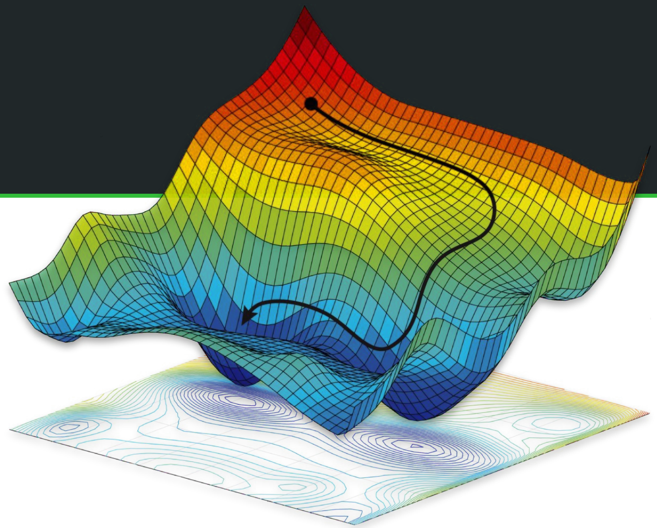
Continuous Normalizing Flows

for Lattice Gauge Theories



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Outline

arXiv:2212.08469

Learning Trivializing Gradient Flows for Lattice Gauge Theories

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(Dated: December 19, 2022)

First application of Continuous Normalizing Flows to Lattice Gauge Theories

Realistic application of Machine Learning in Lattice QCD

arXiv:2305.07932

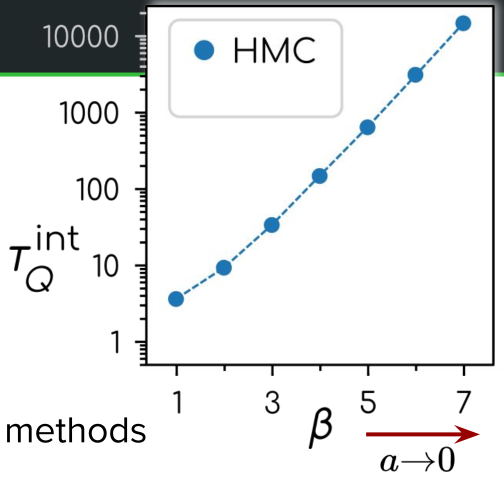
A novel approach for computing gradients of physical observables

Simone Bacchio[1]
[1] *Computation-based Science and Technology Research Center, The Cyprus Institute, Nicosia, Cyprus*
(Dated: May 21, 2023)

Motivation: Critical slowing down

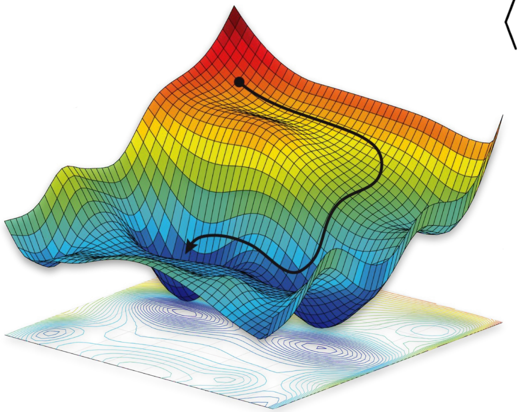
In Lattice Gauge Theories, the expectation value of an observable is defined as

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



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

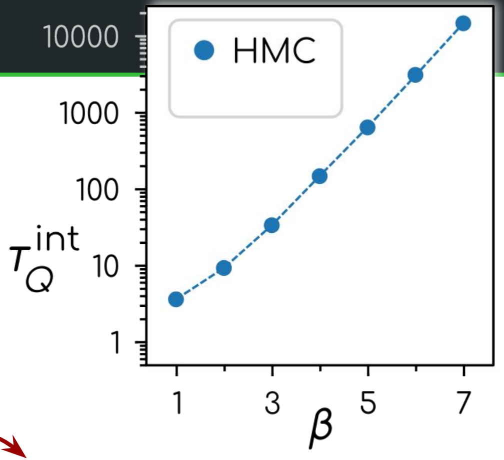
$$\langle \mathcal{O} \rangle = \frac{1}{N} \sum_i^N O(U_i) \quad \textit{with} \quad p(U) = \frac{1}{\mathcal{Z}} \exp(-S(U))$$



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

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

Motivation: Critical slowing down



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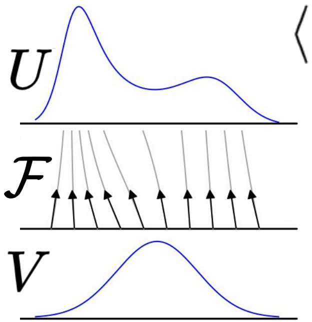
$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathrm{D}[U]\, \mathcal{O}(U)\, \exp(-S(U))$$

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

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



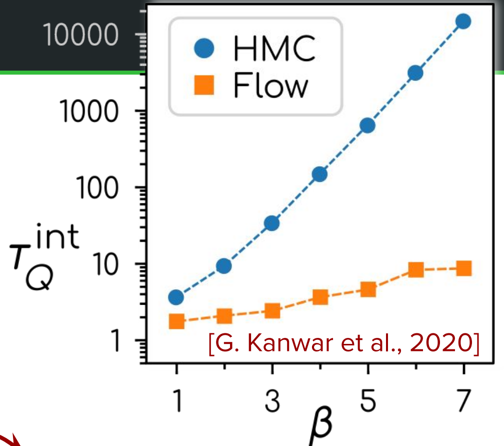
$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathrm{D}[V]\, \mathcal{O}(\mathcal{F}(V))\, \exp(-S_{\mathcal{F}}(V))$$

$$S_{\mathcal{F}}(V) = S(\mathcal{F}(V)) - \log\det \mathcal{F}_*(V)$$

The action is modified by the log-det. of the Jacobian of the transformation

Our goal, then, is to find a *flow*, $\mathcal{F}$, such that $S_{\mathcal{F}}(V)$ is easier to simulate / sample

Motivation: Critical slowing down



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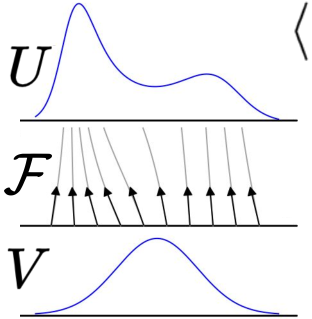


$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathrm{D}[V]\, \mathcal{O}(\mathcal{F}(V))\, \exp(-S_{\mathcal{F}}(V))$$

$$S_{\mathcal{F}}(V) = S(\mathcal{F}(V)) - \log \det \mathcal{F}_*(V) = \text{const.}$$

Ultimate goal

Loss function

Our goal, then, is to find a *flow*, $\mathcal{F}$, such that $S_{\mathcal{F}}(V)$ is easier to simulate / sample

How to construct the flow?

Discrete flow

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

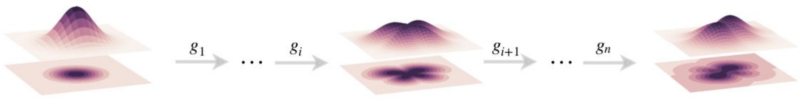
Requirements:

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

Approach:

- RealNVP & Equivariant Normalizing Flows

[G. Kanwar et al., 2020]



Continuous flow

$$U = \mathcal{F}(V) = \text{“}\int f(U_t, t)dt\text{”}$$

$$\dot{U}_t = f(U_t, t)$$

Same requirements…

Approach:

- Gradient flow 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 $\dot{U}_t \equiv \frac{dU_t}{dt} = f(U_t, t)$?

arXiv:0907.5491

Trivializing maps, the Wilson flow and the HMC algorithm

Martin Lüscher

CERN, Physics Department, 1211 Geneva 23, Switzerland

ODEs on manifolds

$$\dot{U}_t = \underbrace{g(U_t, t)}_{Z_t} U_t$$ where $U_t \in$ Group, $Z_t \in$ Algebra

$$U_t = e^{\sum_a c_a(t)\, T_a}$$
$$\dot{U}_t = \left(\textstyle\sum_a \dot{c}_a(t)\, T_a\right) U_t$$

- $Z_t = g(U_t, t)$ is an element of the algebra
- Imposing Gauge invariance:

$$U_\mu(x) \to \Omega(x) U_\mu(x) \Omega^\dagger(x+\mu) \quad \Longrightarrow \quad Z_\mu(x) \to \Omega(x) Z_\mu(x) \Omega^\dagger(x)$$

- Strong constraints on Z_t, **how to satisfy these properties?**

Lüscher’s ansatz

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

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

arXiv:0907.5491

Trivializing maps, the Wilson flow and the HMC algorithm

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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
  - Any force of an action (i.e. gauge invariant quantity) satisfies $Z_\mu(x) \to \Omega(x) Z_\mu(x) \Omega^\dagger(x)$
- $\dot{U}_t = \left(\partial \tilde{S}(U_t, t)\right) U_t$ is the most generic and suitable ODE for lattice gauge theories!

Notation in Continuous Flows

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathrm{D}[V] \, \mathcal{O}(\mathcal{F}(V)) \, \exp(-S_{\mathcal{F}}(V))$$

$$S_{\mathcal{F}}(V) = S(\mathcal{F}(V)) - \log \det \mathcal{F}_*(V)$$

- $U_0 \equiv V$ base field
- $U_T \equiv \mathcal{F}(V) = \int_0^T \dot{U}_t \, dt$ integrated field
- $\dot{U}_t = \left(\partial \tilde{S}(U_t, t)\right) U_t$ flow ODE
- $\log \det \mathcal{F}_*(V) = \int_0^T \mathcal{L}_o \tilde{S}(U_t, t) dt$ with $\mathcal{L}_0 = -\sum_{x,\mu,a} \partial^a_{x,\mu} \partial^a_{x,\mu}$

Summing up on Continuous Flows

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathrm{D}[U_0]\, \mathcal{O}(U_T)\ \exp(-S_0(U_0))$$

$$\underbrace{S_0(U_0)}_{\text{Base action}} = \underbrace{S(U_T)}_{\text{Target action}} - \int_0^T \mathcal{L}_0 \underbrace{\tilde{S}(U_t, t)}_{\text{Flow action}} dt$$

- $S_0(U_0) = \mathrm{const.}/S'(U_0)/\dots$ training condition
- $\tilde{S}(U_t, t) = \sum_i c_i(t) W_i(U_t)$ trainable action with $c_i(t)$ free parameters
- $\mathcal{L}_0 \tilde{S}(U_t, t)$ is always an action-like term, e.g. $\mathcal{L}_0 W_0 = \frac{16}{3} W_0$ (but more complicated for loops with repeated links)

Part 2: Building on Lüscher's idea

How to find $c_i(t)$ *?*

Perturbative approach around $\beta = 0$

arXiv:0907.5491

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Machine Learning approach

arXiv:2212.08469

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(Dated: December 19, 2022)

- … and with CNN [Pim de Haan talk]

Lüscher's t-expansion

$$\tilde{S}(U_t, t) = \sum_i c_i(t) W_i(U_t) = \sum_k t^k \tilde{S}^{(k)}(U_t) = \sum_k t^k \sum_i c_i^{(k)} W_i(U_t)$$

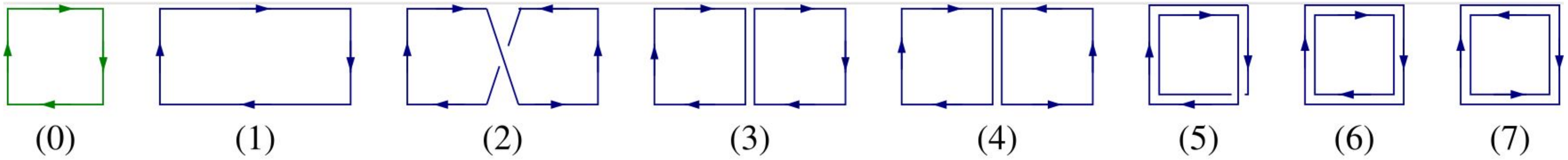
$$c_i(t) = \sum_k c_i^{(k)} t^k$$

- When solving around $\beta = 0$, i.e. $S(U_T) - \int_0^T \mathcal{L}_0 \tilde{S}(U_t, t) dt = \text{const.}$

$$\tilde{S}^{(0)} = \mathcal{L}_0^{-1} S$$

$$\tilde{S}^{(k)} = \mathcal{L}_0^{-1} \sum_{x,\mu,a} \partial^a_{x,\mu} S \, \partial^a_{x,\mu} \tilde{S}^{(k-1)} \quad \text{for } k > 0$$

Lüscher's t-expansion - Wilson action



Terms appearing in the Next-to-Leading order,
i.e. all combinations of two plaquettes sharing a link

- $S = \frac{\beta}{6} W_0$
- $\tilde{S}^{(0)} = \mathcal{L}_0^{-1} S = -\frac{\beta}{32} W_0$
- $\tilde{S}^{(1)} = \mathcal{L}_0^{-1} \sum_{x,\mu,a} \partial^a_{x,\mu} S \, \partial^a_{x,\mu} \tilde{S}^{(0)} = \frac{\beta^2}{192}\Big(-\frac{4}{33}W_1 + \frac{12}{119}W_2 + \frac{1}{33}W_3 - \frac{5}{119}W_4 + \frac{3}{10}W_5 - \frac{1}{5}W_6 + \frac{1}{9}W_7\Big)$
- etc…

Things become very difficult… very fast!

Machine Learning approach

$$\tilde{S}(U_t, t) = \sum_i c_i(t) W_i(U_t) \quad \longrightarrow \quad c_i(t, \vec{\theta})$$

- $\vec{\theta}$ 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

$$\frac{d}{d\vec{\theta}} \Big(\underbrace{S(U_T) - S_0(U_0) - \int_0^T \mathcal{L}_0 \tilde{S}(U_t, t) dt}_{\text{Cost function}} \Big)$$

Gradient of the cost function

$$\frac{\partial}{\partial\vec{\theta}}C(\vec{\theta}) = \underbrace{\frac{d}{d\vec{\theta}}S(U_T)}_{?} - \underbrace{\frac{d}{d\vec{\theta}}S_0(U_0)}_{0} - \int_0^T \underbrace{\frac{d}{d\vec{\theta}}\mathcal{L}_0\tilde{S}(U_t,t)}_{?}dt$$

$$\frac{dU_t}{d\theta_i} = Y_t^{(i)}U_t \longrightarrow \frac{d}{d\theta_i}S(U_t) = \left(\partial S(U_t), Y_t^{(i)}\right)$$

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

$$\frac{\partial}{\partial\vec{\theta}}C(\vec{\theta}) = \int_0^T \left[\left(\lambda_t, \frac{\partial}{\partial\vec{\theta}}\partial\tilde{S}_t \right) - \frac{\partial}{\partial\vec{\theta}}\mathcal{L}_0\tilde{S}_t \right] dt$$

Adjoint State

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

Adjoint State ODE

$$\dot{\lambda}_t = \partial\mathcal{L}_0\tilde{S}_t + [\partial\tilde{S}_t, \lambda_t] - \sum_{y,\nu}\lambda_t^a(y,\nu)\,\partial\,\partial^a_{y,\nu}\tilde{S}_t$$

Second derivative required

$$\lambda_T = \partial S(U_T)$$

The adjoint state is defined at time *T*, so we have to integrate backwards

Part 3: Numerical Results

2 Dimensional SU(3) Yang-Mills Theory

arXiv:2212.08469

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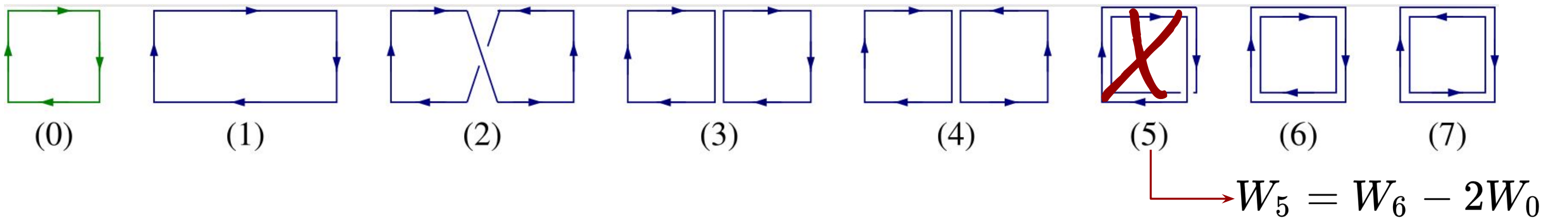
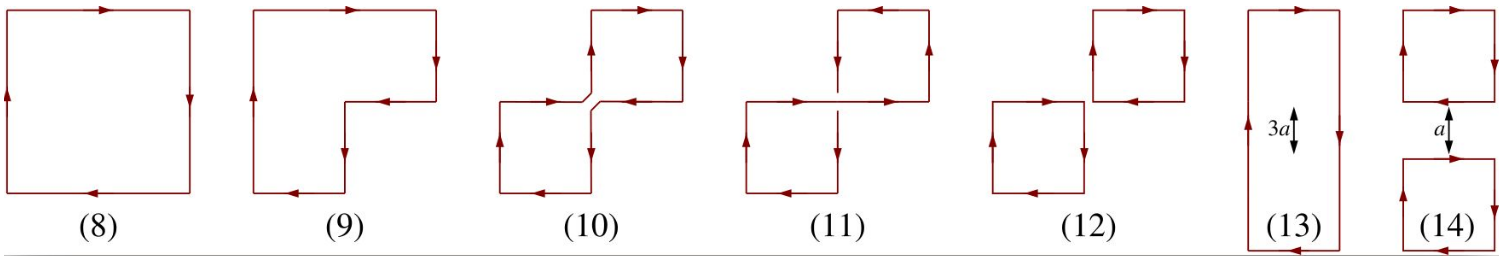
(Dated: December 19, 2022)

Considered Flow Actions

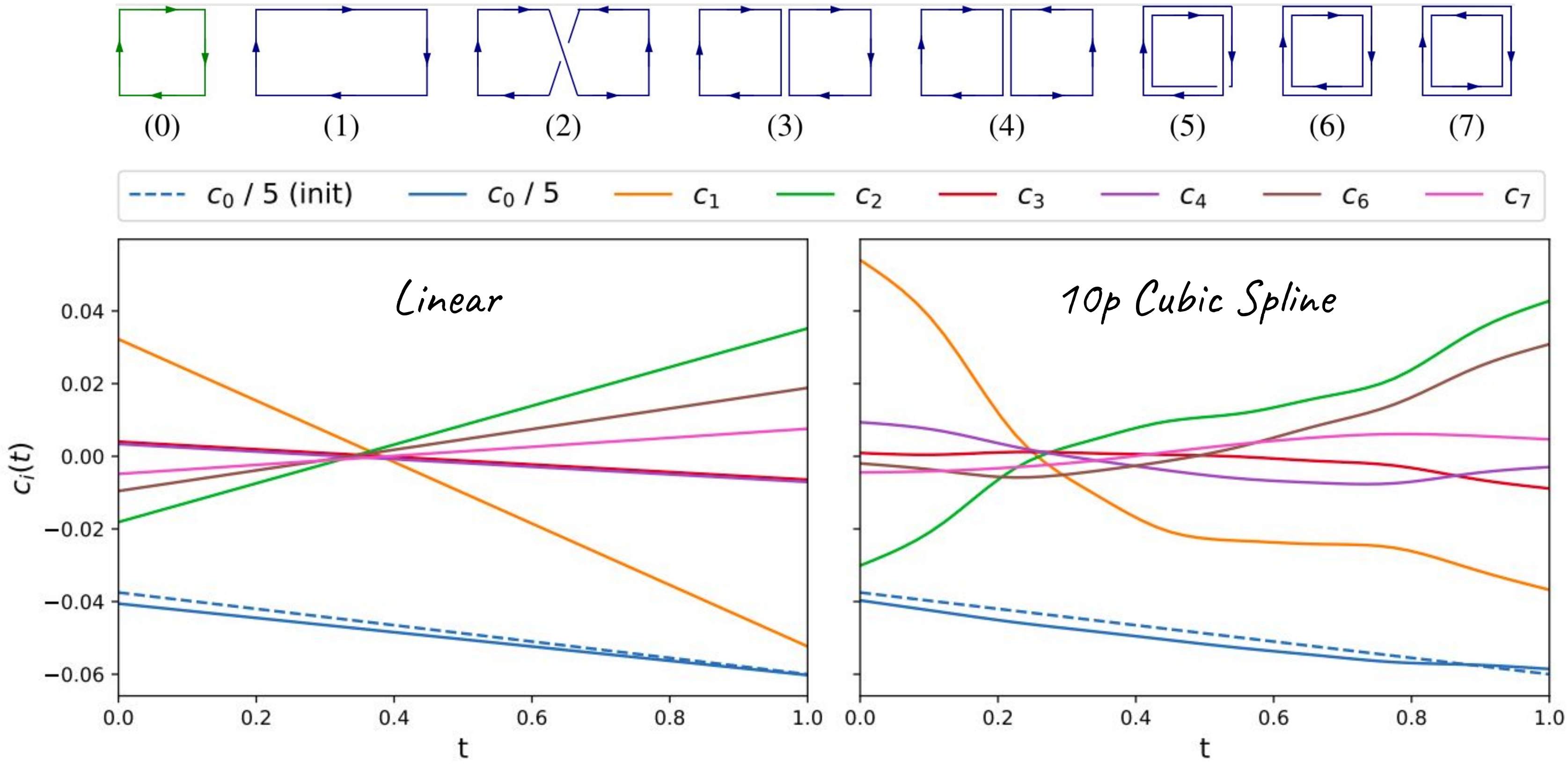
- **Model A:** Next-to-leading order of t-expansion, 7 Loops x Linear coefficients (2 params.)



- **Model B:** 42 Wilson loops x 10 time points (interpolated by a cubic spline)



Time dependence of the coefficients is fundamental



Main Result: Machine-learned Gradient Flows

arXiv:2212.08469

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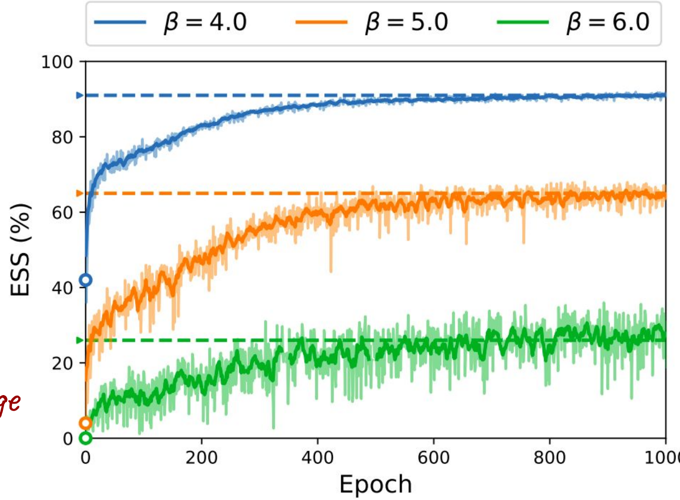
Ref.		N_{params}	ESS at β 4.0	5.0	6.0
Lüscher		8 non-zero values	42%	4%	<1%
Our work	**A**	$14 \equiv 2_t \times 7_W$	91%	65%	26%
	B	$420 \equiv 10_t \times 42_W$	98%	88%	70%
MIT & DeepMind		$\gtrsim 4\,000\,000$	88%	75%	48%

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 16^2 lattice.



Part 4: Towards 4D results

4 Dimensional SU(3) Yang-Mills Theory

Target problem

Results on a 8^4 lattice	β	1.0	2.0	3.0	4.0
	ESS	*91%*	*49%*	*1%*	*0%*

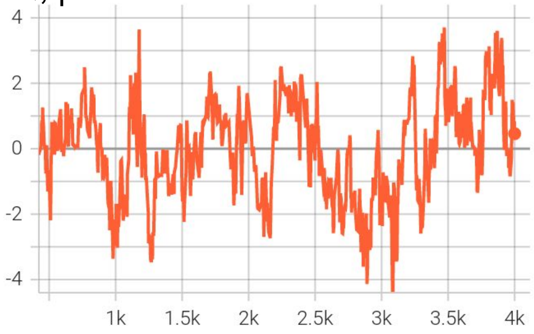
Moving away from toy models, a good target problem is

- **β=6.0** ➔ 0.093 fm lattice spacing [1009.5228]
- **16^4 lattice** ➔ 1.5 fm lattice size
- Long autocorrelation already visible in the smeared Q

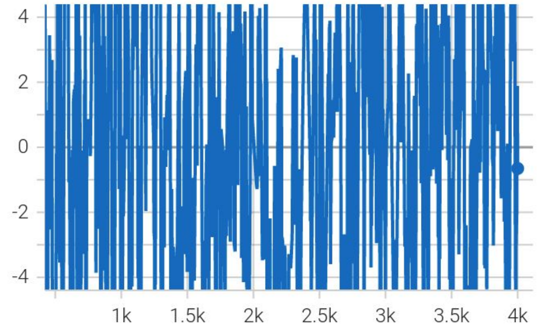
For the base distribution then we can consider

- Ideally, uniform ➔ most probably impossible
- Realistically, β=5.7 ➔ double lattice spacing
- Practically, …

Q, β=6.0



Q, β=5.7



Flowing in β

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

Gradient Flow

$$S_\tau(U_\tau) = S(U) - \int_\tau^1 \mathrm{d}t\, \mathcal{L}_0 \tilde{S}(U_t, t) \quad \begin{cases} \dot{U}_t = -\partial \tilde{S}_t\, U_t \\ U \equiv U_1 \end{cases}$$

Desired base action

$$S_\tau = \tau S = -\tau \frac{\beta}{6} W_0 = -\frac{\beta_0}{6} W_0$$

$\tau = 1$ *Target action*

$\tau = 0$ *Trivial action*

$S = -\frac{\beta}{6} W_0$ *Wilson action*

$\tau = \frac{\beta_0}{\beta}$

Flowing in β

$$S_\tau(U_\tau) = S(U) - \int_\tau^1 \mathrm{d}t\, \mathcal{L}_0 \tilde{S}(U_t, t) \qquad \begin{cases} \dot{U}_t = -\partial \tilde{S}_t\, U_t \\ U \equiv U_1 \end{cases}$$

$$\frac{d}{d\tau}$$

$$\frac{\partial S_\tau}{\partial \tau} - \left(\partial S_\tau, \partial \tilde{S}_\tau\right) = \mathcal{L}_0 \tilde{S}_\tau \qquad S_\tau = \tau S$$

$$S - \tau\left(\partial S, \partial \tilde{S}_\tau\right) = \mathcal{L}_0 \tilde{S}_\tau$$

Wilson action $S = -\frac{\beta}{6} W_0$

$$\mathcal{L}_0 \tilde{S}_\tau - \frac{\tau\beta}{6}\left(\partial W_0, \partial \tilde{S}_\tau\right) + \frac{\beta}{6} W_0 = \text{const.}$$

Flowing in β

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathrm{D}[U]\, \mathcal{O}(U)\, \exp(-S_\beta(U)) = \frac{1}{\mathcal{Z}} \int \mathrm{D}[V]\, \mathcal{O}(U)\, \exp(-S_{\beta_0}(V))$$

Target

$$S_\beta(U) - S_{\beta_0}(V) - \int_{\beta_0/\beta}^{1} \mathrm{d}t\, \mathcal{L}_0 \tilde{S}(U_t, t) = \mathrm{const.}$$

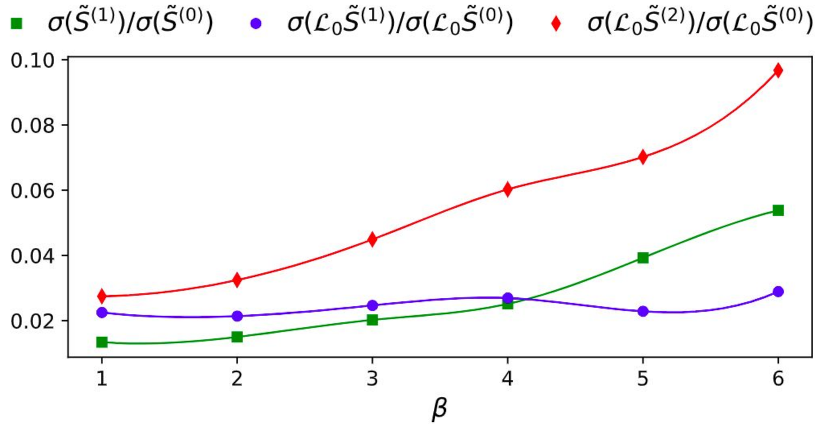
Solution

$$\mathcal{L}_0 \tilde{S}_t - \frac{t\beta}{6} (\partial W_0, \partial \tilde{S}_t) + \frac{\beta}{6} W_0 = \mathrm{const.}$$

$$\tilde{S}(U_t, t) = \frac{\beta}{6} \sum_{k=0}^{\infty} \left(\frac{t\beta}{6} \right)^k \tilde{S}^{(k)}(U_t) \qquad \begin{cases} \tilde{S}^{(0)} = -\mathcal{L}_0^{-1} W_0 = -\frac{3}{16} W_0 \\ \tilde{S}^{(k)} = \mathcal{L}_0^{-1} \left(\partial W_0, \partial \tilde{S}^{(k-1)} \right) \end{cases}$$

Convergence of the flow action

$$\tilde{S}(U_t, t) = \frac{\beta}{6} \sum_{k=0}^{\infty} \left(\frac{t\beta}{6} \right)^k \tilde{S}^{(k)}(U_t)$$



- $t \leq 1$ ✔ Limit of the integral
- $\beta < 6$ ✗ Region of physical interest at $\beta \gtrsim 6$
- Order of magnitude of $\tilde{S}^{(k)}$??

$$\mathcal{L}_0 \tilde{S}^{(2)} = \left(\partial W_0, \partial \tilde{S}^{(1)} \right)$$

- **Our conclusion:** it does not converge!

DEAD END

Final Part: A realistic application

A novel approach for computing gradients

of Physical observables

Opportunity? Calculation of gradients!

arXiv:2305.07932

A novel approach for computing gradients of physical observables

Simone Bacchio[1]

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(Dated: May 21, 2023)

- **Standard finite-difference approach:**

$$\frac{d\langle\mathcal{O}\rangle}{d\theta} = \langle\frac{\partial\mathcal{O}}{\partial\theta} - \underbrace{\mathcal{O}\frac{\partial S}{\partial\theta}\rangle + \langle\mathcal{O}\rangle\langle\frac{\partial S}{\partial\theta}\rangle}$$

→ *noisy disconnected contributions*

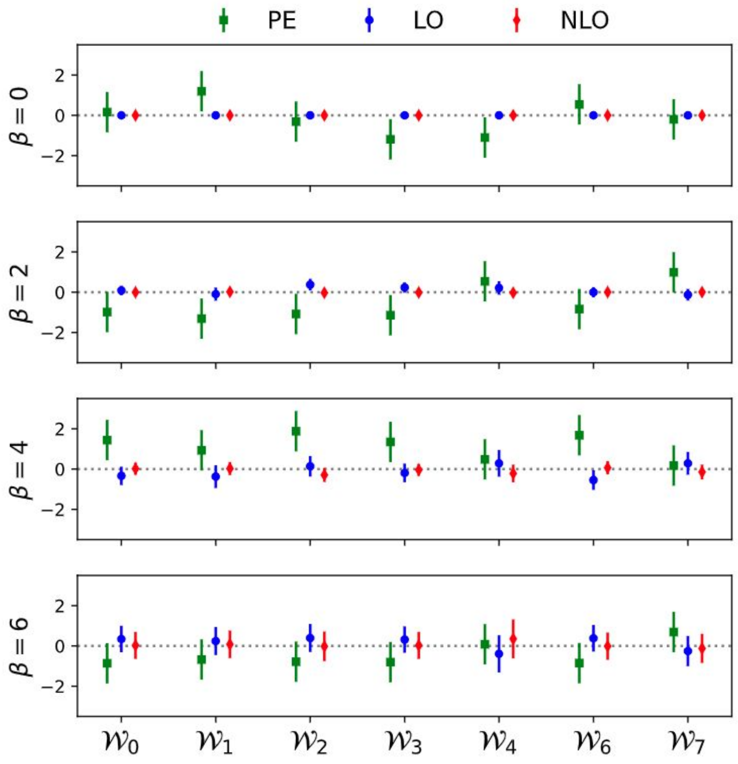
- **Novel approach presented:**

$$\frac{d\langle\mathcal{O}\rangle}{d\theta} = \langle\frac{\partial\mathcal{O}}{\partial\theta} + (\partial\mathcal{O}, \partial\tilde{S})\rangle$$

→ *up to 1000x more precise*

$$\mathcal{L}_0\tilde{S} + (\partial S, \partial\tilde{S}) + \frac{\partial S}{\partial\theta} = \text{const.}$$

→ *condition to be satisfied*



NOTE: Results for 4D pure-gauge SU(3), $V=16^4$

Theorem and Corollaries

The generic formula, demonstrated and valid in any situation, is

$$\frac{d\langle\mathcal{O}\rangle}{d\theta} = \langle\frac{\partial\mathcal{O}}{\partial\theta} + \left(\partial\mathcal{O}, \partial\tilde{S}\right) - \mathcal{O}\mathcal{C}\rangle + \langle\mathcal{O}\rangle\langle\mathcal{C}\rangle$$

where

$$\mathcal{C} = \mathcal{L}_0\tilde{S} + \left(\partial S, \partial\tilde{S}\right) + \frac{\partial S}{\partial\theta}$$

Corollary A: "The new approach"

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

$$\frac{d\langle\mathcal{O}\rangle}{d\theta} = \langle\frac{\partial\mathcal{O}}{\partial\theta} + \left(\partial\mathcal{O}, \partial\tilde{S}\right)\rangle$$

Corollary B: "The standard approach"

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

$$\frac{d\langle\mathcal{O}\rangle}{d\theta} = \langle\frac{\partial\mathcal{O}}{\partial\theta} - \mathcal{O}\frac{\partial S}{\partial\theta}\rangle + \langle\mathcal{O}\rangle\langle\frac{\partial S}{\partial\theta}\rangle$$

Remarks & Outlook

$$\mathcal{L}_0 \tilde{S} + \left(\partial S, \partial \tilde{S}\right) + \frac{\partial S}{\partial \theta} = \text{const.}$$

A new loss function for gradients

Applications:

- Calculation of gradients and leading-order effects (QED, Θ-term, isospin-breaking, etc.)
- Feynman-Hellmann approach for computing observables (g_A, σ-terms, gluons loops, etc.)

Approach:

- Any developed ML for LQCD. This is not a continuous flow anymore, only $\tilde{S}$ is needed!
- Generic analytic solution:

$$\tilde{S} = \sum_{k=0}^{\infty} \tilde{S}^{(k)} \begin{cases} \tilde{S}^{(0)} = -\mathcal{L}_0^{-1} \frac{\partial S}{\partial \theta} \\ \tilde{S}^{(k)} = -\mathcal{L}_0^{-1} \left(\partial S, \partial \tilde{S}^{(k-1)}\right) \end{cases}$$

Can be used as initial guess

Critical for convergence

Remarks & Outlook

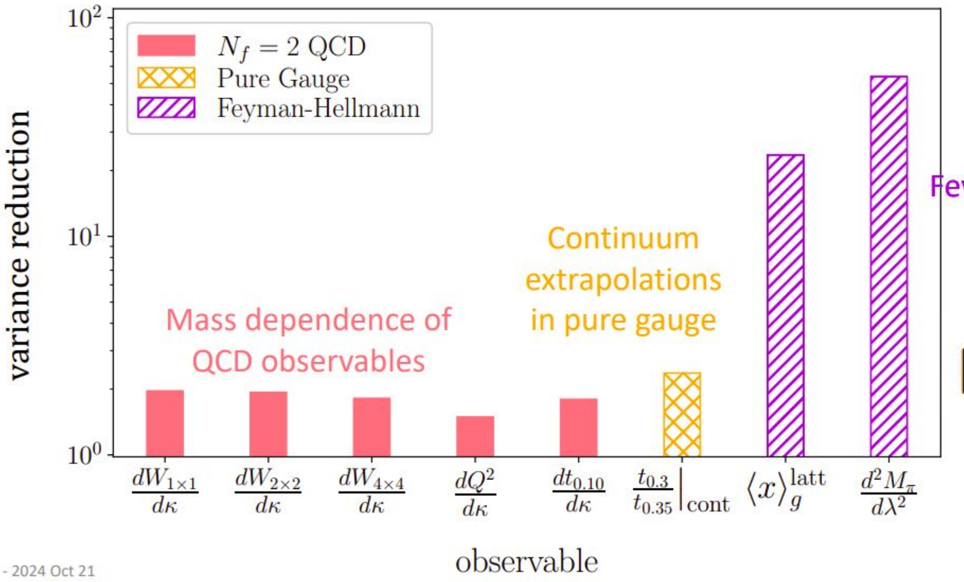
$\mathcal{L}_0 \tilde{S} + (\partial S, \partial \tilde{S}) + \frac{\partial S}{\ldots}$ ... lients

Applicat

- Calc ... king, etc.)
- Feyr ... loops, etc.)

Approac

- Any ... s needed!
- Gene



[2401.10874]

Daniel Hackett, Monday's talk

Can be used as initial guess ... $\sum_{k=0}$ ... $\tilde{S}^{(k)} = -\mathcal{L}_0^{-1}\left(\partial S, \partial \tilde{S}^{(k-1)}\right)$ *Critical for convergence*

Thank you for your attention!

arXiv:2212.08469

Learning Trivializing Gradient Flows for Lattice Gauge Theories

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(Dated: December 19, 2022)

First application of Continuous Normalizing Flows to Lattice Gauge Theories

arXiv:2305.07932

A novel approach for computing gradients of physical observables

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(Dated: May 21, 2023)

Realistic application of Machine Learning in Lattice QCD