# **Continuous Normalizing Flows**

# for Lattice Gauge Theories

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#### arXiv:2212.08469

#### Learning Trivializing Gradient Flows for Lattice Gauge Theories

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arXiv:2305.07932

Realistic application of Machine Learning in Lattice QCD A novel approach for computing gradients of physical observables

Simone Bacchio<sup>1</sup>

<sup>1</sup>Computation-based Science and Technology Research Center, The Cyprus Institute, Nicosia, Cyprus (Dated: May 21, 2023)

# Motivation: Critical slowing down

In Lattice Gauge Theories, the expectation value of an observable is defined as

$$\langle \mathcal{O} 
angle = rac{1}{\mathcal{Z}} \int \mathrm{D}[U] \, \mathcal{O}(U) \, \exp(-S(U))$$

Computed via importance sampling and using Markov-chain Monte Carlo (MCMC) methods

$$|\mathcal{O}
angle = rac{1}{N}\sum_{i}^{N}O(U_{i})$$
 with  $p(U) = rac{1}{\mathcal{Z}} ext{exp}(-S(U))$ 

- Requires independent and identically distributed (IID) samples
- State-of-the-art: Hybrid Monte Carlo (HMC) algorithm

$$\langle \mathcal{O} 
angle = rac{1}{\mathcal{Z}} \int \mathrm{D}[U] \, \mathrm{D}[p] \, \mathcal{O}(U) \, \exp(-p^2/2 - S(U))$$

10000

1000

100

 $au_Q^{\text{int}}$ 

• HMC

3

# Motivation: Critical slowing down

In Lattice Gauge Theories, the expectation value of an observable is defined as

$$\langle \mathcal{O} 
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Alternative: If the field is generated by the transformation  $~~U={\cal F}(V)~~$  –

 $\mathcal{F}_{i}$ 

10000

1000

100

 $au_Q^{\text{int}}$ 

• HMC

3

 $D[U] = D[V] \det \mathcal{F}_*(V)$ 

B <sup>5</sup>

## Motivation: Critical slowing down

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Alternative: If the field is generated by the transformation  $U=\mathcal{F}(V)$  –

10000

1000

100

10

 $\tau_Q^{\text{int}}$ 

HMCFlow

[G. Kanwar et al., 2020

B <sup>5</sup>

3

 $D[U] = D[V] \det \mathcal{F}_*(V)$ 

### How to construct the flow?

#### **Discrete flow**

$$U = \mathcal{F}(V) = f_n \circ \cdots \circ f_2 \circ f_1(V)$$

#### Requirements:

- Cheap calculation of  $\det \mathcal{F}_*(V)$
- Preserve symmetries of the field

#### Approach:

• RealNVP & Equivariant Normalizing Flows [G. Kanwar et al., 2020]



**Continuous flow** 

$$egin{aligned} U &= \mathcal{F}(V) = \hat{\int} f(U_t,t) dt \ egin{aligned} \dot{U}_t &= f(U_t,t) \end{aligned}$$

Same requirements...

#### <u>Approach:</u>

- Trivializing maps by Lüscher [M. Lüscher, 2009]
- ... with machine learning [S.B. et al., 2022]
- Focus of this presentation

### **Part 1: Continuous flows for Lattice Gauge Theories**

How to define 
$${\dot U}_t \equiv {dU_t \over dt} = f(U_t,t)$$
 ?

arXiv:0907.5491

Trivializing maps, the Wilson flow and the HMC algorithm

Martin Lüscher

CERN, Physics Department, 1211 Geneva 23, Switzerland

### **ODEs on manifolds**

$$\dot{U}_t = \underbrace{g(U_t,t)U_t}_{Z_t}$$
 where  $U_t \in ext{Group}$   $U_t = e^{\sum_a c_a(t) T_a}$   
 $Z_t \in ext{Algebra}$   $\dot{U}_t = (\sum_a \dot{c}_a(t) T_a) U_t$ 

• 
$$Z_t = g(U_t,t)$$
 is an element of the algebra

• Imposing Gauge invariance:

$$U_{\mu}(x) o \Omega(x) U_{\mu}(x) \Omega^{\dagger}(x+\mu) ~~ igstarrow \left[~~ Z_{\mu}(x) o \Omega(x) Z_{\mu}(x) \Omega^{\dagger}(x)~
ight]$$

• Strong constraints on  $Z_t$ , how to satisfy these properties?

### Lüscher's ansatz

$$Z_t = \partial ilde{S}(U_t,t)$$

$$ilde{S}(U_t,t) = \sum_i c_i(t) W_i(U_t)$$

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- $Z_t$  is the force of a generic action (i.e. scalar & gauge invariant quantity)
  - Any force (i.e. gradient w.r.t. the field components) is an element of the algebra
  - $\circ$  Any force of an action (i.e. gauge invariant quantity) satisfies  $Z_\mu(x) o \Omega(x) Z_\mu(x) \Omega^\dagger(x)$
- $\dot{U}_t = \left(\partial ilde{S}(U_t,t)
  ight) U_t$  is the most generic and suitable ODE for lattice gauge theories!

### **Notation in Continuous Flows**

$$egin{aligned} \langle \mathcal{O} 
angle &= rac{1}{\mathcal{Z}} \int \mathrm{D}[V] \, \mathcal{O}(\mathcal{F}(V)) \, \exp(-S_\mathcal{F}(V)) \ &S_\mathcal{F}(V) = S(\mathcal{F}(V)) - \log \det \mathcal{F}_*(V) \end{aligned}$$

• 
$$U_0\equiv V$$
 base field

• 
$$U_T\equiv \mathcal{F}(V)=\int_0^T \dot{U}_t \, dt$$
 integrated field

• 
$$\dot{U}_t = \left(\partial ilde{S}(U_t,t)
ight) U_t$$
 flow ode

Caplacian

• 
$$\log\det \mathcal{F}_*(V)=\int_0^T\mathcal{L}_o ilde{S}(U_t,t)dt$$
 with  $\mathcal{L}_0=-\sum_{x,\mu,a}\partial^a_{x,\mu}\partial^a_{x,\mu}$ 

### **Summing up on Continuous Flows**

$$egin{aligned} \langle \mathcal{O} 
angle &= rac{1}{\mathcal{Z}} \int \mathrm{D}[U_0] \, \mathcal{O}(U_T) \, \exp(-S_0(U_0)) \ &S_0(U_0) &= S(U_T) - \int_0^T \mathcal{L}_0 \tilde{S}(U_t,t) dt \ & \overbrace{\mathsf{Base} & \mathsf{Target} & \mathsf{Flow} \ \mathsf{action} & \mathsf{action} & \mathsf{action} \end{aligned}$$

• 
$$S_0(U_0) = \mathrm{const.}/S'(U_0)/\ldots$$
 training condition

$$egin{array}{ll} ullet & ilde S(U_t,t) = \sum_i c_i(t) W_i(U_t) & ext{trainable} ext{ action with } c_i(t) ext{ free parameters} \end{array}$$

•  $\mathcal{L}_0 ilde S(U_t,t)$  is always an action-like term, e.g.  $\mathcal{L}_0 W_0 = rac{16}{3} W_0$  (but more complicated for loops with repeated links)

### Part 2: Building on Lüscher's idea

How to find  $c_i(t)$  ?

<u>Perturbative approach</u> around eta=0

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#### Machine Learning approach

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or with CNN  $c_i\left(t, ec{W}_t(x)
ight)$  [M. Gerdes et al., arXiv:2410.13161]

#### Lüscher's t-expansion

$$egin{aligned} ilde{S}(U_t,t) &= \sum_i c_i(t) W_i(U_t) \ &= \sum_k t^k ilde{S}^{(k)}(U_t) &= \sum_k t^k \sum_i c_i^{(k)} W_i(U_t) \end{aligned} 
ight\} \quad c_i(t) &= \sum_k c_i^{(k)} t^k \ &= \sum_k t^k ilde{S}^{(k)}(U_t) &= \sum_k t^k \sum_i c_i^{(k)} W_i(U_t) \end{aligned}$$

• When solving around ~eta=0 , i.e.  $~S(U_T)-\int_0^T {\cal L}_0 ilde S(U_t,t) dt={
m const.}$ 

$$egin{aligned} & ilde{S}^{(0)} = \mathcal{L}_{0}^{-1}S \ & ilde{S}^{(k)} = \mathcal{L}_{0}^{-1}\sum_{x,\mu,a} \partial^{a}_{x,\mu}S\,\partial^{a}_{x,\mu} ilde{S}^{(k-1)} & ext{ for } k>0 \end{aligned}$$

### Lüscher's t-expansion - Wilson action



•  $S = \frac{\beta}{6}W_0$ •  $\tilde{S}^{(0)} = \mathcal{L}_0^{-1}S = -\frac{\beta}{22}W_0$ Things become very difficult... very fast!

$$\begin{split} \bullet \quad \tilde{S}^{(1)} &= \mathcal{L}_0^{-1} \sum_{x,\mu,a} \partial^a_{x,\mu} S \, \partial^a_{x,\mu} \tilde{S}^{(0)} = \frac{\beta^2}{192} \Big( -\frac{4}{33} W_1 + \frac{12}{119} W_2 + \frac{1}{33} W_3 \\ \bullet \quad \text{etc...} \quad \quad -\frac{5}{119} W_4 + \frac{3}{10} W_5 - \frac{1}{5} W_6 + \frac{1}{9} W_7 \Big) \end{split}$$

### Machine Learning approach

$$ilde{S}(U_t,t) = \sum_i c_i(t) W_i(U_t) \quad \longrightarrow \quad c_i(t,ec{ heta})$$

- $\vec{\theta}$  are coefficients to train for finding the minimum of our tuning condition, i.e. *cost function*.
- Gradients of the cost function are needed for better & faster convergence

$$rac{d}{dec{ heta}} \Big( S(U_T) - S_0(U_0) - \int_0^T \mathcal{L}_0 ilde{S}(U_t,t) dt \Big)$$
Cost function

### Gradient of the cost function

$$\frac{\frac{\partial}{\partial \vec{\theta}}C(\vec{\theta}) = \frac{\frac{d}{d\vec{\theta}}S(U_T) - \frac{\frac{d}{d\vec{\theta}}S_0(U_0) - \int_0^T \frac{\frac{d}{d\vec{\theta}}\mathcal{L}_0\tilde{S}(U_t,t)dt}{\underbrace{\frac{d}{d\vec{\theta}}\mathcal{L}_0\tilde{S}(U_t,t)}dt}$$

$$rac{dU_t}{d heta_i} = Y_t^{(i)} U_t \quad \longrightarrow \quad rac{d}{d heta_i} S(U_t) = \left(\partial S(U_t), Y_t^{(i)}
ight)$$

Coefficients' ODE

Algebra's scalar product

• ISSUE: we have as many fields  $Y_t^{(i)}$  as the number of parameters. Suitable only for few parameters...

#### **Adjoint State method**

• We use the adjoint state method to remove any dependence on  $\,Y_t^{(i)}\,$  See [2212.08469] for details.

$$\begin{split} \lambda_t &= \partial \mathcal{L}_0 \tilde{S}_t + \left[ \partial \tilde{S}_t, \lambda_t \right] - \sum_{y,\nu} \lambda_t^a(y,\nu) \partial \partial_{y,\nu}^a \tilde{S}_t \\ \lambda_T &= \partial S(U_T) & \quad \text{The adjoint state is defined at time } T, \\ \text{so we have to integrate backwards} \end{split}$$

### **Part 3: Numerical Results**

# 2 Dimensional SU(3) Yang-Mills Theory

arXiv:2212.08469

Learning Trivializing Gradient Flows for Lattice Gauge Theories

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### **Considered Flow Actions**

• Model A: Next-to-leading order of t-expansion, <u>7 Loops x Linear coefficients</u> (2 params.)



• Model B: <u>42 Wilson loops x 10 time points</u> (interpolated by a cubic spline)



### Time dependence of the coefficients is fundamental



## Main Result: Machine-learned Gradient Flows

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Dof	N	ESS at $\beta$		
nei.	<sup>1</sup> vparams	4.0	5.0	6.0
Lüscher	8 non-zero values		4%	<1%
Our work A B	$14 \equiv 2_t \times 7_W$	91%	65%	26%
	$420 \equiv 10_t \times 42_W$	98%	88%	70%
MIT & DeepMind	$\gtrsim4000000$	88%	75%	48%

#### [arXiv:2410.13161] obtained ESS compatible to ours

#### We have developed the first continuous flow for Lattice QCD.

Advantages compared to "discrete" flows are

- Highest ESS and better scaling
- 5 orders of magnitude less parameters
- All symmetries of the theory preserved
- Faster training, 100x less iterations
- Initial guess from perturbation theory

NOTE: Results for SU(3) gauge theories on a 2D 16<sup>2</sup> lattice.



### Part 4: Towards 4D results

# 4 Dimensional SU(3) Yang-Mills Theory



### **Target problem**

Results on	β	1.0	2.0	3.0	4.0
a 8 <sup>4</sup> lattice	ESS	91%	49%	1%	0%

Moving away from toy models, a good target problem is

- β=6.0 → 0.093 fm lattice spacing [1009.5228]
- **16<sup>4</sup> lattice →** 1.5 fm lattice size
- Long autocorrelation already visible in the smeared Q

For the base distribution then we can consider

- Ideally, <u>uniform</u> → most probably impossible
- Realistically,  $\beta = 5.7$  double lattice spacing
- Practically, ...





### Flowing in $\beta$

$$\langle \mathcal{O} 
angle = rac{1}{\mathcal{Z}} \int \mathrm{D}[U] \, \mathcal{O}(U) \, \exp(-S(U)) = rac{1}{\mathcal{Z}} \int \mathrm{D}[U_{ au}] \, \mathcal{O}(U) \, \exp(-S_{ au}(U_{ au}))$$

Gradient 
$$S_ au(U_ au) = S(U) - \int_ au^1 \mathrm{d}t\, \mathcal{L}_0 ilde{S}(U_t,t) ~\left\{egin{array}{c} \dot{U}_t = -\partial ilde{S}_t\, U_t \ U \equiv U_1 \end{array}
ight.$$

R

Desired base action

$$S_{ au} = au S = - au rac{eta}{6} W_0$$
  
 $au = 1$  Target action  $S = -rac{eta}{6} W_0$   
 $au = 0$  Trivial action Wilson action

# Flowing in $\beta$

$$egin{aligned} & \left\{ egin{aligned} \dot{S}_{ au}(U_{ au}) &= S(U) - \int_{ au}^{1} \mathrm{d}t\,\mathcal{L}_{0}\, ilde{S}(U_{t},t) & \left\{ egin{aligned} \dot{U}_{t} &= -\partial ilde{S}_{t}\,U_{t} \ U &\equiv U_{1} \end{aligned} 
ight. \ & \left\{ egin{aligned} & \mathcal{U} &\equiv \mathcal{U}_{1} \end{matrix} 
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ight. \ & \left\{ egin{aligned} & \mathcal{U} &\equiv \mathcal{U} &\in \mathcal{U} \\ \mathcal{U} &\equiv \mathcal{U} &\in \mathcal{U}$$

# Flowing in $\beta$

$$egin{aligned} \mathcal{S}_0 \mathcal{I}_t & = rac{teta}{6}ig(\partial W_0,\partial ilde{S}_tig) + rac{eta}{6}W_0 = ext{const.} \ ilde{S}(U_t,t) & = rac{eta}{6}\sum_{k=0}^\inftyig(rac{teta}{6}ig)^k ilde{S}^{(k)}(U_t) & igg\{ egin{aligned} ilde{S}^{(0)} & = -\mathcal{L}_0^{-1}W_0 = -rac{3}{16}W_0 \ ilde{S}^{(k)} & = \mathcal{L}_0^{-1}ig(\partial W_0,\partial ilde{S}^{(k-1)}ig) \end{aligned}$$

### **Convergence of the flow action**

$$\tilde{S}(U_t, t) = \frac{\beta}{6} \sum_{k=0}^{\infty} \left(\frac{t\beta}{6}\right)^k \tilde{S}^{(k)}(U_t)$$
•  $t \leq 1$   $\checkmark$  Limit of the integral
•  $\beta < 6$   $\bigstar$  Region of physical interest at  $\beta \gtrsim 6$ 
• Order of magnitude of  $\tilde{S}^{(k)}$ ??
• Our conclusion: most probably it does not converge!

 $(\tilde{c}(1)) (\tilde{c}(0)) = (\tilde{c}(1)) (\tilde{c}(0)) = (\tilde{c}(2)) (\tilde{c}(0))$ 

### **Final Part: A realistic application**

# A novel approach for computing gradients of Physical observables



When taking a gradient of a physical observable, we have three contributions:

Alternatively, we can compute gradients in the gradient flow formulation:

$$egin{aligned} &\langle \mathcal{O} 
angle &= rac{1}{\mathcal{Z}_{d heta}} \int \mathrm{D}[U_{d heta}] \, \mathcal{O}(U) \, \exp(-S_{d heta}(U_{d heta})) \ & S_{d heta}(U_{d heta}) &= S(U) - \int_{0}^{d heta} \mathcal{L}_{0} \tilde{S}(U_{t},t) dt \end{aligned}$$

### **Theorem and Corollaries**

#### The generic formula, demonstrated in the paper, is

$$\frac{d\langle \mathcal{O} \rangle}{d\theta} = \langle \frac{\partial \mathcal{O}}{\partial \theta} + \left( \partial \mathcal{O}, \partial \tilde{S} \right) - \mathcal{OC} \rangle + \langle \mathcal{O} \rangle \langle \mathcal{C} \rangle \quad \text{with} \\ \mathcal{C} = \mathcal{L}_0 \tilde{S} + \left( \partial S, \partial \tilde{S} \right) + \frac{\partial S}{\partial \theta}$$

#### Corollary A: "The new approach"

If  $\mathcal{C}$  = const. then

$$rac{d\langle \mathcal{O} 
angle}{d heta} = \langle rac{\partial \mathcal{O}}{\partial heta} + ig( \partial \mathcal{O}, \partial ilde{S} ig) 
angle$$

Corollary B: "The standard approach"

If 
$$\, {\tilde S}$$
 = const. then

$$rac{d\langle \mathcal{O} 
angle}{d heta} = \langle rac{\partial \mathcal{O}}{\partial heta} - \mathcal{O} rac{\partial S}{\partial heta} 
angle + \langle \mathcal{O} 
angle \langle rac{\partial S}{\partial heta} 
angle$$

# **Opportunity?** Calculation of gradients!



$$\mathcal{L}_0 ilde{S} + ig(\partial S,\partial ilde{S}ig) + rac{\partial S}{\partial heta} = ext{const.}$$
 A new loss function for ML approaches

#### **Applications:**

- Calculation of gradients and leading-order effects (QED, Θ-term, isospin-breaking, etc.)
- Feynman-Hellmann approach for computing observables ( $g_{\Delta}$ ,  $\sigma$ -terms, gluons loops, etc.)

#### Approach:

- Any ML tools developed for LQCD. This is not a flow anymore, only one  $\hat{S}$  is needed!
- Generic analytic solution:  $\tilde{S} = \sum_{k=0}^{\infty} \tilde{S}^{(k)} \begin{cases} \tilde{S}^{(0)} = -\mathcal{L}_0^{-1} \frac{\partial S}{\partial \theta} \quad \text{Can be used as initial guess} \\ \tilde{S}^{(k)} = -\mathcal{L}_0^{-1} \left( \partial S, \partial \tilde{S}^{(k-1)} \right) \quad \text{Critical for convergence} \end{cases}$

# Comparison with related work

Similar benefits have been shown by R. Abbott et al. in the generation of correlated ensembles.



The two approaches are same in principle, i.e. where one works the other will work too, with few key differences:

- $\checkmark$  It is an exact gradients, no small  $\lambda$  needs to be introduced
- $\checkmark$  We have an analytics solution that can be used as initial guess for the training
- / We require to compute the force of the observable, of the flow action and its Laplacian



# Thank you for your attention!

#### arXiv:2212.08469

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