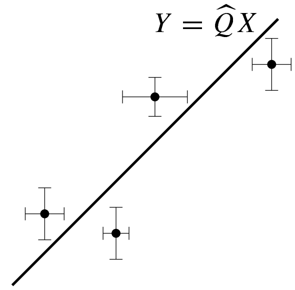
Difference between LS and TLS

- WLS approach assumes that there are errors only on y_i measurements and not on x_i measurements
- TLS approach assumes that there are errors on both x_i and y_i measurements, and models data as

$$(\mathbf{y} - \Delta\mathbf{y}) = Q(\mathbf{x} - \Delta\mathbf{x})$$

- In figure, error bars illustrate uncertainties in each dimension, which are proportional to σ_{x_i} and σ_{y_i}
- We assume $\Delta\mathbf{x} \sim \mathcal{N}(0, \sigma_{x_i}^2)$ and $\Delta\mathbf{y} \sim \mathcal{N}(0, \sigma_{y_i}^2)$, where $\sigma_{x_i}^2$ and $\sigma_{y_i}^2$ are known but not necessarily equal or related in any way to each other

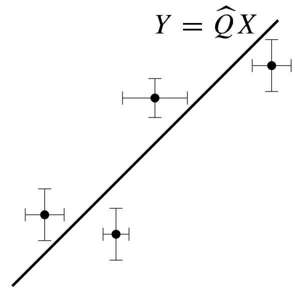


First attempt at cost function for WTLS

- TLS finds $\widehat{Q}$ to minimizes sum of squared errors Δx_i plus the sum of squared errors Δy_i
- We generalize here to weight data points according to uncertainty of the measurement
- That is, we desire to find a $\widehat{Q}$ that minimizes the weighted total least squares (WTLS) cost function

$$\chi^2_{\mathrm{WTLS}} = \sum_{i=1}^{N} \frac{(x_i - X_i)^2}{\sigma_{x_i}^2} + \frac{(y_i - Y_i)^2}{\sigma_{y_i}^2}$$

where X_i and Y_i are the points $Y_i = \widehat{Q}X_i$ mapping noisy measured data pair (x_i, y_i)



Augmented cost function for WTLS

- As both x_i and y_i have noise, must handle this optimization problem differently from how we handled WLS problem
- Augment cost function with Lagrange multipliers λ_i to enforce constraint $Y_i = \widehat{Q}X_i$

$$\chi^2_{\mathrm{WTLS},a} = \sum_{i=1}^{N} \frac{(x_i - X_i)^2}{\sigma_{x_i}^2} + \frac{(y_i - Y_i)^2}{\sigma_{y_i}^2} - \lambda_i(Y_i - \widehat{Q}X_i)$$

- We set the partial derivatives of $\chi^2_{\mathrm{WTLS},a}$ with respect to X_i, Y_i, and λ_i to zero

$$\frac{\partial \chi^2_{\mathrm{WTLS},a}}{\partial \lambda_i} = -(Y_i - \widehat{Q}X_i) = 0 \qquad \Rightarrow \qquad \boxed{Y_i = \widehat{Q}X_i}$$

$$\vdots$$

Simplifying augmented cost function...

- Continuing to set partial derivatives to zero...

$$\frac{\partial \chi^2_{\mathrm{WTLS},a}}{\partial Y_i} = \frac{-2(y_i - Y_i)}{\sigma^2_{y_i}} - \lambda_i = 0 \quad \Rightarrow \quad \boxed{\lambda_i = \frac{-2(y_i - Y_i)}{\sigma^2_{y_i}}}$$

$$\frac{\partial \chi^2_{\mathrm{WTLS},a}}{\partial X_i} = \frac{-2(x_i - X_i)}{\sigma^2_{x_i}} + \lambda_i \widehat{Q} = 0$$

$$0 = -\frac{2(x_i - X_i)}{\sigma^2_{x_i}} - \frac{2(y_i - Y_i)}{\sigma^2_{y_i}}\widehat{Q} = \sigma^2_{y_i}(x_i - X_i) + \sigma^2_{x_i}(y_i - Y_i)\widehat{Q}$$

$$= \sigma^2_{y_i} x_i - \sigma^2_{y_i} X_i + \sigma^2_{x_i} y_i \widehat{Q} - \sigma^2_{x_i} X_i \widehat{Q}^2 \quad \Rightarrow \quad \boxed{X_i = \frac{x_i \sigma^2_{y_i} + \widehat{Q} y_i \sigma^2_{x_i}}{\sigma^2_{y_i} + \widehat{Q}^2 \sigma^2_{x_i}}}$$

...simplifying augmented cost function...

- Can now rewrite cost function in terms of known quantities

$$\chi^2_{\mathrm{WTLS}} = \sum_{i=1}^{N} \frac{(x_i - X_i)^2}{\sigma^2_{x_i}} + \frac{(y_i - Y_i)^2}{\sigma^2_{y_i}}$$

$$= \sum_{i=1}^{N} \left(x_i - \frac{x_i \sigma^2_{y_i} + \widehat{Q} y_i \sigma^2_{x_i}}{\sigma^2_{y_i} + \widehat{Q}^2 \sigma^2_{x_i}} \right)^2 \Bigg/ \sigma^2_{x_i} + \left(y_i - \widehat{Q}\frac{x_i \sigma^2_{y_i} + \widehat{Q} y_i \sigma^2_{x_i}}{\sigma^2_{y_i} + \widehat{Q}^2 \sigma^2_{x_i}} \right)^2 \Bigg/ \sigma^2_{y_i}$$

$$= \sum_{i=1}^{N} \frac{\left(x_i(\sigma^2_{y_i} + \widehat{Q}^2\sigma^2_{x_i}) - (x_i\sigma^2_{y_i} + \widehat{Q} y_i \sigma^2_{x_i})\right)^2}{\sigma^2_{x_i}\left(\sigma^2_{y_i} + \widehat{Q}^2\sigma^2_{x_i}\right)^2} + \frac{\left(y_i(\sigma^2_{y_i} + \widehat{Q}^2\sigma^2_{x_i}) - \widehat{Q}(x_i\sigma^2_{y_i} + \widehat{Q} y_i \sigma^2_{x_i})\right)^2}{\sigma^2_{y_i}\left(\sigma^2_{y_i} + \widehat{Q}^2\sigma^2_{x_i}\right)^2}$$

...simplifying augmented cost function

- Continuing by expanding squares, collecting like terms...

$$\chi^2_{\mathrm{WTLS}} = \sum_{i=1}^{N} \frac{\widehat{Q}^2\sigma^4_{x_i}\left(y_i - \widehat{Q}x_i\right)^2}{\sigma^2_{x_i}\left(\sigma^2_{y_i} + \widehat{Q}^2\sigma^2_{x_i}\right)^2} + \frac{\sigma^4_{y_i}\left(y_i - \widehat{Q}x_i\right)^2}{\sigma^2_{y_i}\left(\sigma^2_{y_i} + \widehat{Q}^2\sigma^2_{x_i}\right)^2}$$

$$= \sum_{i=1}^{N} \frac{\left(\widehat{Q}^2\sigma^2_{x_i} + \sigma^2_{y_i}\right)\left(y_i - \widehat{Q}x_i\right)^2}{\left(\widehat{Q}^2\sigma^2_{x_i} + \sigma^2_{y_i}\right)^2}$$

$$= \sum_{i=1}^{N} \frac{\left(y_i - \widehat{Q}x_i\right)^2}{\widehat{Q}^2\sigma^2_{x_i} + \sigma^2_{y_i}}$$

- Now we have a cost function in terms of known quantities, ready to optimize...

Summary

- WLS approach assumes that there are errors only on y_i measurements and not on x_i measurements
- WTLS approach assumes that there are errors on both x_i and y_i measurements
- Setting up cost function to optimize for WTLS a little tricky, since must also find mapping between (x_i, y_i) and (X_i, Y_i) as part of the optimization
  - We did so using a Lagrange-multiplier approach
- But, finally, we have a cost function in terms only of known quantities
  - We can now proceed to solve for $\widehat{Q}$