Machine Learning the Density of States: Neural Wang-Landau Sampling

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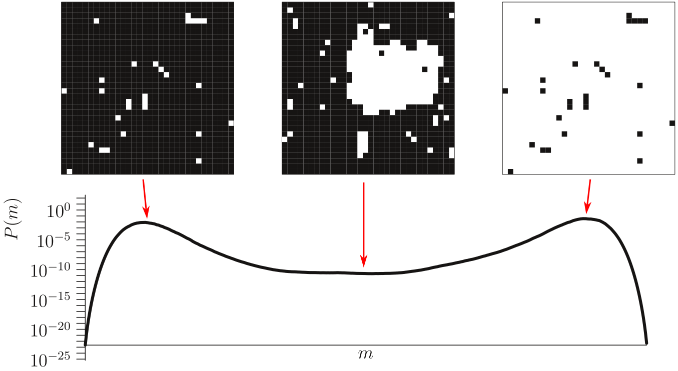
Rare events in statistical physics

Consider for example states in the coexistence region of a first-order phase transition



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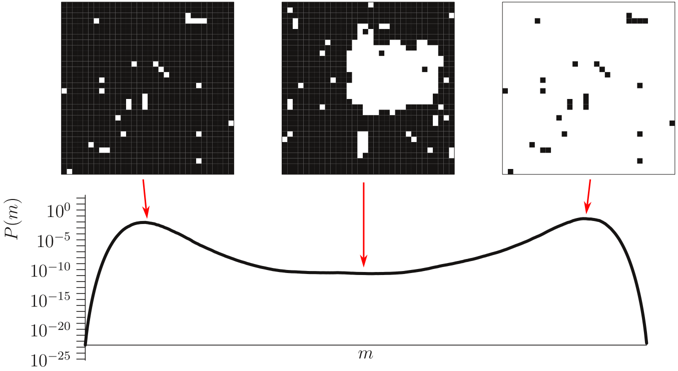

These are practically invisible in standard Monte Carlo simulations.

Rare events in statistical physics

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Other examples:

- transition states in biomolecules
- rare events in distributions of random graphs
- distribution tails in Griffiths phases
- ...

Multicanonical and Wang-Landau simulations

Generalized ensembles

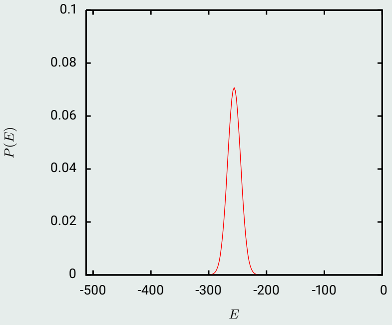
Instead of simulating the canonical distribution,

$$P_\beta(E) = \frac{1}{Z_\beta}\Omega(E)e^{-\beta E},$$

consider using a more general distribution

$$P_{\rm mc}(E) = \frac{\Omega(E)/W(E)}{Z_{\rm muca}} = \frac{\Omega(E)e^{-\omega(E)}}{Z_{\rm muca}},$$

engineered to overcome barriers, improve sampling speed and extend the reweighting range.

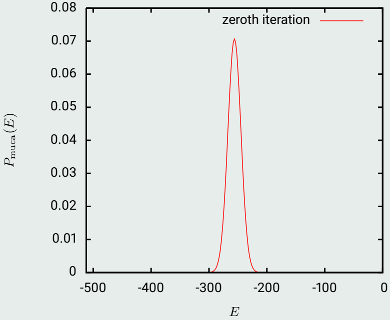


Multicanonical and Wang-Landau simulations

Muca iteration

Determine muca weights/density of states iteratively:

1. Use, e.g., a $K = 0$ canonical simulation to get initial estimate $\hat{S}_0(E) = \ln \hat{\Omega}_0(E)$.



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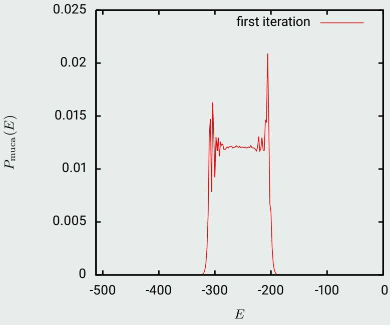

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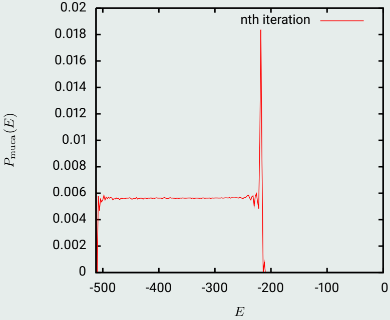
3. Iterate.

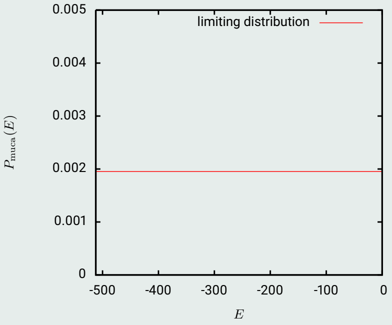


Multicanonical and Wang-Landau simulations

Muca iteration

Advantages:

- always in equilibrium
- arbitrary distributions possible
- system ideally performs an unbiased random walk in energy space $\rightarrow$ fast(er) dynamics

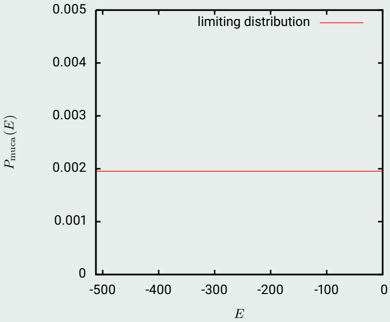


Multicanonical and Wang-Landau simulations

Multicanonical simulations

Variants:

- umbrella sampling, entropic sampling (identical)
- multiple Gaussian modified ensemble
- (broad histogram method)
- transition-matrix Monte Carlo
- metadynamics
- Wang-Landau sampling
- ...



Multicanonical and Wang-Landau simulations

Wang-Landau sampling

Muca weights are updated as

$$\omega_{i+1}(E) - \omega_i(E) = \mathrm{const} + \ln \hat{H}_i(E),$$

i.e., if an energy E is visited more often than others, it receives *less* weight in future iterations.

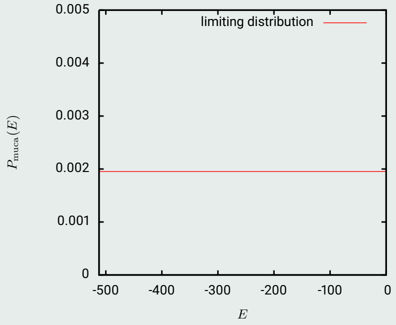
This behavior can be imitated in a one-step iteration: simulate

$$P_{\mathrm{WL}}(E) \propto \Omega(E) e^{-\omega(E)},$$

but update

$$\omega_{i+1}(E) - \omega_i(E) = \phi,$$

each time an energy E is seen.



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WL iteration

1. Start with $\omega(E) = 0 \; \forall E$.
2. Simulate "sufficiently long" while continuously updating $\omega(E)$.
3. Reduce modification factor, e.g.,

$$\phi \to \phi/2$$

4. Iterate till $\phi < \phi_{\text{thres}}$.

Multicanonical and Wang-Landau simulations

Use and justification

Different possible interpretations of this scheme:

- Rather efficient way of calculating muca weights.
- Standalone algorithm for estimating the density of states (convergence?).
- Violates detailed balance for any $\phi > 0$, but convergence can be proved as a stochastic approximation (instead of MCMC) algorithm for

$$\phi = \frac{t_0}{\max(t, t_0)} \sim \frac{1}{t}, \quad t > t_0$$

instead of

$$\phi = \phi_0 \, 2^{-t}$$

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Problem

Multicanonical simulations are very expensive. Samples in Markov chains suffer from autocorrelations of consecutive samples.

Sampling with neural networks

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$$\langle O \rangle_\beta = \frac{\sum_t O(\{s_t\}) P_\beta(\{s_t\})/P_{\rm gen}(\{s_t\})}{\sum_t P_\beta(\{s_t\})/P_{\rm gen}(\{s_t\})}$$

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Standard architectures achieving this: **autoregressive networks** and **normalizing flows**.

Autoregressive networks

Autoregressive networks (`Wu, Wang + Zhang, 2019`): based on factorization property

$$q(\{s_i\}) = \prod_{i=1}^{N} P(s_i|s_{<i}), \quad P(s_i|s_{<i}) = \begin{cases} q_i & s_i = +1, \\ 1 - q_i & s_i = -1. \end{cases}$$

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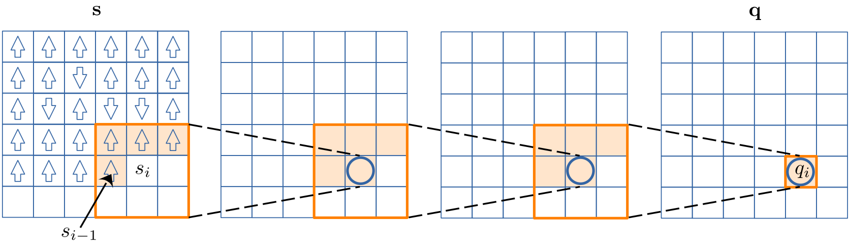

Normalizing flows

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does not work for discrete variables

Wang-Landau sampling with autoregressive network

We consider the 2D Potts model with Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \delta_{s_i,s_j}, \quad s_i = 0, \ldots, q-1.$$

as test system: first-order transitions of increasing strength for $q > 4$.

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How about the task of learning the density of states? Possible algorithm:

1. Initialize a preliminary estimate for the DoS $g(E) \equiv 1$ and a constant $f > 1$.
2. Generate a batch of M states $\{\mathbf{s}^{(k)}\}$ with probabilities $\{q(\mathbf{s}^{(k)})\}$.
3. Minimize $D_{\mathsf{KL}}(q\|p)$ for the current batch with $p(\mathbf{s}) \propto g(H(\mathbf{s}))^{-1}$.
4. Compute relative, not normalized weights $\hat{w}(\mathbf{s}^{(k)}) = g(H(\mathbf{s}^{(k)}))^{-1}/q(\mathbf{s}^{(k)})$ and update $g(H(\mathbf{s}^{(k)})) \leftarrow g(H(\mathbf{s}^{(k)})) \cdot f^{w(\mathbf{s}^{(k)})}$ with $w(\mathbf{s}^{(k)}) = \hat{w}(\mathbf{s}^{(k)}) / \sum_{k=1}^{M} \hat{w}(\mathbf{s}^{(k)})$.
5. Repeat from step 2 until histogram “broad” or “flat”.

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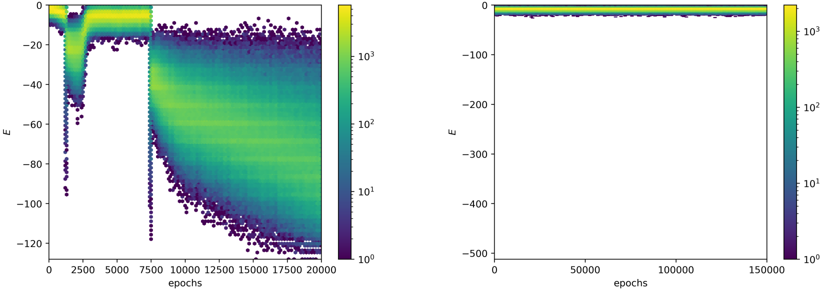

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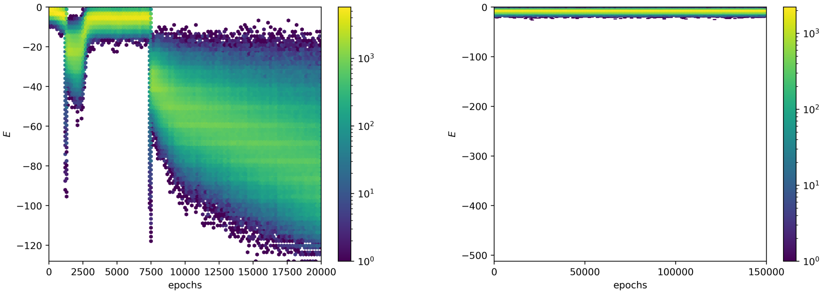

Observations:

- is not able to sample broad energy range
- shows signs of **catastrophic forgetting**
- shows very bad scaling behavior in system size

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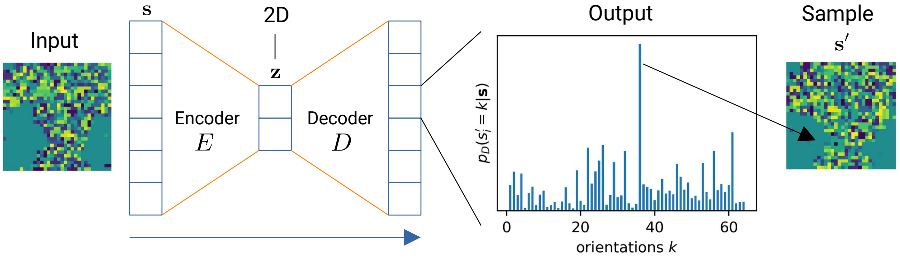

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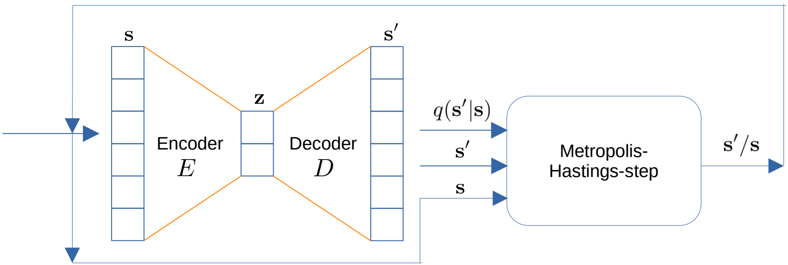

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- possibly complement with supervised training

Neural Wang-Landau sampling

This leads to the following algorithm:

Neural Wang-Landau sampling

1. Generate a batch of M initial states $\{s_i\}$ and initialize $g(E) = 1\ \forall E$, $F > 1$.
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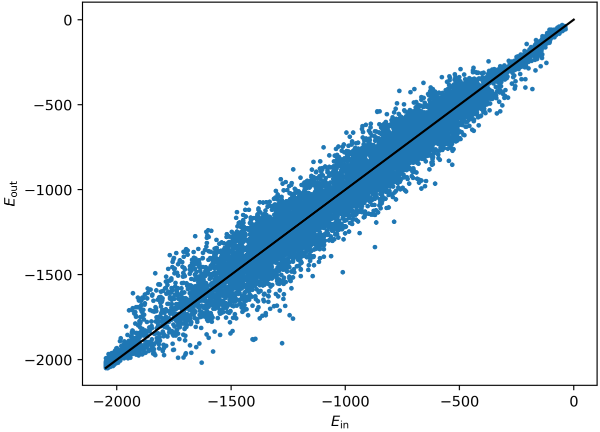
Notably, at this stage it is *not* required to systematically reduce f.

Network training

VAE leads to semi-local updates, ensuring reasonable acceptance rates.



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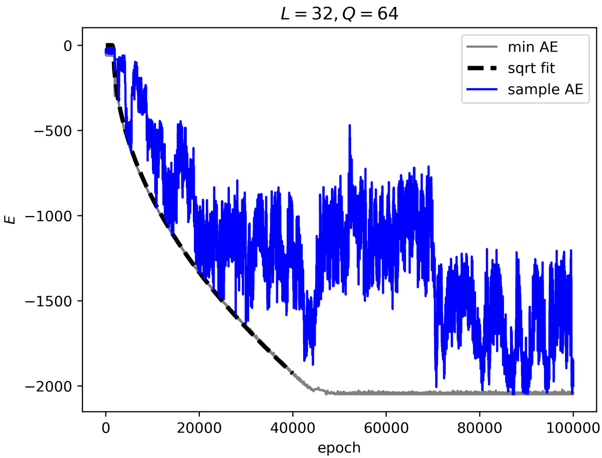

52 h GPU time

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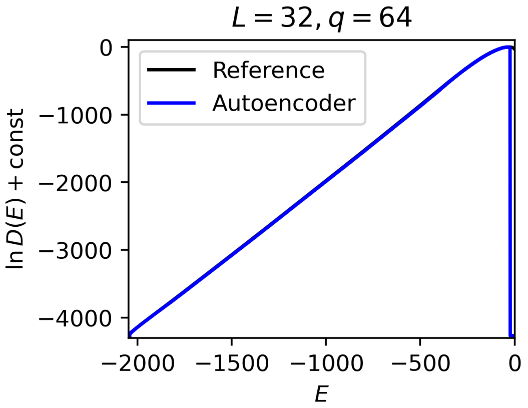

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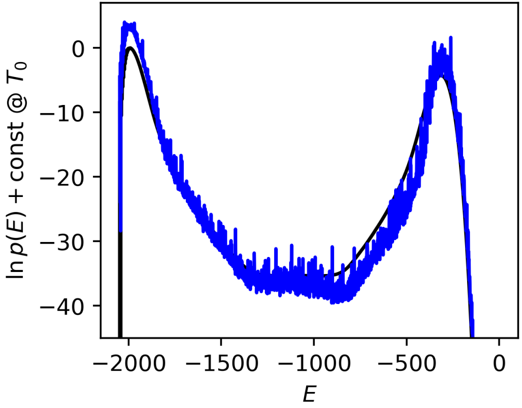
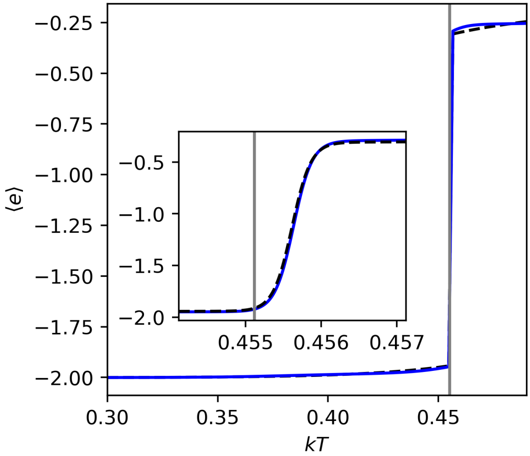


Canonical observables

We can easily estimate canonical averages, such as the mean energy and the free energy.



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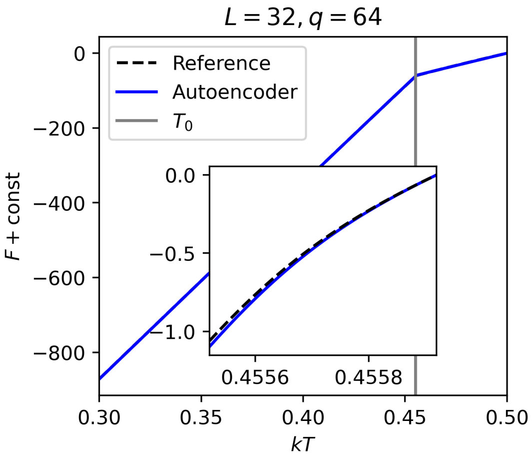
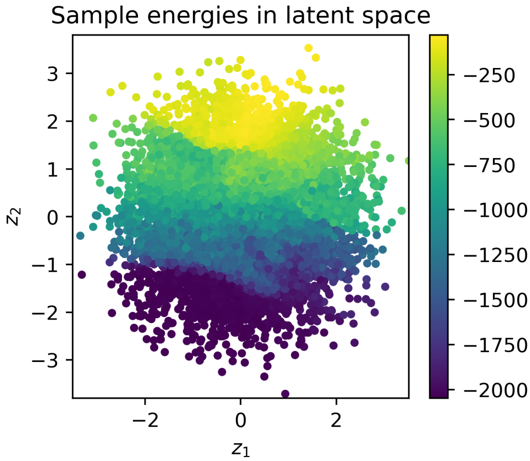


Conditioning in latent space

Use additional term in loss function to tie, e.g., energy to latent space variable.



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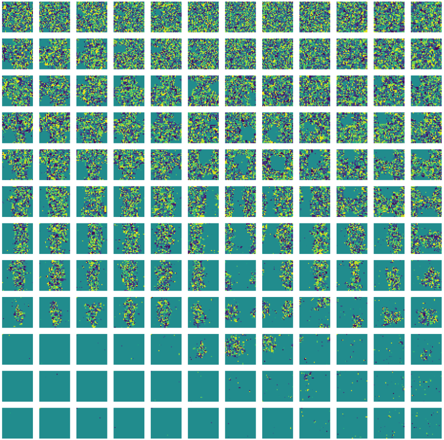

Mode collapse

A general problem with such ANN architectures is contraction to one or a few modes of the distribution: mode collapse

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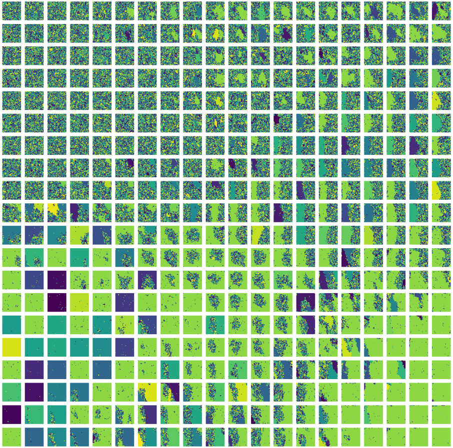
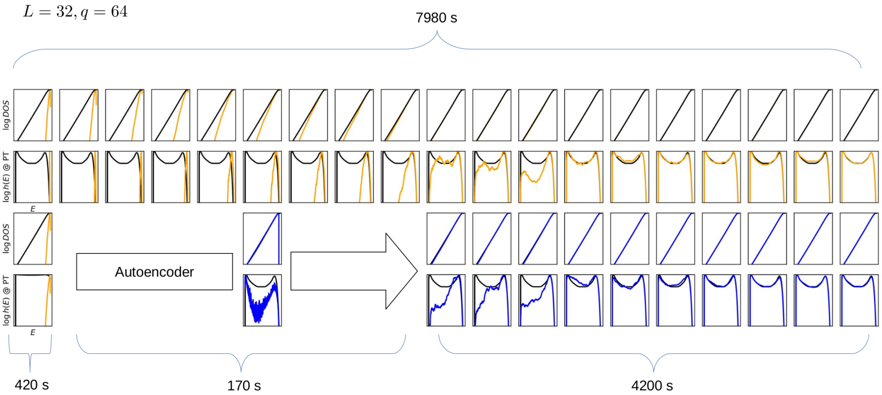
Can be improved by explicitly symmetrizing the training samples.



Hybrid sampling

Combine advantages of traditional and neural WL sampling.



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Thank you for your attention!

Mode collapse (2)