Sum of Squared Errors - Sanity Check

INM431 week 5 - daniel.sikar@city.ac.uk + big sister Given a line equation:

$$y = b + mx$$

where b is the intercept, and m is the slope. We change this into the form:

$$\hat{y} = \hat{\beta_0} + \hat{\beta_1} x \tag{1}$$

and define an error function:

$$E = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \tag{2}$$

where y_i is the *i*th observation of y, and corresponds to the input x_i , and \hat{y}_i is the corresponding prediction. Substituting (1) in (2):

$$E = \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2$$

We want to minimize the error E and can see it is a function of $\hat{\beta}_0$ and $\hat{\beta}_1$ so give it a more descriptive name:

$$SSE(\hat{\beta}_0, \hat{\beta}_1) = \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2$$
 (3)

We take two derivatives, one with respect to $\hat{\beta}_0$ and the other with respect to $\hat{\beta}_1$. Since our error function consists of two functions, one outside function (exponentiation) and one inside function, we apply the chain rule for a general case:

$$g(f(x)) = \frac{\partial g}{\partial f} \cdot \frac{\partial f}{\partial x}$$

For $\hat{\beta_0}$ we have:

$$\frac{\partial g}{\partial f} \cdot \frac{\partial f}{\partial \hat{\beta}_0} = \frac{\partial g}{\partial f} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2 \cdot \frac{\partial f}{\partial \hat{\beta}_0} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)$$

We apply the derivative sum rule - the derivative of the sum is equal to the sum of the derivatives:

$$\frac{\partial g}{\partial f} \cdot \frac{\partial f}{\partial \hat{\beta}_0} = \sum_{i=1}^n \frac{\partial g}{\partial f} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2 \cdot \frac{\partial f}{\partial \hat{\beta}_0} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)$$

$$= 2 \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) \cdot (-1)$$

$$= -2 \sum_{i=1}^n y_i + 2 \sum_{i=1}^n \hat{\beta}_0 + 2 \sum_{i=1}^n \hat{\beta}_1 x_i$$

Since we are trying to minimize:

$$\frac{\partial}{\partial \hat{\beta}_0} SSE(\hat{\beta}_0, \hat{\beta}_1)$$

we set the result to zero and solve for $\hat{\beta}_0$:

$$-2\sum_{i=1}^{n} y_{i} + 2\sum_{i=1}^{n} \hat{\beta_{0}} + 2\sum_{i=1}^{n} \hat{\beta_{1}} x_{i} = 0$$

$$2\sum_{i=1}^{n} \hat{\beta_{0}} = 2\sum_{i=1}^{n} y_{i} - 2\sum_{i=1}^{n} \hat{\beta_{1}} x_{i}$$

$$n\bar{y} = \sum_{i=1}^{n} y_{i}$$

$$2\sum_{i=1}^{n} \hat{\beta_{0}} = 2n\bar{y} - 2\sum_{i=1}^{n} \hat{\beta_{1}} x_{i}$$

$$2\sum_{i=1}^{n} \hat{\beta_{0}} = 2n\bar{y} - \hat{\beta_{1}} 2\sum_{i=1}^{n} x_{i}$$

$$n\bar{x} = \sum_{i=1}^{n} x_{i}$$

$$2\sum_{i=1}^{n} \hat{\beta_{0}} = 2n\bar{y} - \hat{\beta_{1}} 2n\bar{x}$$

$$2n\hat{\beta_{0}} = 2n\bar{y} - \hat{\beta_{1}} 2n\bar{x}$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} \tag{4}$$

For $\hat{\beta_1}$ we have:

$$\frac{\partial g}{\partial f} \cdot \frac{\partial f}{\partial \hat{\beta}_1} = \sum_{i=1}^n \frac{\partial g}{\partial f} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2 \cdot \frac{\partial f}{\partial \hat{\beta}_1} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)$$

$$= 2 \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) \cdot (-x_i)$$

$$= -2 \sum_{i=1}^n x_i y_i + 2 \sum_{i=1}^n \hat{\beta}_0 x_i + 2 \sum_{i=1}^n \hat{\beta}_1 x_i^2$$

Setting result equal to zero:

$$-2\sum_{i=1}^{n} x_i y_i + 2\sum_{i=1}^{n} \hat{\beta_0} x_i + 2\sum_{i=1}^{n} \hat{\beta_1} x_i^2 = 0$$
$$-\sum_{i=1}^{n} x_i y_i + \sum_{i=1}^{n} \hat{\beta_0} x_i + \sum_{i=1}^{n} \hat{\beta_1} x_i^2 = 0$$
$$-\sum_{i=1}^{n} x_i y_i + \hat{\beta_0} \sum_{i=1}^{n} x_i + \hat{\beta_1} \sum_{i=1}^{n} x_i^2 = 0$$

Substituting $\hat{\beta_0}$ from (4):

$$-\sum_{i=1}^{n} x_{i} y_{i} + (\bar{y} - \hat{\beta}_{1} \bar{x}) \sum_{i=1}^{n} x_{i} + \hat{\beta}_{1} \sum_{i=1}^{n} x_{i}^{2} = 0$$

$$-\sum_{i=1}^{n} x_{i} y_{i} + \bar{y} \sum_{i=1}^{n} x_{i} - \hat{\beta}_{1} \bar{x} \sum_{i=1}^{n} x_{i} + \hat{\beta}_{1} \sum_{i=1}^{n} x_{i}^{2} = 0$$

$$-\sum_{i=1}^{n} x_{i} y_{i} + \bar{y} \sum_{i=1}^{n} x_{i} - \hat{\beta}_{1} (\bar{x} \sum_{i=1}^{n} x_{i} - \sum_{i=1}^{n} x_{i}^{2}) = 0$$

$$\hat{\beta}_{1} (\bar{x} \sum_{i=1}^{n} x_{i} - \sum_{i=1}^{n} x_{i}^{2} x_{i} y_{i}) = -\sum_{i=1}^{n} x_{i} y_{i} + \bar{y} \sum_{i=1}^{n} x_{i}$$

$$\hat{\beta}_{1} (\bar{x} \sum_{i=1}^{n} x_{i} - \sum_{i=1}^{n} x_{i}^{2}) = \bar{y} \sum_{i=1}^{n} x_{i} - \sum_{i=1}^{n} x_{i} y_{i}$$

$$\hat{\beta_1} = \frac{\bar{y} \sum_{i=1}^n x_i - \sum_{i=1}^n x_i y_i}{\bar{x} \sum_{i=1}^n x_i - \sum_{i=1}^n x_i^2}$$

$$\sum_{i=1}^n x_i = n\bar{x}$$

$$\hat{\beta_1} = \frac{\bar{y} n\bar{x} - \sum_{i=1}^n x_i y_i}{\bar{x} n\bar{x} - \sum_{i=1}^n x_i^2}$$

$$\hat{\beta_1} = \frac{n\bar{y} \bar{x} - \sum_{i=1}^n x_i y_i}{n\bar{x}^2 - \sum_{i=1}^n x_i^2}$$

$$\hat{\beta_1} = \frac{n\bar{y} \bar{x} - \sum_{i=1}^n x_i y_i}{n\bar{x}^2 - \sum_{i=1}^n x_i y_i} \cdot \frac{-1}{-1}$$

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n x_i y_i - n\bar{y}\bar{x}}{\sum_{i=1}^n x_i^2 - n\bar{x}^2}$$
 (5)

Removing n term from nominator in (5):

$$\begin{split} \sum_{i=1}^{n} x_{i}y_{i} - n\bar{x}\bar{y} &= \sum_{i=1}^{n} x_{i}y_{i} - n\bar{x}\bar{y} - n\bar{x}\bar{y} + n\bar{x}\bar{y} \\ n\bar{x}\bar{y} &= \sum_{i=1}^{n} \bar{x}\bar{y} \\ &= \sum_{i=1}^{n} x_{i}y_{i} - n\bar{x}\bar{y} - n\bar{x}\bar{y} + \sum_{i=1}^{n} \bar{x}\bar{y} \\ \bar{x} &= \frac{\sum_{i=1}^{n} x_{i}}{n} \\ &= \sum_{i=1}^{n} x_{i}y_{i} - n\frac{\sum_{i=1}^{n} x_{i}}{n} \bar{y} - n\bar{x}\bar{y} + \sum_{i=1}^{n} \bar{x}\bar{y} \\ &= \sum_{i=1}^{n} x_{i}y_{i} - \sum_{i=1}^{n} x_{i}\bar{y} - n\bar{x}\bar{y} + \sum_{i=1}^{n} \bar{x}\bar{y} \\ &= \sum_{i=1}^{n} x_{i}y_{i} - \sum_{i=1}^{n} x_{i}\bar{y} - \bar{x}n\bar{y} + \sum_{i=1}^{n} \bar{x}\bar{y} \\ \bar{y} &= \frac{\sum_{i=1}^{n} y_{i}}{n} \\ &= \sum_{i=1}^{n} x_{i}y_{i} - \sum_{i=1}^{n} x_{i}\bar{y} - \bar{x}n\frac{\sum_{i=1}^{n} y_{i}}{n} + \sum_{i=1}^{n} \bar{x}\bar{y} \\ &= \sum_{i=1}^{n} x_{i}y_{i} - \sum_{i=1}^{n} x_{i}\bar{y} - \bar{x}\sum_{i=1}^{n} y_{i} + \sum_{i=1}^{n} \bar{x}\bar{y} \\ &= \sum_{i=1}^{n} x_{i}y_{i} - \sum_{i=1}^{n} x_{i}\bar{y} - \sum_{i=1}^{n} \bar{x}y_{i} + \sum_{i=1}^{n} \bar{x}\bar{y} \\ &= \sum_{i=1}^{n} (x_{i}y_{i} - x_{i}\bar{y} - \bar{x}y_{i} + \bar{x}\bar{y}) \\ &= \sum_{i=1}^{n} (x_{i}y_{i} - x_{i}\bar{y} - \bar{x}y_{i} + \bar{x}\bar{y}) \end{split}$$

Substituting in (5):

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n x_i^2 - n\bar{x}^2}$$
 (6)

Removing n term from denominator in (6):

$$\sum_{i=1}^{n} x_i^2 - n\bar{x}^2 = \sum_{i=1}^{n} x_i^2 - 2n\bar{x}^2 + n\bar{x}^2$$

$$= \sum_{i=1}^{n} x_i^2 - 2\bar{x}n\bar{x} + n\bar{x}^2$$

$$n\bar{x} = \sum_{i=1}^{n} x_i$$

$$= \sum_{i=1}^{n} x_i^2 - 2\bar{x}\sum_{i=1}^{n} x_i + n\bar{x}^2$$

$$= \sum_{i=1}^{n} x_i^2 - \sum_{i=1}^{n} 2x_i\bar{x} + n\bar{x}^2$$

$$= \sum_{i=1}^{n} x_i^2 - \sum_{i=1}^{n} 2x_i\bar{x} + \sum_{i=1}^{n} \bar{x}^2$$

$$= \sum_{i=1}^{n} (x_i^2 - 2x_i\bar{x} + \bar{x}^2)$$

$$= \sum_{i=1}^{n} (x_i - \bar{x})^2$$

Substituting in (6):

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}$$
 (7)

Solving for example given in class:

```
% line of best fit
% y = 74.2307692308 - 4.23076923077 * x

% prediction y for x = 5
% y = 53.0769230769mph

% MATLAB solution for b and m
glmfit([2 4 10], [75 45 35]) % coefficient estimates ans =

74.2308
-4.2308
```