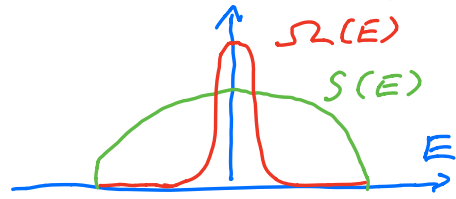


Wang-Landau Algorithm (Entropic Sampling)

Simulate microcanonical potential

$$S(E) = \ln \Omega(E)$$



Relative probability to randomly create state E vs. E' :

$$P(E')/P(E) = \Omega(E')/\Omega(E) = e^{(S(E') - S(E))}$$

← up to unknown factor

∴ Could obtain $\Omega(E)$ by random sampling

How to improve sampling away from peak of $\Omega(E)$?

W-L Algorithm:

- init. {
- Guess some $S(E)$ (e.g. $S(E) = 0$)
 - Create arbitrary initial configuration c with energy E
 - Set $\delta = \ln e = 1$

- Zero out a histogram $H(E)$
- by a spin flip or any other method
- Flatten {
- Create new config c' with energy E'
 - Accept $c' \rightarrow c$ with probability $e^{(S(E) - S(E'))}$
 - If accepted, increment $S(E_f)$ by δ
 - Increment $H(E_f)$ by 1
- ↑ $E_f = E$ or E'
- $= \Omega(E)/\Omega(E')$ if $S(E)$ is exact, thus cancelling $P(E')/P(E)$, and favoring low entropy energies
- Reinit. {
- Reduce $\delta \rightarrow \delta/2$

Green loop: until $H(E)$ "flat enough" \Rightarrow visit full range of E

Pink loop: until $S(E)$ converges (up to added constant)