Weighted Histogram Analysis Method (WHAM) algorithm notes

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https://bougui505.github.io/science/2014/10/23/wham-the-weighted-histogram-analysis-method.html

WHAM equations

Optimal estimate of unbiased probability distribution:

$$\mathcal{P}_0(\dot{w}) = \frac{\sum_{\alpha'} n_{\alpha'}(\dot{w})}{\sum_{\alpha''} N_{\alpha''} f_{\alpha''} c_{\alpha''}(\dot{w})} \tag{1}$$

- $n_{\alpha'}(\dot{w})$: histogram count for $\dot{w}$ values at α'
- $N_{\alpha''}$: total number of snapshots (clones???) at α''
- $f_{\alpha''}$: normalization constant (solve for it iteratively)
- $c_{\alpha''}(\dot{w}) = \exp\left[-\beta\alpha'' \int_0^\tau \dot{w}\, dt\right]$: biasing factor

$$f_{\alpha''}^{-1} = \sum_{\dot{w}} c_{\alpha''} \mathcal{P}_0(\dot{w}) \tag{2}$$

$\beta = 1$ in our simulations

"We discretize the samples into M bins" https://bougui505.github.io/assets/wham_derivation.pdf

- The samples are the $\dot{w}$ values from each clone
- Number of samples then is $n_{\text{frames}} \cdot n_{\text{clones}}$???

Solve iteratively:

- Arbitrary set of starting values for $f_{\alpha''}$ (e.g. set all equal to 1)
- Calculate $\mathcal{P}_0(\dot{w})$
- Use calculated $\mathcal{P}_0(\dot{w})$ to update $f_{\alpha''}$
- Repeat until convergence is achieved

Algorithm

Set $f_{\alpha''}$

Initial guess: 1 for all α''

Calculate $\mathcal{P}_0(\dot{w})$

Numerator

- For each α, histogram $\dot{w}$ values (for all clones???)
  - Input: bin size, value of α
  - File: `wDots.txt`
- Combine histograms

Denominator

- $c_{\alpha''}(\dot{w}) = \exp\left[-\beta\alpha'' \int_0^\tau \dot{w}\, dt\right]$: calculate for each clone and sum
  - Input: value of α
  - File: `wDotIntegral.txt`
  - Scalar value independent of $\dot{w}$??
- Multiply by $f_{\alpha''}$ and $N_{\alpha''}$
  - Input: $N_{\alpha''}$ (number of clones * number of frames)
    - Number of clones: number of `clone*` directories
    - Number of frames: number of lines in `wDots.txt` - 1 ?
- Take sum over all values of α''

Calculate $\mathcal{P}_0(\dot{w})$

Calculate $f_{\alpha''}$

- Sum over all $\dot{w}$ bins: $c_{\alpha''}(\dot{w})\mathcal{P}_0(\dot{w})$
  - Input:
- Take inverse

Monitor convergence ?