MATH-UA 140 - Linear Algebra

Lecture 16: Least Squares Approximations

The purpose of this lecture is to show how linear algebra can be used to find the best fit of a model for a given set of data points. This is of course useful in all fields of science, social sciences, economics, etc.

We start with a relatively simple situation, namely fitting a line to a set of three points, and generalize from there.

I] Fitting a straight line

1) Set up of the problem

Imagine someone made a measurement at 3 different times, $t_1=0$, $t_2=1$, and $t_3=2$, and found the value $b_1=1$ at t_1, $b_2=0$ at t_2, and $b_3=2$ at t_3. The person knows that the phenomenon under study should follow the linear law $b=Ct+D$, and would like to find C and D that best match the data.

It is clear that there does not exist values for C and D for which all three points are on the line.

Here is a linear algebra way to see this. Applying $b=Ct+D$ to each data point, we get the following system for C and D:

$$\begin{cases} D = 1 \\ C + D = 0 \\ 2C + D = 2 \end{cases}$$

This system has more equations than unknowns, and the equations are not compatible with one another, so the system does not have solutions.

Let $A = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 2 & 1 \end{bmatrix}$, $\vec{x} = \begin{bmatrix} C \\ D \end{bmatrix}$, $\vec{b} = \begin{bmatrix} 1 \\ 0 \\ 2 \end{bmatrix}$

$A\vec{x} = \vec{b}$ is not solvable, because $\vec{b}$ is not in $C(A)$. Still, one may still look for a C and a D such that the distance from the data points to the line is minimized.

In the language of linear algebra, we want to make the error $\vec{e} = \vec{b} - A\vec{x}$ as small as possible by finding the optimal $\hat{\vec{x}}$.

2) Minimizing the error

Let us split $\vec{b}$ into $\vec{p}$ in $C(A)$ plus $\vec{e}$ in $N(A^T)$ (the letters $\vec{p}$ and $\vec{e}$ are chosen on purpose here, as we will soon see). $\vec{b} = \vec{p} + \vec{e}$

$A\vec{x} = \vec{b}$ does not have a solution, as we saw. However, $A\hat{\vec{x}} = \vec{p}$ does, since $\vec{p} \in C(A)$.

Furthermore, $\hat{\vec{x}}$ is precisely the vector which minimizes $\| A\vec{x} - \vec{b} \|^2$ as small as possible.

Indeed, $\|A\vec{x}-\vec{b}\|^2 = (A\vec{x}-\vec{b})\cdot(A\vec{x}-\vec{b})$

$$= (A\vec{x}-\vec{p}-\vec{e})\cdot(A\vec{x}-\vec{p}-\vec{e})$$

$$= \Big[(A\vec{x}-\vec{p})\cdot(A\vec{x}-\vec{p}) - 2\underbrace{\underbrace{\vec{e}}_{\text{in } N(A^T)}\cdot\underbrace{(A\vec{x}-\vec{p})}_{\text{in } C(A)}}_{\Rightarrow\, =0} + \vec{e}\cdot\vec{e}\Big]$$

$$= \|A\vec{x}-\vec{p}\|^2 + \|\vec{e}\|^2$$

No choice of $\vec{x}$ will change $\vec{e}$. However, by choosing $\vec{x}$ to be the solution $\hat{\vec{x}}$ to $A\hat{\vec{x}} = \vec{p}$, we can at least set the first term to 0. This is the way to minimize $\|A\vec{x}-\vec{b}\|^2$.

The least squares solution $\hat{\vec{x}}$ makes $E = \|A\vec{x}-\vec{b}\|$ as small as possible.

From the previous lecture, we know that $\vec{p}$ here is the projection of $\vec{b}$ onto $C(A)$, so we know that the equation for $\hat{\vec{x}}$ is

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

Returning to our example, $A^TA = \begin{bmatrix} 0 & 1 & 2 \\ 1 & 1 & 1 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 2 & 1 \end{bmatrix} = \begin{bmatrix} 5 & 3 \\ 3 & 3 \end{bmatrix}$

$$A^T\vec{b} = \begin{bmatrix} 0 & 1 & 2 \\ 1 & 1 & 1 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \\ 2 \end{bmatrix} = \begin{bmatrix} 4 \\ 3 \end{bmatrix}$$

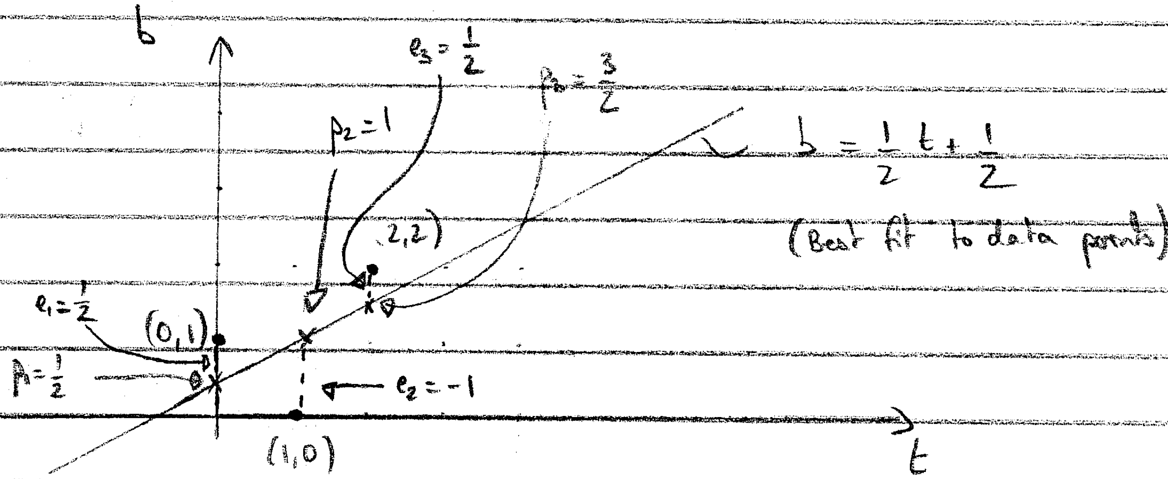
The augmented matrix to find $\hat{\vec{x}}$ is $\begin{bmatrix} 5 & 3 & 4 \\ 3 & 3 & 3 \end{bmatrix}$

$$\rightarrow \begin{bmatrix} 5 & 3 & 4 \\ 0 & \frac{6}{5} & \frac{3}{5} \end{bmatrix} \rightarrow \begin{bmatrix} 1 & \frac{3}{5} & \frac{4}{5} \\ 0 & 1 & \frac{1}{2} \end{bmatrix}$$

$$\longrightarrow \begin{bmatrix} 1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \end{bmatrix}$$

We conclude that the best fit is given by $\hat{\vec{x}} = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}$

which means the line $b = \frac{1}{2}t + \frac{1}{2}$. See figure below:



We can compute $A\hat{\vec{x}} = \begin{bmatrix} \frac{1}{2} \\ 1 \\ \frac{3}{2} \end{bmatrix} = \vec{p}$, so $\vec{e} = \vec{b} - A\hat{\vec{x}} = \begin{bmatrix} \frac{1}{2} \\ -1 \\ \frac{1}{2} \end{bmatrix}$

$\vec{p}$ gives the height of the line at t_1, t_2, and t_3, and $\vec{e}$ measures the difference between $\vec{b}$ and $\vec{p}$, so it corresponds to the vertical dashed line in the figure.

- Geometric viewpoint

Here is another way to understand what we have just done: $A\vec{x}$ lies in the plane spanned by $C(A)$, i.e $\begin{bmatrix} 0 \\ 1 \\ 2 \end{bmatrix}$ and $\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$. In that plane, we look for the point closest to $\vec{b}$; as we saw in the last lecture, this is $\vec{p}$. So the best choice for $\vec{x}$ is $\hat{\vec{x}}$ such that $A\hat{\vec{x}} = \vec{p}$

3) Fitting a straight line: general case

In most applications, we are in fact fitting a line to a very large number m of data points $b_1, \ldots, b_m$ corresponding to times $t_1, \ldots, t_m$. The system of equations for C and D in $b = Ct + D$ is:

$$\begin{cases} Ct_1 + D = b_1 \\ Ct_2 + D = b_2 \\ \vdots \\ Ct_{m-1} + D = b_{m-1} \\ Ct_m + D = b_m \end{cases} \iff A\vec{x} = \vec{b} \text{ with } A = \begin{bmatrix} t_1 & 1 \\ t_2 & 1 \\ \vdots & \vdots \\ t_{m-1} & 1 \\ t_m & 1 \end{bmatrix}, \vec{x} = \begin{bmatrix} C \\ D \end{bmatrix}$$

$$\text{and } \vec{b} = \begin{bmatrix} b_1 \\ \vdots \\ \vdots \\ b_m \end{bmatrix}$$

When $\vec{b}$ is not in the column space of A, which is very likely since A is so tall and so thin, the best one can do is look for $\hat{x} = \begin{bmatrix} C \\ D \end{bmatrix}$ which minimizes $\|\vec{b} - A\vec{x}\|^2$

Following the same arguments as in the previous section, one would find that $\hat{x}$ satisfies

$$\underline{A^T A \hat{\vec{x}} = A^T \vec{b}}$$

The components p_i of $\vec{p} = A\hat{\vec{x}}$ give the heights of the line $Ct + D$ for each t_i, and the error is $e_i = b_i - p_i = b_i - Ct_i - D$

Let us now see how it actually looks in practice

$$A^T A = \begin{bmatrix} t_1 & \cdots & t_m \\ 1 & \cdots & 1 \end{bmatrix} \begin{bmatrix} t_1 & 1 \\ \vdots & \vdots \\ t_m & 1 \end{bmatrix} = \begin{bmatrix} \sum_i t_i^2 & \sum_i t_i \\ \sum_i t_i & m \end{bmatrix}$$

where $\sum_i t_i$ means sum of all t_i, and $\sum_i t_i^2$ means sum of all t_i^2. $\sum$ is the symbol for sum.

$$A^T \vec{b} = \begin{bmatrix} t_1 & \cdots & t_m \\ 1 & \cdots & 1 \end{bmatrix} \begin{bmatrix} b_1 \\ \vdots \\ b_m \end{bmatrix} = \begin{bmatrix} \sum_i b_i t_i \\ \sum_i b_i \end{bmatrix}$$

We can state the general result:

The line $Ct + D$ which is the best fit to $\vec{b} = (b_1, \ldots, b_m)$ measured at time $t_1, \ldots, t_m$ is given by

$$\begin{bmatrix} \sum_i t_i^2 & \sum_i t_i \\ \sum_i t_i & m \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} \sum_i b_i t_i \\ \sum_i b_i \end{bmatrix}$$

- Observe that when the measurement times t_i add to zero, i.e $\sum_i t_i = 0$, $A^T A$ becomes $\begin{bmatrix} \sum_i t_i^2 & 0 \\ 0 & m \end{bmatrix}$: it is diagonal! Then C and D can be solved immediately:

$$C = \frac{\sum_i b_i t_i}{\sum_i t_i^2}, \quad D = \frac{\sum_i b_i}{m}$$

This is really convenient!
What is beautiful is that it is always possible to reduce a problem to this situation. Here is how it works:

A) Compute the average time $\bar{t} = \frac{\sum_i t_i}{m}$

B) Define the shifted times $T_i = t_i - \bar{t}$

Note that $\sum_i T_i = \sum_i t_i - \sum_i \bar{t} = m\bar{t} - \bar{t}\sum_i 1 = m\bar{t} - m\bar{t} = 0$

so for these times T_i, A^TA is diagonal, and we can write

$$C = \frac{\sum_i b_i T_i}{\sum_i T_i^2}, \quad D = \frac{\sum_i b_i}{m}$$

The line corresponding to the best fit is $CT + D = Ct + D - C\bar{t}$

II) Fitting by a parabola

If one would like to fit a curve to the trajectory followed by a golf ball, a straight line is most likely not a good approximation, except perhaps locally. A parabola, on the other hand, is likely to be a better approximation. The good thing is that much of what we have learned caries over to this case.

Imagine we have $m > 3$ measurements $b_1, \ldots, b_m$ at times $t_1, \ldots, t_m$ and we would like to fit the data with the parabola $b = Ct^2 + Dt + E$
The system of equations is as follows:

$$\begin{cases} Ct_1^2 + Dt_1 + E = b_1 \\ \vdots \\ Ct_m^2 + Dt_m + E = b_m \end{cases} \iff A\vec{x} = \vec{b} \text{ with } A = \begin{bmatrix} t_1^2 & t_1 & 1 \\ \vdots & \vdots & \vdots \\ t_m^2 & t_m & 1 \end{bmatrix}$$

$$\vec{x} = \begin{bmatrix} C \\ D \\ E \end{bmatrix} \text{ and } \vec{b} = \begin{bmatrix} b_1 \\ \vdots \\ b_m \end{bmatrix}$$

In general, the system does not have a solution. But we can look for $\hat{x} = \begin{bmatrix} C \\ D \\ E \end{bmatrix}$ which minimizes $\|A\hat{x} - \vec{b}\|^2$.

It is given by $\underline{A^T A \hat{\vec{x}} = A^T \vec{b}}$

QUESTION: Consider the points $(0,1)$, $(1,0)$, $(2,2)$ and $(3,3)$. Give the equation of the parabola corresponding to the best fit of these points.

III] The big picture

Let us look at what the computation of the least squares approximation means in the context of the orthogonal subspaces.

* The columns of A are independent, so its nullspace is the zero vector $\{\vec{0}\}$

* In general, $\vec{b}$ is not in the column space of A, so $A\vec{x} = \vec{b}$ does not have a solution

* We can however split $\vec{b}$ into $\vec{b} = \vec{p} + \vec{e}$, with $\vec{p}$ in $C(A)$ and e in $N(A^T)$

* Then there exists an $\hat{\vec{x}}$ in $\mathbb{R}^n$, which is $C(A^T)$ since $N(A)=\{\vec{0}\}$, such that $A\hat{\vec{x}} = \vec{p}$

$\hat{\vec{x}}$ is the vector in $C(A^T)$ minimizing $\|A\vec{x} - \vec{b}\|^2$.

This can be represented with the following figure: