Field Transformation HMC

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Contents

Versions

- April 20, 2021, version 0
  Some text borrowed from the previous 1D XY model report.

1 Introduction

Following the arguments of "Trivializing maps" [1], to evaluate,

$$\langle O \rangle = 1/Z \int \mathrm{d}x O(x) e^{-S(x)}, \tag{1}$$

we perform a change of variable,

$$x = F(y) \tag{2}$$

with a vector functions F, we have

$$\langle O \rangle = \frac{1}{Z} \int \mathrm{d}y \left|\det[J(y)]\right| O\left(F(y)\right) e^{-S(F(y))}, \tag{3}$$

where the Jacobian matrix,

$$J(y) = \frac{\partial F(y)}{\partial y}. \tag{4}$$

F has to satisfy,

- Injective (1 to 1), from the new integration domain to the old.
- Continuously differentiable (or differentiable and have continuous inverse).

Rewrite the integral as,

$$\langle O\rangle = \frac{1}{Z}\int \mathrm{d}y O\left(F(y)\right) e^{-S(F(y))+\ln|\det[J(y)]|}. \tag{5}$$

F is a trivializing map, when

$$S(F(y)) - \ln|\det[J(y)]| = \text{constant} \tag{6}$$

and our expectation value simplifies to

$$\langle O\rangle = \frac{1}{Z}\int \mathrm{d}y O\left(F(y)\right). \tag{7}$$

In terms of HMC, we add the conjugate momenta, π, and use the equations of motion derived from the Hamiltonian,

$$\mathscr{H}(y,\pi) = \tfrac{1}{2}\pi^2 + S\left(F(y)\right) - \ln|\det[J(y)]|, \tag{8}$$

as

$$\frac{\mathrm{d}}{\mathrm{d}t}\pi = -\frac{\partial}{\partial y}\mathscr{H} = -J(y)S'\left(F(y)\right) + \mathrm{tr}\left[J^{-1}\frac{\mathrm{d}}{\mathrm{d}y}J\right], \tag{9}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}y = \frac{\partial}{\partial y}\mathscr{H} = \pi. \tag{10}$$

This is separable and can use the usual explicit, symplectic and symmetric discrete integrators.

Consider a change of variable for π and y,

$$\pi = J(y)p = J\left(F^{-1}(x)\right)p, \tag{11}$$

$$y = F^{-1}(x), \tag{12}$$

with the Jacobian matrix of determinant 1,

$$\mathscr{J}(p,x) = \begin{bmatrix} J\left(F^{-1}(x)\right) & \frac{\partial}{\partial x}J\left(F^{-1}(x)\right)p \\ 0 & \frac{\partial}{\partial x}F^{-1}(x)\end{bmatrix}, \tag{13}$$

$$\det[\mathscr{J}] = 1. \tag{14}$$

We get a new Hamiltonian from equation (8),

$$\tilde{\mathscr{H}}(x,p) = \tfrac{1}{2}p^\dagger M p + S(x) - \ln|\det[J]| \tag{15}$$

where the positive definite M,

$$M(x) = J^\dagger\left(F^{-1}(x)\right)J\left(F^{-1}(x)\right) \tag{16}$$

is the kernel of the kinetic term considered Duane et al [2, 3].

2 Generalized field transformation

For a generic field transformation, we can take inspiration from an MD update, where

$$U' \leftarrow U \exp[dt * \mathrm{Proj}_{\mathrm{TAH}}(M)]. \tag{17}$$

U is covariant and M (being sum of loops) is invariant under gauge transformation.

The most generic form of a field transformation could be

$$U(x,\mu)' \leftarrow \mathrm{Proj}_{\mathrm{SU}} \sum_L a_L \prod_{\mathrm{ord}} [L(x,\mu)], \tag{18}$$

where $L(x,\mu)$ is any line connecting gauge links from x to $x+\hat{\mu}$, a_L is a scalar coefficient. $L(x,\mu)$ may or may not need to go through $U(x,\mu)$. wet may also have loops in it, and results in a polynomial of such loop after sum.

The $\mathrm{Proj}_{\mathrm{SU}}$ has to satisfy the constraint that

$$X \,\mathrm{Proj}_{\mathrm{SU}}(M) Y = \mathrm{Proj}_{\mathrm{SU}}(XMY) \tag{19}$$

for any X and Y in the group.

We can, however, rewrite the equation to be similar to the MD update,

$$U(x,\mu)' \leftarrow \mathrm{Proj}_{\mathrm{SU}} \sum_L a_L U(x,\mu) U(x,\mu)^\dagger \prod_{\mathrm{ord}} [L(x,\mu)], \tag{20}$$

such that

$$U(x,\mu)^\dagger \prod_{\mathrm{ord}} [L(x,\mu)] \tag{21}$$

becomes a complete loop, which is gauge invariant. We then have it in a simplified form,

$$U' \leftarrow \mathrm{Proj}_{\mathrm{SU}} \sum_R a_R U R, \tag{22}$$

where R is any loop that start and stop at $x+\hat{\mu}$.

We may write it in terms of

$$U' \leftarrow \mathrm{Proj}_{\mathrm{SU}} \sum_{LR} a_{LR} L U R, \tag{23}$$

such that L is any loop that start and stop at x, but since we can always pull the U to the left by multiplying $UU^\dagger$, the most generic form is simply,

$$U' \leftarrow \mathrm{Proj}_{\mathrm{SU}}[U(\sum_R a_R R)], \tag{24}$$

where R is any loop that start and stop at $x+\hat{\mu}$, and may or may not go through U.

We can multiply $UU^\dagger$ again, so it becomes

$$U' \leftarrow UU^\dagger \,\mathrm{Proj}_{\mathrm{SU}}[U(\sum_R a_R R)]. \tag{25}$$

If we had a $\mathrm{Proj}_{\mathrm{SU}}$ that satisfies

$$X \,\mathrm{Proj}_{\mathrm{SU}}(M) Y = \mathrm{Proj}_{\mathrm{SU}}(XMY) \tag{26}$$

the above update would become

$$U' \leftarrow U \,\mathrm{Proj}_{\mathrm{SU}}[\sum_R a_R R] \tag{27}$$

though we need $\mathrm{Proj}_{\mathrm{SU}}$ satisfy a different constraint,

$$X \,\mathrm{Proj}_{\mathrm{SU}}(M) X^\dagger = \mathrm{Proj}_{\mathrm{SU}}(XMX^\dagger) \tag{28}$$

If we were allowed to do the above change of constraint to $\mathrm{Proj}_{\mathrm{SU}}$, it seems we could just use the projection in MD update,

$$U' \leftarrow U \exp[\mathrm{Proj}_{\mathrm{TAH}}(\sum_R a_R R)] \tag{29}$$

It looks like we are only one step away from

$$U' \leftarrow U \exp\left[\frac{\mathrm{d}}{\mathrm{d}U} F(\mathrm{ReTr}\, A, \mathrm{ReTr}\, B, \mathrm{ReTr}\, C, \ldots)\right] \tag{30}$$

where F is any analytical function or neural network, and A, B, C, ... are any closed loops may or may not passing U.

We can simplify it by moving the U independent loops out and keeping the U dependent loops simple,

$$U' \leftarrow U \exp\left[c \,\mathrm{atan}\left[F(\mathrm{ReTr}\, X, \mathrm{ReTr}\, Y, \ldots)\right] \left[\frac{\mathrm{d}}{\mathrm{d}U} \mathrm{ReTr}[W]\right]\right] \tag{31}$$

so that $F(\mathrm{ReTr}\, X, \mathrm{ReTr}\, Y, \ldots)$ only depends on U independent loops, while W contains U dependent loops, $c * \mathrm{atan}(F)$ is for restricting the Jacobian to be positive definite, and W is a sum of any loop and its symmetrized versions including U. The arbitrary function F can take the form of a neural network.

For a transformation to be usable in HMC, we want a tractable Jacobian determinant. One way to achieve this is updating gauge links in subsets, such that each update to the subset of U has a Jacobian matrix, where the only nonzero entries are on its diagonal.

3 Test with 2D U(1) model without explicit neural networks

This test uses F in equation (31) as a simple sum of similar loops, specifically plaquettes and rectangles.

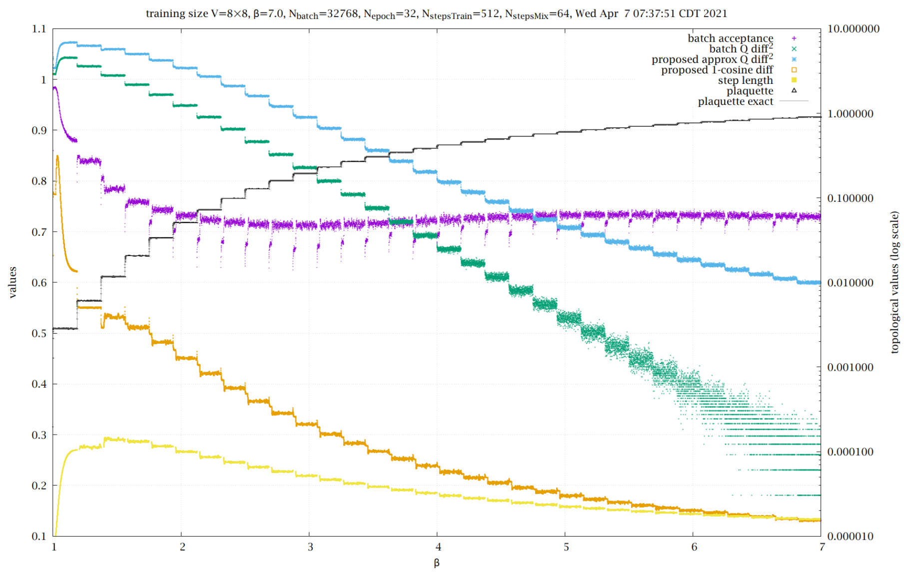

Figure 1: Annealed training steps for $V = 8 \times 8$ for HMC with 10 leapfrog steps, The only trainable parameter is the step size.

The loss function is

$$
\begin{aligned}
l(y', \pi' | y, \pi) = -\frac{1}{N_{\text{batch}}} \sum_{\text{batch}} \max\left\{1, e^{H(y,\pi) - H(y',\pi')}\right\} \\
\left(\lambda \frac{1}{N} \sum_x \left[1 - \cos\left(P'_x - P_x\right)\right]\right. \\
\left. + \rho \left[\sum_x \sin(P'_x) - \sum_x \sin(P_x)\right]^2\right),
\end{aligned}
\tag{32}
$$

where (y', π') and (y, π) are respectively the proposed and initial configuration in the MD evolution, $P_x = \theta_{x,\hat{1}} + \theta_{x+\hat{1},\hat{2}} - \theta_{x+\hat{2},\hat{1}} - \theta_{x,\hat{2}}$ is the plaquette phase at site x, and the sum of sin is an approximate of the topological charge. The test here uses $\lambda = 0.1$ and $\rho = 1.0$.

4 Discussions and plans

- Test equation (31) with F parametrized by neural networks.
- Compute and monitor forces during HMC.
- Compute and monitor changes of momenta (integrated forces) during HMC.

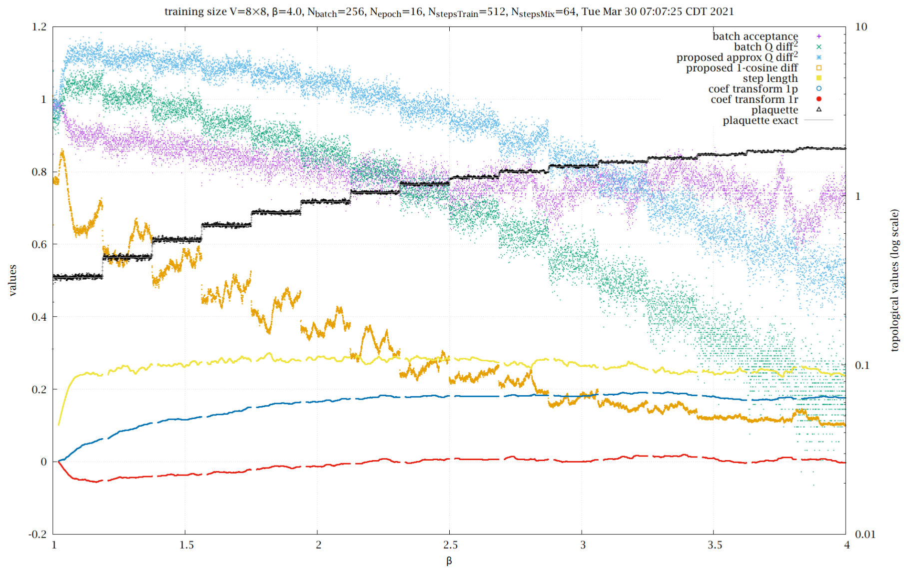

Figure 2: Annealed training steps for $V = 8 \times 8$ with 10 leapfrog steps.

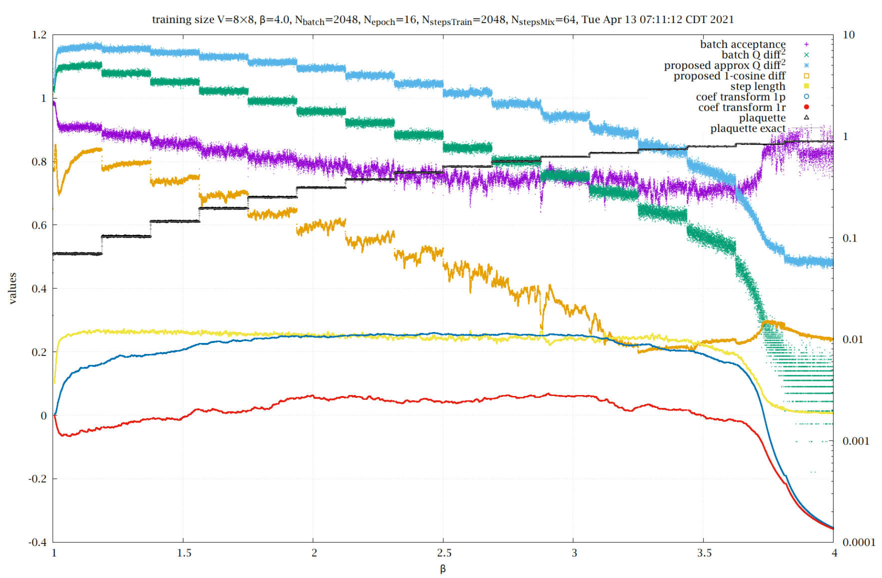

Figure 3: Annealed training steps for $V = 8 \times 8$ with 10 leapfrog steps.

- Vary the number of leapfrog steps.

References

[1] Martin Luscher. “Trivializing maps, the Wilson flow and the HMC algorithm”. In: *Commun. Math. Phys.* 293 (2010), pp. 899–919. DOI: 10.1007/s00220-009-0953-7. arXiv: 0907.5491 [hep-lat] (cit. on p. 1).

[2] Simon Duane et al. “Acceleration of Gauge Field Dynamics”. In: *Phys. Lett.* B176 (1986), p. 143. DOI: 10.1016/0370-2693(86)90940-8 (cit. on p. 2).

[3] Simon Duane and Brian J. Pendleton. “GAUGE INVARIANT FOURIER ACCELERATION”. In: *Phys. Lett.* B206 (1988), pp. 101–106. DOI: 10.1016/0370-2693(88)91270-1 (cit. on p. 2).