Continuous Normalizing Flows

for Lattice Gauge Theories

Dr. Simone Bacchio

Associate Research Scientist CaSToRC, The Cyprus Institute

10/12/24 -NGT Algorithm Workshop, CERN

arXiv:[2212.08469](https://arxiv.org/abs/2212.08469)

Learning Trivializing Gradient Flows for Lattice Gauge Theories

Simone Bacchio.¹ Pan Kessel.^{2, 3} Stefan Schaefer.⁴ and Lorenz Vaitl²

¹ Computation-based Science and Technology Research Center, The Cyprus Institute, Nicosia, Cyprus ² Machine Learning Group, Technische Universität Berlin, Berlin, Germany ³BIFOLD—Berlin Institute for the Foundations of Learning and Data, Berlin, Germany ⁴ John von Neumann-Institut für Computing NIC. Deutsches Elektronen-Synchrotron DESY, Germany (Dated: December 19, 2022)

First application of Continuous Normalizing Flows to Lattice Gauge Theories

[arXiv:2305.07932](https://arxiv.org/abs/2305.07932)

Realistic application of Machine Learning in Lattice QCD

A novel approach for computing gradients of physical observables

Simone Bacchio¹

 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

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

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

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

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

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

Motivation: Critical slowing down

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

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

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

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

 \bullet HMC

 $\mathcal{S}_{\mathcal{S}}$

5 β

10000

1000

100

 τ_Q^{int}

$$
\underbrace{U}{\mathcal{F}}
$$
\n
$$
\underbrace{\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int D[V] \, \mathcal{O}(\mathcal{F}(V)) \, \exp(-S_{\mathcal{F}}(V))}_{\text{The action is modified by}
$$
\n
$$
S_{\mathcal{F}}(V) = S(\mathcal{F}(V)) - \log \det \mathcal{F}_*(V) \longleftarrow \text{the log-det. of the Jacobian}
$$
\n
$$
V
$$
\nOur goal, then, is to find a flow, \mathcal{F} , such that $S_{\mathcal{F}}(V)$ is easier to simulate / sample

Motivation: Critical slowing down

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

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

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

$$
\underbrace{U}{\mathcal{F}}
$$
\n
$$
\begin{array}{c}\n\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int D[V] \, \mathcal{O}(\mathcal{F}(V)) \, \exp(-S_{\mathcal{F}}(V)) \\
\downarrow \qquad \qquad \text{Utimate goal} \\
\downarrow \qquad \qquad S_{\mathcal{F}}(V) = S(\mathcal{F}(V)) - \log \det \mathcal{F}_*(V) = \text{const.} \\
\downarrow \qquad \qquad \downarrow \qquad \qquad \text{Coss function} \\
\downarrow \qquad \qquad \text{Our goal, then, is to find a flow, } \mathcal{F}, \text{ such that } S_{\mathcal{F}}(V) \text{ is easier to simulate } \text{'sample}\n\end{array}
$$

[G. Kanwar et al., 2020

5 β

3

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

 \bullet HMC \blacksquare Flow

10000

1000

100

 10

 τ_Q^{int}

How to construct the 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]

Discrete flow Continuous flow

$$
U = \mathcal{F}(V) = \r \int f(U_t,t) dt^{\r \r}
$$

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

Same requirements…

Approach:

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

[arXiv:0907.5491](https://arxiv.org/abs/0907.5491)

Trivializing maps, the Wilson flow and the HMC algorithm

Martin Lüscher

CERN, Physics Department, 1211 Geneva 23, Switzerland

ODEs on manifolds

$$
\dot U_t = g(U_t,t)U_t \quad \text{where} \quad \begin{array}{c} U_t \in \text{ Group} \\ \hline Z_t \in \text{ Algebra} \end{array} \quad \left| \begin{array}{c} U_t = e^{\sum_a c_a(t) \, T_a} \\ \dot U_t = (\sum_a \dot c_a(t) \, T_a) \, U_t \end{array} \right|
$$

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

Imposing Gauge invariance:

$$
U_\mu(x)\to \Omega(x)U_\mu(x)\Omega^\dagger(x+\mu)\;\;\longrightarrow\;\left[\;Z_\mu(x)\to \Omega(x)Z_\mu(x)\Omega^\dagger(x)\;\right]
$$

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

Lüscher's ansatz

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

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

[arXiv:0907.5491](https://arxiv.org/abs/0907.5491)

Trivializing maps, the Wilson flow and the HMC algorithm

Martin Lüscher

CERN, Physics Department, 1211 Geneva 23, Switzerland

- 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 $\;Z_\mu(x)\to \Omega(x)Z_\mu(x)\Omega^\dagger(x)$
- $\bullet~~\dot{U}_{t}=\left(\partial\tilde{S}(U_{t},t)\right)U_{t}$ is the most generic and suitable ODE for lattice gauge theories!

Notation in Continuous Flows

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

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

$$
\bullet\ \ U_0\equiv V\ \text{base field}
$$

$$
\quad \bullet \ \ U_{T} \equiv \mathcal{F}(V) = \textstyle \int_{0}^{T} \dot{U}_{t} \ dt \quad \text{\scriptsize{\text{integrated field}}}
$$

$$
\bullet\ \ \dot{U}_t=\left(\partial\tilde{S}(U_t,t)\right)U_t\;\;{\scriptstyle \text{{\small flow ODE}}}\ \ \,
$$

Laplacian

$$
\quad \bullet \quad \log \det \mathcal{F}_*(V)=\int_0^T \mathcal{L}_o \tilde{S}(U_t,t)dt \quad \text{with} \quad \mathcal{L}_0=-\sum_{x,\mu,a}\partial_{x,\mu}^a \partial_{x,\mu}^a
$$

Summing up on Continuous Flows

$$
\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}}\int \mathrm{D}[U_0] \, \mathcal{O}(U_T) \, \exp(-S_0(U_0)) \\ \underbrace{S_0(U_0)}_\text{Base} = \underbrace{S(U_T)}_\text{Target} - \int_0^T \mathcal{L}_0 \, \tilde{S}(U_t,t) dt_\text{Flow} \\ \underbrace{\sum_{\text{Plow}}^\text{Elow}}_\text{action} \nonumber
$$

$$
\bullet \quad S_0(U_0)={\rm const.}/S'(U_0)/.\ . \ . \quad \text{training condition}
$$

$$
\bullet \quad \tilde{S}(U_t,t)=\textstyle\sum_i c_i(t)W_i(U_t) \text{ \ \textsf{trainable action with} \ } c_i(t) \text{ \textsf{free parameters} }
$$

 $\bullet\quad \mathcal{L}_0\tilde{S}(U_t,t)$ is always an action-like term, e.g. $\mathcal{L}_0W_0=\frac{16}{3}W_0$ (but more complicated for loops with repeated links)

Part 2: Building on Lüscher's idea

How to find $c_i(t)$?

Perturbative approach around $\beta=0$ \qquad Machine Learning approach

[arXiv:0907.5491](https://arxiv.org/abs/0907.5491)

Trivializing maps, the Wilson flow and the HMC algorithm

Martin Lüscher

CERN, Physics Department, 1211 Geneva 23, Switzerland

arXiv:[2212.08469](https://arxiv.org/abs/2212.08469)

Learning Trivializing Gradient Flows for Lattice Gauge Theories

Simone Bacchio.¹ Pan Kessel.^{2, 3} Stefan Schaefer.⁴ and Lorenz Vaitl² ¹ Computation-based Science and Technology Research Center, The Cyprus Institute, Nicosia, Cyprus ² Machine Learning Group, Technische Universität Berlin, Berlin, Germany ³BIFOLD-Berlin Institute for the Foundations of Learning and Data, Berlin, Germany ⁴ John von Neumann-Institut für Computing NIC. Deutsches Elektronen-Synchrotron DESY, Germany (Dated: December 19, 2022)

or with CNN $c_i\left(t, {\vec W}_t(x)\right)$ [M. Gerdes et al., <u>arXiv:2410.13161</u>]

Lüscher's t-expansion

$$
\begin{aligned} \tilde{S}(U_t,t) & = \sum_i c_i(t) W_i(U_t) \\ & = \sum_k t^k \tilde{S}^{(k)}(U_t) = \sum_k t^k \sum_i c_i^{(k)} W_i(U_t) \end{aligned} \bigg\} \quad c_i(t) = \sum_k c_i^{(k)} t^k
$$

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

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

Lüscher's t-expansion - Wilson action

Terms appearing in the Next-to-Leading order,

Machine Learning approach

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

- $\vec{\theta}$ 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

$$
\frac{\frac{d}{d\tilde{\theta}}\left(S(U_T)-S_0(U_0)-\int_0^T\mathcal{L}_0\tilde{S}(U_t,t)dt\right)}{\mathcal{C}{\it{ost\,function}}}
$$

Gradient of the cost function

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

$$
\frac{dU_t}{d\theta_i} = Y_t^{(i)}U_t \quad \xrightarrow{\hspace{2cm}} \frac{d}{d\theta_i} S(U_t) = \left(\partial S(U_t), Y_t^{(i)} \right)
$$

Coefficients' ODE Algebra's scalar product

 \bullet **ISSUE:** we have as many fields $\ Y^{(i)}_t$ 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

 \bullet We use the adjoint state method to remove any dependence on $\,Y^{(i)}_t\,$ See [\[2212.08469\]](https://arxiv.org/abs/2212.08469) for details.

$$
\lambda_T = \partial S(U_T) \longrightarrow_{\text{Sov}} \text{The adjoint state is defined at time } T,
$$
\n
$$
\lambda_T = \partial S(U_T) \longrightarrow_{\text{Sov}} \text{The adjoint state is defined at time } T,
$$
\n
$$
\lambda_T = \partial S(U_T) \longrightarrow_{\text{Sov}} \text{The adjoint state is defined at time } T,
$$

Part 3: Numerical Results

2 Dimensional SU(3) Yang-Mills Theory

arXiv:[2212.08469](https://arxiv.org/abs/2212.08469)

Learning Trivializing Gradient Flows for Lattice Gauge Theories

Simone Bacchio.¹ Pan Kessel.^{2, 3} Stefan Schaefer.⁴ and Lorenz Vaitl²

 1 Computation-based Science and Technology Research Center, The Cyprus Institute, Nicosia, Cyprus ² Machine Learning Group, Technische Universität Berlin, Berlin, Germany 3 BIFOLD—Berlin Institute for the Foundations of Learning and Data, Berlin, Germany ⁴ John von Neumann-Institut für Computing NIC. Deutsches Elektronen-Synchrotron DESY, Germany (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](https://arxiv.org/abs/2212.08469)

[\[arXiv:2410.13161](https://arxiv.org/abs/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 16² lattice.

Part 4: Towards 4D results

4 Dimensional SU(3) Yang-Mills Theory

Target problem

Moving away from toy models, a good target problem is

- **β=6.0 →** 0.093 fm lattice spacing [\[1009.5228](https://arxiv.org/abs/1009.5228)]
- \bullet **16⁴ lattice** \rightarrow 1.5 fm lattice size
- Long autocorrelation already visible in the smeared Q

For the base distribution then we can consider

- Ideally, $uniform \rightarrow most probably impossible$
- Realistically, $\beta = 5.7$ + double lattice spacing
- Practically, ...

Flowing in β

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

$$
\textit{Gradient}\qquad S_{\tau}(U_{\tau})=S(U)-\int_{\tau}^{1}\mathrm{d}t\,\mathcal{L}_0\tilde{S}(U_t,t)\;\;\left\{\begin{array}{c}\dot{U}_t=-\partial \tilde{S}_t\,U_t\\\ U\equiv U_1\end{array}\right.
$$

Desired base action

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

\n
$$
\tau = 1
$$
 Target action
\n
$$
S = -\frac{\beta}{6} W_0
$$

\n
$$
S = -\frac{\beta}{6} W_0
$$

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

\nWilson action

Flowing in β

$$
\begin{aligned} S_{\tau}(U_{\tau}) &= S(U) - \int_{\tau}^{1} \mathrm{d}t \, \mathcal{L}_{0} \tilde{S}(U_{t},t) \, \begin{array}{l} \left\{ \begin{array}{l} \dot{U}_{t} &= -\partial \tilde{S}_{t} \, U_{t} \\ \ & U \equiv U_{1} \end{array} \right. \\ \\ \left. \frac{\partial S_{\tau}}{\partial \tau} - \left(\partial S_{\tau}, \partial \tilde{S}_{\tau} \right) &= \mathcal{L}_{0} \, \tilde{S}_{\tau} \, \sum_{\mathcal{S}^{\tau} = \tau S} S_{\tau} \\ \\ \text{\tiny Wilson action} \,\, S &= -\frac{\beta}{6} W_{0} \, \end{array} \right. \\ \left. \mathcal{L}_{0} \, \tilde{S}_{\tau} - \frac{\tau \beta}{6} \left(\partial W_{0}, \partial \tilde{S}_{\tau} \right) + \frac{\beta}{6} W_{0} \, = \, \mathrm{const}. \end{aligned} \right. \end{aligned}
$$

Flowing in β

$$
\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathrm{D}[U] \, \mathcal{O}(U) \, \exp(-S_\beta(U)) \, = \frac{1}{\mathcal{Z}} \int \mathrm{D}[V] \, \mathcal{O}(U) \, \exp(-S_{\beta_0}(V))
$$
\n
$$
\mathcal{V}_{\mathcal{A} \mathcal{C} \mathcal{G} \mathcal{C} \mathcal{F}} \quad S_\beta(U) - S_{\beta_0}(V) - \int_{\beta_0/\beta}^1 \mathrm{d}t \, \mathcal{L}_0 \, \tilde{S}(U_t, t) = \mathrm{const.}
$$

$$
\mathcal{G} \textsf{olution} \qquad \mathcal{L}_0 \tilde{S}_t - \tfrac{t \beta}{6} \big(\partial W_0 , \partial \tilde{S}_t \big) + \tfrac{\beta}{6} W_0 = \text{const.} \\ \tilde{S}(U_t,t) = \tfrac{\beta}{6} \sum_{k=0}^\infty \left(\tfrac{t \beta}{6} \right)^k \tilde{S}^{(k)}(U_t) \quad \left\{ \begin{array}{l} \tilde{S}^{(0)} = - \mathcal{L}_0^{-1} W_0 = - \tfrac{3}{16} W_0 \\ \tilde{S}^{(k)} = \mathcal{L}_0^{-1} \left(\partial W_0 , \partial \tilde{S}^{(k-1)} \right) \end{array} \right.
$$

Convergence of the flow action

$$
\tilde{S}(U_t,t) = \frac{\beta}{6} \sum_{k=0}^{\infty} \left(\frac{t\beta}{6}\right)^k \tilde{S}^{(k)}(U_t)
$$
\n• $t \leq 1$ *l l* <

 $N(1)$, $N(0)$, $N(1)$, $N(0)$,

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:

$$
\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int D[U] \, \mathcal{O}(U) \, \exp(-S(U))
$$
\n
$$
\frac{d\langle \mathcal{O} \rangle}{d\theta} = \langle \frac{\partial \mathcal{O}}{\partial \theta} - \mathcal{O} \frac{\partial S}{\partial \theta} \rangle + \langle \mathcal{O} \rangle \langle \frac{\partial S}{\partial \theta} \rangle
$$
\n
$$
\text{Value contribution} \quad \text{See contribution} \quad \text{(usually connected)} \quad \text{(disconnected)}
$$

The novel approach for computing gradients

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

$$
\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}_{d\theta}} \int \mathrm{D}[U_{d\theta}] \, \mathcal{O}(U) \, \exp(-S_{d\theta}(U_{d\theta}))
$$
\n
$$
S_{d\theta}(U_{d\theta}) = S(U) - \int_0^{d\theta} \mathcal{L}_0 \, \tilde{S}(U_t, t) dt
$$
\n
$$
S_{d\theta}(U_{d\theta}) - S(U) = d\theta \, \frac{\partial S}{\partial \theta} + d\theta \, (\partial S, \partial \tilde{S})
$$
\n
$$
\int_0^{d\theta} \mathcal{L}_0 \, \tilde{S}(U_t, t) dt = d\theta \, \mathcal{L}_0 \, \tilde{S} + \text{const.}
$$
\n
$$
\mathcal{L}_0 \tilde{S} + (\partial S, \partial \tilde{S}) + \frac{\partial S}{\partial \theta} = \text{const.}
$$
\n
$$
\text{New loss function}
$$

Theorem and Corollaries

The generic formula, demonstrated in the paper, is

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

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

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

Corollary A: "The new approach" **Corollary B:** "The standard approach"

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

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

Opportunity? Calculation of gradients!

$$
\mathcal{L}_0 \tilde{S} + \left(\partial S, \partial \tilde{S} \right) + \tfrac{\partial S}{\partial \theta} = \text{const.} \quad \text{A new loss function for ML approaches}
$$

Applications:

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

Approach:

- Any ML tools developed for LQCD. This is not a flow anymore, only one S is needed!
- Generic analytic solution: Can be used as initial guess Critical for convergence

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 λ needs to be introduced
- We have an analytics solution that can be used as initial quess 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](https://arxiv.org/abs/2212.08469)

Learning Trivializing Gradient Flows for Lattice Gauge Theories

Simone Bacchio.¹ Pan Kessel.^{2, 3} Stefan Schaefer.⁴ and Lorenz Vaitl²

¹ Computation-based Science and Technology Research Center, The Cyprus Institute, Nicosia, Cyprus ² Machine Learning Group, Technische Universität Berlin, Berlin, Germany ³BIFOLD—Berlin Institute for the Foundations of Learning and Data, Berlin, Germany ⁴ John von Neumann-Institut für Computing NIC. Deutsches Elektronen-Synchrotron DESY, Germany (Dated: December 19, 2022)

First application of Continuous Normalizing Flows to Lattice Gauge Theories

[arXiv:2305.07932](https://arxiv.org/abs/2305.07932)

Realistic application of Machine Learning in Lattice QCD

A novel approach for computing gradients of physical observables

 $Simone$ Bacchio¹

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