Normalizing flows for SU(n) gauge theories employing singular value decomposition

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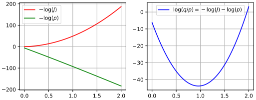
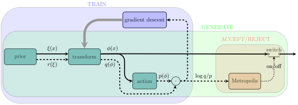
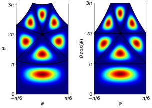
Outline

1. *Trivializing maps as continuous NFs*

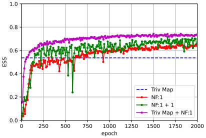


2. *NFs for SU(n) gauge theories employing SVD*





3. *Simulation results & discussion*



Lattice Gauge Theory & Trivializing Maps

Trivializing Maps, the Wilson Flow and the HMC Algorithm

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Abstract: In lattice gauge theory, there exist field transformations that map the theory to the trivial one, where the basic field variables are completely decoupled from one another. Such maps can be constructed systematically by integrating certain flow equations in field space. The construction is worked out in some detail and it is proposed to combine the Wilson flow (which generates approximately trivializing maps for the Wilson gauge action) with the HMC simulation algorithm in order to improve the efficiency of lattice QCD simulations.

4.1. Trivializing flows. If the generator $Z_t(U)$ of the flow (3.2) is such that

$$\int_0^t \mathrm{d}s \sum_{x,\mu} \left\{\partial^a_{x,\mu}[Z_s(U)]^a(x,\mu)\right\}_{U=U_s} = t\,S(U_t) + C_t, \tag{4.1}$$

the substitution $U \to V$ of the integration variables in the functional integral maps the theory to the trivial one where the link variables are completely decoupled from one another. The expectation values (2.1) are then given by

$$\langle \mathcal{O} \rangle = \int \mathrm{D}[V]\,\mathcal{O}(\mathcal{F}(V)). \tag{2.9}$$

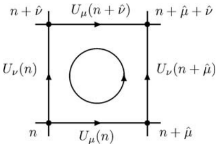
Such trivializing maps thus contain the entire dynamics of the theory.

Although the remark is likely to remain an academic one, an intriguing observation is that the integral (2.9) can be simulated simply by generating uniformly distributed random gauge fields. Subsequent field configurations are uncorrelated in this case and

Leading Order Trivializing Map for Wilson Action

- The Wilson action for SU(n_c) gauge theory

$$S_{\text{Wilson}}[U] = -\frac{\beta}{2n_c}\sum_{x\in\Lambda}\sum_{\mu\neq\nu} \text{Tr Plaq}_{\mu\nu}(x)$$



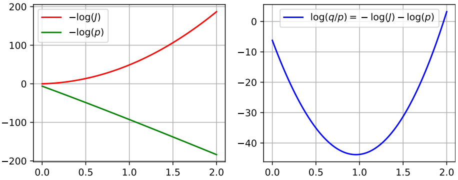
- Lüscher's trivializing map at leading order is a matrix integration as:

$$V(t) = V(0) - \frac{n_c}{2(n_c^2-1)}\frac{\beta}{2n_c}\int_0^t d\tau \mathcal{P}\Big\{V(\tau)\Gamma(\tau)\Big\}V(\tau)$$

where $V(0) = U_\mu(x)$, $\Gamma(\tau)$ is the corresponding sum of staples, and $\mathcal{P}$ is a projection operator to anti-hermitian traceless space.

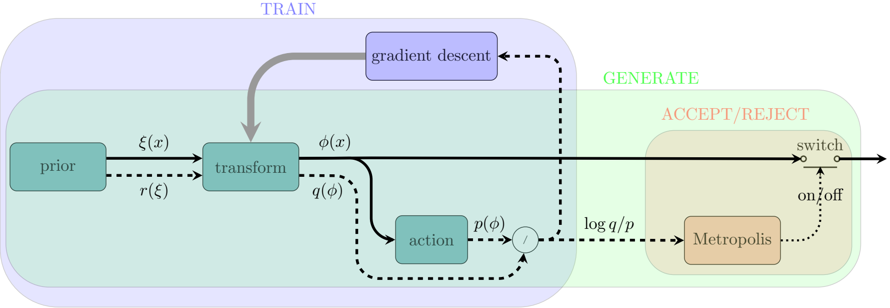
- The Jacobian of transformation is $\log J(t) = -\int_0^t d\tau S_{\text{Wilson}}[V_\tau]$.

- The flow terminates at $t = 1$, $\sim$ the minimum of *KL divergence.*



Normalizing Flows & Machine Learning

- In a nutshell, for the method of normalizing flows, one should provide three essential components:
  - a prior distribution to draw initial samples,
  - a map (e.g. with deep neural networks) to perform a series of invertible transformations on the samples,
  - an action that specifies the target distribution, defining the goal of the generative model; $p \propto \exp(-\text{action})$
- The model is fitted (trained) by minimizing KL divergence: $\mathbb{E}\left[\log(q/p)\right]$
- For exactness, one can impose an accept/reject step or....



NFs for Gauge Theories & Gauge Equivariance

- Gauge theories are invariant under a huge class of gauge transformations

$$U_\mu(x) \;\rightarrow\; \Omega(x)\, U_\mu(x)\, \Omega^\dagger(x+\hat{\mu})$$

- In principle, one can incorporate gauge symmetries in the flow functions in order to improve the training.
- Gauge-equivariant functions incorporate the gauge symmetry; see [Kanwar, et.al., arXiv:2003.06413] & [Boyda, et.al., arXiv:2008.05456].
- Any transformation that involves gauge-invariant quantities by construction is gauge equivariant.

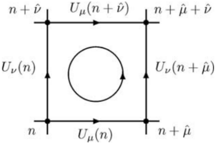
Wilson Action & Gauge Invariant Quantities

- Wilson action for SU(n_c) gauge:

$$S[U] = -\frac{\beta}{2n_c}\sum_{x\in\Lambda}\sum_{\mu\neq\nu}\text{Re Tr }P_{\mu\nu}(x)$$

$$\Rightarrow$$

$$S[U] = -\frac{\beta}{2n_c}\sum_{x\in\Lambda}\sum_{\mu}\text{Re Tr }U_\mu(x)\Gamma_\mu(x)$$



$$\Gamma_\mu(x) = \sum_{\nu\neq\mu}\Big\{U_\nu(x+\hat{\mu})U_\mu^\dagger(x+\hat{\nu})U_\nu^\dagger(x) - U_\nu^\dagger(x+\hat{\mu}-\hat{\nu})U_\mu^\dagger(x-\hat{\nu})U_\nu(x-\hat{\nu})\Big\}$$

- The action is invariant under gauge transformation:

$$U_\mu(x) \;\rightarrow\; \Omega(x)\,U_\mu(x)\,\Omega^\dagger(x+\hat{\mu})$$

- Other gauge-invariant quantities:
  - Eigenvalues of $P_{\mu\nu}$
  - Singular values of Γ_μ, i.e. Σ_μ in $\Gamma_\mu = W_\mu\Sigma_\mu V_\mu^\dagger$
  - Eigenvalues of $\breve{U}_\mu = V_\mu^\dagger U_\mu W_\mu$
- We use gauge-invariant quantities to build gauge equivariant transformations.

Gauge-Equivariant Flows (two methods that we tried)

- (Plaquette) spectral flow:
  Flow eigenvalues of $P_{\mu\nu}$ & push the changes to designated links
  see, e.g., [Kanwar, et.al. arXiv:2003.06413] & [Abbott, et.al., arXiv:2305.02402]

- We calculate the sum of adjacent staples of links, then:

SVD) $\Gamma_\mu = W_\mu \Sigma_\mu V_\mu^\dagger$
Def) $\tilde{U}_\mu = V_\mu^\dagger U_\mu W_\mu$
Eig) $\tilde{U}_\mu = Q \Lambda Q^\dagger$
Flow1) $\Lambda \to \Lambda'(\Lambda, S)$
Flow2) $\Omega \to \Omega' = \Omega e^{ih(\Omega, \Lambda', S)}$
.) $\tilde{U}'_\mu = Q' \Lambda' Q'^\dagger$
.) $U'_\mu = V_\mu \tilde{U}'_\mu W_\mu^\dagger$

Transformation is

  - gauge equivariant,
  - reversible if we update links from even & odd sites in sequence.

A block of transformation contains $2n_{\text{dim}}$ layers covering μ directions and even&odd sites.

Parametrization of Eigenvalues of SU(3) Matrix Model

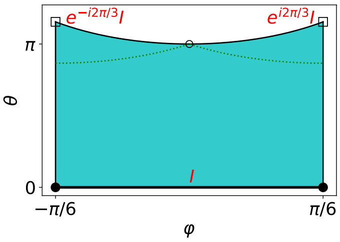
$$Z = \int dU e^{-\frac{\beta}{3}\mathrm{Re}\,\mathrm{Tr}\,U}; \quad (dU \text{ is the Haar measure})$$

$$= \int_{\text{principal}} d\theta_1 d\theta_2 V_{conj}(\theta_1,\theta_2) e^{-\frac{\beta}{3}\mathrm{Re}\left(e^{i\theta_1}+e^{i\theta_2}+e^{i\theta_3}\right)}; \quad (\theta_3 = -\theta_1 - \theta_2)$$

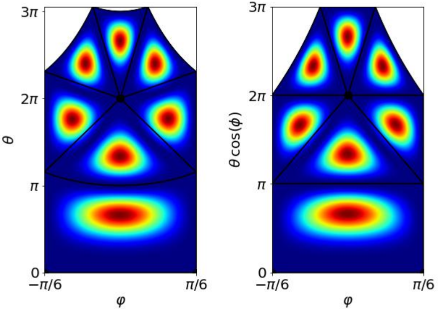
Two variables θ & φ to parameterize three eigenvalues

$$e^{i\theta_k} = e^{i\theta s_k}, \quad s_k = \frac{2}{\sqrt{3}}\sin\left(\varphi + \frac{2\pi}{3}k\right), \quad s_1+s_2+s_3=0$$

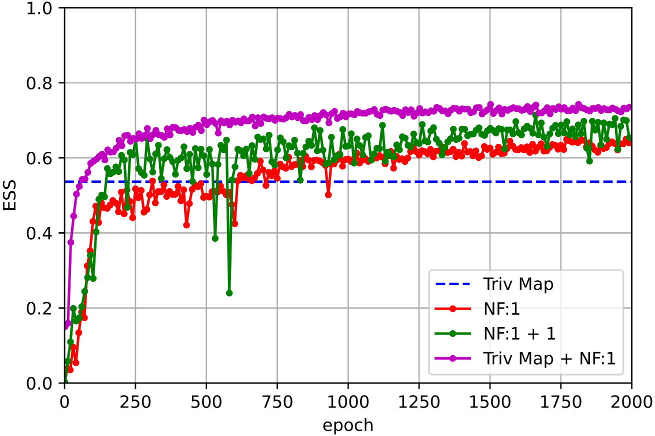
principal/canonic cell



More cells & conjugacy volume



Results for SU(3) on a 4^4 Lattice with $\beta = 1$



0) Lüscher's leading order trivializing map as a reference point; no parameter
1) One block of changing all links as proposed with SVD; 1288 parameters
2) Two blocks of changing all links as proposed with SVD; 2 x 1288 parameters
3) Employing #0 & #1; 1288 parameters

Concluding Remarks & Outlook

- We observe that using SVD at higher dimensions can improve the training compared to (plaquette) spectral flow.
- Continuous & discreet flows can be used together to improve the training.

- We are developing a package...
  https://github.com/jkomijani/normflow_

```
from normflow import Model
from normflow.prior import SUnPrior  # SU(n) uniform dist.
from normflow.action import WilsonGaugeAction
from normflow.nn import WilsonTrivMap_


def make_model(beta, n_c=3, lat_shape=(4, 4, 4, 4)):

    prior = SUnPrior(n_c, shape=(4, *lat_shape))
    action = WilsonGaugeAction(beta, n_c=n_c, ndim=4)
    net_ = WilsonTrivMap_(action)  # default: Leading Order

    return Model(prior=prior, action=action, net_=net_)
```

Thanks for Your Attention!