Search for an effective change of variable in QCD simulations

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Lattice calculations of quantum chromodynamics (QCD) suffers from the critical slowing down as the continuum limit is approached. Furthermore, the topological sectors in the gauge field space become apparent due to the separation by potential barriers in this limit, and this fact makes it difficult to explore the entire field space in the simulation.

To circumvent these issues, Lüscher proposed[1)] using the *trivializing map*[2)] in lattice QCD. The idea is to map the system of interest to a trivial system, where the simulation can be performed efficiently. Precisely, we evaluate the expectation value expressed in terms of the following path integral:

$$\langle \mathcal{O} \rangle_S \equiv \frac{\int \mathcal{D}U\, e^{-S(U)} \mathcal{O}(U)}{\int \mathcal{D}U\, e^{-S(U)}}, \tag{1}$$

where $S(U)$ is the lattice QCD action. The trivializing map[1)] $U = \mathcal{F}(V)$ is defined such that

$$\begin{aligned}\langle \mathcal{O} \rangle_S &= \frac{\int \mathcal{D}V\ \det \mathcal{F}_*(V)\, e^{-S(\mathcal{F}(V))} \mathcal{O}(\mathcal{F}(V))}{\int \mathcal{D}V\ \det \mathcal{F}_*(V)\, e^{-S(\mathcal{F}(V))}} \\ &= \int \mathcal{D}V\, \mathcal{O}(\mathcal{F}(V)),\end{aligned} \tag{2}$$

where $\mathcal{F}_*(V)$ is the Jacobian matrix of the map $\mathcal{F}$. In other words, we construct a map $\mathcal{F}$ that makes the effective action

$$S_{\mathcal{F}}(V) \equiv S(\mathcal{F}(V)) - \ln \det \mathcal{F}_*(V) \tag{3}$$

the target action $S_{\rm tg}(V) \equiv$ const: $S_{\mathcal{F}} = S_{\rm tg}$.

Lüscher explicitly constructed the trivializing map as a flow $\mathcal{F}_t$ for the pure Yang-Mills theory, which was given in the form of an expansion with the flow time t. To the zeroth order in t, this map becomes the *Wilson flow*, the gradient flow for the Wilson action. Combining the Hybrid Monte Carlo (HMC) with the Wilson flow[1)] seems promising, based on the observation of positive effects in the topological tunneling rate.[4)] The subject of this study is to investigate the effectiveness of the field transformation in lattice QCD along this line, extending the code to cover more general flow kernels for the trivializing maps.

To design an approximated map, we consider a different strategy from that of Lüscher's. We first prepare a finite basis $\{W_i\}$ and define the truncated effective action:

$$S'_{\mathcal{F}} \equiv {\sum_i}' \beta'_i W_i, \tag{4}$$

where the prime indicates quantities for the finite basis. The coefficients β'_i can be determined with the Schwinger-Dyson equation:[5,6)]

$${\sum_j}' \beta'_j \langle \partial^A W_j \partial^A W_i \rangle_{S_{\mathcal{F}}} = \langle (\partial^A)^2 W_i \rangle_{S_{\mathcal{F}}}. \tag{5}$$

This determination gives the best approximation of $S_{\mathcal{F}}$ in the sense that it minimizes the norm

$$||S_{\mathcal{F}} - S'_{\mathcal{F}}||^2 \equiv \langle (\partial^A S_{\mathcal{F}} - \partial^A S'_{\mathcal{F}})^2 \rangle_{S_{\mathcal{F}}}. \tag{6}$$

This is a calculable norm of the HMC force.

We use Eq. (5) to design the approximated map. We define the infinitesimal map $\mathcal{F}_{t,\epsilon}$, which evolves the parameter t by ϵ as

$$\mathcal{F}_{t,\epsilon}(V)_{x,\mu} \equiv e^{\epsilon T^a Z^a_{t,x,\mu}(V)}\, V_{x,\mu}. \tag{7}$$

Here $Z^a_{x,\mu}$ is the kernel

$$Z^A_t \equiv -{\sum_i}' \gamma_{i,t}\, \partial^A W_i, \tag{8}$$

where the label A corresponds to (x, μ, a). Since γ_i can be related to β'_i by

$$\begin{aligned}&{\sum_k}' \gamma_{k,t} \big\langle \partial^A W_k \partial^A [-(\partial^B)^2 W_i + \partial^B S'_{\mathcal{F}} \partial^B W_i] \big\rangle_{S_{\mathcal{F}}} \\ &\quad = -(d\beta'_{j,t}/dt) \langle \partial^B W_j \partial^B W_i \rangle_{S_{\mathcal{F}}},\end{aligned} \tag{9}$$

we can determine $\gamma_{i,t}$ by specifying the functional form of $\beta'_{i,t}$, or equivalently the target action $S_{{\rm tg},t}$ for all t. In the case where the truncation error is negligible, the above framework provides a way to construct the trivializing map with a large freedom of choosing the intermediate trajectory in the space of actions.[7)] The authors thank the US DOE for the resources, which have been necessary for the work.

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