

TODO...

- *New items (added 09/11/2019):*

- ☐ Monitor tunneling rate during training.
- ☐ Try increasing the batch size.
- ☐ Try changing the number of leapfrog steps.
- ☐ Try different annealing schedule.
- ☐ Modify the **loss function** as follows:

Let $\Lambda \equiv \Lambda(\xi, \xi') = \delta(\xi', \xi) A(\xi' | \xi)$.

In terms of Λ , we can write the $\ell_\lambda(\xi, \xi', A(\xi' | \xi))$ (Eq. 7 from the L2HMC paper) as

$$\ell_\lambda(\xi, \xi', A(\xi' | \xi)) = \frac{\lambda^2}{\Lambda(\xi, \xi')} - \frac{\Lambda(\xi, \xi')}{\lambda^2}. \quad (1)$$

We are interested to see how the model behaves if we replace ℓ_λ with a Quadratic Gaussian, i.e.

$$\ell_\lambda(\xi, \xi', A(\xi' | \xi)) \longrightarrow \exp \left[\frac{(\Lambda - \Lambda_0)^T (\Lambda - \Lambda_0)}{2 \sigma_\Lambda^2} \right] \quad (2)$$

where Λ_0 is a parameter related to the “average distance” between the initial and proposed configuration and σ_Λ^2 controls the width of the Gaussian.

- *Previous items:*

- ☐ Get a reasonable estimate of the **integrated autocorrelation length**.
- ☐ Look at [Neal's](#) proof and see if there's anything in the L2HMC algorithm that might violate reversibility.
- ☐ Try reducing the step size ε during inference by some multiplicative factor $\varepsilon \rightarrow \alpha \cdot \varepsilon$ so that the acceptance probability $p_x \rightarrow 1$.
 - In doing so we need to increase the number of run steps by $1/\alpha$.
 - See if the bias in the average plaquette scales with ε^2 .
- ☐ Try and figure out why the Jacobian isn't (*exactly*) the same for the forward and backward updates.

- ☐ Try removing the forward/backward masks during inference (i.e. run strictly forward or run strictly backward)
- ☐ Try eliminating either the first x update (i.e. $x \rightarrow x'$) or second x update ($x' \rightarrow x''$) when running inference by setting either $m^t = [1, 1, \dots, 1]$ and $\bar{m}^t = [0, 0, \dots, 0]$ or vice versa (i.e. removing the mask when running inference).

- *Completed:*

- ☒ Implement reversibility checker that ensures that the reversibility condition holds (for both position and momentum)
- ☒ Try with 'float64'. (*Error still present.*)
- ☒ Try as few as 10 hidden nodes and see if the error persists. (*It does.*)
- ☒ Try anti-symmetric Gaussian Mixture Model and see if the trained model is an accurate representation of the target distribution (e.g. by looking at the locations of the means) ([link to post](#)).
- ☒ Loop over `net_weights = [scale_w, translation_w, transformation_w]` from $[0, 0, 0]$ up to $[2, 0, 0]$, $[0, 2, 0]$, $[0, 0, 2]$, and see how the error in the average plaquette changes ([link to post](#)).