares**

Topic : **Least Squares**

Concept : **Supplementary –** Proving Solutions of Normal Equation are Least Square Solutions

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TAs: **Zhang Su, Vishal Choudhari**

Rev: 2nd July 2020

Proving Solutions of Normal Equation are Least Square Solutions

The set of least-squares solutions of $A\mathbf{x} = \mathbf{b}$ coincides with the nonempty set of solutions of the normal equations $A^TA\mathbf{x} = A^T\mathbf{b}$.

Proofs by:

1. Gilbert Strang, MIT (2 Proofs)
2. Jeffrey Chasnov, HKUST
3. Alex Townsend, MIT
4. Alexey Grigorev
5. Quora

Gilbert Strang (Proof 1)

In Strang's Lecture 15 video, Strang: 18.06

Projection onto Subspace

https://youtu.be/Y_Ac6KiQ1t0?t=951

1. 3-D, projecting a point b onto a plane span by A's columns (2-D) (18:50)
   - Vector b is not in the plane (span by A's columns). (Fig a)
   - What is that plane? (19:40)
     - The plane is span by columns of A: a_1 and a_2 and hence, form the basis for the subspace.
     - The columns of A are independent, and need NOT be perpendicular.
   - (22:20) $e = b - p$ (is orthogonal to the plane of A) (crucial fact)

2. What is small p (the projected vector of b on subspace spanned by A's columns)?
   - 23:45: p is some linear combination of columns of A. (Fig b)
   - $p = A\hat{x}$, we are looking for $\hat{x}$ such that error vector e is orthogonal to plane.

3. Now e is orthogonal to the column space of A. (26:00)
   - We have 2 equations to solve for 2 unknowns (fig c)
   - Reducing it to $A^T(b - A\hat{x}) = 0$ (fig d) -> The normal equation

Fig (a)

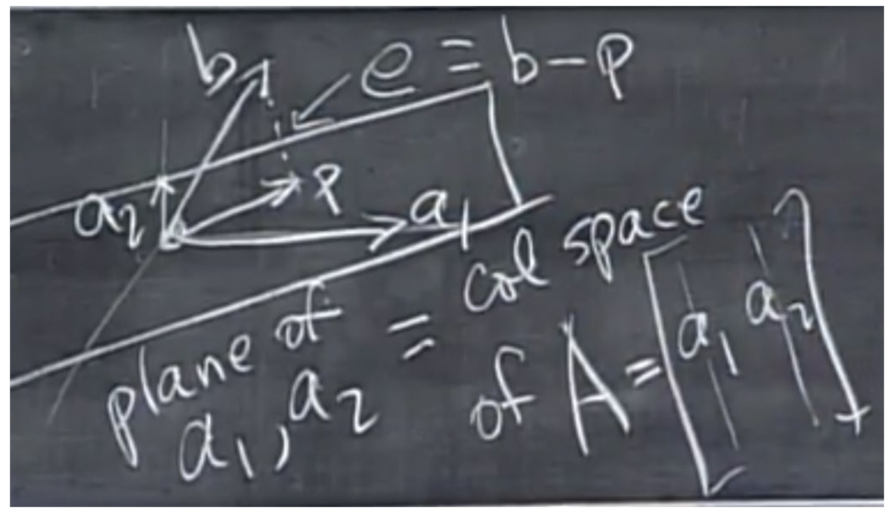


Fig (b)

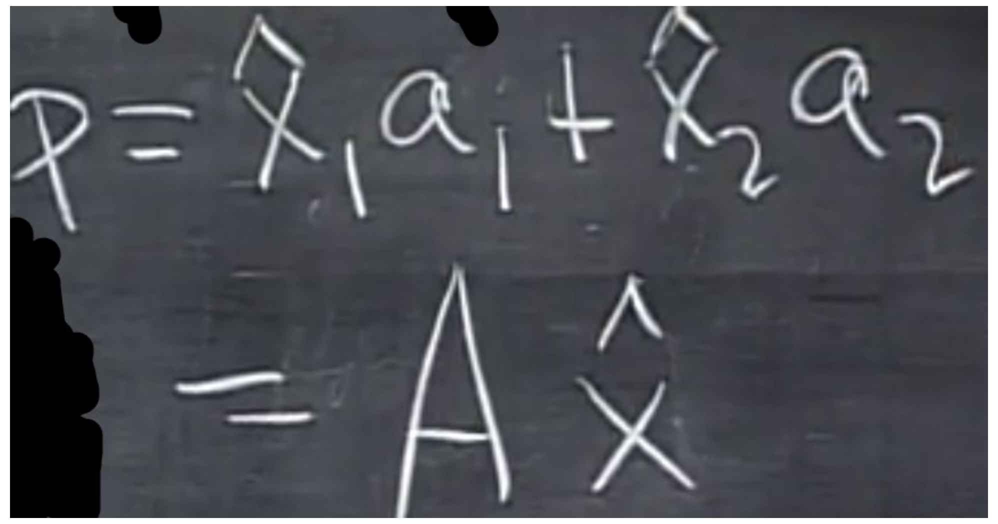


Fig (c)

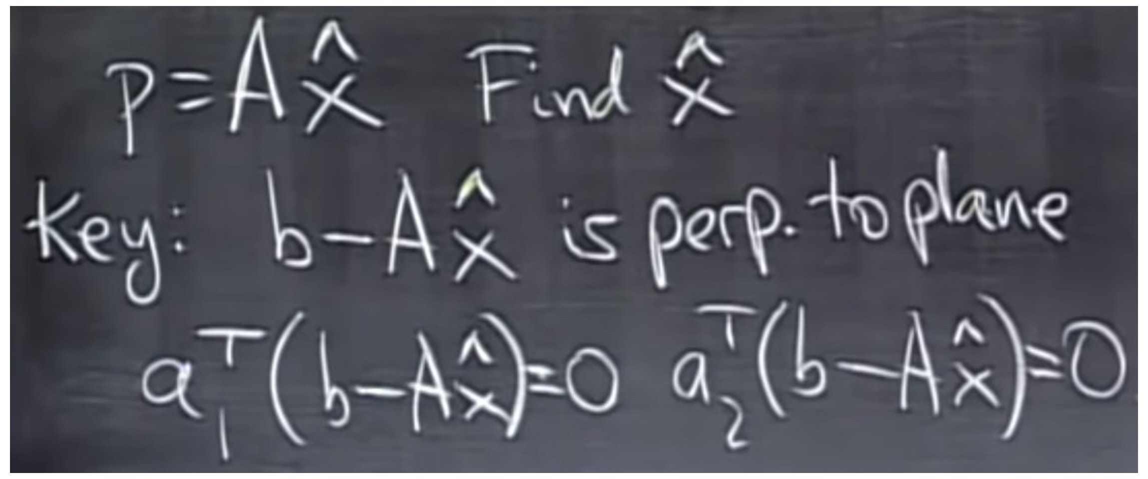
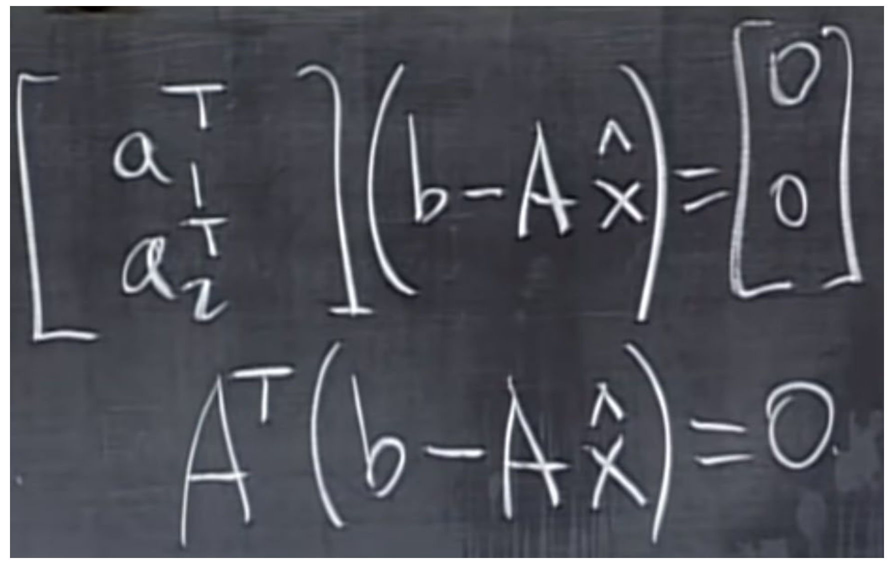
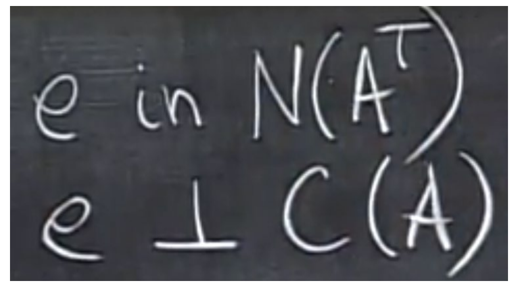


Fig (d)





Gilbert Strang (Proof 2 - Using Dot Product)

Projections onto subspaces

Projections

If we have a vector **b** and a line determined by a vector **a**, how do we find tl point on the line that is closest to **b**?

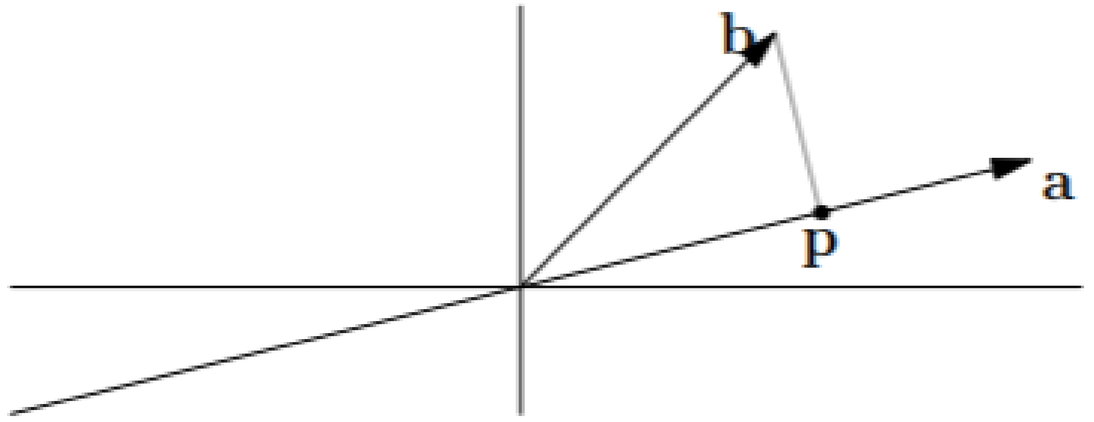


Figure 1: The point closest to **b** on the line determined by **a**.

We can see from Figure 1 that this closest point **p** is at the intersectio formed by a line through **b** that is orthogonal to **a**. If we think of **p** as a approximation of **b**, then the length of $\mathbf{e} = \mathbf{b} - \mathbf{p}$ is the error in that approx mation.

We could try to find **p** using trigonometry or calculus, but it's easier to u linear algebra. Since **p** lies on the line through **a**, we know $\mathbf{p} = x\mathbf{a}$ for son number x. We also know that **a** is perpendicular to $\mathbf{e} = \mathbf{b} - \mathbf{xa}$:

$$\begin{aligned} \mathbf{a}^T(\mathbf{b} - x\mathbf{a}) &= 0 \\ x\mathbf{a}^T\mathbf{a} &= \mathbf{a}^T\mathbf{b} \\ x &= \frac{\mathbf{a}^T\mathbf{b}}{\mathbf{a}^T\mathbf{a}}, \end{aligned}$$

and $\mathbf{p} = \mathbf{a}x = \mathbf{a}\frac{\mathbf{a}^T\mathbf{b}}{\mathbf{a}^T\mathbf{a}}$. Doubling **b** doubles **p**. Doubling **a** does not affect **p**.

Why project?

As we know, the equation $A\mathbf{x} = \mathbf{b}$ may have no solution. The vector $A\mathbf{x}$ is always in the column space of A, and **b** is unlikely to be in the column space. So, we project **b** onto a vector **p** in the column space of A and solve $A\hat{\mathbf{x}} = \mathbf{p}$.

Projection in higher dimensions

In $\mathbb{R}^3$, how do we project a vector **b** onto the closest point **p** in a plane?

If $\mathbf{a}_1$ and $\mathbf{a}_2$ form a basis for the plane, then that plane is the column space of the matrix $A = \begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 \end{bmatrix}$.

We know that $\mathbf{p} = \hat{x}_1\mathbf{a}_1 + \hat{x}_2\mathbf{a}_2 = A\hat{\mathbf{x}}$. We want to find $\hat{\mathbf{x}}$. There are many ways to show that $\mathbf{e} = \mathbf{b} - \mathbf{p} = \mathbf{b} - A\hat{\mathbf{x}}$ is orthogonal to the plane we're projecting onto, after which we can use the fact that **e** is perpendicular to $\mathbf{a}_1$ and $\mathbf{a}_2$:

$$\mathbf{a}_1^T(\mathbf{b} - A\hat{\mathbf{x}}) = 0 \quad \text{and} \quad \mathbf{a}_2^T(\mathbf{b} - A\hat{\mathbf{x}}) = 0.$$

In matrix form, $A^T(\mathbf{b} - A\hat{\mathbf{x}}) = \mathbf{0}$. When we were projecting onto a line, A only had one column and so this equation looked like: $a^T(\mathbf{b} - x\mathbf{a}) = \mathbf{0}$.

Note that $\mathbf{e} = \mathbf{b} - A\hat{\mathbf{x}}$ is in the nullspace of A^T and so is in the left nullspace of A. We know that everything in the left nullspace of A is perpendicular to the column space of A, so this is another confirmation that our calculations are correct.

We can rewrite the equation $A^T(\mathbf{b} - A\hat{\mathbf{x}}) = \mathbf{0}$ as:

$$A^TA\hat{\mathbf{x}} = A^T\mathbf{b}.$$

When projecting onto a line, A^TA was just a number; now it is a square matrix. So instead of dividing by $\mathbf{a}^T\mathbf{a}$ we now have to multiply by $(A^TA)^{-1}$

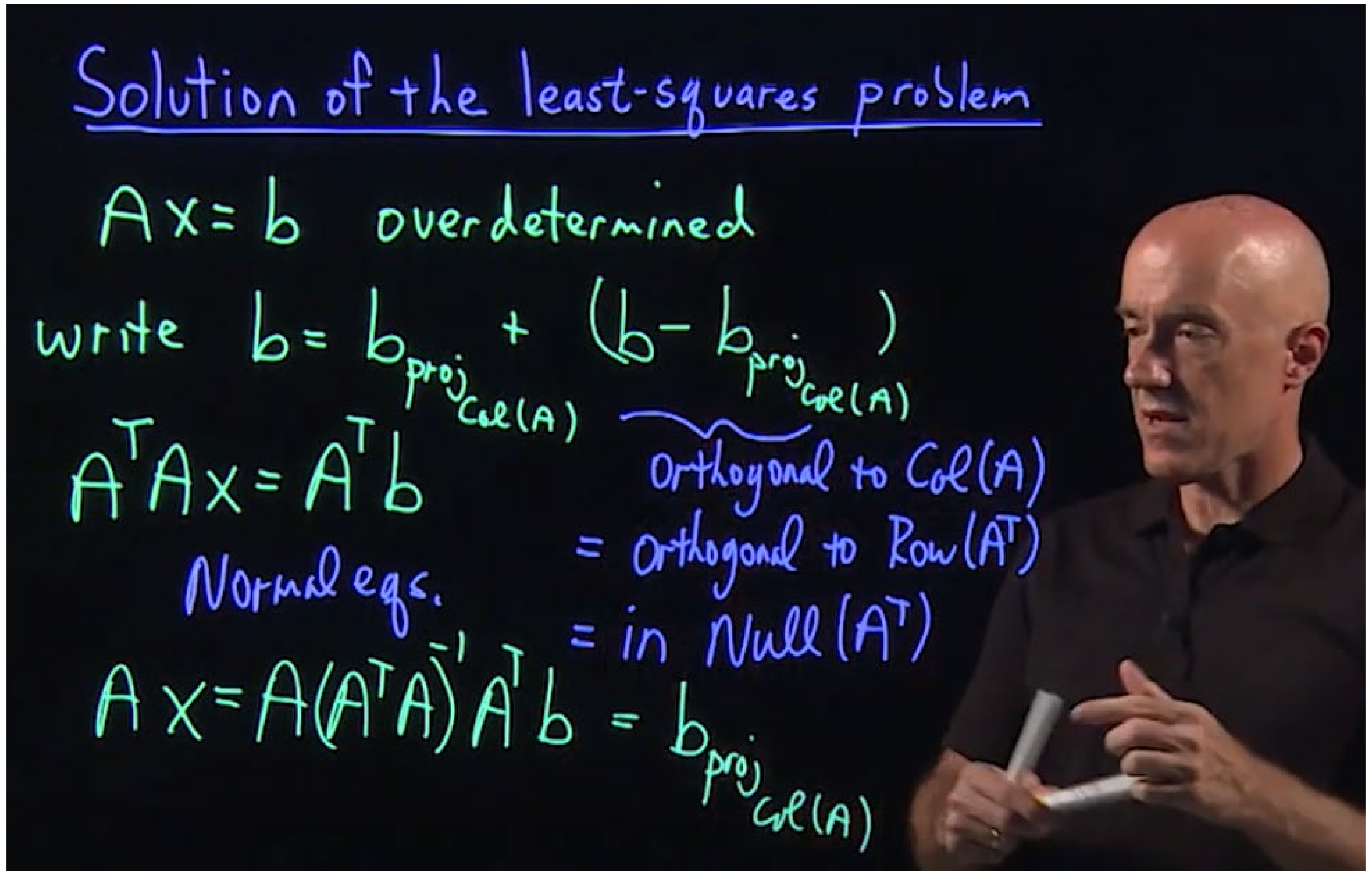
In n dimensions,

$$\begin{aligned} \hat{\mathbf{x}} &= (A^TA)^{-1}A^T\mathbf{b} \\ \mathbf{p} = A\hat{\mathbf{x}} &= A(A^TA)^{-1}A^T\mathbf{b} \\ P &= A(A^TA)^{-1}A^T. \end{aligned}$$

Ref: Lecture Writeup
https://ocw.mit.edu/courses/mathematics/18-06sc-linear-algebra-fall-2011/least-squares-determinants-and-eigenvalues/projections-onto-subspaces/MIT18_06SCF11_Ses2.2sum.pdf

Jeffrey Chasnov

If you understand Strang's proof,
Chasnov repeats it in the first 4 minutes.



Ref: https://www.youtube.com/watch?v=WABC6wmuLOk

Alex Townsend

Townsend's slide:
https://math.mit.edu/classes/18.085/summer2016/handouts/LeastSquares.pdf

Another way to show the same thing:
- https://theclevermachine.wordpress.com/2012/09/01/derivation-of-ols-normal-equations/
- https://sites.math.washington.edu/~burke/crs/308/LeastSquares.pdf

Online tool to perform differentiation of matrix:
http://www.matrixcalculus.org/

Matrix calculus reference (Advance):
- https://atmos.washington.edu/~dennis/MatrixCalculus.pdf
- https://www.comp.nus.edu.sg/~cs5240/lecture/matrix-differentiation.pdf
- https://www.math.uwaterloo.ca/~hwolkowi/matrixcookbook.pdf

NORMAL EQUATIONS:

$$A^T Ax = A^T b$$

Why the normal equations? To find out you will need to be slightly crazy and totally comfortable with calculus.

In general, we want to minimize[1]

$$f(x) = \|b - Ax\|_2^2 = (b - Ax)^T(b - Ax) = b^T b - x^T A^T b - b^T Ax + x^T A^T Ax.$$

If x is a global minimum of f, then its gradient $\nabla f(x)$ is the zero vector. Let's take the gradient of f remembering that

$$\nabla f(x) = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}.$$

We have the following three gradients:

$$\nabla(x^T A^T b) = A^T b, \quad \nabla(b^T Ax) = A^T b, \quad \nabla(x^T A^T Ax) = 2A^T Ax.$$

To calculate these gradients, write out $x^T A^T b$, $b^T Ax$, and $x^T A^T Ax$, in terms of sums and differentiate with respect to $x_1, \ldots, x_n$ (this gets very messy).

Thus, we have

$$\nabla f(x) = 2A^T Ax - 2A^T b,$$

just like we saw in the example. We can solve $\nabla f(x) = 0$ or, equivalently $A^T Ax = A^T b$ to find the least squares solution. Magic.

Is this the global minimum? Could it be a maximum, a local minimum, or a saddle point? To find out we take the "second derivative" (known as the Hessian in this context):

$$Hf = 2A^T A.$$

Next week we will see that $A^T A$ is a positive semi-definite matrix and that this implies that the solution to $A^T Ax = A^T b$ is a global minimum of $f(x)$. Roughly speaking, $f(x)$ is a function that looks like a bowl.

Alexey Grigorev

Alexey Grigorev

A personal page

ML Wiki

Home   Page Info

Normal Equation

Contents [hide]

Projection onto Subspaces

Contents [hide]

Ref: http://mlwiki.org/index.php/Normal_Equation

Sometimes Quora has the Answer!

Terry Moore, PhD in statistics
Answered February 1, 2018

How complex is the proof / derivation of the normal equation in linear regression?

It's quite simple once you have learned how to differentiate vector equations. If you don't use vectors and matrices it can become a bit messy.

You can also do it by completing the square. I think this is more straightforward.

You have the model $y = X\beta + \epsilon$ where X is a matrix and the rest vectors. We want to minimise $\epsilon^T\epsilon$.

Now

$$\epsilon^T\epsilon = (y - X\beta)^T(y - X\beta) = y^Ty - y^TX\beta - \beta^TX^Ty + \beta^TX^TX\beta.$$

We want the terms containing β to be in the form $(\beta - k)^TA(\beta - k)$. Multiply this out: $\beta^TA\beta - k^TA\beta - \beta^TAk + k^TAk$.

This works if $A = X^TX$ and $Ak = X^Ty$, i.e. $X^TXk = X^Ty$, i.e. $k = (X^TX)^{-1}X^Ty$.

Thus

$$\epsilon^T\epsilon = (\beta - k)^TX^TX(\beta - k) + y^T(I - X(X^TX)^{-1}X^T)y.$$

The first term is zero (a minimum because it is the sum of squares of the components of $X(\beta - k)$) if $\beta = k = (X^TX)^{-1}X^Ty$. The term $y^T(I - X(X^TX)^{-1}X^T)y$ is the sum of squared residuals.

The normal equations come from this by multiplying $k = (X^TX)^{-1}X^Ty$ on the left by X^TX. Note that I assumed that the latter matrix is non-singular. If not it is possible to use a generalised inverse (G is a generalised inverse of A if $AGA = A$. Such an inverse always exists but is not unique except if it is an ordinary inverse.)

Yes, pretty trivial.

Ref: https://www.quora.com/How-complex-is-the-proof-derivation-of-the-normal-equation-in-linear-regression