# Least Squares Method MATH 3512, BCIT

Matrix Methods and Statistics for Geomatics

October 12, 2018

The projection  $u_H$  of a vector u onto a hyperplane H is the vector in the hyperplane that is "most similar" to u. The formal definition for  $u_H$  requires that

- $\mathbf{0}$  u is in H
- $(u u_H)$  is orthogonal to all basis vectors of H

**Example 1: Finding a Projection.** Let H be the line spanned by  $\vec{v} = (-1, 1)^{\mathsf{T}}$  in  $\mathbb{R}^2$ . What is the projection  $\vec{w}$  of  $\vec{u} = (3, -2)^{\mathsf{T}}$ ?



Let  $\vec{w} = (w_1, w_2)^{\mathsf{T}}$ . Then (1)  $\vec{u} - \vec{w}$  is orthogonal to  $\vec{v}$  and (2)  $\vec{w} = \alpha \vec{v}$  for some  $\alpha \in \mathbb{R}$ .

$$\begin{array}{rcl}
 w_1 & - & w_2 & = & 5 \\
 w_1 & + & w_2 & = & 0
 \end{array}$$
 (1)

Cramer's rule tells us that  $\vec{w} = (2.5, -2.5)^{T}$ .

Let  $u = (u_1, ..., u_n)^{\mathsf{T}}$  be a vector and H be a k-dimensional hyperplane in the vector space  $\mathbb{R}^n$ . Let  $x_1, ..., x_k$  be a basis for H. Then it is true for all vectors v in the hyperplane that

$$||u-v|| \ge ||u-u_H||$$
 (2)

Proof: use the theorem of Pythagoras for

$$||u - v||^2 = ||u - u_H||^2 + ||u_H - v||^2 \ge ||u - u_H||^2$$
 (3)

The claim follows. It illustrates what I mean when I say that  $u_H$  is the vector in H that is most similar to u.

**Example 2: Finding Another Projection.** What is the projection of  $\vec{u} = (5, 2, 10)^{\mathsf{T}}$  onto the plane T characterized by 2x + y + 3z = 0?

First we find two linearly independent vectors in H to form a basis of H, for example  $\vec{v_1} = (1,1,-1)^{\mathsf{T}}$  and  $\vec{v_2} = (0,-3,1)^{\mathsf{T}}$ . The conditions

- $\mathbf{0}$   $u_H \in T$
- ②  $(u u_H) \perp v_1$
- **③**  $(u u_H) ⊥ v_2$

give us the system of linear equations

$$\begin{bmatrix} 2 & 1 & 3 \\ -1 & 1 & 1 \\ 0 & 3 & -1 \end{bmatrix} \cdot \begin{bmatrix} \hat{x} \\ \hat{y} \\ \hat{z} \end{bmatrix} = \begin{bmatrix} 0 \\ 3 \\ -4 \end{bmatrix} \tag{4}$$

for which the solution is  $u_H = (\hat{x}, \hat{y}, \hat{z})^{\mathsf{T}} = (-1, -1, 1)^{\mathsf{T}}$ .

Let there be two linearly independent vectors u and v in  $\mathbb{R}^n$ . Then the formula for the projection  $u_v$  of u onto the line spanned by v is

$$u_{v} = \left(\frac{u \cdot v}{v \cdot v}\right) v \tag{5}$$

To verify the formula, note that  $u_v = av$  for some real number a. Therefore

$$(u-av)\perp v \tag{6}$$

Isolate a in the equation  $(u - av) \cdot v = 0$  to yield the formula.

Formula (5) only works when the hyperplane is a line. You can scale up the idea in terms of dimensions by the following theorem.

#### Formula for Projection Onto Plane with Orthogonal Basis

Let  $\{u, v\}$  be an orthogonal basis for H. Then the projection of w onto H is the sum of  $w_u$  and  $w_v$ , the projections of w onto the lines spanned by u and v, respectively.

Proof: check the following

- ②  $(w (w_u + w_v)) \perp u$  (use the fact that  $u \perp v$ )

Consider the following table of measurements for the length of shoe prints and the height of the person wearing the shoes.

Shoe Print (cm)	Height (cm)		
29.7	175.3		
29.9	177.8		
31.4	185.4		
31.8	175.3		
27.6	172.7		

In the statistics portion of this course, we will learn whether the paired data provide evidence of a linear relationship. In the linear algebra portion, we will learn how to find the line which is closest to the data points in the least squares sense.



#### Least Squares Method

If L is a given line, the error for each data point is the vertical distance from that point to the line. The squared error is the sum of the squares of the errors. The line that best fits the data in the least squares sense is the line that minimizes the squared error.

You can find the regression line using calculus optimization. However, there is also an elegant method using linear algebra.

Let L be a line with slope m and y-intercept b. Let  $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$  be a set of paired data. Then the following equations hold:

$$y_{1} = mx_{1} + b + \epsilon_{1}$$

$$y_{2} = mx_{2} + b + \epsilon_{2}$$

$$\vdots$$

$$y_{n} = mx_{n} + b + \epsilon_{n}$$

$$(7)$$

where the  $\epsilon_i$  are the errors (i = 1, ..., n). This system is equivalent to the following vector equation,

$$Y = AV + E \tag{8}$$

where Y, A, V, E are defined on the next slide.

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, A = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix}, V = \begin{bmatrix} m \\ b \end{bmatrix}, E = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

E is called the error vector. According to (8), it is

$$E = Y - AV \tag{9}$$

We are trying to choose m, b so that

$$||E||^2 = ||Y - AV||^2 \tag{10}$$

is minimal.

Let

$$X = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \text{ and } B = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$
 (11)

Then AV = mX + bB. The set  $S = \{AV | m, b \in \mathbb{R}\}$  is a plane in n-dimensional space. The ordered pair (m, b) that minimizes the squared error corresponds to the projection  $Y_S$  of Y onto S.

Let C be  $B - B_X$ , where  $B_X$  is the projection of B onto the line spanned by X. Then

$$C = B - \left(\frac{B \cdot X}{X \cdot X}\right) X \tag{12}$$

Note that  $X \perp C$ . X and C form an orthogonal basis for S. We have chosen C by a process called successive orthogonal selection. Consequently,

$$Y_S = Y_X + Y_C = \left(\frac{Y \cdot X}{X \cdot X}\right) X + \left(\frac{Y \cdot C}{C \cdot C}\right) C$$
 (13)

Replace the rightmost C by  $B - \left(\frac{B \cdot X}{X \cdot X}\right) X$  for

$$Y_{S} = \left(\frac{Y \cdot X}{X \cdot X} - \left(\frac{Y \cdot C}{C \cdot C}\right) \left(\frac{B \cdot X}{X \cdot X}\right)\right) X + \left(\frac{Y \cdot C}{C \cdot C}\right) B \qquad (14)$$

or alternatively

$$m = \frac{Y \cdot X}{X \cdot X} - \left(\frac{Y \cdot C}{C \cdot C}\right) \left(\frac{B \cdot X}{X \cdot X}\right) \tag{15}$$

$$b = \frac{Y \cdot C}{C \cdot C} \tag{16}$$

with

$$C = B - \left(\frac{B \cdot X}{X \cdot X}\right) X \tag{17}$$

**Example 3: Shoe Print and Height.** Recall

Shoe Print (cm)	Height (cm)		
29.7	175.3		
29.9	177.8		
31.4	185.4		
31.8	175.3		
27.6	172.7		

Which regression line best represents a possible linear relationship between shoe print and height? In this case, the shoe print is the independent variable x, on the basis of which we are trying to predict the dependent variable y, the height.

$$X = \begin{bmatrix} 29.7 \\ 29.9 \\ 31.4 \\ 31.8 \\ 27.6 \end{bmatrix}, Y = \begin{bmatrix} 175.3 \\ 177.8 \\ 185.4 \\ 175.3 \\ 172.7 \end{bmatrix}, B = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$
(18)

Calculate C using the formula

$$C = B - \left(\frac{B \cdot X}{X \cdot X}\right) X = \begin{bmatrix} 0.0150340 \\ 0.0084012 \\ -0.0413445 \\ -0.0546101 \\ 0.0846780 \end{bmatrix}$$
(19)

Now calculate m and b

$$m = \frac{Y \cdot X}{X \cdot X} - \left(\frac{Y \cdot C}{C \cdot C}\right) \left(\frac{B \cdot X}{X \cdot X}\right) = 1.7528 \tag{20}$$

$$b = \frac{Y \cdot C}{C \cdot C} = 124.58 \tag{21}$$



**Example 4: Angles at Gray Cliff.** This example is from Oscar S. Adams's *Application of the Theory of Least Squares to the Adjustment of Triangulation* (1915), a "working manual for the computer in the office." You measure the following angles.

from	to	angle
Boulder	Tower	65°6′29.3″
Tower	Tyonek	19°46′26.9″
Tyonek	Round Point	8°39′14.2″
Round Point	Boulder	266°27′47.9″

Notice that the angles do not add up to  $360^{\circ}$ . We are missing 1.7''. How should we adjust these numbers?

Basic assumptions underlying least squares theory in surveying are

- mistakes and systematic errors have been eliminated
- the number of observations being adjusted is large
- the frequency distribution of the errors is normal

Convert the angles to real numbers

$$\hat{a} = 65.108, \hat{b} = 19.774, \hat{c} = 8.6539, \hat{d} = 266.46$$
 (22)

The sum is 359.999527778. Here is a system of equations with measurement errors, exploiting the fact that d is supposed to be  $360^{\circ} - (a + b + c)$ 

$$\begin{array}{rcl}
a & = & 65.108 + \epsilon_1 \\
b & = & 19.774 + \epsilon_2 \\
c & = & 8.6539 + \epsilon_3 \\
360 - (a+b+c) & = & 266.46 + \epsilon_4
\end{array} \tag{23}$$

The system of equations is equivalent to the following matrix equation.

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ -1 & -1 & -1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 65.108 \\ 19.774 \\ 8.6539 \\ -93.537 \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \end{bmatrix}$$
(24)

In symbols,

$$AV = Y + E \tag{25}$$

Again, we want to minimize

$$||Y - AV||^2 = ||E||^2 \tag{26}$$

The minimization is achieved by projecting Y onto the hyperplane S

$$a\begin{bmatrix} 1\\0\\0\\-1\end{bmatrix} + b\begin{bmatrix} 0\\1\\0\\-1\end{bmatrix} + c\begin{bmatrix} 0\\0\\1\\-1\end{bmatrix}$$
 (27)

These three vectors  $\alpha, \beta, \gamma$  form a basis of S, but the basis vectors are not orthogonal to each other. We will search for a different basis of S that is orthonormal by successive orthogonal selection.

Start with a non-zero vector  $b_1$  in S, for example  $b_1 = \alpha = (1, 0, 0, -1)^{\mathsf{T}}$ . This is our first basis vector. The second basis vector  $b_2$  must fulfill

- **1**  $b_2 \cdot b_1 = 0$  (which is equivalent to  $b_2 \perp b_1$ )
- ②  $b_2$  ∈ S

For example,  $b_2 = (1, -1, -1, 1)^{\mathsf{T}}$  qualifies. Follow the same procedure for  $b_3 = (0, 1, -1, 0)^{\mathsf{T}}$ .

Let  $Y_i$  be the projection of Y onto the line spanned by  $b_i$ , for example.

$$Y_{1} = \left(\frac{Y \cdot b_{1}}{b_{1} \cdot b_{1}}\right) b_{1} = \begin{bmatrix} 79.32242 \\ 0 \\ 0 \\ -79.32242 \end{bmatrix}$$
 (28)

Then the projection  $Y_5$  equals  $Y_1 + Y_2 + Y_3 =$ 

$$\begin{bmatrix} 79.32242 \\ 0 \\ 0 \\ -79.32242 \end{bmatrix} + \begin{bmatrix} -14.214 \\ 14.214 \\ 14.214 \\ -14.214 \end{bmatrix} + \begin{bmatrix} 0 \\ 5.56010 \\ -5.56010 \\ 0 \end{bmatrix} = \begin{bmatrix} 65.1083 \\ 19.7743 \\ 8.6541 \\ -93.5366 \end{bmatrix}$$

The least squares adjusted angles are  $65^{\circ}6'29.7'', 19^{\circ}46'27.3'', 8^{\circ}39'14.6''$  compared to the original  $65^{\circ}6'29.3'', 19^{\circ}46'26.9'', 8^{\circ}39'14.2''$ .

## Abigail, Ben, and Charlie

**Example 5: Abigail, Ben, and Charlie.** Here is an example adapted from Paul R. Wolf's *Survey Measurement Adjustments by Least Squares*. Abigail measures a length  $\overline{XY}$  to be 211.52 units. Ben measures a length  $\overline{YZ}$  to be 220.10 units. Charlie measures the length  $\overline{XZ}$  to be 431.71 units. What lengths should they report to their supervisor?

We will solve this problem three different ways.

- use calculus
- use projection
- use a matrix formula based on projection

# Abigail, Ben, and Charlie [Calculus]

Here are the three equations with errors:

$$a = 211.52 + \epsilon_1$$
  
 $b = 220.10 + \epsilon_2$  (29)  
 $a + b = 431.71 + \epsilon_3$ 

Define the function

$$F(a,b) = ||E||^2 = (a-211.52)^2 + (b-220.10)^2 + (a+b-431.71)^2 =$$

$$2a^2 + 2ab + 2b^2 - 1286.46a - 1303.62b + 279558.2445$$
 (30)

We want to minimize F. The partial derivatives are

$$\frac{\partial F}{\partial a} = 4a + 2b - 1286.46 \tag{31}$$

$$\frac{\partial F}{\partial b} = 2a + 4b - 1303.62 \tag{32}$$

# Abigail, Ben, and Charlie [Calculus]

Setting the partial derivatives to zero gives us the following system of linear equations.

$$\begin{bmatrix} 4 & 2 \\ 2 & 4 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1286.46 \\ 1303.62 \end{bmatrix}$$
 (33)

The solution is a=211.55, b=220.13 for Abigail and Ben's least squares adjusted measurements, compared to the original  $\hat{a}=211.52, \hat{b}=220.10$ . Charlie's measurement is adjusted from 431.71 to 431.68.

# Abigail, Ben, and Charlie [Projection]

Equation (29) translates into the following matrix equation.

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 211.52 \\ 220.10 \\ 431.71 \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \end{bmatrix}$$
(34)

or

$$AV = Y + E$$
 and therefore  $E = Y - AV$  (35)

# Abigail, Ben, and Charlie [Projection]

Find the projection  $Y_S$  of Y onto the hyperplane S defined by AV with free variables a, b.  $u = (1,0,1)^{\mathsf{T}}$  and  $v = (0,1,1)^{\mathsf{T}}$  are not orthogonal. Find the projection  $v_u$  of v onto the line spanned by u and define  $w = v - v_u$  (successive orthogonal selection).

$$w = v - v_u = v - \left(\frac{v \cdot u}{u \cdot u}\right) u = \begin{bmatrix} -\frac{1}{2} \\ 1 \\ \frac{1}{2} \end{bmatrix}$$
 (36)

Consequently,

$$Y_S = Y_u + Y_w = \left(\frac{Y \cdot u}{u \cdot u}\right) u + \left(\frac{Y \cdot w}{w \cdot w}\right) w = \begin{bmatrix} 211.55 \\ 220.13 \\ 431.68 \end{bmatrix}$$
(37)

The solution found by using projection agrees with the solution found by using calculus.

On a rainy day, you may not be in the mood to remember the projection procedure. You just want to use a formula. Here it is for Abigail, Ben, and Charlie:

$$V_0 = \begin{bmatrix} a \\ b \end{bmatrix} = (A^{\mathsf{T}}A)^{-1}A^{\mathsf{T}}Y = \begin{bmatrix} 211.55 \\ 220.13 \end{bmatrix}$$
 (38)

Why does this formula work?

Let  $V_0$  be the solution to the least squares problem,  $AV_0$  is the projection  $Y_S$  of Y onto the hyperplane S defined by AV when the variables in V are still free.  $Y-AV_0$  is orthogonal to S. S is the hyperplane  $\{AU|U$  is a vector with the right dimensions $\}$ . Consequently,

$$(Y - AV_0) \cdot AU = 0 \tag{39}$$

for some U with the right dimensions. Rewrite

$$Y \cdot AU = AV_0 \cdot AU \tag{40}$$

For column vectors u and v, it is generally true that  $u \cdot v = u^{\mathsf{T}} v$ . Also recall that for any two matrices A and B

$$(AB)^{\mathsf{T}} = B^{\mathsf{T}}A^{\mathsf{T}} \tag{41}$$

Using these two facts, continue with

$$Y \cdot AU = Y^{\mathsf{T}}AU = (A^{\mathsf{T}}Y)^{\mathsf{T}}U \tag{42}$$

and

$$AV_0 \cdot AU = (AV_0)^{\mathsf{T}} AU = (A^{\mathsf{T}} AV_0)^{\mathsf{T}} U \tag{43}$$

Combine (40), (42) and (43) for

$$(A^{\mathsf{T}}Y)^{\mathsf{T}}U = (A^{\mathsf{T}}AV_0)^{\mathsf{T}}U \tag{44}$$

Because this is true for all well-dimensioned vectors U, it must be true that

$$(A^{\mathsf{T}}Y)^{\mathsf{T}} = (A^{\mathsf{T}}AV_0)^{\mathsf{T}} \tag{45}$$

If  $A^{T}A$  is invertible (this can be shown to be true), it follows that

$$V_0 = (A^{\mathsf{T}}A)^{-1}A^{\mathsf{T}}Y \tag{46}$$

Now that we have a formula, let us return to the problem of shoe print and height.

Shoe Print (cm)	Height (cm)
29.7	175.3
29.9	177.8
31.4	185.4
31.8	175.3
27.6	172.7

The yave setup Y - AV = E is

$$\begin{bmatrix} 175.3 \\ 177.8 \\ 185.4 \\ 175.3 \\ 172.7 \end{bmatrix} - \begin{bmatrix} 29.7 & 1 \\ 29.9 & 1 \\ 31.4 & 1 \\ 31.8 & 1 \\ 27.6 & 1 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \end{bmatrix}$$
(47)

Use

$$V_0 = (A^{\mathsf{T}}A)^{-1}A^{\mathsf{T}}Y = \begin{bmatrix} 1.7528 \\ 124.5754 \end{bmatrix}$$
 (48)

As we already know, the slope m of the regression line is 1.7528 and the y-intercept b is 124.5754.

**Exercise 1:** Find the quadratic of best fit for the data

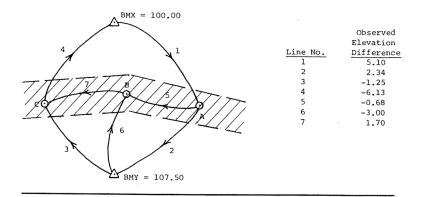
Х	0	1	2	3	4	
у	9.1	2.8	1.2	3.1	8.7	_

**Exercise 2:** At 6327 ft (or 6.327 thousand feet), Mario Triola recorded the temperature. Find the best predicted temperature at that altitude based on other measurements, assuming a linear relationship. How does the result compare to the actual recorded value of 48°F?

Altitude	3	10	14	22	28	31	33
Temperature	57	37	24	-5	-30	-41	-54

**Exercise 3:** You measure the four angles in a quadrilateral  $\hat{a} = 8.490426^{\circ}$ ,  $\hat{b} = 182.029154^{\circ}$ ,  $\hat{c} = 119.148088^{\circ}$ ,  $\hat{d} = 50.32948$ . What are the least squares adjusted measurements?

**Exercise 4:** Consider the following leveling network.



The objective is to determine elevations of A, B, and C, which are to serve as temporary project bench marks to control construction of a highway through the crosshatched corridor.

Obviously, it would have been possible to obtain elevations for *A*, *B*, and *C* by beginning at *BMX* and running a single closed loop consisting of only courses 1, 5, 7, and 4. Alternatively, a single closed loop could have been initiated at *BMY* and consist of courses 2, 5, 7, and 3.

However, by running all seven courses, redundancy is achieved that enables checks to be made, blunders to be isolated, and precision to be increased. Having run all seven courses, it would be possible to compute the adjusted elevation of B, for example, using several different single closed circuits. Loops 1-5-6, 2-5-6, 3-7-6, and 4-7-6 could each be used, but it is almost certain that each would yield a different elevation for B.

A more logical approach, which will produce only one adjusted value for *B*—its most probable one—is to use all seven courses in a simultaneous least squares adjustment. In adjusting level networks, the observed difference in elevation for each course is treated as one observation containing a single random error.

This single random error is the total of the individual random errors in backsight and foresight readings for the entire course. In the figure, the arrows indicate the direction of leveling. Thus, for course number 1, leveling proceeded from BMX to A and the observed elevation difference was +5.10 feet.

Try to find the equations yourself (before looking at the next slide to check if they are correct) and then calculate the least square adjusted elevations of A, B, and C.

The first set of equation for the seven courses is

$$A = BMX + 5.10 + \epsilon_{1}$$

$$BMY = A + 2.34 + \epsilon_{2}$$

$$C = BMY - 1.25 + \epsilon_{3}$$

$$BMX = C - 6.13 + \epsilon_{4}$$

$$B = A - 0.68 + \epsilon_{5}$$

$$B = BMY - 3.00 + \epsilon_{6}$$

$$C = B + 1.70 + \epsilon_{7}$$
(49)

The resulting yave setup is

$$A = 105.10 + \epsilon_{1}$$

$$A = 105.16 + \epsilon_{2}$$

$$C = 106.25 + \epsilon_{3}$$

$$C = 106.13 + \epsilon_{4}$$

$$A - B = 0.68 + \epsilon_{5}$$

$$B = 104.50 + \epsilon_{6}$$

$$B - C = -1.70 + \epsilon_{7}$$
(50)

#### End of Lesson

Next Lesson: Eigenvalues and Eigenvectors