Can model the data as being a function of the i observations x_i and a vector a of the fitting parameters,

$$y = y(x; a_i), \text{ given some params } a_i.$$
$$= mx_i + c$$

$$a = \begin{bmatrix} m \\ c \end{bmatrix}$$

The overall quality of the fit can be measured using chi-squared.

$$x^2 = \sum r_i^2$$
$$= \sum (y_i - mx_i - c)^2$$

The residual is the difference between y and the predicted items.

$$r_i = y_i - (mx_i + c)$$

· squaring
① ensures equal penalty to positive and negative residuals
② weighted penalties to greater residuals.

The goal is to find the lowest chi-squared possible — that is the best fitting parameters. This is an optimization problem!
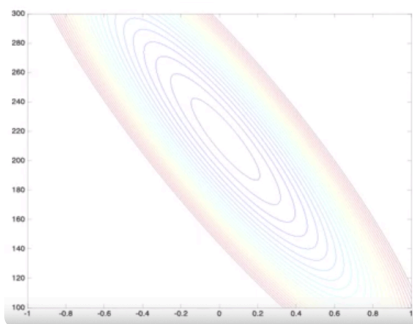
This is what the chi-squared looks like for many different values of m and c. The min is around $m = 215, c = 0$.

There is some relationship between m and c, as m gets bigger c must get smaller — and vice versa.

(*) Also this function has a really shallow gradient/trough the min. This makes steepest descent have to perform more computations — and is a slower process.

The minimum of the chi-squared function can be found when the chi-sq. gradient is zero. Solution is to find chi-sq. with respect to the fitting params.

This can be solved explicitly,
   • can also be solved by linear descent.
   • can also — by non-explicit solution.

$$\nabla x^2 = \begin{bmatrix} \dfrac{\partial x^2}{\partial m} \\[2ex] \dfrac{\partial x^2}{\partial c} \end{bmatrix} = \begin{bmatrix} 0 \\[2ex] 0 \end{bmatrix} = \begin{bmatrix} -2\sum_i x_i(y_i - mx_i - c) \\[2ex] -2\sum_i(y_i - mx_i - c) \end{bmatrix}$$

In manipulating the second partial derivative, $-2\sum_i(y_i - mx_i - c)$, can find an expression for c,

$$\frac{\partial x^2}{\partial c} = -2\sum_i(y_i - mx_i - c)$$

$$0 = -2\sum_i(y_i - mx_i) + 2Nc, \text{ where N is the number of observations.}$$

$$-2Nc = -2\sum_i y_i + 2\sum_i mx_i$$

$$Nc = \sum_i y_i - \sum_i mx_i$$

$$c = \frac{\sum_i y_i}{N} - \frac{\sum_i mx_i}{N}$$

$$c = \bar{y} - m\bar{x}, \text{ where } \bar{y} \text{ is avg } y \text{ and } \bar{x} \text{ is avg } x.$$
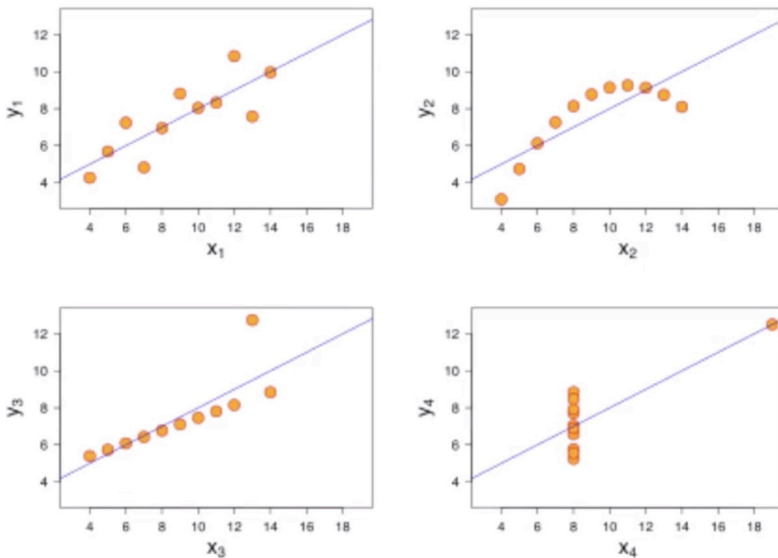
By then solving for m, can find,

$$m = \frac{\sum (x - \bar{x}) y}{\sum (x - \bar{x})^2}$$

Uncertainties are,

$$\sigma_c \simeq \sigma_m \sqrt{x^2 + \frac{1}{n} \sum_i (x - \bar{x})^2}$$

$$\sigma_m^2 \simeq \frac{x^2}{\sum (x - \bar{x})^2 (n-2)}$$

Anscombe's quartet

It's important to validate that your model correctly expresses the nature of your data — in general that your description via descriptive stat. matches the description of your data.

The relationships of your model are important too — and if you introduce unneeded complexity

$C = \bar{y} - m \bar{x}$, is dependent on the m param.

Can remove this dependency by expressing observations as deviations from the centre of mass (i.e $\bar{x}$) and the intercept is the centre of mass $\bar{y}$. This produces a linear formulation where c is no longer afflicted by the gradient!
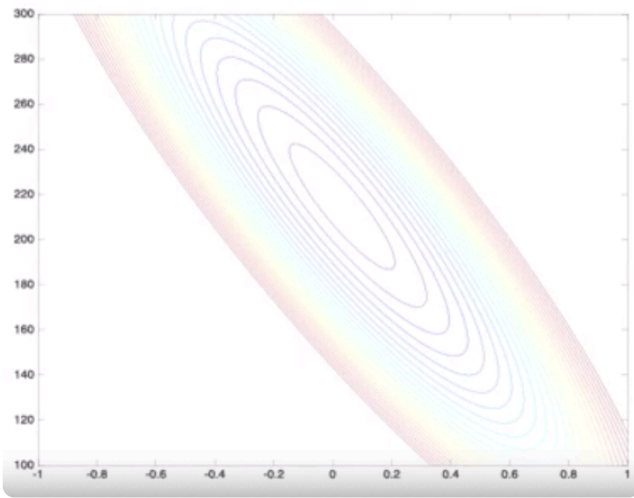
$$y = (m \pm \sigma_m)(x - \bar{x}) + (b \pm \sigma_b)$$

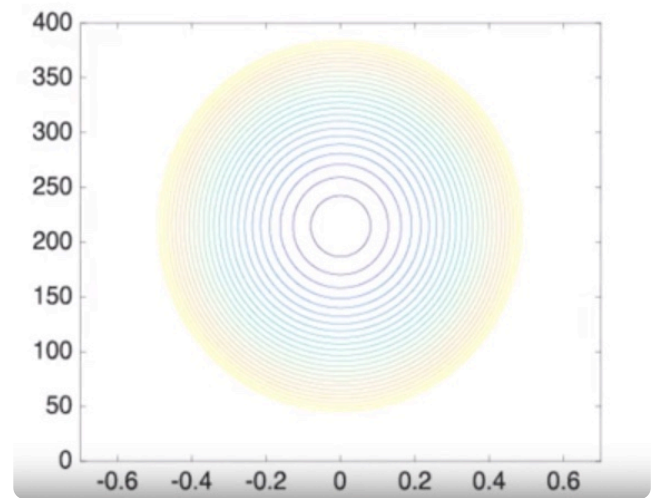$$m = \frac{\sum(x - \bar{x})y}{\sum(x - \bar{x})^2}$$

$$b = \bar{y}$$

$$\sigma_m^2 \simeq \frac{x^2}{\sum(x - \bar{x})^2 (n-2)}$$

$$\sigma_b^2 \simeq \frac{x^2}{n(n-2)}$$

By reformulating the linear models to remove the dependencies between parameter definitions, the minimization problem simplifies.

 $\Rightarrow$

Contour map of Chi^2 test when $c = \bar{y} - m\bar{x}$, and deviation is based on origin $x = 0$.

Contour map of Chi^2 test when $c = \bar{y}$ and linear model is based off deviation from centre-mass.

All of this minimization was to answer —

"how to fit a line to some data".

Chi squared measures goodness of fit by squares and deviations of fit from the data.