Confidence limits on estimated total capacity

- When computing $\widehat{Q}$, important to know certainty of estimate
- Would like to know variance $\sigma^2_{\widehat{Q}}$ to compute confidence intervals within which the true cell total capacity Q lies, with high certainty
  - For example, three-sigma bounds: $Q \in (\widehat{Q} - 3\sigma_{\widehat{Q}}, \widehat{Q} + 3\sigma_{\widehat{Q}})$
- To derive confidence limits, must re-cast least-squares type problem as maximum-likelihood optimization problem
- Then, Cramer–Rao theorem will give us confidence bounds

Recasting WLS as maximum-likelihood

- First, recast problem as maximum-likelihood optimization
- Assuming all errors are Gaussian, this is straightforward
- If we form a vector $\mathbf{y}$ comprising elements y_i, and a vector $\mathbf{x}$ comprising corresponding elements x_i and a diagonal matrix $\Sigma_{\mathbf{y}}$ having corresponding diagonal elements $\sigma^2_{y_i}$, then minimizing χ^2_{WLS} is equivalent to maximizing

$$
\begin{aligned}
ML_{\mathrm{WLS}} &= \frac{1}{(2\pi)^{N/2}|\Sigma_{\mathbf{y}}|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{y} - \widehat{Q}\mathbf{x})^T \Sigma_{\mathbf{y}}^{-1}(\mathbf{y} - \widehat{Q}\mathbf{x})\right) \\
&= \frac{1}{(2\pi)^{N/2}|\Sigma_{\mathbf{y}}|^{1/2}} \exp\left(-\frac{1}{2}\chi^2_{\mathrm{WLS}}\right),
\end{aligned}
$$

  which is a maximum-likelihood problem
- Constant multiplying exponential causes ML_{WLS} to integrate to 1, yielding valid pdf

Recasting WTLS as maximum-likelihood

- If we form vector $\mathbf{d}$ concatenating $\mathbf{y}$ and $\mathbf{x}$, and vector $\widehat{\mathbf{d}}$ concatenating corresponding elements Y_i and X_i, and diagonal matrix $\Sigma_{\mathbf{d}}$ having diagonal elements $\sigma^2_{y_i}$ followed by $\sigma^2_{x_i}$, then minimizing χ^2_{WTLS} is equivalent to maximizing

$$
\begin{aligned}
ML_{\mathrm{WTLS}} &= \frac{1}{(2\pi)^{N}|\Sigma_{\mathbf{d}}|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{d} - \widehat{\mathbf{d}})^T \Sigma_{\mathbf{d}}^{-1}(\mathbf{d} - \widehat{\mathbf{d}})\right) \\
&= \frac{1}{(2\pi)^{N}|\Sigma_{\mathbf{d}}|^{1/2}} \exp\left(-\frac{1}{2}\chi^2_{\mathrm{WTLS}}\right)
\end{aligned}
$$

- The maximum-likelihood formulation makes it possible to determine confidence intervals on $\widehat{Q}\ldots$

Application of Cramer–Rao theorem

- Cramer–Rao theorem, a tight lower bound on variance of $\widehat{Q}$ is given by the negative inverse of second derivative of argument of the exponential function, evaluated at the $\widehat{Q}$ that optimizes the cost function
- That is, for the cost functions we have investigated so far,

$$\sigma^2_{\widehat{Q}} \geq 2 \left(\frac{\partial^2 \chi^2_{\mathrm{WLS}}}{\partial Q^2} \right)^{-1} \Bigg|_{Q=\widehat{Q}} \qquad \text{for WLS}$$

$$\sigma^2_{\widehat{Q}} \geq 2 \left(\frac{\partial^2 \chi^2_{\mathrm{WTLS}}}{\partial Q^2} \right)^{-1} \Bigg|_{Q=\widehat{Q}} \qquad \text{for WTLS}$$

Finding the Hessians

- The second partial derivatives (*i.e.*, Hessians) of WTLS and FMWTLS cost functions have already been described in the context of a Newton–Raphson iteration
- For WLS and FMWLS, the situation is easier:

$$\frac{\partial^2 \chi^2_{\mathrm{WLS}}}{\partial Q^2} = 2 \sum_{i=1}^{N} \frac{x_i^2}{\sigma^2_{y_i}} \qquad \text{and} \qquad \frac{\partial^2 \chi^2_{\mathrm{FMWLS}}}{\partial Q^2} = 2 \sum_{i=1}^{N} \gamma^{N-i} \frac{x_i^2}{\sigma^2_{y_i}}$$

- These may be computed using the previously defined recursive parameters as

$$\frac{\partial^2 \chi^2_{\mathrm{WLS}}}{\partial Q^2} = 2 c_{1,n} \qquad \text{and} \qquad \frac{\partial^2 \chi^2_{\mathrm{FMWLS}}}{\partial Q^2} = 2 \tilde{c}_{1,n}$$

Summary

- Desire to find $\sigma^2_{\widehat{Q}}$ to compute confidence intervals on $\widehat{Q}$
  - For example, three-sigma bounds: $Q \in (\widehat{Q} - 3\sigma_{\widehat{Q}}, \widehat{Q} + 3\sigma_{\widehat{Q}})$
- Recasting xLS problem as ML problem allows invoking Cramer–Rao theorem,

$$\sigma^2_{\widehat{Q}} \geq 2 \left(\frac{\partial^2 \chi^2_{\mathrm{xLS}}}{\partial Q^2} \right)^{-1} \Bigg|_{Q=\widehat{Q}}$$

  - Hessians for WTLS/FMWTLS were already known
  - Hessians for WLS/FMWLS trivial to compute using already-existing quantities