

3.3 Projections and Least Squares

A system of equations $Ax = b$ has a solution iff $b \in C(A)$.

$$\begin{aligned}
 a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= b_1 \\
 a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n &= b_2 \\
 &\vdots \\
 a_{m1}x_1 + a_{m2}x_2 + \cdots + a_{mn}x_n &= b_m
 \end{aligned} \tag{1}$$

Equation (1) can be written as

$$\begin{pmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{m1} \end{pmatrix} x_1 + \begin{pmatrix} a_{12} \\ a_{22} \\ \vdots \\ a_{m2} \end{pmatrix} x_2 + \cdots + \begin{pmatrix} a_{1n} \\ a_{2n} \\ \vdots \\ a_{mn} \end{pmatrix} x_n = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{pmatrix}.$$

Let the co-efficient vector of x_i be a_i . Now, $b \in C(A)$, i.e., there exists c_1, c_2, \dots, c_n such

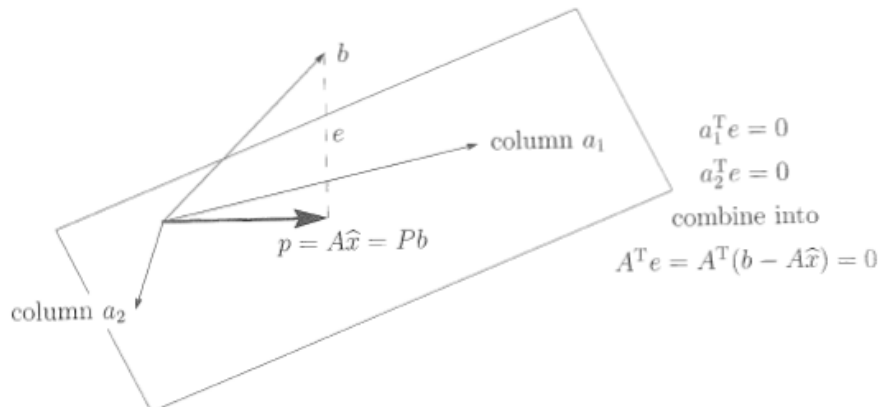
that $b = \sum_{i=1}^n c_i a_i$. Then for $x_i = c_i$, $x = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$ is a solution of (1).

If x is a solution of (1), then $c_i = x_i$, i.e., b is a linear combination of columns of A , i.e., $b \in C(A)$.

Consider a system of linear equations

$$Ax = b \tag{2}$$

with $b \notin C(A)$. Then (2) has no solution. Then one must choose \hat{x} a best fit solution of it.



As $b \notin C(A)$, let us obtain a column vector p in $C(A)$, which is the most closest vector of b in $C(A)$ such that the error $e = b - p$ is of minimum length .i.e., $\|e\|^2 = \|b - p\|^2$ is minimum. Hence it is called least square approximation.

$$\|e\|^2 \text{ is minimum}$$

$$\iff e \perp C(A)$$

$$\iff e \in N(A^T)$$

$$\iff A^T e = 0$$

$$\iff A^T(b - p) = 0$$

$$\iff A^T(b - A\hat{x}) = 0$$

$$\iff A^T b = A^T A\hat{x}$$

i.e., Normal equations $A^T A\hat{x} = A^T b$.

Best estimate: $\hat{x} = (A^T A)^{-1} A^T b$.

Projection $p = A\hat{x} = A(A^T A)^{-1} A^T b$.

Projection matrix $P = A(A^T A)^{-1} A^T$.

Remark 1 1. Suppose b is actually in the column space of A it is a combination $b = Ax$ of the columns. Then the projection of b is still b : b in column space

$$p = A(A^T A)^{-1} A^T Ax = Ax = b :$$

The closest point p is just b itself, which is obvious.

2. At the other extreme, suppose b is perpendicular to every column, so $A^T b = 0$. In this case b projects to the zero vector: b in left nullspace, i.e., $b \in N(A^T)$

$$p = A(A^T A)^{-1} A^T b = A(A^T A)^{-1} 0 = 0 :$$

3. When A is square and invertible, the column space is the whole space. Every vector projects to itself, p equals b , and $\hat{x} = x$: If A is invertible

$$p = A(A^T A)^{-1} A^T b = AA^{-1}(A^T)^{-1} A^T b = b :$$

This is the only case when we can take apart $(A^T A)^{-1}$, and write it as $A^{-1}(A^T)^{-1}$.

When A is rectangular that is not possible.

4. Suppose A has only one column, containing a . Then the matrix $A^T A$ is the number $a^T a$ and \hat{x} is $a^T b / a^T a$.

5. $A^T A$ has the same nullspace as A .

If $Ax = 0$, then $A^T Ax = 0$. Vectors x in the nullspace of A are also in the nullspace of $A^T A$. To go in the other direction, start by supposing that $A^T Ax = 0$, and take the inner product with x to show that $Ax = 0$:

$$x^T A^T Ax = 0 \Rightarrow \|Ax\|^2 = 0 \Rightarrow Ax = 0.$$

Hence, the two nullspaces are identical.

6. If A has independent columns, then $N(A^T A) = N(A) = \{0\}$.

7. If A has independent columns, then $A^T A$ is square, symmetric, and invertible.

Projection Matrices

$$\begin{aligned} P &= \text{Projection matrix, which projects a vector onto } C(A) \\ &= A(A^T A)^{-1} A^T \end{aligned}$$

i.e, $p = Pb$.

Note that

$$\begin{aligned} P^2 &= A(A^T A)^{-1} A^T A(A^T A)^{-1} A^T \\ &= A(A^T A)^{-1} (A^T A) (A^T A)^{-1} A^T \\ &= A(A^T A)^{-1} A^T \\ &= P \end{aligned}$$

and

$$\begin{aligned} P^T &= [A(A^T A)^{-1} A^T]^T \\ &= (A^T)^T [(A^T A)^{-1}]^T A^T \\ &= A(A^T A)^{-1} A^T \\ &= P. \end{aligned}$$

Suppose that A is invertible. Then,

$$\begin{aligned} P &= A(A^T A)^{-1} A^T \\ &= AA^{-1} (A^T)^{-1} A^T \\ &= I. \end{aligned}$$

Hence, $p = Pb = Ib = b$. Therefore, $\text{error} = p - b = 0$.

Exercise-3.3

1. Solve $Ax = b$ by least squares and find $p = A\hat{x}$, if $A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{pmatrix}$ and $b = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$.

Verify that the error $b - p$ is perpendicular to the columns of A .

Solution:

$$\begin{aligned}\hat{x} &= (A^T A)^{-1} A^T b \\ &= \frac{1}{3} \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{3} \\ \frac{1}{3} \end{pmatrix}\end{aligned}$$

and

$$\begin{aligned}P &= A\hat{x} \\ &= (A^T A)^{-1} A^T b \\ &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{3} \\ \frac{1}{3} \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{3} \\ \frac{1}{3} \\ \frac{2}{3} \end{pmatrix}.\end{aligned}$$

$$\text{Here, Error} = b - p = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} - \begin{pmatrix} \frac{1}{3} \\ \frac{1}{3} \\ \frac{2}{3} \end{pmatrix} = \begin{pmatrix} \frac{2}{3} \\ \frac{2}{3} \\ -\frac{2}{3} \end{pmatrix}.$$

$b - p$ is perpendicular to the column of the matrix.

$$(b-p)^T C_1 = \begin{pmatrix} \frac{2}{3} & \frac{2}{3} & -\frac{2}{3} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} = \frac{2}{3} - \frac{2}{3} = 0 \text{ and}$$

$$(b-p)^T C_2 = \begin{pmatrix} \frac{2}{3} & \frac{2}{3} & -\frac{2}{3} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} = \frac{2}{3} - \frac{2}{3} = 0.$$

4. The following system has no solution: $Ax = \begin{pmatrix} 1 & -1 \\ 1 & 0 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} 4 \\ 5 \\ 9 \end{pmatrix} = b.$

Sketch and solve a straight-line fit that leads to the minimization of the quadratic $(C - D - 4)^2 + (C - 5)^2 + (C + D - 9)^2$. What is the projection of b onto the column space of A ?

Solution:

$$\begin{aligned} \hat{x} &= (A^T A)^{-1} A^T b \\ &= \begin{pmatrix} \frac{1}{3} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 \\ -1 & 0 & 1 \end{pmatrix} \begin{pmatrix} 4 \\ 5 \\ 9 \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 4 \\ 5 \\ 9 \end{pmatrix} \\ &= \begin{pmatrix} 6 \\ 5 \\ \frac{2}{2} \end{pmatrix}. \end{aligned}$$

Now,

$$\begin{aligned} P &= A\hat{x} \\ &= \begin{pmatrix} 1 & -1 \\ 1 & 0 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 6 \\ 5 \\ \frac{2}{2} \end{pmatrix} \\ &= \begin{pmatrix} \frac{7}{2} \\ 6 \\ \frac{17}{2} \end{pmatrix}. \end{aligned}$$

Assignments

Exercise-3.3, Q. 2,9,12,24.