Overdetermined Systems, Least Squares Fit

Suppose A is an $m \times n$ matrix and c is a $m \times 1$ column. If $m > n$, the system

$$Ax = c$$

is called overdetermined. There may be no exact solution. The method of Least Squares Fit is to find x which minimizes the length of $Ax - c$.

- The equations for x are $(A^T \cdot A) \cdot x = A^T \cdot c.$, These are called the "Normal Equations."

(**Ex 1**) A is a column: $A = \begin{bmatrix} 1 \\ 2 \\ 5 \end{bmatrix}$ and $c = \begin{bmatrix} 6 \\ 7 \\ 8 \end{bmatrix}$. We want the value of x that minimizes the length of the vector $Ax - c$. This will be the value of x that makes the vector $Ax - c$ perpendicular to the vector A. This happens when

$$\begin{aligned} A^T \cdot (Ax - c) &= 0 \\ A^T \cdot A \cdot x - A^T \cdot c &= 0 \\ A^T \cdot A \cdot x &= A^T \cdot c \end{aligned}$$

$A^T \cdot A = (1 \cdot 1 + 2 \cdot 2 + 5 \cdot 5) = 30;$ $\quad c = A^T \cdot c = (1 \cdot 6 + 2 \cdot 7 + 5 \cdot 8 = 60.$

The "normal equation" $A^T \cdot A \cdot x = A^T \cdot c$ becomes $30x = 60;$ $x = 2.$

Let L be the line through the origin in the direction of $\begin{bmatrix} 1 \\ 2 \\ 5 \end{bmatrix}$. The point on L closest to $\begin{bmatrix} 6 \\ 7 \\ 8 \end{bmatrix}$ is $\begin{bmatrix} 1 \\ 2 \\ 5 \end{bmatrix} \cdot 2 = \begin{bmatrix} 2 \\ 4 \\ 10 \end{bmatrix}$. The vector of errors is $E = \begin{bmatrix} 1 \\ 2 \\ 5 \end{bmatrix} \cdot 2 - \begin{bmatrix} 6 \\ 7 \\ 8 \end{bmatrix} = \begin{bmatrix} -2 \\ -3 \\ 2 \end{bmatrix}$

(**Ex 2**) Find the "best" solution to:
$$\begin{array}{rcrcr} -x_1 & + & x_2 & = & -2 \\ 0 & + & 2x_2 & = & 6 \\ x_1 & + & 3x_2 & = & 8 \end{array}$$

Here A is the 3×2 matrix $A = \begin{bmatrix} -1 & 1 \\ 0 & 2 \\ 1 & 3 \end{bmatrix}$ and $c = \begin{bmatrix} -2 \\ 6 \\ 8 \end{bmatrix}$.

We want the vector $x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ that makes the vector $Ax - c$ perpendicular to the plane containing the columns of A. That is $A^T \cdot (Ax - c) = 0$ which is $A^T \cdot A \cdot x = A^T \cdot c$

$$A^T \cdot A = \begin{bmatrix} -1 & 0 & 1 \\ 1 & 2 & 3 \end{bmatrix} \cdot \begin{bmatrix} -1 & 1 \\ 0 & 2 \\ 1 & 3 \end{bmatrix} = \begin{bmatrix} 2 & 2 \\ 2 & 14 \end{bmatrix}$$

and $A^T \cdot c = \begin{bmatrix} -1 & 0 & 1 \\ 1 & 2 & 3 \end{bmatrix} \cdot \begin{bmatrix} -2 \\ 6 \\ 8 \end{bmatrix} = \begin{bmatrix} 10 \\ 34 \end{bmatrix}$.

The normal equations are $\begin{bmatrix} 2 & 2 \\ 2 & 14 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 10 \\ 34 \end{bmatrix}$ The solution is $\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 3 \\ 2 \end{bmatrix}$

The vector of errors is $E = \begin{bmatrix} -1 & 1 \\ 0 & 2 \\ 1 & 3 \end{bmatrix} \cdot \begin{bmatrix} 3 \\ 2 \end{bmatrix} - \begin{bmatrix} -2 \\ 6 \\ 8 \end{bmatrix} = \begin{bmatrix} -1 \\ 4 \\ 9 \end{bmatrix} - \begin{bmatrix} -2 \\ 6 \\ 8 \end{bmatrix} = \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}$

(**Ex 3**)) Find the equation of the form $y = b + mt$ which best fits the data:

t	0	2	4
y	2.9	4.2	4.9

We want b and m so that $\begin{array}{ccccc} b & + & 0m & = & 2.9 \\ b & + & 2m & = & 4.2 \\ b & + & 4m & = & 4.9 \end{array}$. This is an overdetermined system.

Here $A = \begin{bmatrix} 1 & 0 \\ 1 & 2 \\ 1 & 4 \end{bmatrix}$, $c = \begin{bmatrix} 2.9 \\ 4.2 \\ 4.9 \end{bmatrix}$. We want $x = \begin{bmatrix} b \\ m \end{bmatrix}$ that minimizes the vector $Ax - c$.

$A^T \cdot A = \begin{bmatrix} 1 & 1 & 1 \\ 0 & 2 & 4 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 \\ 1 & 2 \\ 1 & 4 \end{bmatrix} = \begin{bmatrix} 3 & 6 \\ 3 & 20 \end{bmatrix}$, and $A^T \cdot c = \begin{bmatrix} 1 & 1 & 1 \\ 0 & 2 & 4 \end{bmatrix} \cdot \begin{bmatrix} 2.9 \\ 4.2 \\ 4.9 \end{bmatrix} = \begin{bmatrix} 12 \\ 28 \end{bmatrix}$.

The normal equations are: $\begin{bmatrix} 3 & 6 \\ 3 & 20 \end{bmatrix} \cdot \begin{bmatrix} b \\ m \end{bmatrix} = \begin{bmatrix} 12 \\ 28 \end{bmatrix}$. The solution is $\begin{bmatrix} b \\ m \end{bmatrix} = \begin{bmatrix} 3 \\ 0.5 \end{bmatrix}$

The "best" line is $y = 3 + 0.5t$. The vector of errors is $E = \begin{bmatrix} 3 \\ 4 \\ 5 \end{bmatrix} - \begin{bmatrix} 2.9 \\ 4.2 \\ 4.9 \end{bmatrix} = \begin{bmatrix} 0.1 \\ -0.2 \\ 0.1 \end{bmatrix}$

(**Ex 4**) Find the equation of the form $y = Ae^{kt}$ which best fits the data:

t	1	2	4	7
y	12	14	22	41

Take logarithms of the y values to get

t	1	2	4	7
w	2.48	2.64	3.09	3.70

We want the line $w = b + mt$ which best fits this data.

We want b and m so that $\begin{array}{ccccc} b & + & 1m & = & 2.48 \\ b & + & 2m & = & 2.64 \\ b & + & 4m & = & 3.09 \\ b & + & 7m & = & 3.70 \end{array}$, an overdetermined system for b and m.

Here $A = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 4 \\ 1 & 7 \end{bmatrix}$, $c = \begin{bmatrix} 2.48 \\ 2.64 \\ 3.09 \\ 3.70 \end{bmatrix}$. Want $x = \begin{bmatrix} b \\ m \end{bmatrix}$ that minimizes the vector $Ax - c$.

$$A^T \cdot A = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 2 & 4 & 7 \end{bmatrix} \cdot \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 4 \\ 1 & 7 \end{bmatrix} = \begin{bmatrix} 4 & 14 \\ 14 & 70 \end{bmatrix}, \quad \text{and}$$

$$A^T \cdot w = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 4 & 7 \end{bmatrix} \cdot \begin{bmatrix} 2.48 \\ 2.64 \\ 3.09 \\ 3.70 \end{bmatrix} = \begin{bmatrix} 11.91 \\ 46.02 \end{bmatrix}.$$

The normal equations are $\begin{bmatrix} 4 & 14 \\ 14 & 70 \end{bmatrix} \cdot \begin{bmatrix} b \\ m \end{bmatrix} = \begin{bmatrix} 11.9 \\ 46.0 \end{bmatrix}$

The solution is $\begin{bmatrix} b \\ m \end{bmatrix} = \begin{bmatrix} 2.3 \\ 0.2 \end{bmatrix}$, (numbers rounded off).

The "best" line is $w = 2.3 + 0.2t$ The exponential is $y = e^{2.3}e^{0.2t} = 10e^{0.2t}$

(Ex 5) The table shows the length-weight relation for a species of Salmon. Find a power function $W = \alpha L^{\beta}$ which best fits the data.

L	0.5	1.0	2.0
W	1.77	10	56.6

Taking logarithms, we have $\ln(W) = \ln(\alpha) + \beta \ln(L)$. The change of variable is $w = \ln(W)$, $u = \ln(L)$, $b = \ln(\alpha)$. Taking logarithms of the L and the W values, we get

u	-.693	0	.693
w	.57	2.30	4.04

We want the line $w = b + mu$ which best fits this data.

To find b and m so that $\begin{array}{rcrcl} b & - & 0.693m & = & .57 \\ b & + & 0 & = & 2.30 \\ b & + & 0.693m & = & 4.04 \end{array}$, an overdetermined system

Here $A = \begin{bmatrix} 1 & -.693 \\ 1 & 0 \\ 1 & .693 \end{bmatrix}$, $c = \begin{bmatrix} .57 \\ 2.30 \\ 4.04 \end{bmatrix}$. Want $x = \begin{bmatrix} b \\ m \end{bmatrix}$ that minimizes the vector $Ax - c$.

$$A^T \cdot A = \begin{bmatrix} 1 & 1 & 1 \\ -.693 & 0 & .693 \end{bmatrix} \cdot \begin{bmatrix} 1 & -.693 \\ 1 & 0 \\ 1 & .693 \end{bmatrix} = \begin{bmatrix} 3 & 0 \\ 0 & .96 \end{bmatrix}, \text{ and}$$

$$A^T \cdot c = \begin{bmatrix} 1 & 1 & 1 \\ -.693 & 0 & .693 \end{bmatrix} \cdot \begin{bmatrix} .57 \\ 2.3 \\ 4.04 \end{bmatrix} = \begin{bmatrix} 6.91 \\ 2.40 \end{bmatrix}.$$

The normal equations are $\begin{bmatrix} 3 & 0 \\ 0 & .96 \end{bmatrix} \cdot \begin{bmatrix} b \\ m \end{bmatrix} = \begin{bmatrix} 6.91 \\ 2.40 \end{bmatrix}$ (numbers rounded off).

The solution is $\begin{bmatrix} b \\ m \end{bmatrix} = \begin{bmatrix} 2.3 \\ 2.5 \end{bmatrix}$, The "best" line is $w = 2.3 + 2.46u$

The power law is $W = e^{2.3} L^{2.46} = 10L^{2.46}$

(Ex 6) The velocity of an enzymatic reaction with Michaelis-Menton kinetics is given by

$$v(s) = \frac{\alpha s}{1 + \beta s}$$

Inverting this gives the Lineweaver-Burke equation:

$$\frac{1}{v} = \frac{1}{\alpha}\frac{1}{s} + \frac{\beta}{\alpha}$$

With the change of variables $\frac{1}{v} = w$ and $\frac{1}{s} = u$, this becomes: $w = \frac{1}{\alpha}u + \frac{\beta}{\alpha}$.

Find the Michaelis-Menton equation which best fits the data:

s	1	4	6	16
v	4	10	12	16

Take $w = \frac{1}{s}$ and $u = \frac{1}{v}$

u	1	.25	.167	.0625
w	.25	0.1	.083	.0625

Here $A = \begin{bmatrix} 1 & 1 \\ 1 & .25 \\ 1 & .167 \\ 1 & .0625 \end{bmatrix}$, $c = \begin{bmatrix} .25 \\ .1 \\ .083 \\ .0625 \end{bmatrix}$. Want $x = \begin{bmatrix} b \\ m \end{bmatrix}$ that minimizes $Ax - c$.

$$A^T \cdot A = \begin{bmatrix} 1 & 1 & 1 & 1 \\ .25 & .1 & .083 & .0625 \end{bmatrix} \cdot \begin{bmatrix} 1 & 1 \\ 1 & .25 \\ 1 & .167 \\ 1 & .0625 \end{bmatrix} = \begin{bmatrix} 4 & 1.48 \\ 1.48 & 1.09 \end{bmatrix}, \text{ and}$$

$$A^T \cdot c = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & .25 & .167 & .0625 \end{bmatrix} \cdot \begin{bmatrix} .25 \\ .1 \\ .083 \\ .0625 \end{bmatrix} = \begin{bmatrix} .496 \\ .293 \end{bmatrix}.$$

The normal equations are $\begin{bmatrix} 4 & 1.48 \\ 1.48 & 1.09 \end{bmatrix} \cdot \begin{bmatrix} b \\ m \end{bmatrix} = \begin{bmatrix} .496 \\ .293 \end{bmatrix}$

The solution is $\begin{bmatrix} b \\ m \end{bmatrix} = \begin{bmatrix} .05 \\ 0.2 \end{bmatrix}$, (numbers rounded off). $\alpha = 5$, $\beta = 0.25$

The M-M equation is: $y = \dfrac{5s}{1 + 0.25s}$

M146 Sample Quiz #06 for Thursday, May 4, 2006

(1) Let $C = \begin{bmatrix} 1 \\ 2 \\ 5 \end{bmatrix}$. Find the point on the line $x = Ct$ closest to the point $b = \begin{bmatrix} 3 \\ 4 \\ 7 \end{bmatrix}$.

(2) $A = \begin{bmatrix} 1 & 3 \\ 2 & 2 \\ 5 & 1 \end{bmatrix}$; $b = \begin{bmatrix} 3 \\ 4 \\ 7 \end{bmatrix}$. Find the best (least squares) solution to $Ax = b$

(3) The following data were obtained for the length y in centimeters of a human fetus versus the age t in weeks. Find a linear function $y = b + mt$ which best fits the data.

Age t	12	20	28	40
Length y	10	25	38	53

(4) Radioactive sample Y is decaying exponentially. The data shows the amount (y in grams) of Y at times (t in days). Find an exponential function $y = Ae^{rt}$ which best fits the data.

t	0	1	2	3	4	5
y	100	82	67	55	45	37

(5) The table shows the length-weight relation for Pacific halibut. Find an power function $W = \alpha L^{\beta}$ which best fits the data.

L	0.5	1.0	1.5	2.0	2.5
W	1.3	10.4	35	82	163

(6) The velocity of an enzymatic reaction with Michaelis-Menton kinetics is given by

$$v(s) = \frac{\alpha s}{1 + \beta s}$$

Find the Michaelis-Menton equation which best fits the data:

s	1	2.5	5	10	20
v	4.1	6.1	9.3	12.9	17.1