Biostatistics

Week #16 6/16/2020

Chapter 17 – Correlation & Regression

- Correlation (Pearson's correlation coefficient)
- Linear Regression
- Multiple Regression

Introduction

- To determine whether there is an association between two variables (one independent and one dependent)
- If so, ***what is the association***?
- Can we use it to ***predict*** the weight of a male bear given his body length?

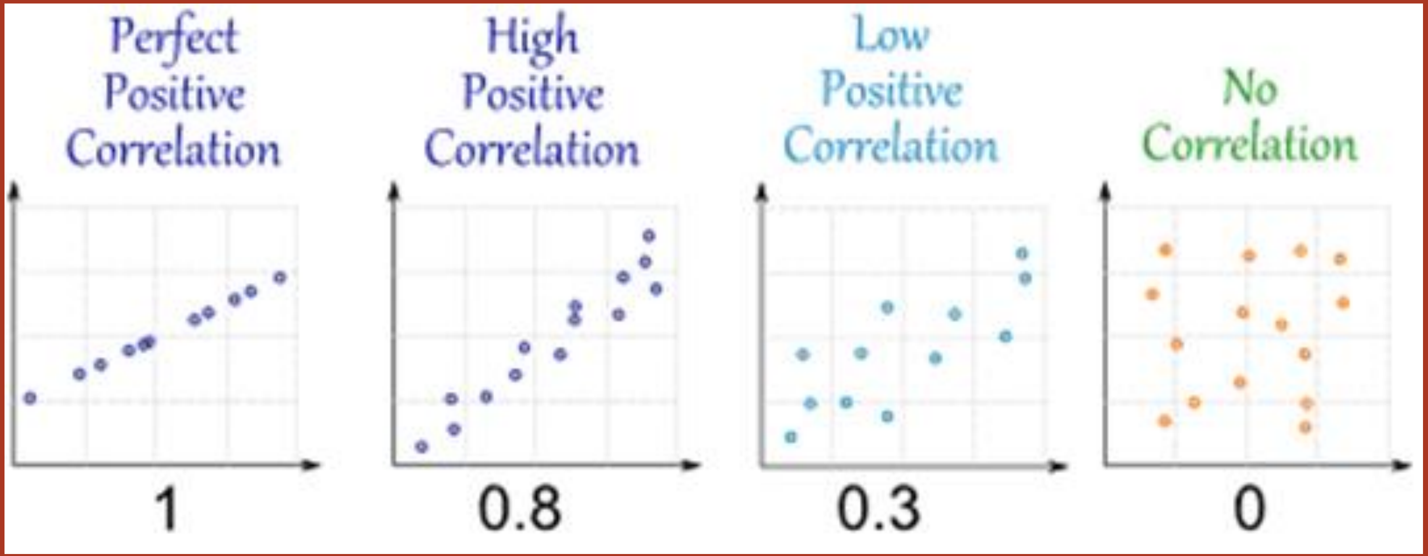
Lengths and Weights of Male Bears								
x Length	**53.0**	**67.5**	**72.0**	**72.0**	**73.5**	**68.5**	**73.0**	**37.0**
y Weight	**80**	**344**	**416**	**348**	**262**	**360**	**332**	**34**

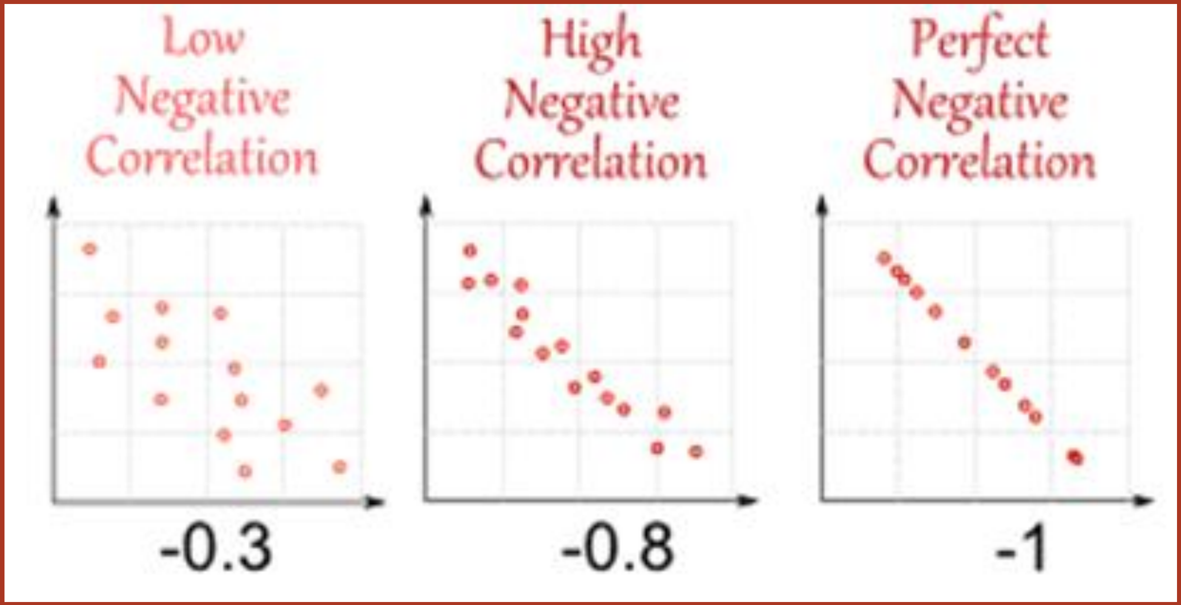
Correlation

- A “correlation” can help determining whether there is a “statistically significant” association between two variables.
- A scatter plot can help visually assessing whether the paired data (x, y) might be correlated.
- Such correlation could be “linear” or in other nonlinear forms (such as exponential, etc.)

Linear correlation

- The ***linear correlation coefficient r*** measures the strength of the linear association between the paired x- and y- quantitative values in a sample.
- It is sometimes called ***Pearson product moment correlation coefficient***.
- ***r*** ranges between -1 and 1.


Perfect Positive Correlation
1
High Positive Correlation
0.8
Low Positive Correlation
0.3
No Correlation
0


Low Negative Correlation
-0.3
High Negative Correlation
-0.8
Perfect Negative Correlation
-1

Basic requirements before computing r

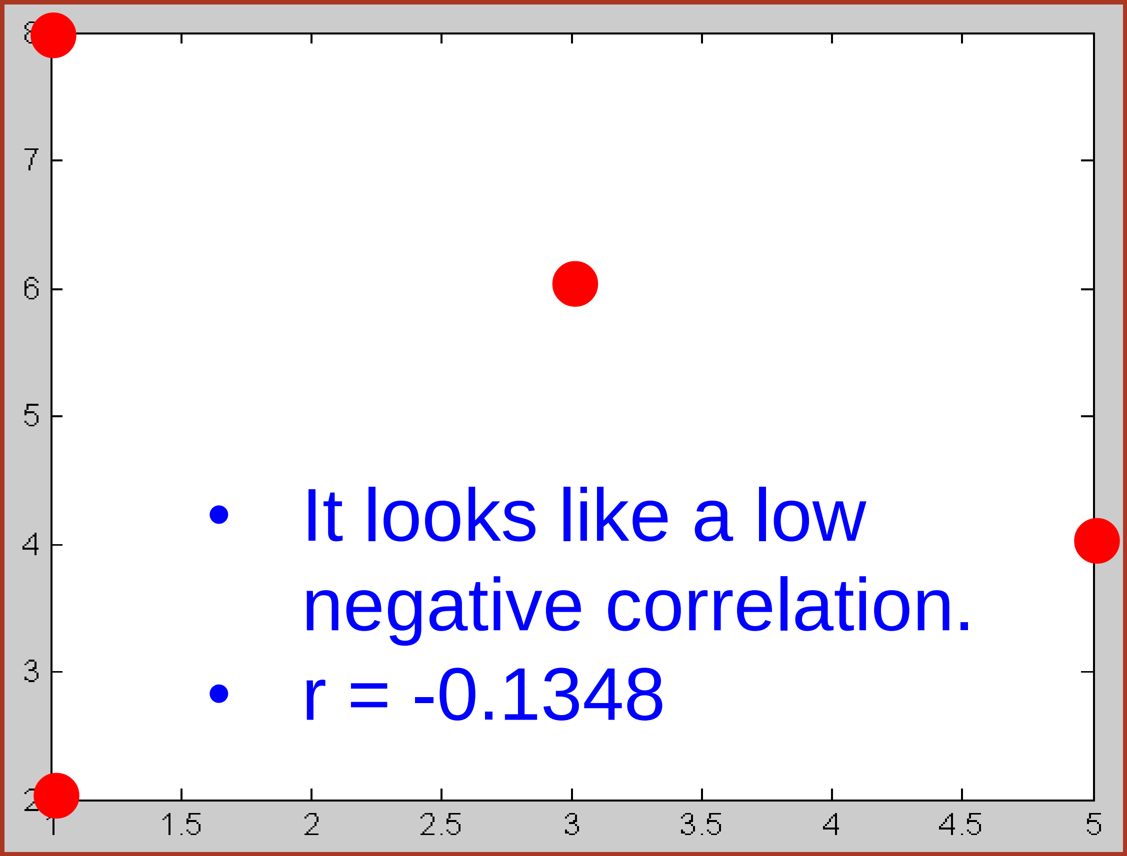
1. paired data (x, y) are randomly sampled.
2. visual scatter plot be approximately a straight line.
3. outliners be firstly removed

$$r = \frac{n(\sum xy) - (\sum x)(\sum y)}{\sqrt{[n(\sum x^2) - (\sum x)^2]\,[n(\sum y^2) - (\sum y)^2]}}$$

Example 1

Given the following 4 paired data, compute the correlation coefficient r.

x	1	1	3	5
y	2	8	6	4



- It looks like a low negative correlation.
- $r = -0.1348$

```
>> x=[1 1 3 5];y=[2 8 6 4];n=4;
>> r=(n*sum(x.*y)-
sum(x)*sum(y))/sqrt((n*sum(x.*x)-
sum(x)^2)*(n*sum(y.*y)-sum(y)^2))

r = -0.1348


>>
```

$$r = \frac{n(\sum xy) - (\sum x)(\sum y)}{\sqrt{[n(\sum x^2) - (\sum x)^2]\,[n(\sum y^2) - (\sum y)^2]}}$$

```
>> x=[1 1 3 5];y=[2 8 6 4];n=4;
>> r=(n*sum(x.*y)-sum(x)*sum(y))/sqrt((n*sum(x.*x)-sum(x)^2)*(n*sum(y.*y)-sum(y)^2))

r = -0.1348

>>
```

Pay special attention to the usage of computing those summations.

$$r = \frac{n\boxed{\left(\sum xy\right)} - \boxed{\left(\sum x\right)\left(\sum y\right)}}{\sqrt{\left[n\left(\sum x^2\right) - \left(\sum x\right)^2\right]\left[n\left(\sum y^2\right) - \left(\sum y\right)^2\right]}}$$

```
>> x=[1 1 3 5];y=[2 8 6 4];n=4;
>> r=(n*sum(x.*y)-sum(x)*sum(y))/sqrt((n*sum(x.*x)-sum(x)^2)*(n*sum(y.*y)-sum(y)^2))

r = -0.1348

>>
```

Pay special attention to the usage of computing those summations.

$$r = \frac{n\left(\sum xy\right) - \left(\sum x\right)\left(\sum y\right)}{\sqrt{\left[n\boxed{\left(\sum x^2\right)} - \boxed{\left(\sum x\right)^2}\right]\left[n\left(\sum y^2\right) - \left(\sum y\right)^2\right]}}$$

Interpreting *r*

- *r* is between -1 (perfect negative correlation) and +1 (perfect positive correlation).
- *r* = 0 means no correlation.
- Then what defines a “strong” correlation?
- The absolute value of r should be no less than ***a critical value***?
- Is *r* a random variable having its own probability density function?

Hypothesis testing for *r*

- H_0: ***no*** significant linear correlation
- Test statistic *t*:
- This is a 2-tailed t test
- DF = n-2
- α = 0.05 (usually)
- p-value can be computed based on computed t on a t distribution of specific DF.
- Reject if p <= 0.05.

$$t = \frac{r}{\sqrt{\frac{1-r^2}{n-2}}}$$

Back to example 1 (n=4)

- A critical t value that cuts 0.025 off the left tail of $t_{DF=2}$ is "tinv(0.025, 2) = -4.3027".
- The t-statistic computed based on previously computed r = -0.1348 now becomes -0.1925.

$$t = \frac{r}{\sqrt{\frac{1-r^2}{n-2}}}$$

- -0.1925 is not as extreme or more extreme than -4.3027. We thus do not reject the null hypothesis of no significant linear correlation. 【There exists NO significant correlation~~~】
- P-value = 2*tcdf(-0.1925,2)=0.8652, much greater than α=0.05.

```
>> x=[1 1 3 5];y=[2 8 6 4];
>> n=4;
>> r=(n*sum(x.*y)-sum(x)*sum(y))/sqrt((n*sum(x.*x)-sum(x)^2)*(n*sum(y.*y)-sum(y)^2))

r =   -0.1348
```

```
>> t=r/sqrt((1-r^2)/(n-2))
t =   -0.1925

>> 2*tcdf(t,n-2)
ans =    0.8652
```

Conclusion – No correlation between the two variables.

Example 2

- Find the linear correlation coefficient r for the following data.
- Determine whether the correlation is significant or not by computing a critical r value and a p-value.

Lengths and Weights of Male Bears								
x Length	53.0	67.5	72.0	72.0	73.5	68.5	73.0	37.0
y Weight	80	344	416	348	262	360	332	34

- The computed r = **0.8974**.
- The computed t-statistic = 4.9807.
- DF=8-2=6
- A critical r cutting off 0.025 of the right tail of $t_{DF=6}$ is “tinv(0.975, 6)=2.4469”. This is smaller than 4.9807. So our t-statistic is more extreme than expected.
- P-value = “2*(1-tcdf(4.9807,6))=**0.0025**”.
- We thus reject the null hypothesis, suggesting a significant linear correlation exists between the length and weight for male bears.

```
>> y=[80 344 416 348 262 360 332 34];y=[80 344 416 348 262 360 332 34];n=8;
>> r=(n*sum(x.*y)-sum(x)*sum(y))/sqrt((n*sum(x.*x)-sum(x)^2)*(n*sum(y.*y)-sum(y)^2))
```

r = 0.8974

$$r = \frac{n(\sum xy) - (\sum x)(\sum y)}{\sqrt{[n(\sum x^2) - (\sum x)^2]\,[n(\sum y^2) - (\sum y)^2]}}$$

```
>> t=r/sqrt((1-r^2)/(n-2))
```

t = 4.9807

$$t = \frac{r}{\sqrt{\frac{1-r^2}{n-2}}}$$

```
>> 2*(1-tcdf(t,6))
```

ans = 0.0025

```
>>
```

Using MATLAB's "corrcoef" function

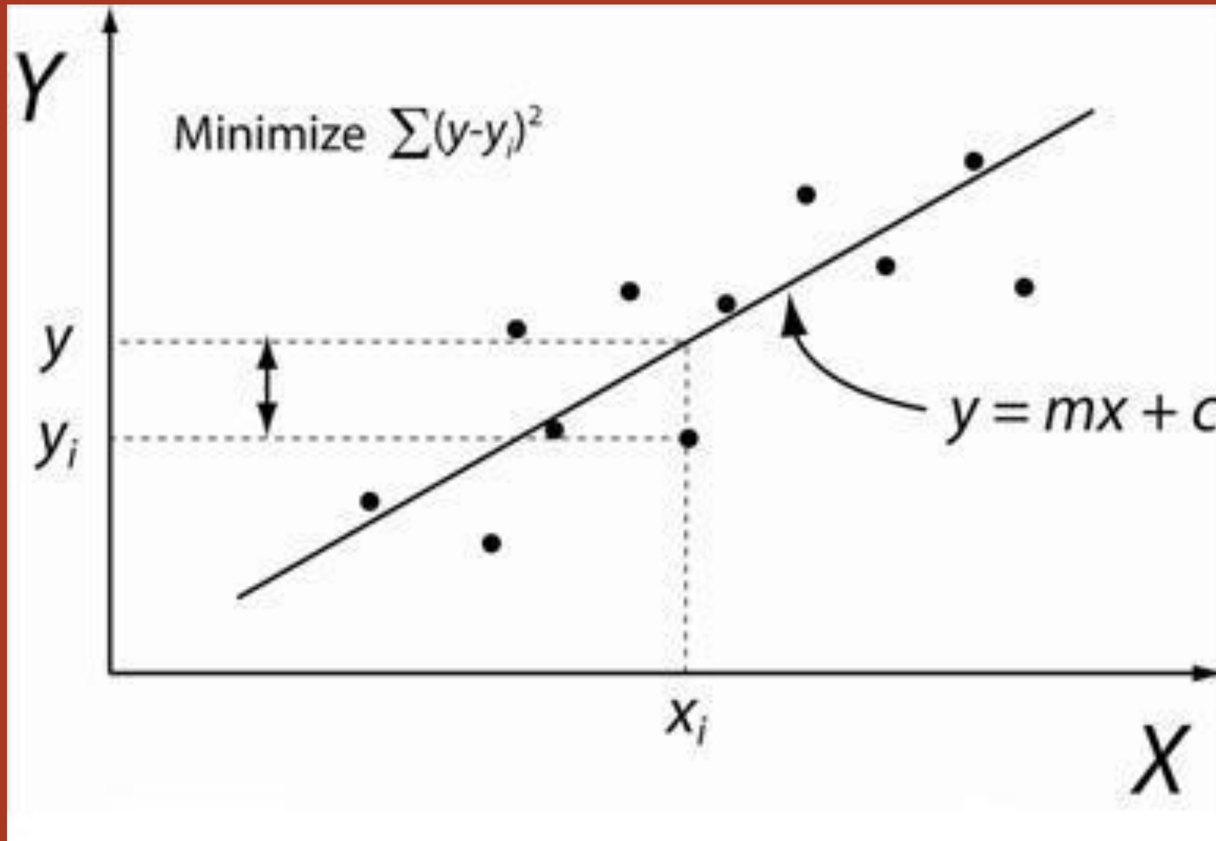
```
>> x=[53 67.5 72 72 73.5 68.5 73 37];
>> y=[80 344 416 348 262 360 332 34];
>> [R, P] = corrcoef(x,y)
R =
    1.0000    0.8974
    0.8974    1.0000
P =
    1.0000    0.0025
    0.0025    1.0000
```

Pearson coefficient

P-value in supporting the linear correlation at α=0.05.

Linear Regression

- To find a graph and an equation of the straight line that represents the association.
- The straight line is called “regression line”.
- The equation is called “regression equation”.



It's all about finding the slope *m* and the y-intercept *c* of the straight line.

Example 3

- Find the regression equation for the following data.
- Predict the weight of a bear with x = 71.0.

Lengths and Weights of Male Bears								
x Length	53.0	67.5	72.0	72.0	73.5	68.5	73.0	37.0
y Weight	80	344	416	348	262	360	332	34

MATLAB's "polyfit" (based on minimizing the least-squares of the errors) will serve the purpose.

```
>> x=[53 67.5 72 72 73.5 68.5 73 37];
>> y=[80 344 416 348 262 360 332 34];
>> polyfit(x,y,1)
ans =
   9.6598 -351.6599
>>
```

The equation is $y = 9.6598x - 351.6599$

MATLAB's "polyval" can be used to evaluate a value of a polynomial function.

```
>> x=[53 67.5 72 72 73.5 68.5 73 37];
>> y=[80 344 416 348 262 360 332 34];
>> polyfit(x,y,1)
ans =
   9.6598 -351.6599
>> polyval(polyfit(x,y,1), 71.0)
ans = 334.1849

>>
```

A male bear of length 71.0 in would weigh 334.1849 pounds.

Multiple regression

- Two or more independent variables.

Data from Male Bears								
y Weight	80	344	416	348	262	360	332	34
x2 Age	19	55	81	115	56	51	68	8
x3 Head L	11.0	16.5	15.5	17.0	15.0	13.5	16.0	9.0
x4 Head W	5.5	9.0	8.0	10.0	7.5	8.0	9.0	4.5
x5 Neck	16.0	28.0	31.0	31.5	26.6	27.0	29.0	13.0
x6 Length	53.0	67.5	72.0	72.0	73.5	68.5	73.0	37.0
x7 Chest	26	45	54	49	41	49	44	19

$y = b1 + b2*x2 + b3*x3 + \ldots + b6*x6 + b7*x7$

Example 4

- Find b1, b3 and b6.

Data from Male Bears								
y Weight	**80**	**344**	**416**	**348**	**262**	**360**	**332**	**34**
x2 Age	**19**	**55**	**81**	**115**	**56**	**51**	**68**	**8**
x3 Head L	**11.0**	**16.5**	**15.5**	**17.0**	**15.0**	**13.5**	**16.0**	**9.0**
x4 Head W	**5.5**	**9.0**	**8.0**	**10.0**	**7.5**	**8.0**	**9.0**	**4.5**
x5 Neck	**16.0**	**28.0**	**31.0**	**31.5**	**26.6**	**27.0**	**29.0**	**13.0**
x6 Length	**53.0**	**67.5**	**72.0**	**72.0**	**73.5**	**68.5**	**73.0**	**37.0**
x7 Chest	**26**	**45**	**54**	**49**	**41**	**49**	**44**	**19**

y = b1 + b3*x3 + b6*x6

b1 + b3*x3 + b6*x6 = y

b1 + 11.0*b3 + 53.0*b6 = 80
b1 + 16.5*b3 + 67.5*b6 = 344
b1 + 15.5*b3 + 72.0*b6 = 416
b1 + 17.0*b3 + 72.0*b6 = 348
b1 + 15.0*b3 + 73.5*b6 = 262
b1 + 13.5*b3 + 68.5*b6 = 360
b1 + 16.0*b3 + 73.0*b6 = 332
b1 + 9.0*b3 + 37.0*b6 = 34

This is called an ***over-determined system****. We have 8 equations, more than needed to solve 3 unknowns (b1, b3 and b6).*

$$\begin{bmatrix} 1 & 11.0 & 53.0 \\ 1 & 16.5 & 67.5 \\ 1 & 15.5 & 72.0 \\ 1 & 17.0 & 72.0 \\ 1 & 15.0 & 73.5 \\ 1 & 13.5 & 68.5 \\ 1 & 16.0 & 73.0 \\ 1 & 9.0 & 37.0 \end{bmatrix} \begin{bmatrix} b1 \\ b3 \\ b6 \end{bmatrix} = \begin{bmatrix} 80 \\ 344 \\ 416 \\ 348 \\ 262 \\ 360 \\ 332 \\ 34 \end{bmatrix}$$

or **AX = y**

$AX = y$

$[8 \text{ by } 3][3 \text{ by } 1] = [8 \text{ by } 1]$

- The problem is – matrix A is not square. We cannot find its inverse and solve the equation as $X=A^{-1}y$.

Pseudo-inverse of matrix A

$X = \text{pinv}(A)y$

[3 by 1] = [3 by **8**] [8 by 1]

- I need to have a "3 by 8" matrix which serves like an inverse of A. We call it a pseudo-inverse of matrix A, or **$\text{pinv}(A) = (A^tA)^{-1}A^t$** .
- See Appendix for the definition of pinv(A)

```
>> y=[80 344 416 348 262 360 332 34]';
>> x3=[11 16.5 15.5 17 15 13.5 16 9]';
>> x6=[53 67.5 72 72 73.5 68.5 73 37]';
>> A=[ones(size(x3))   x3   x6]

A =

   1.0000   11.0000   53.0000
   1.0000   16.5000   67.5000
   1.0000   15.5000   72.0000
   1.0000   17.0000   72.0000
   1.0000   15.0000   73.5000
   1.0000   13.5000   68.5000
   1.0000   16.0000   73.0000
   1.0000    9.0000   37.0000
```

Note that y, x3 and x6 must be column vectors.

[8 by 3]

>> A'*A

ans =

1.0e+004 *

0.0008	0.0114	0.0517
0.0114	0.1667	0.7565
0.0517	0.7565	3.4526

>> pinvA=inv(ans)*A'

A' * A

[3 by 8] [8 by 3] = [3 by 3]

$\boxed{\mathrm{pinv}(A) = (A^tA)^{-1}A^t}$

$(A^tA)^{-1}$ * A^t

[3 by **8**] = [3 by 3] [3 by 8]

pinvA =

0.8763	-0.2719	-0.2571	-0.4628	-0.2293	0.1123	-0.3528	1.5853
-0.0983	0.1962	-0.0209	0.1501	-0.1123	-0.1686	0.0132	0.0405
0.0100	-0.0370	0.0105	-0.0239	0.0302	0.0373	0.0045	-0.0315

>> b=pinvA*y

b =

-374.3035

18.8204

5.8748

>>

[3 by 1] = [3 by **8**] [8 by 1]

y = -374.3035 + 18.8204*x3 + 5.8748*x6

MATLAB's "regress"

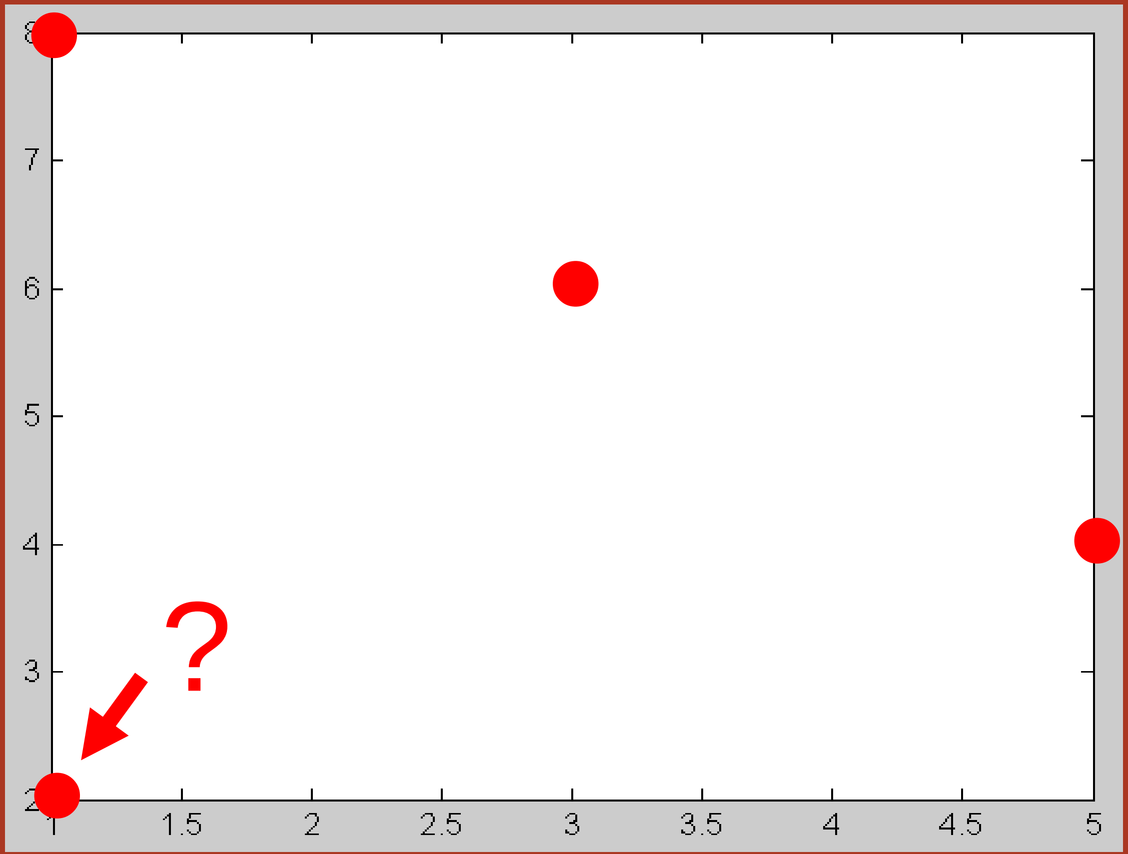
```
>> y=[80 344 416 348 262 360 332 34]';
>> x3=[11 16.5 15.5 17 15 13.5 16 9]';
>> x6=[53 67.5 72 72 73.5 68.5 73 37]';
>> A=[ones(size(x3)) x3 x6];
>> b=regress(y, A)
b =
 -374.3035
   18.8204
    5.8748
>>
```

Note that y, x3 and x6 must be column vectors in order to build the 8x3 matrix A.

In class practice – 1

- What if we treat the first data point in Example 1 as an outlier?

x	1	1	3	5
y	2	8	6	4



Cont'd

- Compute the correlation coefficient r.
- Compute the corresponding t-statistic t.
- Compute the p-value for the null hypothesis that the two variables are not correlated.
- Your conclusion?

In class practice – 2

- Find b1, b2 and b6.

Data from Male Bears								
y Weight	**80**	**344**	**416**	**348**	**262**	**360**	**332**	**34**
x2 Age	**19**	**55**	**81**	**115**	**56**	**51**	**68**	**8**
x3 Head L	11.0	16.5	15.5	17.0	15.0	13.5	16.0	9.0
x4 Head W	5.5	9.0	8.0	10.0	7.5	8.0	9.0	4.5
x5 Neck	16.0	28.0	31.0	31.5	26.6	27.0	29.0	13.0
x6 Length	**53.0**	**67.5**	**72.0**	**72.0**	**73.5**	**68.5**	**73.0**	**37.0**
x7 Chest	26	45	54	49	41	49	44	19

y = b1 + b2*x2 + b6*x6

APPENDIX – LEAST SQUARE METHOD FROM LINEAR ALGEBRA

Least-Squares Curves

- A system $A\mathbf{x} = \mathbf{y}$ of n equations in n variables, where A is invertible, has the unique solution $\mathbf{x} = A^{-1}\mathbf{y}$.
- However, if the system has n equations and m variables, with $n > m$, the system does not, in general, have a solution and it is said to be **over-determined**.
- A is not a square matrix, thus A^{-1} does not exist.
- A matrix called the **pseudoinverse** of A, denoted pinv(A), leads to a least-squares solution $\mathbf{x} =$ pinv(A)$\mathbf{y}$ for an over-determined system.
- This is not a true solution, but in some sense the closest we can get in order to have a true solution.

DEFINITION：

Let A be a matrix, then the matrix $(A^tA)^{-1}A^t$ is called a **pseudoinverse** of A and is denoted pinv(A).

Example 1 Find the pseudoinverse of $A = \begin{bmatrix} 1 & 2 \\ -1 & 3 \\ 2 & 4 \end{bmatrix}$

Solution

$$A^tA = \begin{bmatrix} 1 & -1 & 2 \\ 2 & 3 & 4 \end{bmatrix}\begin{bmatrix} 1 & 2 \\ -1 & 3 \\ 2 & 4 \end{bmatrix} = \begin{bmatrix} 6 & 7 \\ 7 & 29 \end{bmatrix}$$

$$(A^tA)^{-1} = \frac{1}{|A^tA|}\operatorname{adj}(A^tA) = \frac{1}{125}\begin{bmatrix} 29 & -7 \\ -7 & 6 \end{bmatrix}$$

$$\operatorname{pinv}(A) = (A^tA)^{-1}A^t = \frac{1}{125}\begin{bmatrix} 29 & -7 \\ -7 & 6 \end{bmatrix}\begin{bmatrix} 1 & -1 & 2 \\ 2 & 3 & 4 \end{bmatrix} = \frac{1}{25}\begin{bmatrix} 3 & -10 & 6 \\ 1 & 5 & 2 \end{bmatrix}$$

System of Equations $A\mathbf{x} = \mathbf{y}$

$$A\mathbf{x} = \mathbf{y} \qquad \mathbf{x} = \mathrm{pinv}(A)\mathbf{y}$$

system least-squares solution

Let $A\mathbf{x} = \mathbf{y}$ be a system of n linear equations in m variables with $n > m$, **where A is of rank m**.

(1) This system has a least-squares solution.

(2) If the system has a unique solution, the least –squares solution is that unique solution.

(3) If the system is over-determined, the least-squares solution is the closest we can get to a true solution.

(4) The system cannot have many solutions.

Example 2

Find the least-squares solution to the following over-determined system of equations. Sketch the solution.

$$x+y=6$$
$$-x+y=3$$
$$2x+3y=9$$

(m=3, n=2)

Solution

We have

$$A=\begin{bmatrix}1 & 1\\ -1 & 1\\ 2 & 3\end{bmatrix} \text{ and } \mathbf{y}=\begin{bmatrix}6\\ 3\\ 9\end{bmatrix}$$

$$A^tA=\begin{bmatrix}1 & -1 & 2\\ 1 & 1 & 3\end{bmatrix}\begin{bmatrix}1 & 1\\ -1 & 1\\ 2 & 3\end{bmatrix}=\begin{bmatrix}6 & 6\\ 6 & 11\end{bmatrix}$$

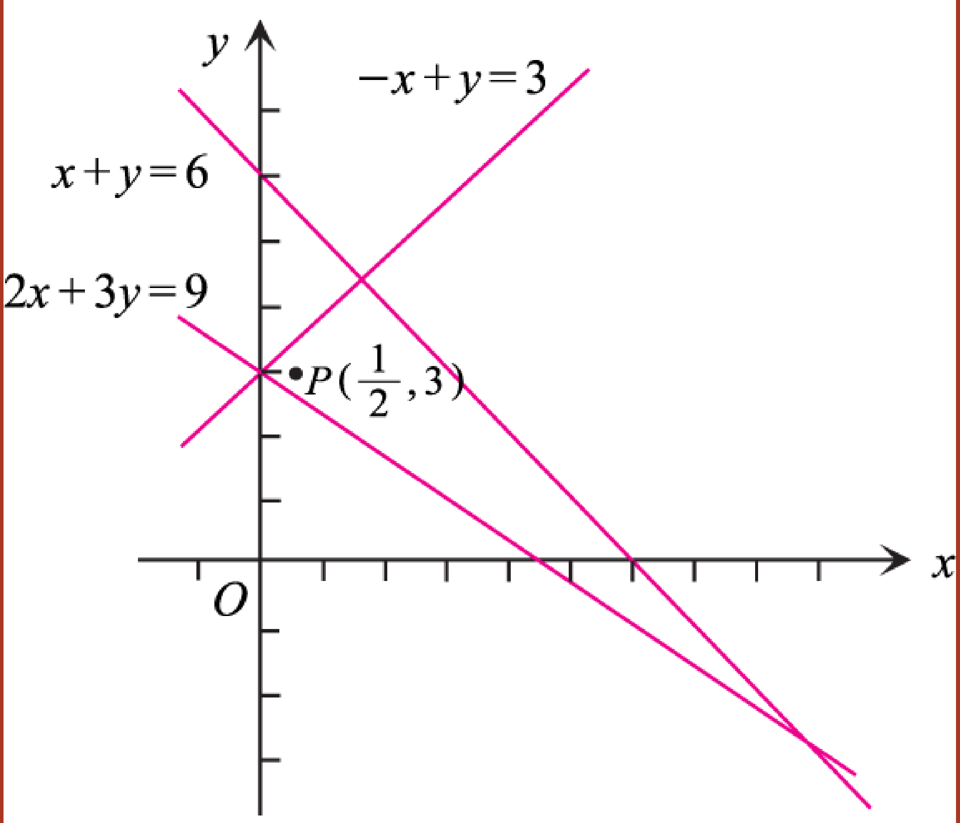
$$(A^tA)^{-1}=\frac{1}{|A^tA|}\operatorname{adj}(A^tA)=\frac{1}{30}\begin{bmatrix}11 & -6\\ -6 & 6\end{bmatrix}$$

$$\operatorname{pinv}(A)=(A^tA)^{-1}A^t=\frac{1}{30}\begin{bmatrix}11 & -6\\ -6 & 6\end{bmatrix}\begin{bmatrix}1 & -1 & 2\\ 1 & 1 & 3\end{bmatrix}=\frac{1}{30}\begin{bmatrix}5 & -17 & 4\\ 0 & 12 & 6\end{bmatrix}$$

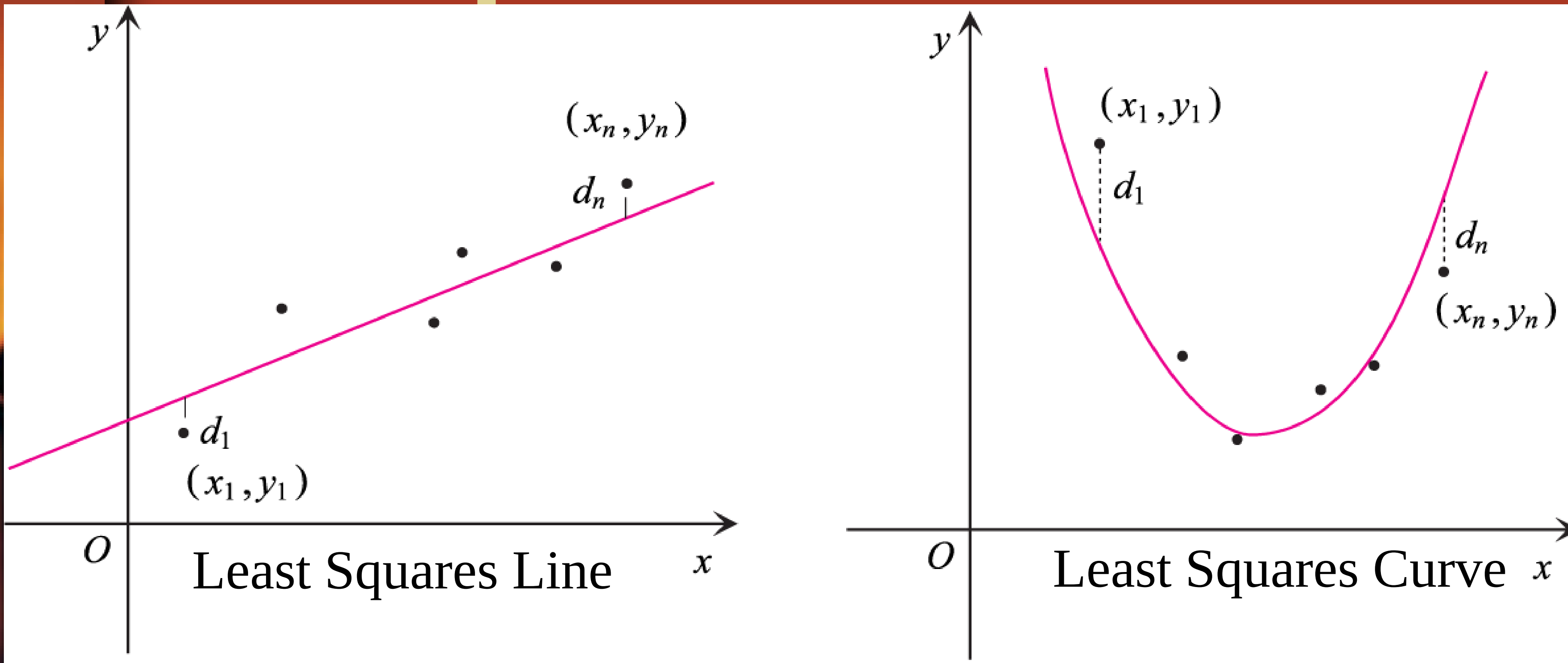
Then the least-squares solution is

$$\text{pinv}(A)\mathbf{y} = \frac{1}{30}\begin{bmatrix} 5 & -17 & 4 \\ 0 & 12 & 6 \end{bmatrix}\begin{bmatrix} 6 \\ 3 \\ 9 \end{bmatrix} = \begin{bmatrix} 1/2 \\ 3 \end{bmatrix}$$

The solution is shown below as point $P(\frac{1}{2}, 3)$.



Least Squares Curves



The least squares line or curve can be found by solving a over-determined system. This is found by minimizing the sum of $d_1^2 + d_2^2 + \ldots + d_n^2$

That's where we get the name "least squares" from.

Example 3

Find the least-squares line for the following data points.

(1, 1), (2, 2.4), (3, 3.6), (4, 4)

Solution

Let the equation of the line be ***y* = *a* + *bx***. Substituting for these points into the equation, we get an over-determined system:

$$\begin{aligned} a+b&=1\\ a+2b&=2.4\\ a+3b&=3.6\\ a+4b&=4 \end{aligned}$$

To solve for the least-squares solution, we have

$$A=\begin{bmatrix}1&1\\1&2\\1&3\\1&4\end{bmatrix} \quad \text{and} \quad \mathbf{y}=\begin{bmatrix}1\\2.4\\3.6\\4\end{bmatrix}$$

Thus

$$\mathrm{pinv}(A)=(A^tA)^{-1}A^t=\frac{1}{20}\begin{bmatrix}20&10&0&-10\\-6&-2&2&6\end{bmatrix}$$

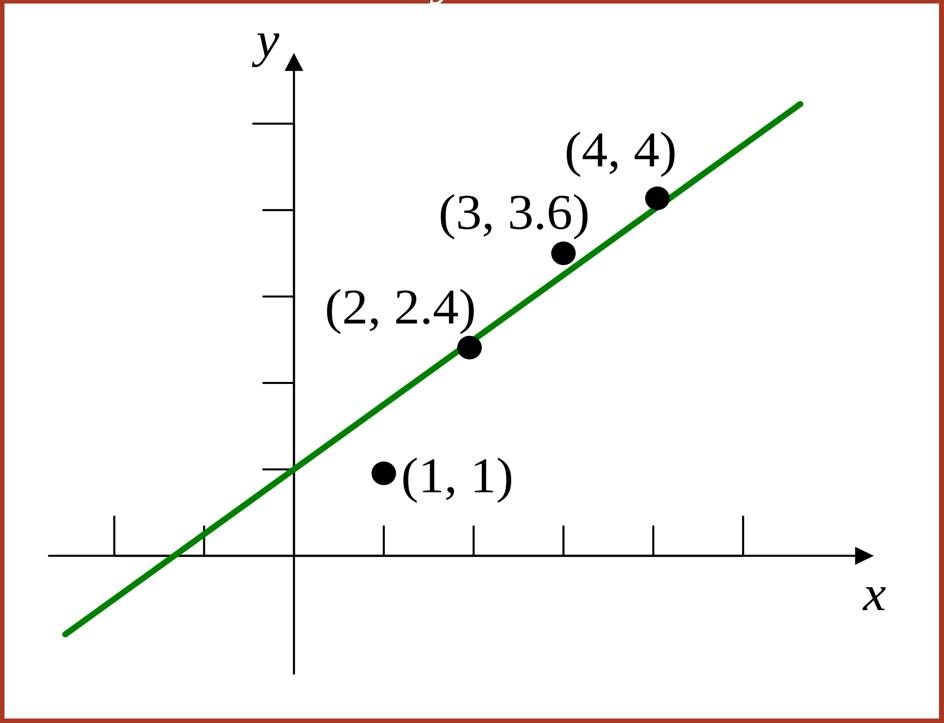
And the least-squares solution is

$$[(A^tA)^{-1}A^t]\mathbf{y} = \frac{1}{20}\begin{bmatrix} 20 & 10 & 0 & -10 \\ -6 & -2 & 2 & 6 \end{bmatrix}\begin{bmatrix} 1 \\ 2.4 \\ 3.6 \\ 4 \end{bmatrix} = \begin{bmatrix} 0.2 \\ 1.02 \end{bmatrix}$$

Thus $a = 0.2$, $b = 1.02$.

And the equation is

$$y = 0.2 + 1.02x$$



Example 4

Find the least-squares **parabola** for the following data points.

(1, 7), (2, 2), (3, 1), (4, 3)

Solution

Let the parabola be $y = a + bx + cx^2$. Substituting data points:

$$\begin{aligned} a+b+c&=7\\ a+2b+4c&=2\\ a+3b+9c&=1\\ a+4b+16c&=3 \end{aligned}$$

$$A=\begin{bmatrix}1&1&1\\1&2&4\\1&3&9\\1&4&16\end{bmatrix} \text{ and } \mathbf{y}=\begin{bmatrix}7\\2\\1\\3\end{bmatrix}$$

We have

$$\operatorname{pinv}(A)=(A^tA)^{-1}A^t=\frac{1}{20}\begin{bmatrix}45&-15&-25&15\\-31&23&27&-19\\5&-5&-5&5\end{bmatrix}$$

Finally we have the solution

$$[(A^tA)^{-1}A^t]\mathbf{y} = \frac{1}{20}\begin{bmatrix} 45 & -15 & -25 & 15 \\ -31 & 23 & 27 & -19 \\ 5 & -5 & -5 & 5 \end{bmatrix}\begin{bmatrix} 7 \\ 2 \\ 1 \\ 3 \end{bmatrix} = \begin{bmatrix} 15.25 \\ -10.05 \\ 1.75 \end{bmatrix}$$

Thus $a = 15.25$, $b = -10.05$, $c = 1.75$.

Or

$y = 15.25 - 10.05x + 1.75x^2$