Field Transformation HMC

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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

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

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

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

Consider a change of variable in π,

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

we get a new Hamiltonian,

$$H(x,p) = \tfrac{1}{2}p^\dagger M p + S(x) - \ln|\det[J]| \tag{12}$$

where the positive definite M,

$$M(x) = J^\dagger\left(F^{-1}(x)\right)J\left(F^{-1}(x)\right) \tag{13}$$

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

2 Test in one dimensional model

We consider a one dimensional spin chain from complete fixing of the temporal links of a two dimensional gauge theory with action,

$$S(U) = -\sum_x \beta \,\mathrm{Re}\,\mathrm{tr}[U_x^\dagger U_{x+1}]. \tag{14}$$

With $U(1)$ gauge group, we use phase angle, $\theta \in [-\pi, \pi)$, and

$$U = e^{i\theta}, \tag{15}$$

$$S(U) = -\sum_x \beta \cos[\theta_{x+1} - \theta_x], \tag{16}$$

which is a one dimensional $O(2)$ model. With open boundary conditions, we can perform a change of variable for a chain of N spins,

$$\varphi_x = \theta_{x+1} - \theta_x, \tag{17}$$

$$Z = \int \mathrm{d}\theta \prod_x e^{\beta \cos[\theta_{x+1} - \theta_x]} \tag{18}$$

$$= \int \mathrm{d}\varphi \prod_x e^{\beta \cos[\varphi_x]} \tag{19}$$

$$= \prod_x \int_{-\pi}^{\pi} \mathrm{d}\varphi e^{\beta \cos\varphi}, \tag{20}$$

where all the spins decouple. This gives us the expectation value of the plaquette, exactly the same as for the 2D $U(1)$ gauge theory in the limit,

$$\langle P \rangle = \frac{I_1(\beta)}{I_0(\beta)}, \tag{21}$$

where I is the modified Bessel function of the first kind,

$$I_n(z) = \frac{1}{2\pi i} \oint e^{(t+1/t)z/2} t^{-n-1} dt \tag{22}$$

$$= \frac{1}{\pi} \int_0^{\pi} e^{z\cos\theta} \cos(n\theta) d\theta \quad \text{for } n \in \mathbb{Z}. \tag{23}$$

We can define the topological charge the same as in the 2D U(1) model,

$$Q = \frac{1}{2\pi} \sum_x \mathrm{Arg}[\theta_{x+1} - \theta_x]. \tag{24}$$

For the field transformation, we use "stout smearing" [4] style update, which is also used in the perturbative treatment in reference [1]. Given the 1D analogy of n cycle Wilson loops of length d,

$$W_{ndx}^{\text{even/odd}}(\theta) = -\frac{\gamma_{nd}^{\text{even/odd}}}{n^2} \cos\left[n(\theta_{x+d} - \theta_x)\right], \tag{25}$$

our smearing update from θ to θ' is

$$\theta'_x = F^{\text{even/odd}}_{ndx}(\theta) = \theta_x + \frac{\partial}{\partial \theta_x} W^{\text{even/odd}}_{ndy}(\theta). \tag{26}$$

In order to have a tractable Jacobian determinant, we update "even" and "odd" sites separately,

$$\text{even: } x \mod 2d < d, \tag{27}$$

$$\text{odd: } x \mod 2d \geq d. \tag{28}$$

This defines a series of diffeomorphism with positive definite Jacobian determinant with

$$-0.5 < \gamma < 0.5. \tag{29}$$

We optimize the coefficients, γ, during HMC, by minimize the loss function defined as,

$$\begin{aligned} l(\theta', \pi' | \theta, \pi) = -\frac{1}{N_{\text{batch}}} \sum_{\text{batch}} \max\left\{1, e^{H(\theta,\pi) - H(\theta',\pi')}\right\} \\ \left(\lambda \frac{1}{N} \sum_x \left[1 - \cos\left((\theta'_{x+1} - \theta'_x) - (\theta_{x+1} - \theta_x)\right)\right]\right. \\ \left. + \mu \left[\sum_x \sin(\theta'_{x+1} - \theta'_x) - \sum_x \sin(\theta_{x+1} - \theta_x)\right]^2\right), \end{aligned} \tag{30}$$

where (θ', π') and (θ, π) are respectively the proposed and initial configuration in the MD evolution, and the sum of sin is an approximate of the topological charge.

In the following test, we apply a chain of 48 transformations twice,

$$F^{\text{odd}}_{ndx} \circ F^{\text{even}}_{ndx} \circ \cdots, \tag{31}$$

with $n \in [1, 2, 3, 4]$ and $d \in [1, 2, 4, 8, 16, 32]$. There are 96 free parameters, γ, in total. In addition we also train the leapfrog step size. We train these 97 parameters during HMC with changing β from small to large in steps, everytime allow thermolizating after changing β before starting optimization. We train the model on a system with the number of sites, $N = 64$, and apply the trained model to a system with the number of sites, $N = 256$.

3 Discussions and plans

A chain of "stout smearing" works for 1D. Parameters trained for a chain of size 64 works for a chain of size 256.

Plans: Try optimize the trivializing map directly. Test with 2D U(1) model. Try neural network parametrized smearing.

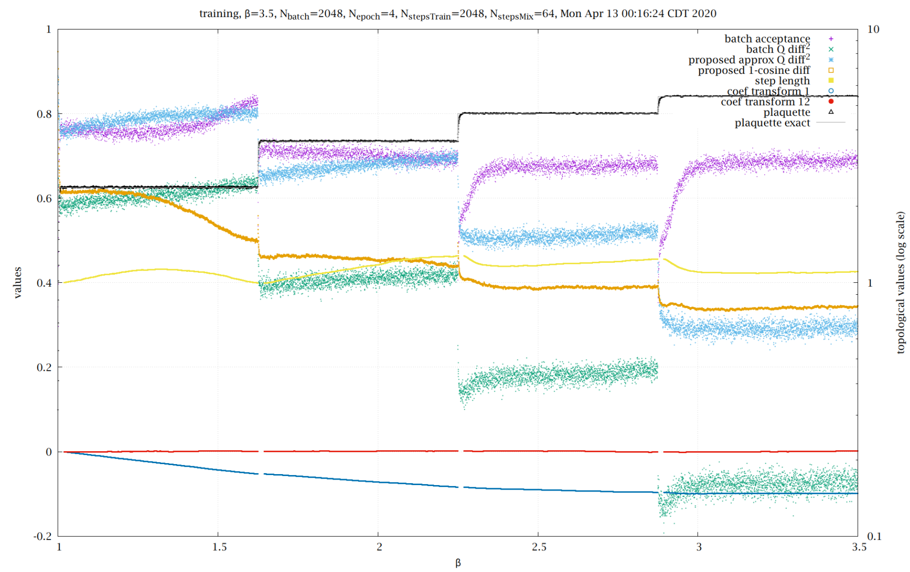

Figure 1: Annealed training steps for $N = 64$.

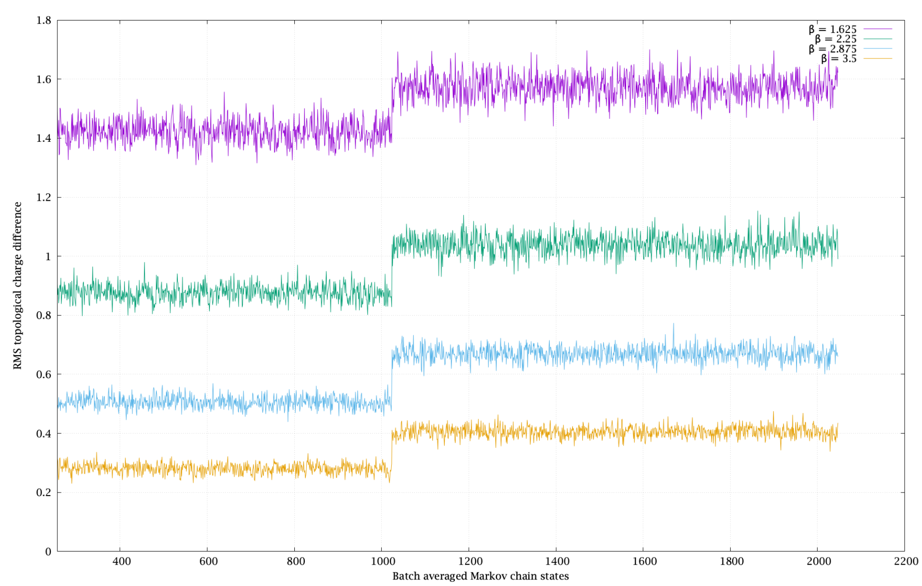

Figure 2: Topological charge change rate at $N = 64$, with traditional HMC and field transformation HMC.

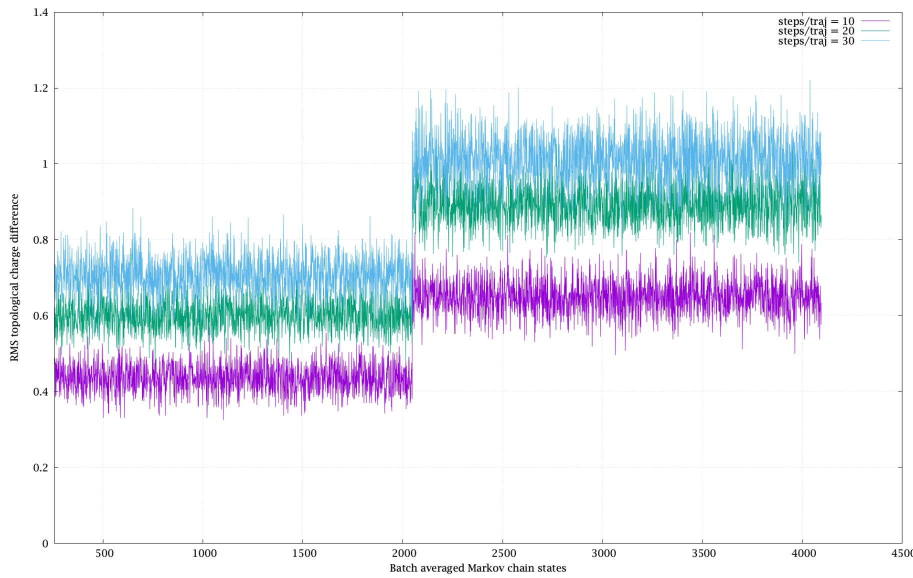

Figure 3: Apply trained parameters from $N = 64$ to $N = 256$, with traditional HMC and field transformation HMC.

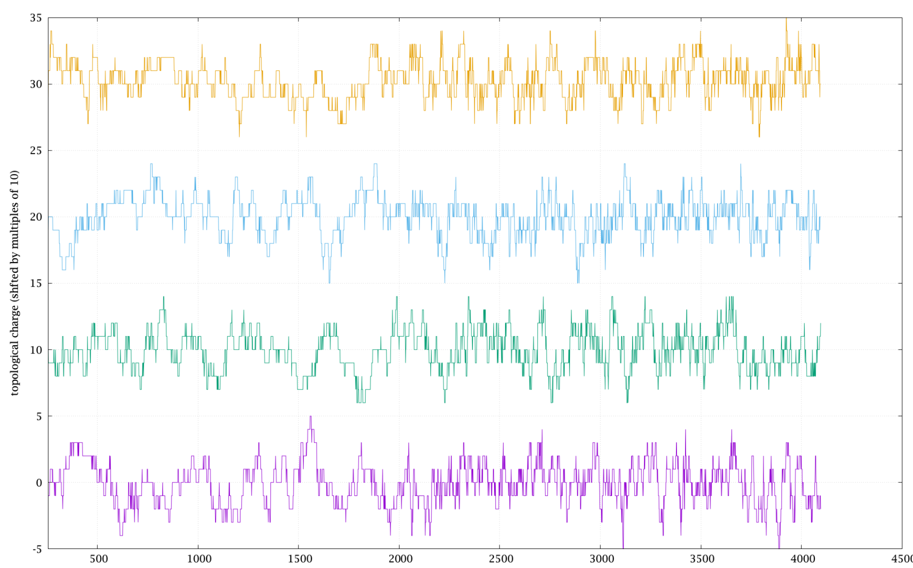

Figure 4: Individual MC evolution after applying trained parameters from $N = 64$ to $N = 256$, with traditional HMC and field transformation HMC.

References

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[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).

[4] Colin Morningstar and Mike J. Peardon. "Analytic smearing of SU(3) link variables in lattice QCD". In: *Phys. Rev.* D69 (2004), p. 054501. DOI: 10.1103/PhysRevD.69.054501. arXiv: hep-lat/0311018 [hep-lat] (cit. on p. 3).