Path gradient estimators for CNFs in Lattice Gauge Theory

Lorenz Vaitl, Simone Bacchio, Pan Kessel, Shinichi Nakajima, Kim Nicoli, Stefan Schaefer



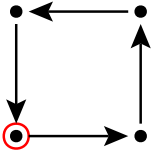



Problem setting

- 4D Yang-Mills Theory:

$$S = \frac{\beta}{3} \sum_{\mu,\nu<\mu,x} Re\mathrm{Tr}\left(I - P(x,\mu,\nu)\right)$$

  - $P(x,\mu,\nu)$: plaquette
  - β: inverse coupling
  - $P(x,\mu,\nu) \in SU(3)$
- Normalizing Flows
  - deep generative model
  - promise embarassingly parallel sampling
  - typically trained with self-sampling



$P(\circ, 1, 2)$

Normalizing Flows

- Diffeomorphism $\mathcal{T}_\theta : \mathcal{Z} \to \mathcal{X}$ from base density $p_0(U_0)$ to approximate target density $p(U)$:

$$q_\theta(U) = p_0(\mathcal{T}_\theta^{-1}(U)) \left| \det \frac{\partial \mathcal{T}_\theta^{-1}(U)}{\partial U} \right|$$

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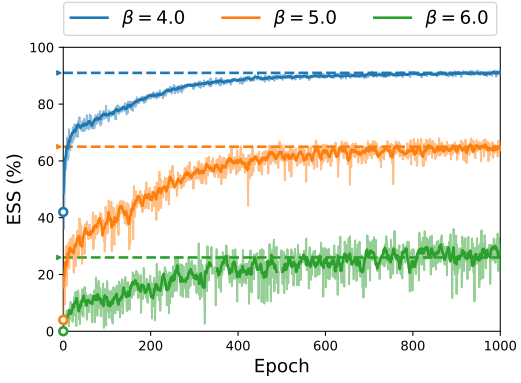
- Can be implemented via ODE (i.e. Continuous Normalizing Flow):

$$\mathcal{T}_\theta(U_0) = U_0 + \int_0^T \mathrm{d}t\, \dot{U}(U_t, t, \theta)$$

$$\left| \det \frac{\partial \mathcal{T}_\theta^{-1}(U)}{\partial U} \right| = \int_0^T \mathrm{tr} \left(\frac{\partial \dot{U}(U_t, t, \theta)}{\partial U_t} \right) \mathrm{d}t$$

Continuous Normalizing Flows

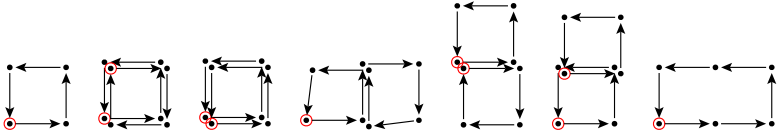
- Easy to incorporate symmetries [Köhler et al., 2020]
- Lüscher proposed continuous flow for LGT with parametrization by perturbative expansion [Lüscher, 2010]
- In recent work [Bacchio et al., 2023] we proposed optimizing the Lüscher's model with gradient descent



2D problem, $L = 16$

Lüscher's approach

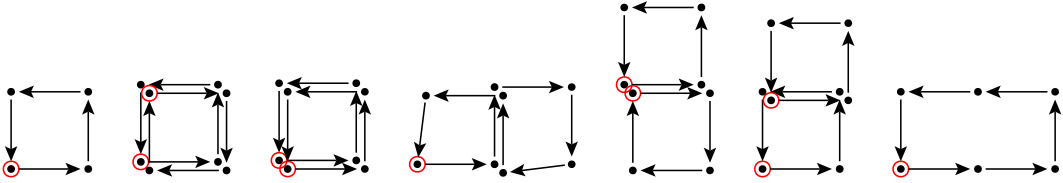
- Define $\dot{U}(U_t, t, \theta) = \partial\tilde{S}(U_t, t) \cdot U_t$, where $\partial\tilde{S}(U_t, t)$ is force of generic action
  - $\tilde{S}$ is scalar & invariant
    - Force equivariant and is element of Lie algebra $\mathfrak{su}(N)$
    - generic ODE for lattice gauge theory
  - $\tilde{S} = \Sigma_i c_i(t) W_i(U_t)$
    - W_i are traces of Wilson loops
    - $c_i(t)$ are time dependent coefficients parametrized by θ
- Lüscher found $W_i \& c_i(t)$ by a perturbative expansion around $t = 0$



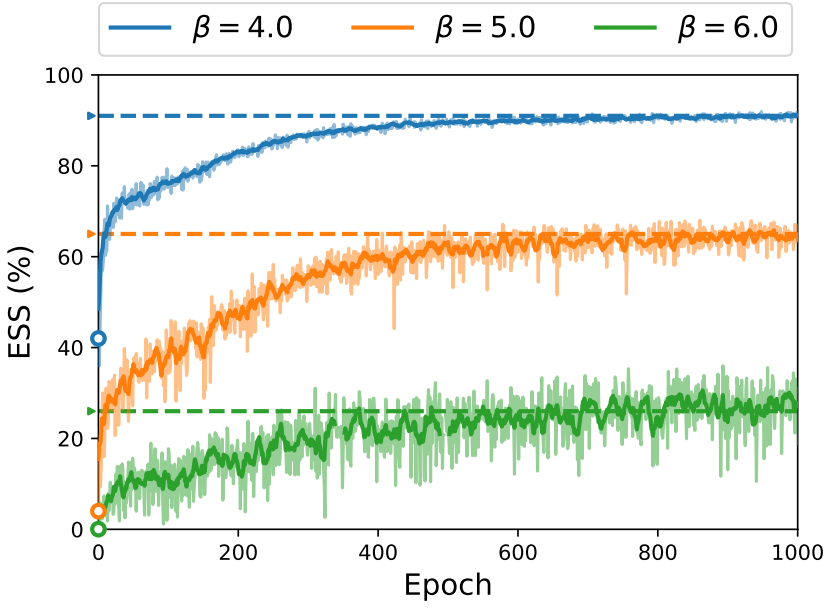
Training Trivializing Maps

- We proposed optimizing θ by minimizing the $\mathrm{KL}(q_\theta|p) \overset{c}{=} \mathbb{E}_{q_\theta(U_T)}\left[\ln q_\theta(U_T) + S(U_T)\right]$
  - Derived adjoint-state method for adjoint state $\in \mathfrak{su}(N)$
  - Implemented CG3 ODE solver, more complex functions for $c_i(t)$
  - Used **path gradients** for low variance gradient estimators

$\Rightarrow$ Expressive model with **few** parameters (14: linear $c_i(t)$ for each Wilson loop W_i)



2D SU(3)
Yang-Mills
Theory, $L = 16$



Path Gradient Estimators

- Low variance [Roeder et al., 2017]
  - efficiently computed with a modified adjoint method [Vaitl et al., 2022b]
- Reverse KL

$$KL(q_\theta|p) = \mathbb{E}_{U_T \sim q_\theta(U_T)} \left[\ln \frac{q_\theta(U_T)}{p(U_T)} \right] = \mathbb{E}_{U_0 \sim p_0} \left[\ln \frac{q_\theta(T_\theta(U_0))}{p(T_\theta(U_0))} \right]$$

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$$\frac{d}{d\theta} KL(q_\theta|p) = \mathbb{E}_{U_0 \sim p_0} \left[\frac{\partial}{\partial T_\theta(U_0)} \left(\ln \frac{q_\theta(T_\theta(U_0))}{p(T_\theta(U_0))} \right) \frac{\partial T_\theta(U_0)}{\partial \theta} + \frac{\partial \ln q_\theta(U_T)}{\partial \theta} \Big|_{U_T = T_\theta(U_0)} \right]$$

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- Path Gradient / Sticking-the-Landing

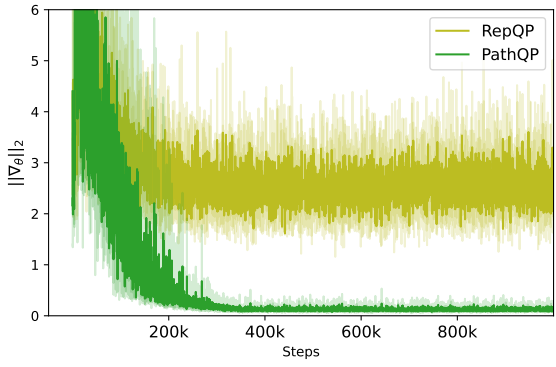
$$\frac{d}{d\theta} KL(q_\theta|p) = \mathbb{E}_{U_0 \sim p_0} \left[\frac{\partial}{\partial T_\theta(U_0)} \left(\ln \frac{q_\theta(T_\theta(U_0))}{p(T_\theta(U_0))} \right) \frac{\partial T_\theta(U_0)}{\partial \theta} + \cancel{\frac{\partial \ln q_\theta(U_T)}{\partial \theta}} \Big|_{U_T = T_\theta(U_0)} \right]$$

[Roeder et al., 2017]

- Path Gradient

$$\frac{d}{d\theta} KL(q_\theta|p) = \mathbb{E}_{U_0 \sim p_0}\left[\frac{\partial}{\partial T_\theta(U_0)} \left(\ln \frac{q_\theta(T_\theta(U_0))}{p(T_\theta(U_0))} \right) \frac{\partial T_\theta(U_0)}{\partial \theta} + \cancel{\frac{\partial \ln q_\theta(U_T)}{\partial \theta}}\Big|_{U_T = T_\theta(U_0)} \right]$$

Favourable behavior seen in many contexts e.g.
[Roeder et al., 2017, Tucker et al., 2019, Agrawal et al., 2020, Vaitl et al., 2022a]



Score term as control variate

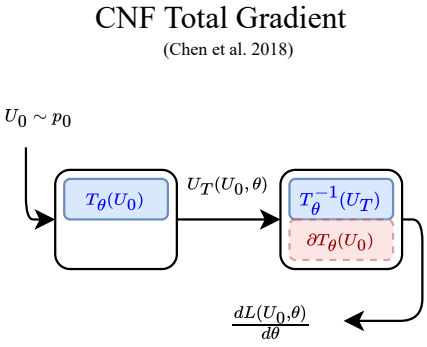
- Path gradients can be seen as akin to using the score term $\mathcal{G}_{\text{score}}$ as a control variate with a constant factor of 1

$$\underbrace{\frac{\partial \left(\ln \frac{q_\theta(T_\theta(U_0))}{p(T_\theta(U_0))} \right)}{\partial T_\theta(U_0)} \frac{\partial T_\theta(U_0)}{\partial \theta}}_{\mathcal{G}_{\text{path}}} = \underbrace{\frac{d}{d\theta} \ln \frac{q_\theta(T_\theta(U_0))}{p(T_\theta(U_0))}}_{\mathcal{G}_{\text{total}}} - 1 \cdot \underbrace{\frac{\partial \ln q_\theta(U_T)}{\partial \theta}\Big|_{U_T = T_\theta(U_0)}}_{\mathcal{G}_{\text{score}}}$$

- Remarks:
  - Empirically we did not see an improvement when estimating cv factor
  - Can also be interpreted as double reparametrization [Tucker et al., 2019]
  - The variance of the score term $\mathcal{G}_{\text{score}}$ is the Fisher Information $\mathcal{I}(\theta)$ divided by the batch-size
  - Path gradients work on a per sample basis

Adjoint state method CNF

- Gradients in standard neural ODEs computed using adjoint state method



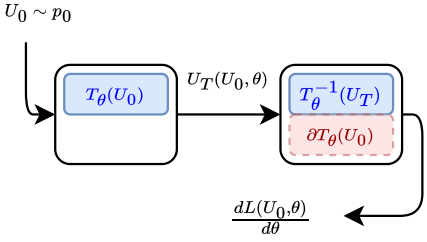
Adjoint state method CNF

- Gradients in standard neural ODEs computed using adjoint state method

$$U_T = U_0 + \int_0^T \dot{U}(U_t, t, \theta)dt \quad \Big\} \quad T_\theta(U_0)$$

CNF Total Gradient

(Chen et al. 2018)



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$$
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\begin{aligned}
U_T &= U_0 + \int_0^T \dot{U}(U_t, t, \theta) dt
\end{aligned}
\right\} \quad T_\theta(U_0)
$$

$$
\left.
\begin{aligned}
\lambda(T) &= \frac{\partial \ln p(U_T)}{\partial U_T} \\
\dot{\lambda}(t) &= -\lambda(t) \frac{\partial \dot{U}(U_t, t, \theta)}{\partial U_t} \\
\frac{dL}{d\theta} &= -\int_T^0 \lambda(t) \frac{\partial \dot{U}(U_t, t, \theta)}{\partial \theta} \\
&\quad -\partial_\theta \mathrm{tr} \left(\frac{\partial \dot{U}(U_t, t, \theta)}{\partial U_t} \right) dt
\end{aligned}
\right\} \quad \partial T_\theta(U_0)
$$

CNF Total Gradient

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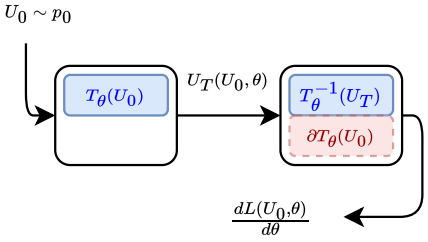
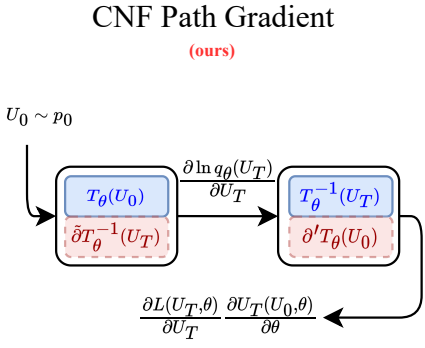


Modified adjoint state method [Vaitl et al., 2022b]



Modified adjoint state method [Vaitl et al., 2022b]

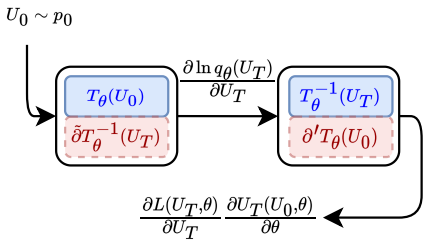
$$\tilde{\lambda}(0) = \partial_{U_0} \ln p_0(U_0)$$

$$\dot{\tilde{\lambda}}(t) = -\tilde{\lambda}(t) \frac{\partial \dot{U}(U_t, t, \theta)}{\partial U_t} - \partial_{U_t} \mathrm{tr} \left(\frac{\partial \dot{U}(U_t, t, \theta)}{\partial U_t} \right)$$

$$\Big\} \; \tilde{\partial} T_\theta^{-1}(U_T)$$

CNF Path Gradient

(ours)



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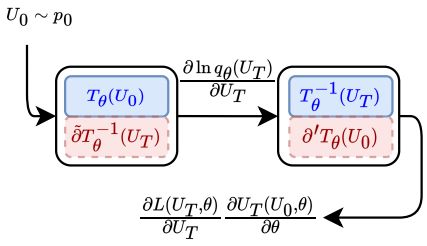
&\quad -\partial_{U_t} \mathrm{tr} \left(\frac{\partial \dot{U}(U_t, t, \theta)}{\partial U_t} \right)
\end{aligned}\right\} \tilde{\partial} T_\theta^{-1}(U_T)$$

$$\left.\begin{aligned}
\lambda'(T) &= \frac{\partial \ln q_\theta(U_T) - \ln p(U_T)}{\partial U_T} \\
\dot{\lambda}'(t) &= -\lambda'(t) \frac{\partial \dot{U}(U_t, t, \theta)}{\partial U_t} \\
\frac{\partial L}{\partial U_T} \frac{\partial U_T}{\partial \theta} &= -\int_T^0 \lambda'(t) \frac{\partial \dot{U}(U_t, t, \theta)}{\partial \theta} dt
\end{aligned}\right\} \partial' T_\theta(U_0)$$

CNF Path Gradient

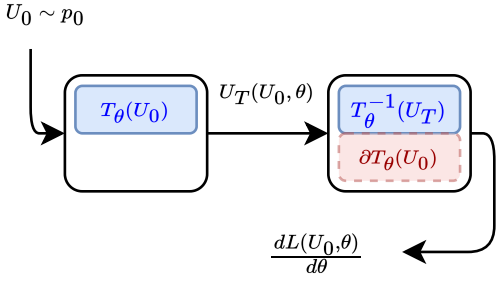
(ours)



Path gradients for CNFs

CNF Total Gradient

(Chen et al. 2018)



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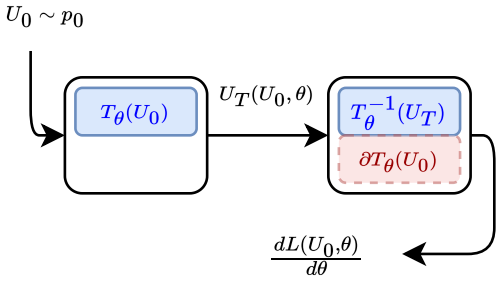

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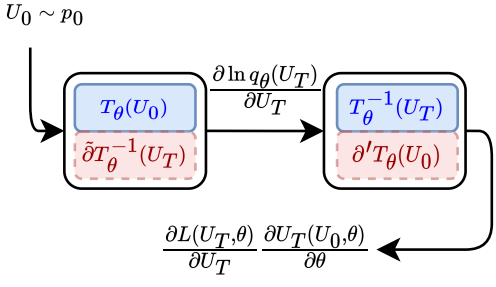

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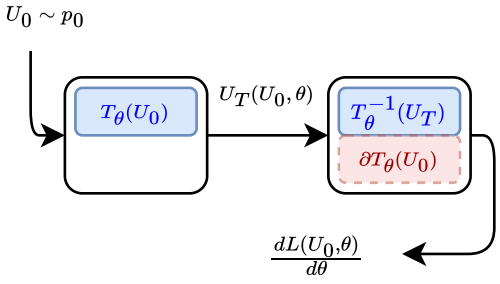

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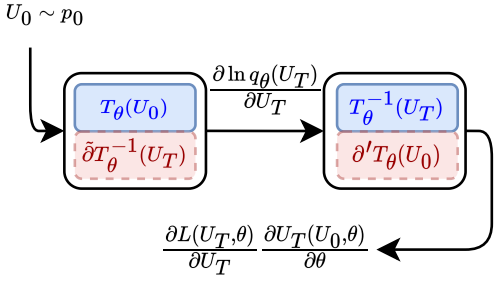
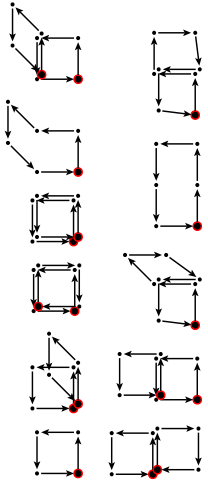


- Same memory requirements, 33% runtime increase per iteration

Results Trivializing Map in 4D

Training

- 4D SU(3) Yang-Mills Theory
- 11 Wilson loops
- Target $\beta \in \{1, 2, 3, 4\}$
  - $c_i(t)$ cubic splines with 2,5,7,10 knots
  - 5,10,15,20 ODE steps
- Lattice size 8, base-density uniform
- Batch-size 1, Adam, learning-rate 10^{-4}, trained on 1 A100
  - Trained on Juwels-Booster

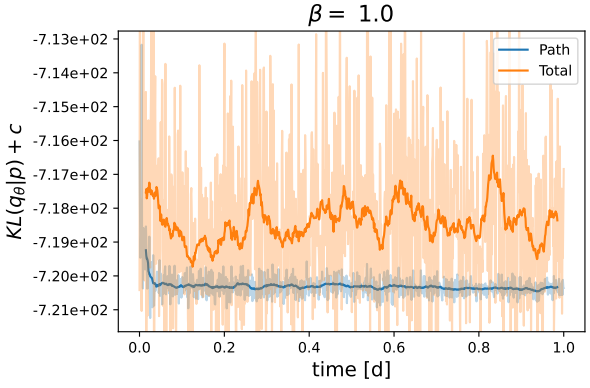


Results in 4D LGT

Effective Sampling Ratio

Estimated on 1k samples

β	Path	Total	days trained
1	96.6 %	13.7 %	1



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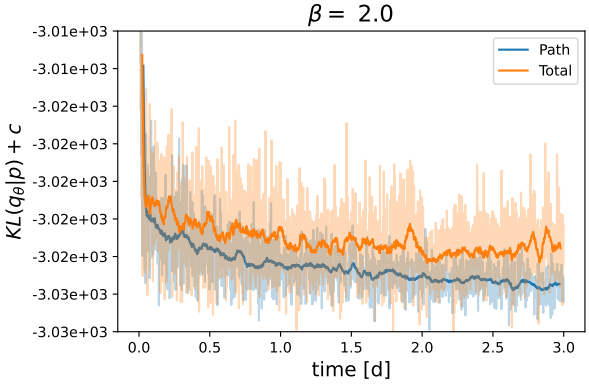

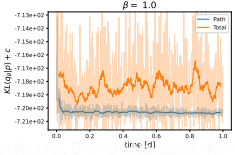

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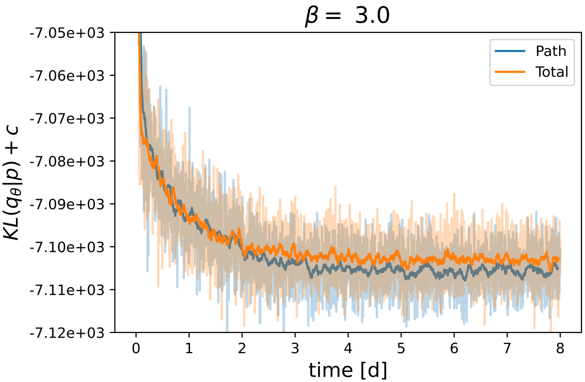
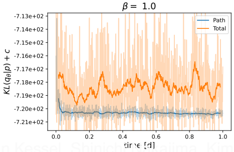
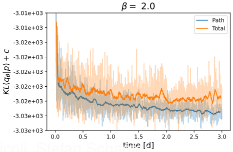
3	00.8 %	00.4 %	8







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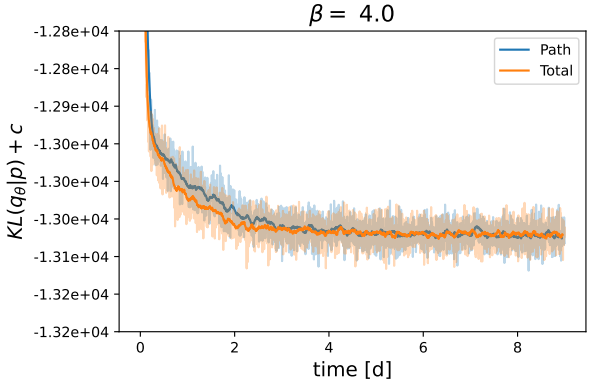
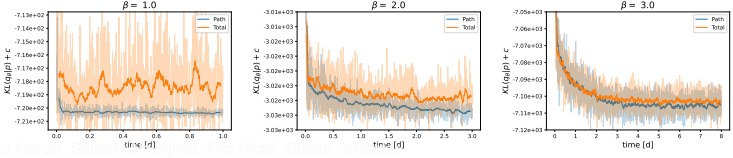
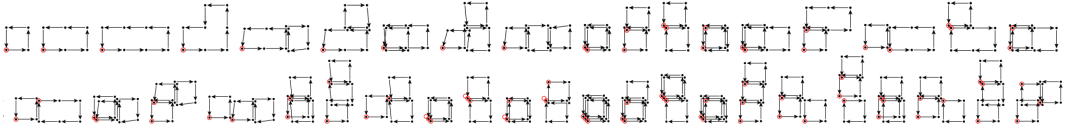




Summary

- Path gradients help training
- As is, the proposed CNF is not able to scale up to interesting β and lattice size
  - Possible to make flow more complex (e.g. NNLO basis), but drastic increase in runtime
  - Problem becomes exponentially more complex with increasing target β and lattice size



Thank you for your attention

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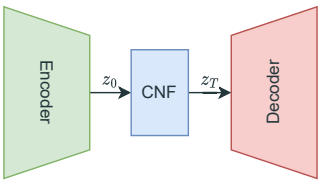
Results VAE



ELBO	Path	Total
MNIST	**82.09** $\pm$ .04	82.82 $\pm$ .01
Omniglot	**96.61** $\pm$ .17	98.33 $\pm$ .09
Caltech Silhouettes	**101.93** $\pm$ .63	104.03 $\pm$ .43
Frey Faces	**4.35** $\pm$ .00	4.39 $\pm$ .01

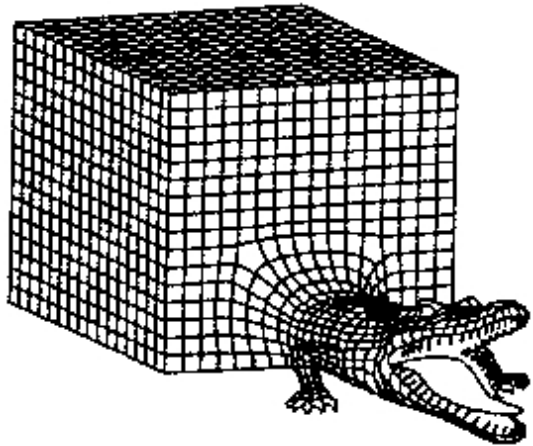
Lattice Field Theory:

- Target

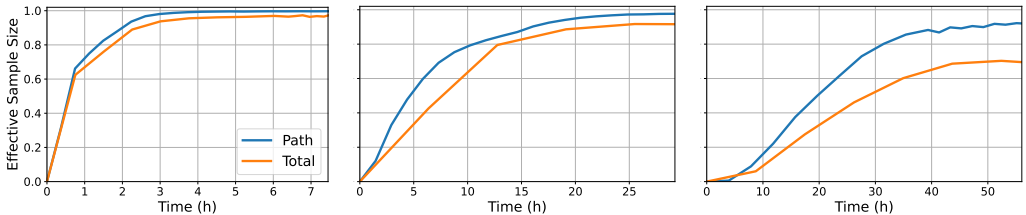
$$p(x) = \frac{1}{Z} e^{-S(x)}$$

  - Intractable
  - Known in closed form

- Can be approximated by CNF with inductive biases
  [de Haan et al., 2021]

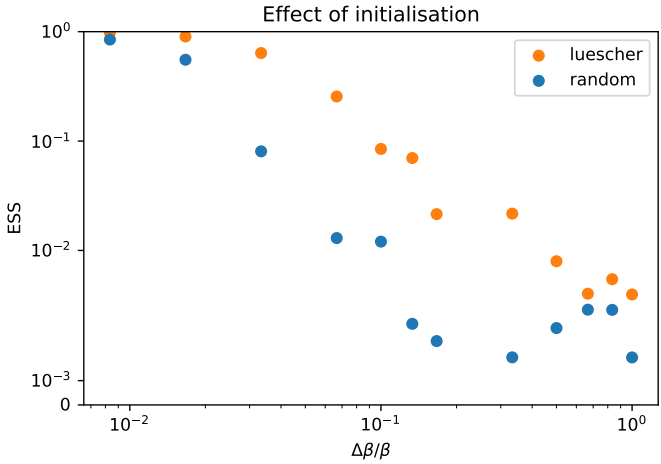


Lattice size	Path	Total
12x12	**99.66**$\% \pm 0.07$	$98.01\% \pm 0.44$
20x20	**97.65**$\% \pm 0.14$	$91.56\% \pm 1.13$
32x32	**91.81**$\% \pm 1.32$	$69.53\% \pm 5.59$



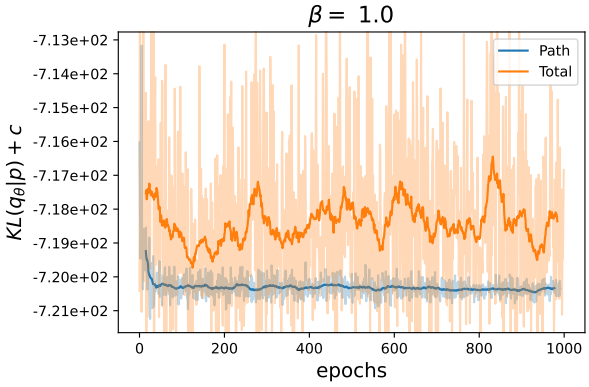
Training from non-trivial distribution

- 2D lattice, $L = 32$, target $\beta = 6$
- 1k epochs, batchsize 512



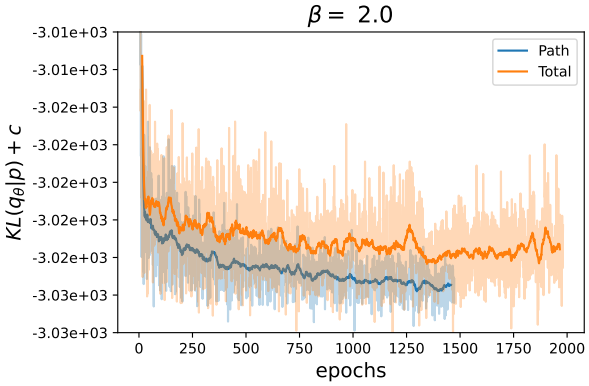
Results in 4D LGT

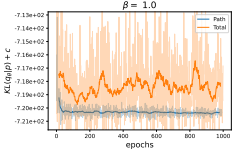
β	Path	Total	days trained
1	96.6 %	13.7 %	1



Results in 4D LGT

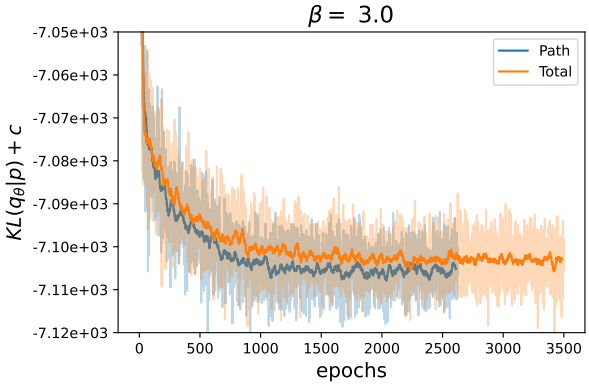
β	Path	Total	days trained
1	96.6 %	13.7 %	1
2	40.1 %	16.7 %	2

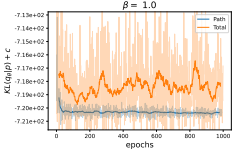


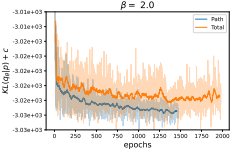


Results in 4D LGT

β	Path	Total	days trained
1	96.6 %	13.7 %	1
2	40.1 %	16.7 %	2
3	00.8 %	00.4 %	8

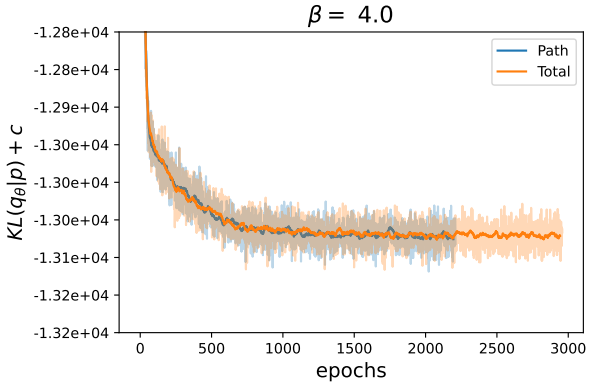


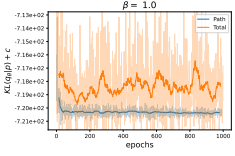


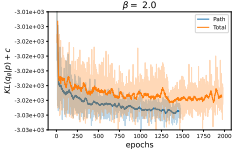


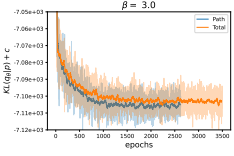
Results in 4D LGT

β	Path	Total	days trained
1	96.6 %	13.7 %	1
2	40.1 %	16.7 %	2
3	00.8 %	00.4 %	8
4	00.2 %	00.1 %	9









Acceptance rate, 4D LGT

Acceptance rate

Estimated on 1k samples

β	Path	Total	days trained
1	91 %	28 %	1
2	49 %	25 %	3
3	1 %	1 %	8
4	0 %	0 %	9

2D coefficients