PROCEEDINGS OF SCIENCE

MLMC: Machine Learning Monte Carlo for Lattice Gauge Theory

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We present a trainable framework for efficiently generating gauge configurations, and discss ongoing work in this direction. In particular, we consider the problem of sampling configurations from a 4D $SU(3)$ lattice gauge theory, and consider a generalized leapfrog integrator in the molecular dynamics update that can be trained to improve sampling efficiency.

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1. Introduction

2. Background

We would like to calculate observables O:

$$\langle O \rangle \propto \int [\mathcal{D}x]\; O(x)\, \pi(x) \tag{1}$$

where $\pi(x) \propto e^{-\beta S(x)})isourtargetdistribution.$
If these were independent, we could approximate the integral as $\langle O \rangle \simeq \frac{1}{N}\sum_{n=1}^{N} O(x_n)$ with variance

$$\sigma_O^2 = \frac{1}{N}\,\mathrm{Var}\left[O(x)\right] \Longrightarrow \sigma_O \propto \frac{1}{\sqrt{N}}. \tag{2}$$

Instead, nearby configurations are correlated, causing us to incur a factor of τ_{int}^{O} in the variance expression

$$\sigma_O^2 = \frac{\tau_{\mathrm{int}}^{O}}{N}\mathrm{Var}\left[O(x)\right] \tag{3}$$

2.1 Hamiltonian Monte Carlo (HMC)

The typical approach [?] is to use Hamiltonian Monte Carlo (HMC) algorithm for generating configurations distributed according to our target distribution $\pi(x)$. Specifically, we want to (sequentially) construct a chain of states:

$$x_0 \to x_1 \to x_i \to \cdots \to x_n \tag{4}$$

such that, as $n \to \infty$:

$$\{x_i, x_{i+1}, x_{i+2}, \ldots, x_n\} \xrightarrow{n\to\infty} \pi(x) \tag{5}$$

To do this, we begin by introducing a fictitious momentum[1] $v \sim \mathcal{N}(0, 1)$ normally distributed, independent of x. We can write the joint distribution $\pi(x, v)$ as

$$\pi(x, v) = \pi(x)\pi(v) \propto e^{-S(x)} e^{-\frac{1}{2}v^T v} \tag{6}$$
$$= e^{-\left[S(x) + \frac{1}{2}v^T v\right]} \tag{7}$$
$$= e^{-H(x,v)} \tag{8}$$

We can evolve the Hamiltonian dynamics of the $(\dot{x}, \dot{v}) = (\partial_v H, -\partial_x H)$ system using operators $\Gamma : v \to v'$ and $\Lambda : x \to x'$. Explicitly, for a single update step of the leapfrog integrator:

$$\tilde{v} := \Gamma(x, v) = v - \frac{\varepsilon}{2}F(x) \tag{9}$$
$$x' := \Lambda(x, \tilde{v}) = x + \varepsilon\tilde{v} \tag{10}$$
$$v' := \Lambda(x', \tilde{v}) = \tilde{v} - \frac{\varepsilon}{2}F(x'), \tag{11}$$

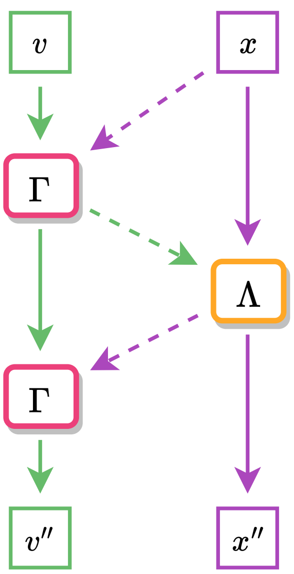


Figure 1: Illustration of the leapfrog update for HMC.

[1]Here ~ means *is distributed according to*.

where we've written the force term as $F(x) = \partial_x S(x)$. Typically, we build a trajectory of N_{LF} leapfrog steps

$$(x_0, v_0) \to (x_1, v_1) \to \cdots \to (x', v'), \tag{12}$$

and propose x' as the next state in our chain. This proposal state is accepted according to the Metropolis-Hastings criteria [**?**].

$$A(x'|x) = \min\left\{1, \frac{\pi(x')}{\pi(x)}\left|\frac{\partial x'}{\partial x}\right|\right\}. \tag{13}$$

3. Method

Unfortunately, HMC is known to suffer from long auto-correlations and often struggles with multi-modal target densities. Instead, we propose building on the approach from [**? ? ?**]. We introduce two (invertible) neural networks (`xNet`, `vNet`):

$$\texttt{vNet} : (x, F) \to (s_v, t_v, q_v) \tag{14}$$
$$\texttt{xNet} : (x, v) \to (s_x, t_x, q_x) \tag{15}$$

where s, t, q are all of the same dimensionality as x and v, and are parameterized by a set of weights θ. These network outputs (s, t, q) are then used in a generalized MD update (as shown in Fig 2) via:

$$\Gamma_\theta^\pm : (x, v) \to (x, v') \tag{16}$$
$$\Lambda_\theta^\pm : (x, v) \to (x', v). \tag{17}$$

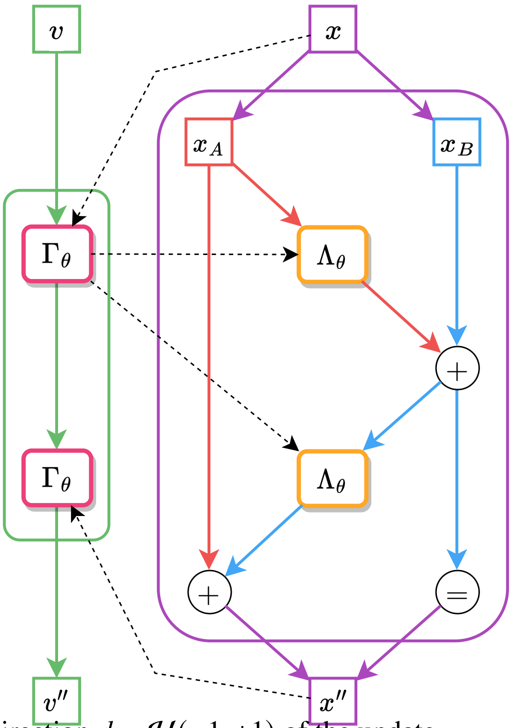


Figure 2: Illustration of the generalized MD update `leapfrog layer` : $(x, v) \to (x'', v'')$.

where the superscript $\pm$ on $\Gamma_\theta^\pm, \Lambda_\theta^\pm$ correspond to the direction $d \sim \mathcal{U}(-1, +1)$ of the update. To ensure that our proposed update remains reversible, we split the x update into two sub-updates on complementary subsets ($x = x_A \cup x_B$):

$$v' = \Gamma_\theta(x, v) \tag{18}$$
$$x' = x_B + \Lambda_\theta(x_A, v') \tag{19}$$
$$x'' = x'_A + \Lambda_\theta(x'_B, v') \tag{20}$$
$$v'' = \Gamma_\theta(x'', v') \tag{21}$$

3.1 Algorithm

1. `input:` x
    - Re-sample $v \sim \mathcal{N}(0, 1)$
    - Construct initial state $\xi := (x, v)$
2. `forward:` Generate proposal ξ' by passing initial ξ through N_{LF} leapfrog layers:

$$\xi \xrightarrow{\text{LF Layer}} \xi_1 \to \cdots \to \xi_{N_{\mathrm{LF}}} = \xi' := (x'', v'') \tag{22}$$

    - Metropolis-Hastings accept / reject:

$$A(\xi'|\xi) = \min\left\{1, \frac{\pi(\xi')}{\pi(\xi)} \left|\mathcal{J}(\xi', \xi)\right|\right\}, \tag{23}$$

      where $|\mathcal{J}(\xi', \xi)|$ is the determinant of the Jacobian.
3. `backward:` (if training)
    - Evaluate the loss function $\mathcal{L}(\xi', \xi)$ and back propagate
4. `return:` x_{i+1}
    - Evaluate MH criteria (Eq. 23) and return accepted config:

$$x_{i+1} \leftarrow \begin{cases} x'' & \text{w/ prob.} \quad A(\xi'|\xi) \\ x & \text{w/ prob.} \quad 1 - A(\xi'|\xi) \end{cases} \tag{24}$$

3.2 4D $SU(3)$ Model

Write link variables $U_\mu(x) \in SU(3)$:

$$U_\mu(x) = \exp\left[i\omega_\mu^k(x)\lambda^k\right] \tag{25}$$

$$= e^{iW}, \quad W \in \mathfrak{su}(3) \tag{26}$$

where $\omega_\mu^k(x) \in \mathbb{R}$ and λ^k are the generators of $SU(3)$. We consider the standard Wilson gauge action

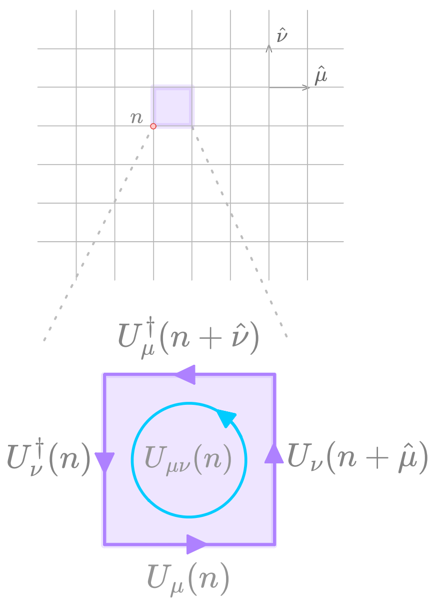
$$S_G = -\frac{\beta}{6} \sum \mathrm{Tr}\left[U_{\mu\nu}(x) + U_{\mu\nu}^\dagger(x)\right] \tag{27}$$

where

$$U_{\mu\nu}(x) = U_\mu(x) U_\nu(x + \hat{\mu}) U_\mu^\dagger(x + \hat{\nu}) U_\nu^\dagger(x).$$

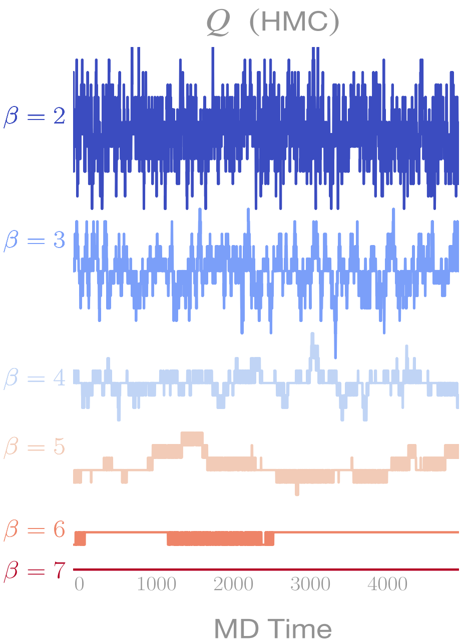
In particular, we are interested in measuring the (scalar) topological charge Q on the lattice. Since different lattice configurations with the same value of Q are related by a gauge transformation, they do not meaningfully

Figure 3: Illustration of the lattice



contribute to our statistics. Because of this, we would like to gneconfigurations from different *topological sectors*[2] to reduce uncertainty in our statistical estimates. By repeating this procedure at increasing spatial resolution ($\beta \propto 1/a^3$), we are able to extrapolate our estimates to the continuum limit where they can be compared with experimental measurements.

Figure 4: $\delta Q \to 0$ with increasing β.



Current approaches (HMC, ...) are known to suffer from auto-correlation times which scale exponentially in this limit, significantly limiting their effectiveness. This phenomenon can be seen in Fig 4, where fluctuations in the topological charge $\delta Q = |Q^{i+1} - Q^i|$ decreases as $\beta = 2 \to 3 \to \cdots$, and disappear completely ($Q = \text{const.}$) by $\beta = 7$.

3.3 MD Updates

As before, we introduce momenta $P_\mu(x) = P^k_\mu(x)\lambda^k$ conjugate to the real fields $\omega^k_\mu(x)$.
We can write the Hamiltonian as

$$H[P, U] = \frac{1}{2}P^2 + S_G[U] \tag{28}$$

by Hamilton's equations

$$\frac{d\omega^k}{dt} = \frac{\partial H}{\partial P^k}, \quad \frac{dP^k}{dt} = -\frac{\partial H}{\partial \omega^k}. \tag{29}$$

To update the gauge field $U_\mu = e^{i\omega^k_\mu \lambda^k}$,

$$\frac{d\omega^k}{dt}\lambda^k = P^k\lambda^k \Longrightarrow \frac{dW}{dt} = P \tag{30}$$

Discretizing with step size ε,

$$W(\varepsilon) = W(0) + \varepsilon P(0) \Longrightarrow \tag{31}$$

$$-i\log U(\varepsilon) = -i\log U(0) + \varepsilon P(0) \tag{32}$$

$$U(\varepsilon) = e^{i\varepsilon P(0)}U(0) \Longrightarrow \tag{33}$$

$$\Lambda : U \to U' = e^{i\varepsilon P}U \tag{34}$$

Similarly for the momentum update,

$$\frac{dP^k}{dt} = -\frac{\partial H}{\partial \omega^k} = -\frac{\partial H}{\partial W} = -\frac{dS}{dW} \Longrightarrow \tag{35}$$

$$P(\varepsilon) = P(0) - \varepsilon \left.\frac{dS}{dW}\right|_{t=0} = P(0) - \varepsilon F[U] \tag{36}$$

$$\Gamma : P \to P' = P - \frac{\varepsilon}{2}F[U] \tag{37}$$

[2]Characterized by different values of Q
[3]Here a is the lattice spacing

where $F[U]$ is the force term. In terms of the operators

$$\Gamma_\theta^\pm : (U, P) \xrightarrow{(s_P, t_P, q_P)} (U, P') \tag{38}$$

$$\Lambda_\theta^\pm : (U, P) \xrightarrow{(s_U, t_U, q_U)} (U', P) \tag{39}$$

and we can write the complete update:

$$P' = \Gamma_\theta^\pm(U, P) \tag{40}$$

$$U' = U_B + \Lambda_\theta^\pm(U_A, P') \tag{41}$$

$$U'' = U'_A + \Lambda_\theta^\pm(U'_B, P') \tag{42}$$

$$P'' = \Gamma_\theta^\pm(U'', P') \tag{43}$$

3.4 Momentum Update

In this case, our `vNet` : $(U, F) = (e^{iW}, F) \longrightarrow (s_P, t_P, q_P)$. We can use this in the momentum update $\Gamma_\theta^\pm$ via[4]:

1. `forward`, $(+)$:

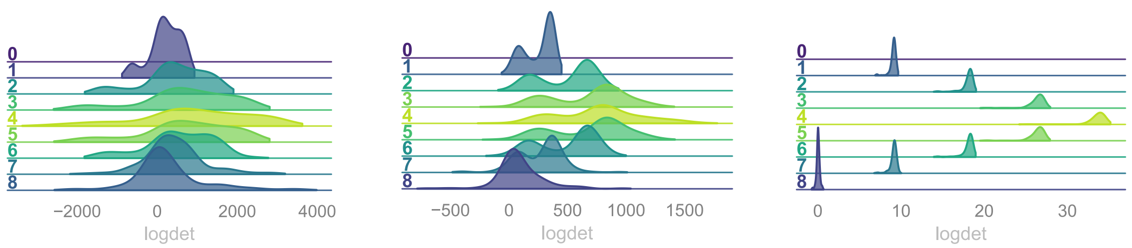
$$\Gamma^+(U, F) = P \cdot e^{\frac{\varepsilon}{2} s_P} - \frac{\varepsilon}{2}\left[F \cdot e^{\varepsilon q_P} + t_P\right] \tag{44}$$

2. `backward`, $(-)$:

$$\Gamma^-(U, F) = e^{-\frac{\varepsilon}{2} s_P}\left\{P + \frac{\varepsilon}{2}\left[F \cdot e^{\varepsilon q_P} + t_P\right]\right\} \tag{45}$$

3.5 Gauge Field Update

4. Results



(a) 100 train iters **(b)** 500 train iters **(c)** 1000 train iters

Figure 5: Evolution of $|\mathcal{J}|$ vs N_{LF} (`logdet`) during the first 1000 training iterations.

5. Conclusion

TODO

[4]Note that $(\Gamma^+)^{-1} = \Gamma^-$, i.e. $\Gamma^+\left[\Gamma^-(U, F)\right] = \Gamma^-\left[\Gamma^+(U, F)\right] = (U, F)$