Progress in Normalizing Flows for 4d Gauge Theories

Ryan Abbott

MIT

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Collaborators

Universität Bern
AEC Albert Einstein Center for Fundamental Physics

Massachusetts Institute of Technology


P. Shanahan

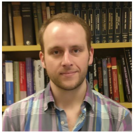

D. Boyda


R. Abbott


J. Urban


F. Romero-López

Fermilab

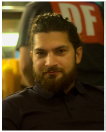

D. Hackett

DeepMind


S. Racanière


D. Rezende


A. Razavi


A. Botev


A. Matthews

Universität Bern
AEC Albert Einstein Center for Fundamental Physics

The University of Edinburgh

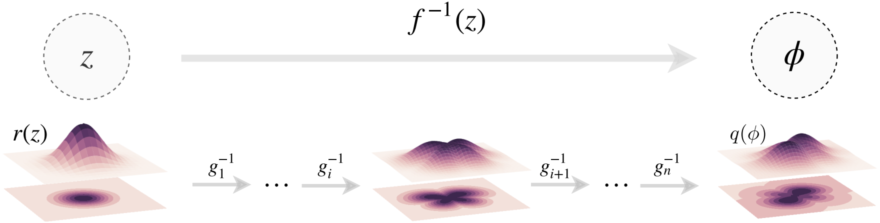

G. Kanwar

New York University

VE RI TAS
Harvard


M. Albergo

Normalizing flows



[Albergo et al., 1904.12072]

- Learned change of variables f maps density $r(z)$

$$q(\phi) = |\det J_f(f(\phi))| r(f(\phi))$$

- $r(z), f^{-1}(z), |\det J_f(z)|$ tractable $\implies$ $q(\phi)$ tractable
- Given (known) target $p(\phi)$, train f so $q \approx p$
  - Can apply corrections for exact/unbiased sampling

Normalizing flows & QCD

- Modern effort began w/ scalar fields [Albergo et al., 1904.12072]
- Required significant effort to get to QCD
  - Working with $\mathrm{U}(1)$ & SU(3), gauge symmetry, pseudofermions, ...
- Have tools for QCD [Abbott et al., 2208.03832]
- Outline today
  - Novel applications past accelerated sampling
  - More recent work on improving models
  - Scaling on Aurora (supercomputer)

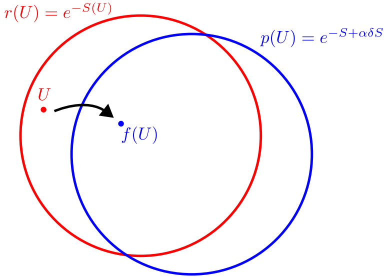
Novel Applications of Flows

[Abbott et al., 2401.10874]

- If $f \approx$ identity (can force), then $f(U)$ and U are correlated
  - $\implies$ correlated differences, improved uncertainties
- Derivatives w/r/t action params
  $S \mapsto S + \alpha\delta S$

$$\frac{d\left\langle \mathcal{O}(U)\right\rangle_{\alpha}}{d\alpha} \approx \left\langle \frac{\mathcal{O}(f(U)) - \mathcal{O}(U)}{\Delta\alpha} \right\rangle_{\alpha=0}$$

- E.g. Feyman-Hellman, continuum limit

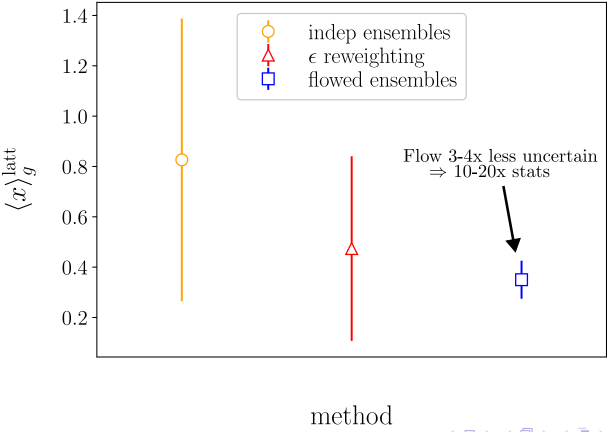


Feynman-Hellman Example

[Abbott et al., 2401.10874]

Gluon momentum fraction (bare):

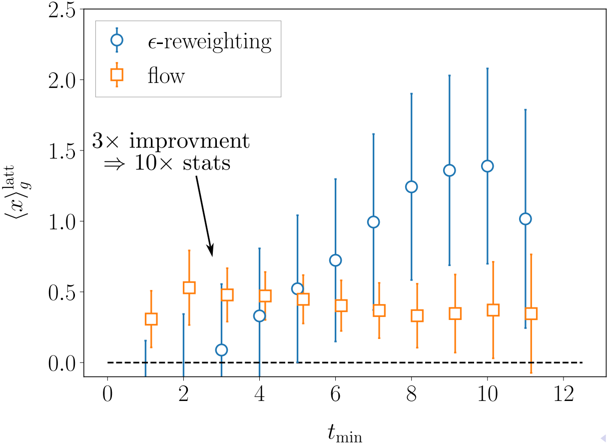
$$\langle x \rangle_g^{\text{latt}} = -\frac{2}{3M_\pi}\frac{dM_\pi}{d\alpha}$$



Dynamical Feynman-Hellman

Gluon momentum fraction (bare):

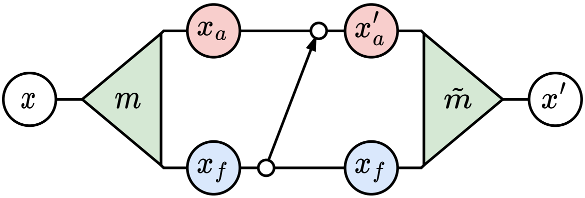
$$\langle x \rangle_g^{\text{latt}} = -\frac{2}{3M_\pi}\frac{dM_\pi}{d\alpha}$$



Twisted mass fermions
$m_\pi \sim 500$ MeV
$L^3 \times T = 12^3 \times 24$
$a = 0.1$ fm

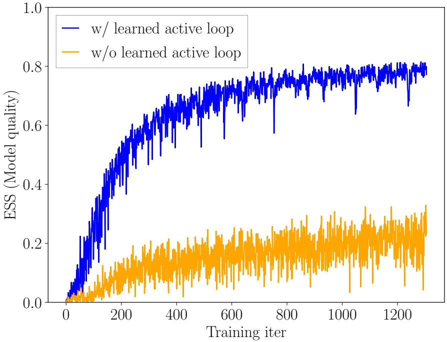
Model improvements

- Two main architectures: spectral & residual
  - See [Abbott et al, 2305.02402]
- Many improvements to both
  - Diagonal features, learned active loops, initialization, ...
  - General theme: more gauge equivariant information
    - E.g. convolutions → parallel transport

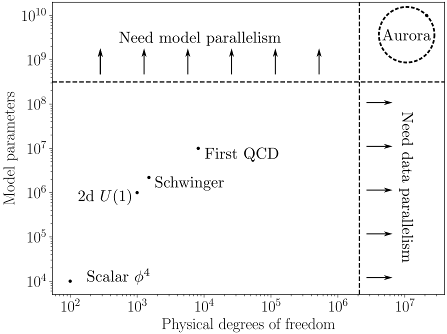


Learned active loops

- Need to choose "active loop" per gauge link
  - Usually plaquette, 2×1 loop
- Idea: use learned linear combination of possible loops
  - Constructed w/ neural net, similar to gauge-equivariant networks [Favoni et al., 2012.12901]
- Small test on 4^4 lattice, $\beta = 2$, 4d SU(3):



Scaling On Aurora



- Aurora is an exascale machine at Argonne
- Significant software effort
  - Porting/checking code on Intel GPUs ✓
  - Distributing model + fields over multiple GPUs ✓
    - Note: training is very memory intensive
  - Model scaling to $O(10,000)$ GPUs – ongoing

Scaling on Aurora (continued)

- Significantly larger models, $\sim 10^9$–10^{10} parameters
  - Current models $\sim 10^6$–10^7 parameters
- Target: dynamical QCD, moderate size lattices
- Note: scaling ML models is highly nonintuitive, context-dependent
  - See [Abbott et al., 2211.07541] for a full discussion

GPT-1 (117 million parameters)
Lattice QCD is on and in the bag's not mine, "ben said. he was lying on the couch, . . .

GPT 3.5 ($\sim$ 175 billion parameters)
Lattice QCD is a numerical approach used in theoretical physics to study the strong interaction between quarks and gluons, which are the fundamental constituents of protons, neutrons, and other hadrons.

Conclusions

- Novel applications of flows (ab)using correlations
- Learned active loops among many improvements for 4d SU(3) flows
- Upcoming/ongoing scaling on Aurora

Conclusions

- Novel applications of flows (ab)using correlations
- Learned active loops among many improvements for 4d SU(3) flows
- Upcoming/ongoing scaling on Aurora
- Thanks! Questions?

Massachusetts Institute of Technology

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Backup

Comments on Scaling

- Reference: [Abbott et al., 2211.07541]
- Scaling depends strongly every aspect of the model
  - E.g. use of flow, architecture choices, training choices
  - Makes extrapolating beyond any particular choice difficult

Use of Flow

- Direct Sampling (Independence Metropolis)
- HMC on trivialized distribution [Lüscher 0907.5491]
- Generalize proposal distribution [Foreman et al., 2112.01582]
- Subdomain updates [Finkenrath, 2201.02216]
- Stochastic Normalizing Flows [Wu et al. 2002.0670]
- CRAFT [Matthews et al. 2201.13117]

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Architecture Choices

- Choice of coupling layers (spectral, residual, continuous)
- Choice of Neural networks (CNN, fully-connected, gauge-equivariant)
  - Gauge-equivariant networks [Favoni et al., 2012.12901]
- Choice of invariant context passed to networks
- Size of model (# layers, NN sizes)

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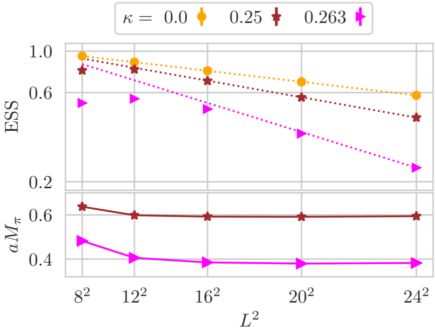
Training Choices

- Optimizer (Adam, SGD, higher-order optimizers)
- Choice of Loss (reverse/forward KL, MSE, ...)
- Computation of gradients (path gradients/control variates)
- Hyperparameter choices (batch size, learning rate)
  - Hyperparameter scheduling
- Volume chosen for training

Exponential Volume Scaling

- For $L/\xi \gg 1$, $\xi =$ correlation length, direct volume transfer
$$ESS(V) = ESS(V_0)^{V/V_0}$$
- Prevents *direct sampling* in thermodynamic limit $L/\xi \to \infty$
  - Does not apply to continuum limit $L/\xi \sim m_\pi L$ fixed, $\xi/a \to \infty$
  - Typically $4 \lesssim m_\pi L \lesssim 10 \implies$ no in principle issue



Spectral Flows

Goal: $h(\Omega X \Omega^\dagger) = \Omega h(X) \Omega^\dagger$

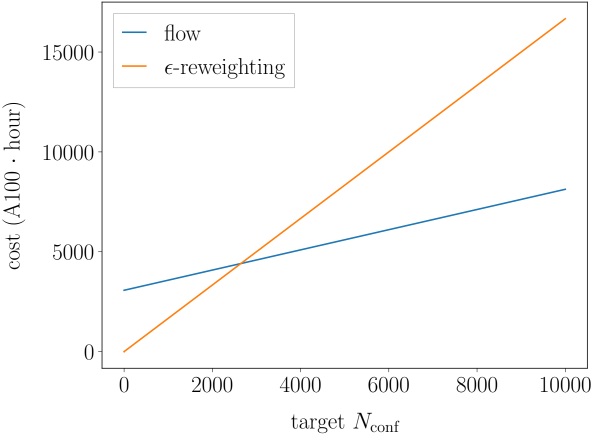
- Conjugation invariant data $\Leftrightarrow$ eigenvalues
- Diagonalize $X \in \mathrm{SU}(N)$ via eigenbasis V:

$$X = V \begin{pmatrix} e^{i\theta_1} & & \\ & \ddots & \\ & & e^{i\theta_N} \end{pmatrix} V^\dagger \mapsto V \begin{pmatrix} e^{i\theta'_1} & & \\ & \ddots & \\ & & e^{i\theta'_N} \end{pmatrix} V^\dagger$$

- Define $h : \mathrm{SU}(N) \to \mathrm{SU}(N)$ by action on $\{\theta_1, \ldots, \theta_N\}$
  - Need to be careful about order $\Rightarrow$ choose canonical order
  - Note: θ_k not independent, $\prod_k e^{i\theta_k} = \det X = 1 \Rightarrow$ remove θ_N

Dynamical Feynman Hellman - Costs

Caveat: flow code is not heavily optimized



Unbiased sampling

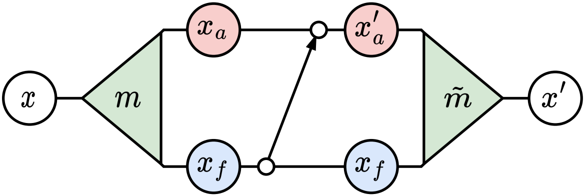
- Independence Metropolis: accept $\phi \to \phi' \sim q(\phi')$ with probability

$$P_{\text{accept}}(\phi \to \phi') = \min\left(1, \frac{p(\phi')}{p(\phi)} \frac{q(\phi)}{q(\phi')}\right)$$

- Hybrid methods
  - Alternate HMC/flow updates
  - HMC on trivialized distribution [Lüscher 0907.5491]
  - Subdomain updates [Finkenrath, 2201.02216]
  - CRAFT/Annealed Importance Sampling [Matthews et al. 2201.13117]
  - ...

SU(N)-Equivariant Flows

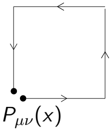
- Two types here
  - Spectral flows - transform untraced plaquettes
    - Reference: [Boyda et al., 2008.05456]
  - Residual flows - parametrized Wilson flow/stout smearing step
    - Reference: [Abbott et al., 2304.XXXXX] (to appear)
- Both based on active/frozen split



Spectral Flows

[Boyda et al., 2008.05456]

- Transform untraced plaquette $P_{\mu\nu}$
- Under gauge transformation $\Omega(x) \in \mathrm{SU}(N)$



$$(\Omega \cdot P)_{\mu\nu}(x) = \Omega(x) P_{\mu\nu}(x) \Omega(x)^\dagger$$

- Given $h : \mathrm{SU}(N) \to \mathrm{SU}(N)$, transform U_μ so $P_{\mu\nu} \mapsto h(P_{\mu\nu})$

$$f(U_\mu) = h(P_{\mu\nu}) P_{\mu\nu}^\dagger U_\mu$$

- Gauge equivariance $\iff$ *conjugation equivariance*:

$$h(\Omega P \Omega^\dagger) = \Omega h(P) \Omega^\dagger$$

- Achieve by transforming eigenvalues for fixed eigenvectors

Residual Flows

- Inspired by Lüscher's trivializing map [Lüscher 0907.5491]
- Transform active links via

$$U_\mu(x) \mapsto e^{\overbrace{i\epsilon\partial_{x,\mu}}^{\text{Lie-algebra-valued derivative}}\phi(U)} U_\mu(x)$$

- Gauge-invariant "potential" $\phi(U)$
  - Example: $\phi(U) \propto S_{\text{Wilson}}(U) \implies$ Wilson flow/stout smearing
  - More complex:

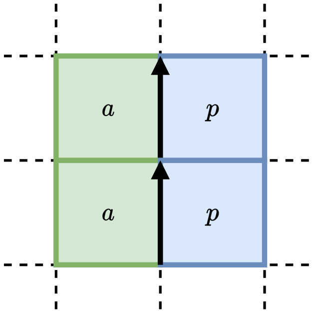
$$\phi(U) = \sum_x \sum_{\mu \neq \nu} c_{\mu\nu}(x; U_{\text{frozen}}) \mathrm{Re}\,\mathrm{Tr}(P_{\mu\nu})$$

- Small but finite ϵ for invertibility ($\epsilon \lesssim 1/8$)

Spectral vs Residual Flows

Spectral flows

- Transform plaquettes
- Limited by passive plaquettes



Residual flows

- Update links
- Denser active mask
- Limited by step size
- Harder to invert
    - Require fixed-point iteration

Continuous Flows

[Bacchio et al. 2212.08469]

- Continuous time
- Unmasked
- Requires ODE integration

Fermions

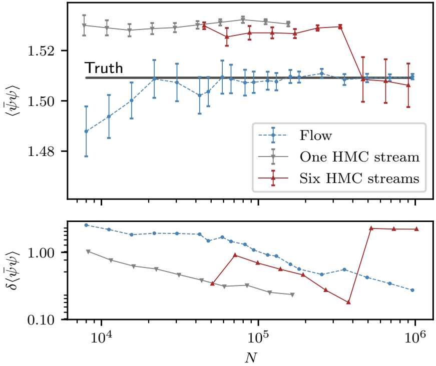
Fermion target:

$$p(U) \propto e^{-S_G[U]} \det M[U]$$

Methods:

- Compute $\det M$ directly
  - Simple, but not scalable
- Estimate $\det M$
  - E.g. pseudofermions

Schwinger model at criticality



[Albergo et al. 2202.11712]

Autoregressive Pseudofermion modeling

Target Distributions:

- Marginal:

$$p_m(U) = e^{-S_G(U)} \det M[U]$$

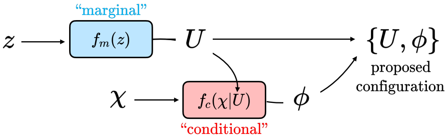
- Conditional:

$$p_c(\phi \mid U) \propto \frac{1}{\det M[U]} e^{-\phi^\dagger M^{-1} \phi}$$

- Joint:

$$\begin{aligned} p_{\text{joint}}(U,\phi) &= p_c(\phi \mid U) p_m(U) \\ &= e^{-S_G(U) - \phi^\dagger M^{-1}\phi} \end{aligned}$$

Models:



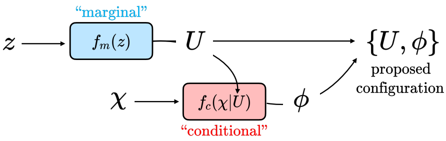
Prior:

- Gauge $z \sim$ Haar, heatbath, ...
- Pseudofermion $\chi \sim e^{-\chi^\dagger \chi}$

[Albergo et al., 2106.05934]
[Abbott et al., 2207.0945]

Conditional Model (2 Flavor Theory)

[Albergo et al., 2106.05934]
[Abbott et al., arxiv:2207.0945]



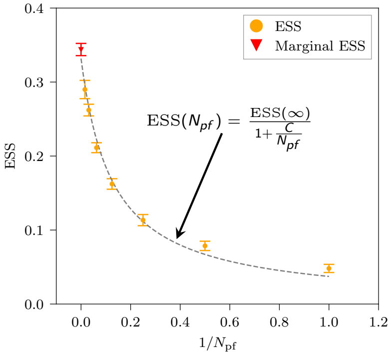
- Prior $\chi \sim e^{-\chi^\dagger \chi}$
- Target $\phi \sim \frac{1}{\det(DD^\dagger)} e^{-\phi^\dagger (DD^\dagger)^{-1} \phi}$
- *Optimal* model: $\phi = f_c(\chi \mid U) = D[U]\chi$
  - But $\det J = \det DD^\dagger$ not tractable
- Estimate optimal model with tractable (gauge-equivariant) layers

$$\phi_a(x) \mapsto A[U](x)\phi_a(x) + B[U](x,y)\phi_f(y)$$
$$\phi_f(x) \mapsto \phi_f(x)$$

- $A[U], B[U]$: (learned) linear operators

Improving Pseudofermion Models

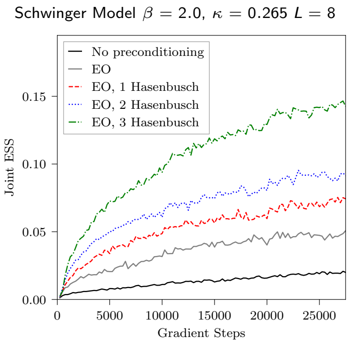
- More pseudofermion draws
    - Improve for fixed model



(ESS $\sim$ acceptance rate)

- Even/Odd preconditioning
- Hasenbusch factorization

$$\det(M) = \frac{\det(M)}{\det(M+\mu)} \det(M+\mu)$$



Future work

- Gauge equivariant flows
  - Currently: Spectral, Residual, Continuous
  - More work needed – particularly on SU(N)
- Fermions
  - Exact determinant works, but not scalable
  - Currently: pseudofermion models
- Scaling – in progress at Aurora
- Hybrid methods – large space to explore
- Beyond sampling
  - Mapping between different actions
  - Contour deformation [Detmold et al., 2101.12668] [Pawlowski+Urban, 2203.01243] [Lawrence et al., 2205.12303]

Training Marginal Models

- Stochastic derivative estimate:

$$\begin{aligned}\nabla \log \det M &= \operatorname{Tr} \nabla \log M \\ &= \operatorname{Tr}\left[M^{-1}\nabla M\right] \\ &= \mathbb{E}_{\chi \sim e^{-\chi^\dagger \chi}}\left[\chi^\dagger M^{-1} \nabla M \chi\right]\end{aligned}$$

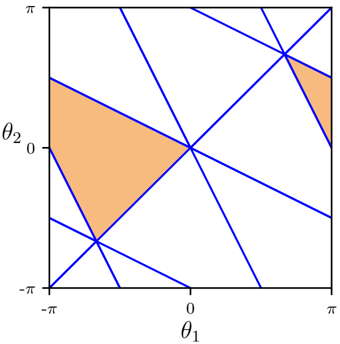
- Requires 1 inversion/sample $\chi^\dagger M^{-1}$
- Does not give access to density

Spectral Flows (continued)

Goal: Permutation equivariant flow

- Perform *maximal torus flow* on $\{\theta_i\}$
- Choose (arbitrary) canonical cell
- Use order of eigenvalues
  - Canonicalization $\sim$ sorting
- In canonical cell: use standard methods
  - e.g. rational quadratic spline

SU(3) example:



Parallel Transport Convolution Networks

Normal Convolution:

$$\phi(x) \mapsto \sum_{\delta} c_\delta \phi(x+\delta)$$

Parallel transport convolution:

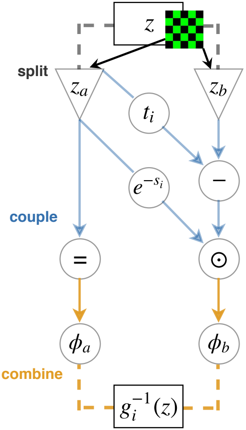
$$PTCL[\phi](x) = \sum_{\delta} c_\delta \overbrace{W(x, x+\delta)}^{\text{Wilson line}}\phi(x+\delta)$$

$$\phi_a(x) \mapsto A[U](x)\phi_a(x) + B[U](x,y)\phi_f(y)$$
$$\phi_f(x) \mapsto \phi_f(x)$$

$$B[U](x,y)\phi_f(y) = PTCL[PTCL[\dots PTCL[\phi]]]$$

Example: Scalar Field Theory

[Dinh et al, 1605.08803] [Albergo e al., 1904.12072]



- Fields $\phi(x) \in \mathbb{R}$, target $p(\phi) \propto e^{-S(\phi)}$
- Split $z \to z_a, z_f$ active/frozen
  - Typically: even/odd checkerboard

Arbitrary functions

$$\phi_f = z_f$$
$$\phi_a = e^{s(z_f)} \odot z_a + t(z_f)$$

- Inverse:

$$z_f = \phi_f$$
$$z_a = e^{-s(\phi_f)} \odot (\phi_a - t(\phi_f))$$

- Tractable Jacobian: $\det J = \prod_i e^{s(\phi_f)_i}$
- Compose alternating transforms $(\phi_a, \phi_f) \leftrightarrow (\phi_f, \phi_a)$

Reverse KL Training

- Model density $q(\phi)$, target $p(\phi) = \frac{1}{Z} e^{-S(\phi)}$
- Reverse Kullback Leibler (KL) loss $\mathcal{L}$:

$$\begin{aligned}\mathcal{L} &= D_{KL}(q||p) \\ &= \int \mathrm{d}\phi \, q(\phi) \log \frac{q(\phi)}{p(\phi)} \\ &= \mathbb{E}_{\phi \sim q} \left[\log q(\phi) + S(\phi)\right] + \log Z\end{aligned}$$

Model samples

Constant
($\Rightarrow$ can ignore)

Key facts

$D_{KL}(q||p) \geq 0$
$D_{KL}(q||p) = 0 \Leftrightarrow q = p$

Symmetries and Sampling

Gauge transformation

- Gauge symmetry $\implies p(\Omega \cdot U) = p(U)$
- Model gauge invariance: $q(\Omega \cdot U) = q(U)$
- Achieve with 2 conditions:
  - Prior gauge invariance: $r(\Omega \cdot U) = r(U)$
  - Gauge Equivariance: $f(\Omega \cdot U) = \Omega \cdot f(U)$