Field Transformation HMC

Xiao-Yong Jin for Lattice QCD ECP

July 28, 2021

Contents

Versions

- April 20, 2021, version 0
  Some text borrowed from the previous 1D XY model report.
- June, 2021, version 1
  Updated section 2.

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

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

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,

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

as

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

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

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,

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

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

We get a new Hamiltonian from equation (8),

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

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 UPDATED

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

$$U' \leftarrow U \exp[\mathrm{d}t\,\mathrm{Proj}_{\mathrm{TAH}}(M)]. \tag{17}$$

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

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

where $\mathscr{F}$ 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,

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

so that $\mathscr{F}(\mathrm{ReTr}\,X, \mathrm{ReTr}\,Y, \ldots)$ only depends on U independent loops, while W contains U dependent loops, $c\,\mathrm{atan}(\mathscr{F})$ 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 $\mathscr{F}$ 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.

Figure 1 shows an example of generic field transformation. We identify the subset of the gauge links to update in red, computing the gauge invariant Wilson loops, and mask out those loops depending on the to-be-updated links. We apply convolutional neural networks, with kernels K_0 for the plaquettes and K_1 for the rectangles, applying to the green unmasked Wilson loops, with their respective kernel sizes in yellow. We then stack the results of the previous networks together and apply further convolutional neural network $\mathscr{F}_c$ to it as a whole. The result of this neural network provides the coefficients, c_0 and c_1, for the local update depending on the plaquette and rectangle terms respectively.

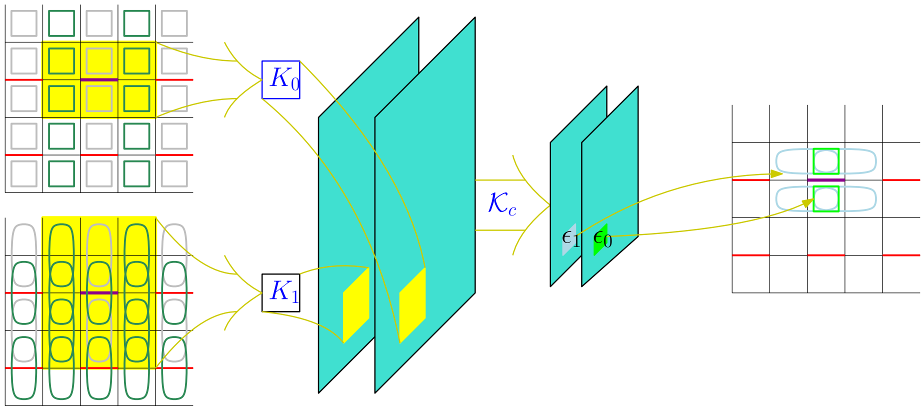

Figure 1: Example generic filters for gauge covariant update of selected links. See text for details.

3 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.
- 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).