Least Squares Solutions/Data Fitting (4/16/16)

***Question*:** Find the least squares solution to

x + y = 1

x - 3y = 4

2x + y = 3.

In[149]:=
```
(*Here are the matrices a, b*)
a = {{1, 1}, {1, -3}, {2, 1}};
b = {{1}, {4}, {3}};
MatrixForm[a]
MatrixForm[b]
```

Out[151]//MatrixForm=

$$\begin{pmatrix} 1 & 1 \\ 1 & -3 \\ 2 & 1 \end{pmatrix}$$

Out[152]//MatrixForm=

$$\begin{pmatrix} 1 \\ 4 \\ 3 \end{pmatrix}$$

In[153]:=
```
(*Here are two ways of obtaining the transpose.*)
Transpose[a] // MatrixForm
aᵀ // MatrixForm
```

Out[153]//MatrixForm=

$$\begin{pmatrix} 1 & 1 & 2 \\ 1 & -3 & 1 \end{pmatrix}$$

Out[154]//MatrixForm=

$$\begin{pmatrix} 1 & 1 & 2 \\ 1 & -3 & 1 \end{pmatrix}$$

In[155]:=
```
(soln = Inverse[Transpose[a].a].Transpose[a].b ) // MatrixForm
```

Out[155]//MatrixForm=

$$\begin{pmatrix} \frac{11}{6} \\ -\frac{8}{11} \end{pmatrix}$$

The least squares solution is y = (11/6)x - 8/11.

In[156]:=
```
N[a.soln]
```
Out[156]=
```
{{1.10606}, {4.01515}, {2.93939}}
```

Note that the output values obtained from our solution are very close to the values of b in the original problem.

Question: Find the line y=ax + b that best fits the data (-1,1), (1,2), (2,-1).

In[157]:=
```
a = {{-1, 1}, {1, 1}, {2, 1}};
MatrixForm[a]
b = {1, 2, -1};
MatrixForm[b]
```
Out[158]//MatrixForm=

$$\begin{pmatrix} -1 & 1 \\ 1 & 1 \\ 2 & 1 \end{pmatrix}$$

Out[160]//MatrixForm=

$$\begin{pmatrix} 1 \\ 2 \\ -1 \end{pmatrix}$$

In[161]:=
```
Inverse[Transpose[a].a].Transpose[a].b  // MatrixForm
```
Out[161]//MatrixForm=

$$\begin{pmatrix} -\frac{1}{2} \\ 1 \end{pmatrix}$$

The line y = -1/2 x + 1 is the best fit line.

Question: Find the parabola that best fits the data points (-1,8), (0,8), (1,4), (2, 16).

Here, I will illustrate how *Mathematica* has built-in commmands for the methods we are using.

In[162]:=
```
data = {{-1, 8}, {0, 8}, {1, 4}, {2, 16}};
MatrixForm[data]
```
Out[163]//MatrixForm=

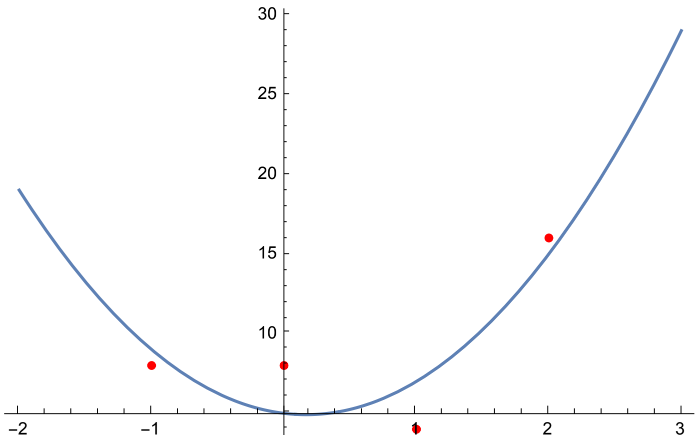
$$\begin{pmatrix} -1 & 8 \\ 0 & 8 \\ 1 & 4 \\ 2 & 16 \end{pmatrix}$$

In[164]:=
```
quad = Fit[data, {1, x, x^2}, x]
```
Out[164]= $5. - 1.\, x + 3.\, x^2$

The parabola that best fits the data is 3x^2 - x + 5. Here is a graph with the data points and the quadratic function.

In[165]:=
```
Show[Plot[quad, {x, -2, 3}], ListPlot[data, PlotStyle → Red]]
```

Out[165]=

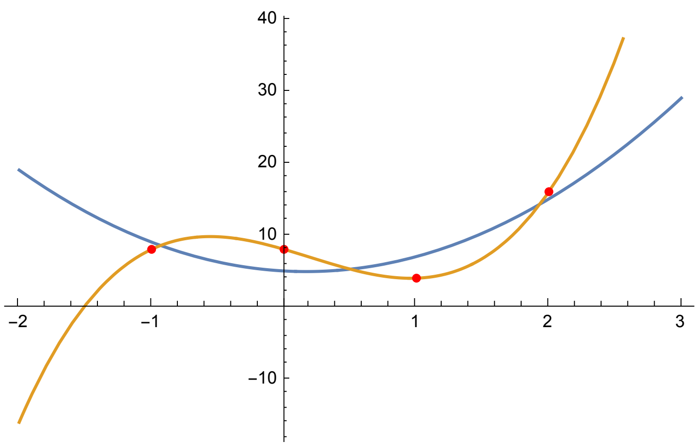


Note that we can find a cubic function going through all 4 data points.

In[166]:=
```
cubic = Fit[data, {x^3, x^2, x, 1}, x]
Show[Plot[{quad, cubic}, {x, -2, 3}], ListPlot[data, PlotStyle → Red]]
```

Out[166]= $8. - 5.33333\, x - 2.\, x^2 + 3.33333\, x^3$

Out[167]=



Finally, here are some tricks for producing and manipulating matrices.

To access the (i,j)th entry in a matrix, you use [[i,j]]. For example, the various entries of data can be accessed as follows.

In[168]:=
```
(data = {{-1, 8}, {0, 8}, {1, 4}, {2, 16}}) // MatrixForm
data[[2, 2]] (*Row 2, Column 2*)
data[[3, 1]] (*Row 3, Column 1*)
data[[3, 3]] (*Row 3, Column 3, which does not exist*)
```

Out[168]//MatrixForm=

$$\begin{pmatrix} -1 & 8 \\ 0 & 8 \\ 1 & 4 \\ 2 & 16 \end{pmatrix}$$

Out[169]= 8

Out[170]= 1

Part: Part 3 of {1, 4} does not exist.

Out[171]= {{-1, 8}, {0, 8}, {1, 4}, {2, 16}}[[3, 3]]

Here is a way we can use the data table to create matrices a, b.

In[172]:=
```
(xvals = Table[data[[i, 1]], {i, 1, 4}])
(b = Table[data[[i, 2]], {i, 1, 4}]) // MatrixForm
(a = Table[ { i^2, i, 1} , {i, xvals}]) // MatrixForm
```

Out[172]= {-1, 0, 1, 2}

Out[173]//MatrixForm=

$$\begin{pmatrix} 8 \\ 8 \\ 4 \\ 16 \end{pmatrix}$$

Out[174]//MatrixForm=

$$\begin{pmatrix} 1 & -1 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 1 \\ 4 & 2 & 1 \end{pmatrix}$$

In[175]:=
```
Inverse[Transpose[a].a].Transpose[a].b  // MatrixForm
```

Out[175]//MatrixForm=

$$\begin{pmatrix} 3 \\ -1 \\ 5 \end{pmatrix}$$

or, there is a built-in command for LeastSquares.

In[176]:=
```
LeastSquares[a, b]
```

Out[176]= {3, -1, 5}

If you are interested in Problem 5: Here is an example of creating a list of (x,y) values for the curve y = x^2 - 1, from x=1 to x=3, with step size of 1/5.

In[177]:=
```
Table[{x, x^2 - 1}, {x, 1, 3, .2}]
```

Out[177]=
```
{{1., 0.}, {1.2, 0.44}, {1.4, 0.96}, {1.6, 1.56}, {1.8, 2.24},
 {2., 3.}, {2.2, 3.84}, {2.4, 4.76}, {2.6, 5.76}, {2.8, 6.84}, {3., 8.}}
```

Here is an example of (x,y) values for y=sin(x), from x=1 to x=3 with step size of .2.

In[178]:=
```
Table[{x, Sin[x]}, {x, 1, 3, .2}]
```

Out[178]=
```
{{1., 0.841471}, {1.2, 0.932039}, {1.4, 0.98545},
 {1.6, 0.999574}, {1.8, 0.973848}, {2., 0.909297}, {2.2, 0.808496},
 {2.4, 0.675463}, {2.6, 0.515501}, {2.8, 0.334988}, {3., 0.14112}}
```