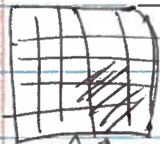
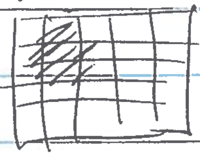
16 FEBRUARY, 2017

How to do WHAM re-weighting

RUN $i=1$  RUN $i=2$ 

j = bins

predicted counts $\quad c_j^{i\,PRED} = z^i f_j w_j^i$

(unknown) normalization: z^i

(unknown) probability density: f_j, $\quad \sum_j f_j = 1$

biasing weight: w_j^i $\quad (e^{-V_j^i/k_BT})$

Poisson ~~likelihood~~ $\quad P(c^{obs}) = \frac{[c^{PRED}]^{c^{obs}}}{c^{obs}!} e^{-c^{PRED}}$

$$\log P = \sum_{i,j} \left[c_j^{i\,obs} \log c_j^{i\,PRED} - c_j^{i\,PRED} \right] + \text{const.}$$

$$0 = \frac{\partial \log P}{\partial z^i} = \sum_{\text{bins } j} \left[\frac{c_j^{i\,OBS}}{z^i} - \frac{c_j^{i\,PRED}}{z^i} \right]$$

$$\Rightarrow \sum_{\text{bins } j} c_j^{PRED} = \sum_{\text{bins } j} c_j^{i\,obs} \Rightarrow \boxed{z^i = \frac{\sum_{\text{bins } j} c_j^{i,OBS}}{\sum_{\text{bins } j} f_j w_j^i}}$$

Similarly, $\quad 0 = \frac{\partial \log P}{\partial f_j} \Rightarrow \boxed{f_j = \frac{\sum_{\text{expts } i} c_j^{i\,OBS}}{\sum_{\text{expts } i} z^i w_j^i}}$

[Solve by iterations, assuming $z^i = 1$ at beginning...]

In 6D potential case I'm using $\quad w_j^i = e^{-\alpha(\vec{x}_j - \vec{x}_0)^2/k_BT}$ (no dependence on rotation),

$\boxed{c_{xyz}^{i\,obs} = \sum_{v_x,v_y,v_z} c^{i\,OBS}_{x,y,z,v_x,v_y,v_z}}$

So do iteration projecting over rotations to get z^i, and f_{xyz},

then infer $\quad f_{x,y,z,v_x,v_y,v_z} = \frac{\sum_{\text{runs } i} c^{i\,OBS}_{x,y,z,v_x,v_y,v_z}}{\sum_{\text{runs } i} z^i w^i_{xyz}}$