Avoiding Using Least Squares

Justification for fitting data visually:

- Large simplifications in model development mean that eyeballing a fit is reasonable.
- ► Mathematical methods do not necessarily imply a *better* fit!
- You can make objective judgements that computers cannot; you know which data points should be taken more seriously.
- ► Mathematics give precise answers; every answer is fallible.

Regression

If we have confidence in our data, we may wish to do a **regression**, a method for fitting a curve through a set of points by following a goodness-of-fit criterion.

Goal: Formulate mathematically what we do internally: Make the discrepancies between the data and the curve small.

► Make the sum of the set of **absolute deviations** small. (Pic!) minimize over all *f* the sum: $\sum_{(x_i, y_i)} |y_i - f(x_i)|$

► Make the largest of the set of absolute deviations small. minimize over all f the value: max |y_i - f(x_i)| (x_i,y_i)

One or the other might make more sense depending on the situation.

Least Squares

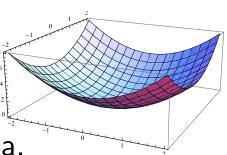
A regression method often used is called *least squares*.

minimize over all
$$f$$
 the sum: $\sum_{(x_i,y_i)} (y_i - f(x_i))^2$

- A middle ground, giving weight to <u>all</u> discrepancies and more weight to those that are further from the curve.
- Easy to analyze mathematically because this is a smooth function.

Calculating minima of smooth functions: (You know how!)

- Differentiate with respect to each variable, and set equal to zero.
- Solve the resulting system of equations.
- Check to see if the solutions are local minima.



Least Squares Example

Example. Use the least-squares criterion to fit a line y = mx + b to the data: {(1.0, 3.6), (2.1, 2.9), (3.5, 2.2), (4.0, 1.7)}. Intution / Expectations?

Solution. We need to calculate the sum $S = \sum_{(x_i, y_i)} [y_i - (mx_i + b)]^2$. $S = (3.6-1.0m-b)^2 + (2.9-2.1m-b)^2 + (2.2-3.5m-b)^2 + (1.7-4.0m-b)^2$ Expanding, $S = 29.1 - 20.8b + 4b^2 - 48.38m + 21.2bm + 33.66m^2$ Calculating the partial derivatives and setting equal to zero: $\begin{cases} \frac{\partial S}{\partial b} = -20.8 + 8b + 21.2m = 0\\ \frac{\partial S}{\partial m} = -48.38 + 21.2b + 67.32m = 0 \end{cases}$

Solving the system of equations gives: $\{b = 4.20332, m = -0.605027\}$

That is, the line that gives the least-squares fit for the data is

$$y = -0.605027x + 4.20332$$

Notes on the Method of Least Squares

- Least squares becomes messy when there are many data points.
- We chose least squares because it was easy. Is it really the "right" method for the job?
- ▶ Least squares isn't always easy, for example: $y = Ce^{kx}$.
- You can use least squares on transformed data, but the result is NOT a least-squares curve for the original data.
- Multivariable least squares can also be done: w = ax + by + cz + d (Would want to minimize:
 .)
- Least squares measures distance vertically.
 A better measure would probably be perpendicular distance.
- You need to understand the concept of least squares and know how to do least squares by hand for small examples.
- ► We'll learn how to use *Mathematica* to do this for us!

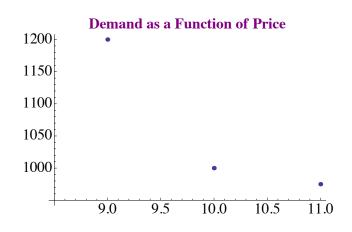
Price – Demand Curve (p. 111–114)

Example. A company is trying to determine how demand for a new product depends on its price and collect the following data:

| price p | \$9 | \$10 | \$11 |
|----------|----------|----------|---------|
| demand d | 1200/mo. | 1000/mo. | 975/mo. |

The company has reason to believe that price and demand are **inversely proportional**, that is, $d = \frac{c}{p}$ for some constant c.

ightarrow Use the method of least squares to determine this constant c.



Price – Demand Curve (p. 111–114)

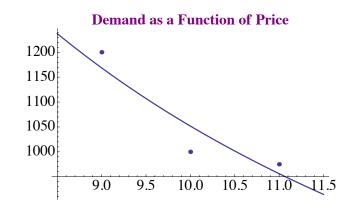
Solution. Since $f(p) = \frac{c}{p}$, then the sum $S = \sum_{(p_i, d_i)} \left[d_i - \left(\frac{c}{p_i} \right) \right]^2$. Specifying datapoints gives

$$S = \left[1200 - \frac{c}{9}\right]^2 + \left[1000 - \frac{c}{10}\right]^2 + \left[975 - \frac{c}{11}\right]^2$$

Setting the derivative equal to zero gives

$$\frac{dS}{dc} = \frac{-2}{9} \left[1200 - \frac{c}{9} \right] + \frac{-2}{10} \left[1000 - \frac{c}{10} \right] + \frac{-2}{11} \left[975 - \frac{c}{11} \right] = 0$$

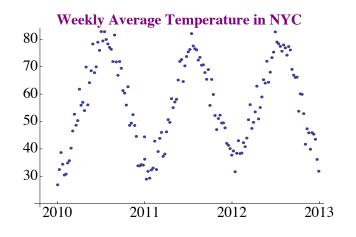
Solving for *c* gives $c \approx 10517$.



New York City Temperature (similar to p. 158)

The graph of average weekly temperature in New York City from Jan. 2010 to Dec. 2012 gives the distinct impression of a _____.

We need to determine the constants in: $Temp(t) = A + B \sin(C(t - D)).$



Mathematica has a hard time finding all four constants at once. Using knowledge of the seasons, we can make assumptions about C and D. We can assume that $C = _$.

For *D*, find when the sine passes through zero. ⁸⁰ Since January is coldest and July is hottest, ⁷⁰ the zero should occur in April; guess $D \approx 0.3$. ⁵⁰

Fitting to $Temp(t) = A + B \sin[2\pi(t - 0.3)]$ gives: $Temp(t) = 56.5 + 20.6 \sin[2\pi(t - 0.3)]$

