

Notation: usually, “ $i$ ” is reserved for integer indices or the imaginary number. Intensity is usually capital “ $I$ ”. Let,  $c$  = concentration (mg/ml),  $M$  = molecular weight (kDa),  $\Delta\rho$  = contrast,  $t$  = exposure time,  $F$  = flux. Variables with a hat “ $\wedge$ ” have dependences factored out.

For simplicity, let  $\kappa = (c \cdot M \cdot \Delta\rho^2)$  and  $\tau = (t \cdot F)$ .

We get  $I(q)$  by subtracting buffer from sample ... which means we add the squares of the errors:  $\sigma^2 = \sigma_{sample}^2 + \sigma_{buffer}^2$ . Sample is really a mix of protein and buffer,  
 $I(q) = I_{protein} + I_{sample\ buffer} - I_{bulk\ buffer}$ .

For a Poisson counting process, variance is equal to counts:

$\sigma^2 = \kappa\tau\hat{\sigma}_{protein}^2 + \tau 2\hat{\sigma}_{buffer}^2$ . Notice that buffer has only time and flux dependence.

We are interested in the linear fit

$$\ln(I(q)) = b \cdot q^2 + a, \quad \text{where } b = -\frac{1}{3}R_g^2 \text{ and } a = \ln(I(0)).$$

To calculate relative error for this equation we need the sigma one would get from  $\ln(I(q))$  rather than  $I(q)$ . The relationship is

$$\sigma_{\ln(I_i)} = \frac{\sigma_i}{I_i} = \frac{1}{\kappa\sqrt{\tau}} \frac{1}{\hat{I}_i} (\kappa\hat{\sigma}_{protein}^2 + 2\hat{\sigma}_{buffer}^2)^{1/2}.$$

In the limit of low concentration, one can neglect the  $\kappa$  dependence of the square root term. Whether this is generally justified or not for determining lower limits of usability should be investigated further.

The terms in the standard error formula become

$$S \equiv \sum_i \frac{1}{\sigma_{\ln(I_i)}^2} = \kappa^2\tau \sum_i \frac{1}{(\hat{\sigma}_i/\hat{I}_i)^2}, \quad S_{q^2} \equiv \sum_i \frac{q_i^2}{\sigma_{\ln(I_i)}^2} = \kappa^2\tau \sum_i \frac{q_i^2}{(\hat{\sigma}_i/\hat{I}_i)^2}$$

$$S_{q^2q^2} \equiv \sum_i \frac{q_i^4}{\sigma_{\ln(I_i)}^2} = \kappa^2\tau \sum_i \frac{q_i^4}{(\hat{\sigma}_i/\hat{I}_i)^2}.$$

$$\Delta \equiv S \cdot S_{q^2q^2} - S_{q^2}^2 = \kappa^4\tau^2 (\hat{S} \cdot \hat{S}_{q^2q^2} - \hat{S}_{q^2}^2) = \kappa^4\tau^2 \hat{\Delta}.$$

So the relative standard error in slope “ $b$ ” is  $\frac{\sigma_b}{b} = \frac{1}{b} \sqrt{\frac{S}{\Delta}}$ .

Remembering that  $R_g = \sqrt{-3b}$ , then  $\sigma_{R_g} = \left| \frac{R_g \sigma_b}{2b} \right|$

$$\text{So, } \frac{\sigma_{R_g}}{R_g} = \frac{\sigma_b}{2b} = \frac{1}{2b} \sqrt{\frac{S}{\Delta}} = \frac{1}{2b} \frac{1}{\kappa\sqrt{\tau}} \sqrt{\frac{\hat{S}}{\hat{\Delta}}}$$