Measures with error bars (here: S_{CH})

$$Q = \sum_{i}^{N} \frac{1}{N} \frac{|S_{CH,exp,i} - S_{CH,sim,i}|}{\sqrt{\Delta_{exp,i}^2 + \Delta_{sim,i}^2}}$$

“How many times the error is the deviation”

Suggestion: cap the scale at 3

Option 1: Average over entire molecule

+ one number
- tails will dominate

Option 2: headgroup Q1 and tails (both) Q2

+ more balanced
- two numbers
-doesn’t separate tails

Option 3: headgroup Q1 + sn1 Q2 + sn2 Q3

+ separates tails
- 3 numbers

Measures without error bars (Form factor)

Can’t use the SIMtoEXP (closest thing to a standard):

$$k_e = \frac{\sum_{i=1}^{N_q} \frac{|F_s(q_i)|\,|F_e(q_i)|}{(\Delta F_e(q_i))^2}}{\sum_{i=1}^{N_q} \frac{|F_e(q_i)|^2}{(\Delta F_e(q_i))^2}}$$

$$\chi^2 = \frac{\sqrt{\sum_{i=1}^{N_q} (|F_s(q_i)| - k_e|F_e(q_i)|)^2/(\Delta F_e(q_i))^2}}{\sqrt{N_q - 1}}$$

- Experimental and simulation accuracy will differ based on curve location. Currently **both** unknown
- Ranking will based on rmse

  - will depend on choise of q cutoff

  - Will depend on choice of how to scale

  + will take heights and zeros into account in “same units”

Suggestions

- Obtain the scaling from fit to first lobe
- Calculate rmse to q=0.5

  + fit based on most reliable data

  - fit and rmse not from same measure

- Obtain the scaling from minimizing the rmse up to q=0.5

  + fit and rmse consistent

  - all points treated as equally accurate in the fit