Fitting a straight line

For a set of data $\left(x_i, y_i\right)$ with error in y direction of σ_i, we'd like to find a straight line $y = a + bx,\ (a:\text{intercept},\ b:\text{slope})$ to describe the relationship of x_i and y_i.

Define $\boxed{\chi^2 = \sum_{i=1}^{N} \frac{\left(y_i - a - bx_i\right)^2}{\sigma_i^2}}$

The best values of a and b occur when χ^2 reach minimum value.

$$\left.\frac{\partial \chi^2}{\partial a'}\right|_{a'=a} = 0 = -2\sum_i \frac{y_i - a - bx_i}{\sigma_i^2} \Rightarrow a\sum_i \frac{1}{\sigma_i^2} + b\sum_i \frac{x_i}{\sigma_i^2} = \sum_i \frac{y_i}{\sigma_i^2} \cdots\cdots(1)$$

$$\left.\frac{\partial \chi^2}{\partial b'}\right|_{b'=b} = 0 = -2\sum_i x_i \frac{y_i - a - bx_i}{\sigma_i^2} \Rightarrow a\sum_i \frac{x_i}{\sigma_i^2} + b\sum_i \frac{x_i^2}{\sigma_i^2} = \sum_i \frac{x_i y_i}{\sigma_i^2} \cdots\cdots(2)$$

Define $S \equiv \sum_i \frac{1}{\sigma_i^2},\ S_x \equiv \sum_i \frac{x_i}{\sigma_i^2},\ S_{xx} \equiv \sum_i \frac{x_i^2}{\sigma_i^2},\ S_y \equiv \sum_i \frac{y_i}{\sigma_i^2},\ S_{xy} \equiv \sum_i \frac{x_i y_i}{\sigma_i^2}$

Thus, the equations become: $\begin{cases} aS + bS_x = S_y \cdots\cdots\cdots(1) \\ aS_x + bS_{xx} = S_{xy} \cdots\cdots(2) \end{cases}$

Let $\Delta = \begin{vmatrix} S & S_x \\ S_x & S_{xx} \end{vmatrix} = S \cdot S_{xx} - S_x^2 \Rightarrow \boxed{a = \frac{S_{xx}S_y - S_x S_{xy}}{\Delta}}, \boxed{b = \frac{SS_{xy} - S_x S_y}{\Delta}}$

Then, what is the error of parameters σ_a, σ_b? Because a, b are functions of y_i

$$\therefore \sigma_a^2 = \sum_i \left(\frac{\partial a}{\partial y_i}\right)^2 \sigma_i^2, \sigma_b^2 = \sum_i \left(\frac{\partial b}{\partial y_i}\right)^2 \sigma_i^2$$

$$\left(\frac{\partial a}{\partial y_i}\right) = \frac{\partial}{\partial y_i} \frac{S_{xx}S_y - S_x S_{xy}}{\Delta} = \frac{1}{\Delta}\left(S_{xx}\frac{\partial S_y}{\partial y_i} - S_x \frac{\partial S_{xy}}{\partial y_i}\right) = \frac{1}{\Delta}\left(\frac{1}{\sigma_i^2} S_{xx} - S_x \frac{x_i}{\sigma_i^2}\right)$$

$$\left(\frac{\partial b}{\partial y_i}\right) = \frac{\partial}{\partial y_i} \frac{SS_{xy} - S_x S_y}{\Delta} = \frac{1}{\Delta}\left(S\frac{\partial S_{xy}}{\partial y_i} - S_x \frac{\partial S_y}{\partial y_i}\right) = \frac{1}{\Delta \sigma_i^2}\left(S \cdot x_i - S_x\right)$$

$\Rightarrow \sigma_a^2 = \frac{S_{xx}}{\Delta}, \sigma_b^2 = \frac{S}{\Delta}$, which is independent of y_i

Suppose $\sigma_i \sim \sigma,\ S_{xx} = \sum_i \frac{x_i^2}{\sigma_i^2} \propto \frac{1}{\sigma^2}.\ \Delta = S \cdot S_{xx} - S_x^2 \propto \left(\frac{1}{\sigma^2}\right)^2 \Rightarrow \sigma_a^2 \propto \sigma^2$

Follow the same way, we can find $\sigma_b^2 \propto \sigma^2$

$\therefore$ The larger measured error $\Rightarrow$ larger errors of a and b

Covariance

$$\sigma_{ab} = \sum_i \left(\frac{\partial a}{\partial y_i}\right)\left(\frac{\partial b}{\partial y_i}\right)\sigma_i^{\,2} = \frac{1}{\Delta^2}\sum_i \frac{1}{\sigma_i^{\,4}}\left(S_{xx} - S_x x_i\right)\left(Sx_i - S_x\right)\sigma_i^{\,2} = -\frac{1}{\Delta^2}\left(S_x S_{xx} S - S_x^{\,3}\right)$$

$$= -\frac{S_x}{\Delta^2}\left(\underbrace{S \cdot S_{xx} - S_x^{\,2}}_{=\Delta}\right) = -\frac{S_x}{\Delta} \cdots \text{independent of } y_i$$

Un-weight Fitting

If we do not know the individual measurement errors (σ_i), and want to estimate the errors of coefficients, then here is the procedure:

1. Set $\sigma_i = 1$
2. Calculate the coefficient a and b
3. Calculate χ^2 with a and b in previous step. Then calculate σ_a, σ_b then multiply them by $\sqrt{\chi^2/(N-M)}$, where N is the number of data points and M is the number of coefficient. For linear fitting, M=2.
4. As a result, the errors can be estimated as:

$$\sigma_a = \sqrt{\frac{S_{xx}}{\Delta}} \cdot \sqrt{\frac{\chi^2}{N-2}}, \quad \sigma_b = \sqrt{\frac{S}{\Delta}} \cdot \sqrt{\frac{\chi^2}{N-2}}$$