

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:
$$\max_{(x_i, y_i)} |y_i - f(x_i)|$$

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

Least Squares

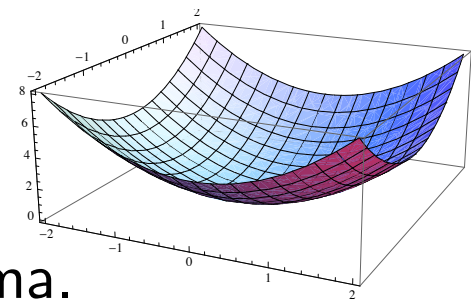
A regression method often used is called *least squares*.

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

- ▶ A middle ground, giving weight to all 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: $\{(1.0, 3.6), (2.1, 2.9), (3.5, 2.2), (4.0, 1.7)\}$.

Intuition / 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!

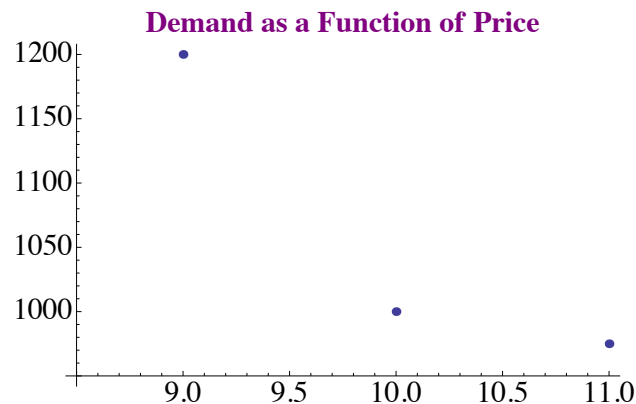
Price – Demand Curve (p. 111–114)

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 .

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



Price – Demand Curve (p. 111–114)

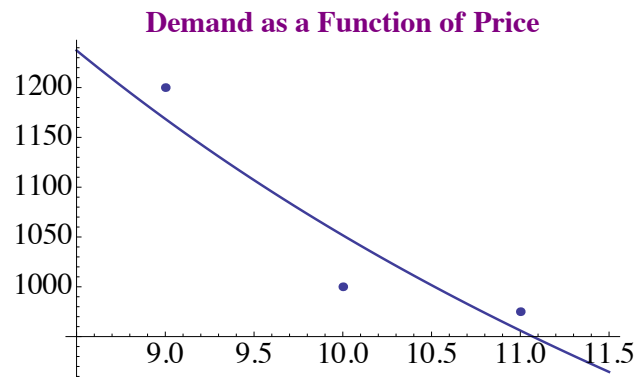
Solution. Since $f(p) = \frac{c}{p}$, then the sum $S = \sum_{(p_i, d_i)} \left[d_i - \left(\frac{c}{p_i} \right) \right]^2$.
Specifying datapoints gives

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

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 $C = \underline{\hspace{2cm}}$.

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

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

