Section 6.6: Other Models

Summary of last time: Given that the matrix equation

$$A\mathbf{x} = \mathbf{b}$$

has no solution, it is possible to find a solution that minimizes the "error":

$$\min_{\mathbf{x}} \|\mathbf{b} - A\mathbf{x}\|^2$$

We know that the error is minimized when we find $\widehat{x}$, so that $A\widehat{\mathbf{x}} = \widehat{\mathbf{b}}$, which is the orthogonal projection of $\mathbf{b}$ into the column space of A.

To actually compute $\widehat{\mathbf{x}}$, we have two choices:

- Use the normal equations: $A^T A\mathbf{x} = A^T\mathbf{b}$.

  In Matlab, this would be:

  ```
  xhat=inv(A'*A)*A'*b
  ```

- If we have the QR factorization of A, then $\widehat{\mathbf{x}} = R^{-1}Q^T\mathbf{b}$:

  $$A\widehat{\mathbf{x}} = AR^{-1}Q^T\mathbf{b} = QRR^{-1}Q^T\mathbf{b} = QQ^T\mathbf{b}$$

  In Matlab, this would be:

  ```
  [Q,R]=qr(A,0);
  xhat=inv(R)*Q'*b;
  ```

Numerically speaking, for large matrices, the QR factorization would lead to a better answer (in terms of less round off error).

Construction of the Matrix A

Now that we know how to solve $A\mathbf{x} = \mathbf{b}$, we have to understand how to get the matrix A and vector $\mathbf{b}$.

Line of Best Fit

Given $\{(x_1, y_1), (x_2, y_2) \cdots, (x_k, y_k)\}$ and the model equation:

$$y = \beta_1 x + \beta_0$$

Then putting in the data leads to a linear equation:

$$A = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_k & 1 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_k \end{bmatrix}$$

(Tell students that you could switch the columns, but remember that you switch the unknowns)

General Linear Model

You can do the same thing if you want to fit any model that is linear in its parameters. Here are some examples with the corresponding matrix- You might even have multidimensional input.

$$\text{Model: } y = \beta_2 x^2 + \beta_1 x + \beta_0 \quad \Rightarrow \quad A\mathbf{x} = \mathbf{b} \Rightarrow \begin{bmatrix} x_1^2 & x_1 & 1 \\ x_2^2 & x_2 & 1 \\ \vdots & \vdots & \\ x_k^2 & x_k & 1 \end{bmatrix} \begin{bmatrix} \beta_2 \\ \beta_1 \\ \beta_0 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_k \end{bmatrix}$$

Example: Find the best fitting parabola to the following set of data:

x	-1	1	2	4	5
y	8	0	2	30	50

In Matlab, we would type:

```
x=[-1 1 2 4 5]';
y=[8 0 2 30 50];
A=[x.^2 x ones(5,1)];
c=inv(A'*A)*A'*y;
xTest=linspace(min(x), max(x))';
yTest=[xTest.^2 xTest ones(100,1)]*c;
plot(x,y,'*',xTest,yTest,'k-');
```

$$\text{Model: } y = \beta_2 \cos(x) + \beta_1 \cos(3x) + \alpha \sin(x) + \gamma \quad \Rightarrow$$

$$A\mathbf{x} = \mathbf{b} \Rightarrow \begin{bmatrix} \cos(x_1) & \cos(3x_1) & \sin(x_1) & 1 \\ \cos(x_2) & \cos(3x_2) & \sin(x_1) & 1 \\ \vdots & \vdots & & \\ \cos(x_k) & \cos(3x_k) & \sin(x_k) & 1 \end{bmatrix} \begin{bmatrix} \beta_2 \\ \beta_1 \\ \alpha \\ \gamma \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_k \end{bmatrix}$$

Note: In Matlab, if `x` is a column vector, then you could write:

```
k= (number of points)
A=[cos(x) cos(3*x) sin(x) ones(k,1)]
```

Other Models

A measurement that comes up often in Biology is the general form:

$$y = Ax^n$$

where A, n are unknowns. In this case, we cannot write down a linear system of equations since this is not a linear relationship.

However, it is possible to transform it into a linear relationship. Take the log (base anything) of both sides:

$$\log(y) = \log(Ax^n) = \log(A) + \log(x^n) = \log(A) + n\log(x)$$

Which is: $z = n\hat{x} + c$, which is linear. The matrices in question:

$$A\mathbf{x} = \mathbf{b} \quad \Rightarrow \quad \begin{bmatrix} \ln(x_1) & 1 \\ \ln(x_2) & 1 \\ \vdots & \vdots \\ \ln(x_k) & 1 \end{bmatrix} \begin{bmatrix} n \\ c \end{bmatrix} = \begin{bmatrix} \ln(y_1) \\ \ln(y_2) \\ \vdots \\ \ln(y_k) \end{bmatrix}$$

The n value is the original value, but recall that $c = \ln(A)$, so that $A = \mathrm{e}^c$.