Least squares derivation of linear regression

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

Define loss function and expand:

$$Q = \sum_{i=1}^{n} (y_i - \hat{y_i})^2, \hat{y_i} = mx_i + b$$

$$Q(m,b) = \sum_{i=1}^{n} (y_i - (mx_i + b))^2$$

$$Q(m,b) = \sum_{i=1}^{n} (y_i - mx_i - b)^2$$

$$Q(m,b) = \sum_{i=1}^{n} (y_i^2 - y_i m x_i - y_i b - y_i m x_i + m^2 x_i^2 + m x_i b - y_i b + m x_i b + b^2)$$

$$Q(m,b) = \sum_{i=1}^{n} y_i^2 - \sum_{i=1}^{n} y_i m x_i - \sum_{i=1}^{n} y_i b - \sum_{i=1}^{n} y_i m x_i + \sum_{i=1}^{n} m^2 x_i^2 + \sum_{i=1}^{n} m x_i b - \sum_{i=1}^{n} y_i b + \sum_{i=1}^{n} m x_i b + \sum_{i=1}^{n} b^2$$

$$Q(m,b) = \sum_{i=1}^{n} y_i^2 + \sum_{i=1}^{n} m^2 x_i^2 + \sum_{i=1}^{n} b^2 - \sum_{i=1}^{n} 2y_i m x_i - \sum_{i=1}^{n} 2y_i b + \sum_{i=1}^{n} 2m x_i b$$

Differentiate with respect to **m** and **b**:

$$\frac{\partial Q}{\partial m} = 2m \sum_{i=1}^{n} x_i^2 - 2 \sum_{i=1}^{n} y_i x_i + 2b \sum_{i=1}^{n} x_i$$

$$\frac{\partial Q}{\partial b} = 2bN - 2\sum y_i + 2m\sum x_i, N = number of points$$

We want to minimize m and b, so set both to 0:

$$2m\sum x_i^2 - 2\sum y_i x_i + 2b\sum x_i = 0$$

$$2bN - 2\sum y_i + 2m\sum x_i = 0$$

Solve for b first:

$$b = \frac{2\sum y_i - 2m\sum x_i}{2N}$$

$$b = \frac{\sum y_i - m \sum x_i}{N}$$

Substitute b and solve for m:

$$2m\sum_{i} x_{i}^{2} - 2\sum_{i} y_{i}x_{i} + 2\frac{\sum_{i} y_{i} - m\sum_{i} x_{i}}{N}\sum_{i} x_{i} = 0$$

$$m\sum_{i} x_{i}^{2} - \sum_{i} y_{i}x_{i} + \frac{\sum_{i} y_{i} - m\sum_{i} x_{i}}{N} \sum_{i} x_{i} = 0$$

$$m\sum_{i} x_{i}^{2} - \sum_{i} y_{i}x_{i} + \frac{\sum_{i} y_{i}\sum_{i} x_{i} - m(\sum_{i} x_{i})^{2}}{N} = 0$$

$$mN\sum_{i} x_{i}^{2} - N\sum_{i} y_{i}x_{i} + \sum_{i} y_{i}\sum_{i} x_{i} - m(\sum_{i} x_{i})^{2} = 0$$

$$mN\sum_{i} x_{i}^{2} - m(\sum_{i} x_{i})^{2} = N\sum_{i} y_{i}x_{i} - \sum_{i} y_{i}\sum_{i} x_{i}$$

$$m(N\sum_{i} x_{i}^{2} - (\sum_{i} x_{i})^{2}) = N\sum_{i} y_{i}x_{i} - \sum_{i} y_{i}\sum_{i} x_{i}$$

$$m = \frac{N\sum_{i} y_{i}x_{i} - \sum_{i} y_{i}\sum_{i} x_{i}}{N\sum_{i} x_{i}^{2} - (\sum_{i} x_{i})^{2}}$$

This solution assumes:

1. Normally distributed residuals.

Least squares derivation of linear regression (abridged)

1. Define loss function and expand:

$$Q(m,b) = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} (y_i - (mx_i + b))^2$$

...

$$Q(m,b) = \sum_{i=1}^{n} y_i^2 + \sum_{i=1}^{n} m^2 x_i^2 + \sum_{i=1}^{n} b^2 - \sum_{i=1}^{n} 2y_i m x_i - \sum_{i=1}^{n} 2y_i b + \sum_{i=1}^{n} 2m x_i b$$

2. Differentiate with respect to **m** and **b** and set to 0 because we want to minimize error:

$$\frac{\partial Q}{\partial m} = 0 = 2m \sum_{i=1}^{n} x_i^2 - 2 \sum_{i=1}^{n} y_i x_i + 2b \sum_{i=1}^{n} x_i$$

$$\frac{\partial Q}{\partial b} = 0 = 2bN - 2\sum y_i + 2m\sum x_i$$

N = number of points

3. Solve for m and b:

$$m = \frac{N \sum y_i x_i - \sum y_i \sum x_i}{N \sum x_i^2 - (\sum x_i)^2}$$
$$b = \frac{\sum y_i - m \sum x_i}{N}$$

Maximum likelihood derivation of linear regression (abridged)

1. PDF for normally-distributed variable: $X \sim \mathcal{N}(\mu, \sigma^2)$

$$PDF(X) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

2. PDF, with linear equation in place of the mean.

$$P(y|x; m, b, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-(y - (mx + b))^2}{2\sigma^2}}$$

3. Likelihood function for all observed points (x, y) is the product of the probability density for each point:

$$L(m, b, \sigma^{2}) = \frac{1}{\sqrt{2\pi\sigma^{2}}} \prod_{i=1}^{n} e^{\frac{-(y_{i} - (mx_{i} + b))^{2}}{2\sigma^{2}}}$$

- 4. Goal: find parameters **b**, **m** and σ that **maximize** L.
- 1. Convert to log likelihood for easier math, maximize log(L):

$$log(L) = log[\frac{1}{\sqrt{2\pi\sigma^2}} \prod_{i=1}^{n} e^{\frac{-(y_i - (mx_i + b))^2}{2\sigma^2}}]$$

..

$$log(L) = -\frac{1}{2}log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - (mx_i + b))^2$$

2. Or, minimize negative log likelihood:

$$-log(L) = \frac{1}{2}log(2\pi\sigma^2) + \frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - (mx_i + b))^2$$

3. Let's imagine that our variance term is a fixed constant.

$$-log(L) = \sum_{i=1}^{n} (y_i - (mx_i + b))^2$$