Approximate full solution: Derivation

- In prior lesson, you learned new AWTLS cost function

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

- Jacobian of AWTLS cost function can be found to be

$$\begin{aligned}\frac{\partial \chi^2_{\text{AWTLS}}}{\partial \widehat{Q}} = \frac{2}{(\widehat{Q}^2+1)^3} \sum_{i=1}^{N} \widehat{Q}^4\left(\frac{x_i y_i}{\sigma^2_{x_i}}\right) + \widehat{Q}^3\left(\frac{2x_i^2}{\sigma^2_{x_i}} - \frac{x_i^2}{\sigma^2_{y_i}} - \frac{y_i^2}{\sigma^2_{x_i}}\right) \\ + \widehat{Q}^2\left(\frac{3x_i y_i}{\sigma^2_{y_i}} - \frac{3x_i y_i}{\sigma^2_{x_i}}\right) + \widehat{Q}\left(\frac{x_i^2 - 2y_i^2}{\sigma^2_{y_i}} + \frac{y_i^2}{\sigma^2_{x_i}}\right) + \left(\frac{-x_i y_i}{\sigma^2_{y_i}}\right)\end{aligned}$$

Recursive solution

- Can be rewritten in terms of recursive summations

$$\begin{aligned}\frac{\partial \chi^2_{\text{AWTLS}}}{\partial \widehat{Q}} = \frac{2}{(\widehat{Q}^2+1)^3}\Big(c_5\widehat{Q}^4 + (2c_4 - c_1 - c_6)\widehat{Q}^3 \\ + (3c_2 - 3c_5)\widehat{Q}^2 + (c_1 - 2c_3 + c_6)\widehat{Q} - c_2\Big)\end{aligned}$$

where

$$\begin{aligned} c_{1,n} &= c_{1,n-1} + x_n^2/\sigma^2_{y_n}; & c_{3,n} &= c_{3,n-1} + y_n^2/\sigma^2_{y_n}; & c_{5,n} &= c_{5,n-1} + x_n y_n/\sigma^2_{x_n} \\ c_{2,n} &= c_{2,n-1} + x_n y_n/\sigma^2_{y_n}; & c_{4,n} &= c_{4,n-1} + x_n^2/\sigma^2_{x_n}; & c_{6,n} &= c_{6,n-1} + y_n^2/\sigma^2_{x_n}\end{aligned}$$

- Roots of the quartic equation, below, are candidate solutions for $\widehat{Q}$

$$c_5\widehat{Q}^4 + (2c_4 - c_1 - c_6)\widehat{Q}^3 + (3c_2 - 3c_5)\widehat{Q}^2 + (c_1 - 2c_3 + c_6)\widehat{Q} - c_2 = 0$$

Initializing recursive solution

- Initialized by setting

$$\begin{aligned} x_0 = 1 \text{ and } y_0 = Q_{\text{nom}} \\ \sigma^2_{y_0} = \text{uncertainty in } Q_{\text{nom}} \text{ versus } Q\end{aligned}$$

- We assume that $\sigma_{x_0} = \sigma_{y_0}$ to be compatible with TLS for $k = 1$ (will generalize for different k later in code)
- Therefore,

$$\begin{aligned} c_{1,0} &= 1/\sigma^2_{y_0}; & c_{3,0} &= Q^2_{\text{nom}}/\sigma^2_{y_0}; & c_{5,0} &= Q_{\text{nom}}/\sigma^2_{y_0} \\ c_{2,0} &= Q_{\text{nom}}/\sigma^2_{y_0}; & c_{4,0} &= 1/\sigma^2_{y_0}; & c_{6,0} &= Q^2_{\text{nom}}/\sigma^2_{y_0}\end{aligned}$$

Selecting solution

- Any root the quartic equation found earlier is a possible solution for the $\widehat{Q}$ that optimizes the cost function
  - Roots may be found using closed-form Ferrari method
  - Roots may also be found via eigenvalues of a “companion matrix”
- However, of the four roots only one is optimal, and no method to decide *a priori* which to solve for
- In my experience, with some sets of data all roots are real, but with other sets of data some can be complex, and some can be negative
- Only foolproof method to determine optimizing root is to evaluate χ^2_{AWTLS} at each of the four candidate solutions, retain the one that gives lowest value (skip for negative and complex roots)

Efficiently computing cost function, Hessian

- Computing the cost function may be very readily done if we rewrite it in terms of the running summations

$$\chi^2_{\text{AWTLS}} = \frac{1}{(\widehat{Q}^2+1)^2}\left(c_4\widehat{Q}^4 - 2c_5\widehat{Q}^3 + (c_1+c_6)\widehat{Q}^2 - 2c_2\widehat{Q} + c_3\right)$$

- When the assumptions made in deriving AWTLS are approximately true, the Hessian yields a good value for the error bounds on the total capacity estimate
- After some straightforward but messy mathematics, we can find the Hessian to be

$$\frac{\partial^2\chi^2_{\text{AWTLS}}}{\partial Q^2} = \frac{2}{(Q^2+1)^4}\Big(-2c_5Q^5 + (3c_1-6c_4+3c_6)Q^4 + (-12c_2+16c_5)Q^3$$
$$+ (-8c_1+10c_3+6c_4-8c_6)Q^2 + (12c_2-6c_5)Q + (c_1-2c_3+c_6)\Big)$$

Summary

- Have now found solution to AWTLS cost function
- Optimizing $\widehat{Q}$ is root of a quartic equation
  - Can be found via Ferrari method or eigenvalue method
- Must substitute solutions into cost function to choose best one
- Made efficient via recursive summations
- Hessian can also be computed using recursive sums to provide confidence bounds