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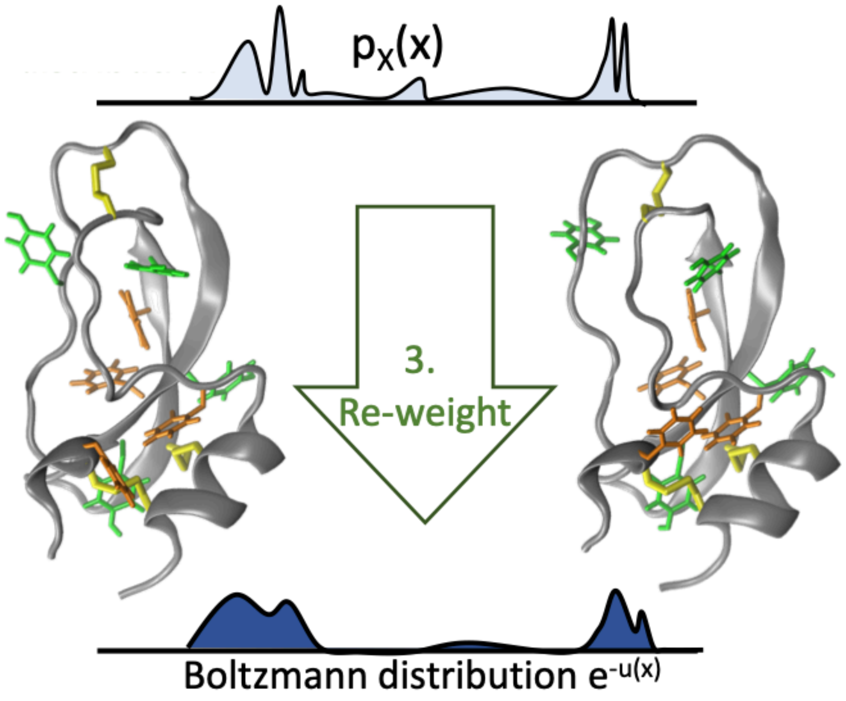
Normalizing Flows for importance sampling in lattice computations

Kim A. Nicoli

TRA Matter, HISKP, Bethe Center, LAMARR

Talk based on PRD 108, 114501 (2023) and prior works PRL 126, 032001 (2021), PRE 101, 023304 (2020)

F. Noé, et al., Science, eaaw1147 (2019)



(Image credits: F. Noé, et al., Science, eaaw1147 (2019))

Generative AI for Physics : Past, Present and Future

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Scalar Field Theories (ϕ^4)

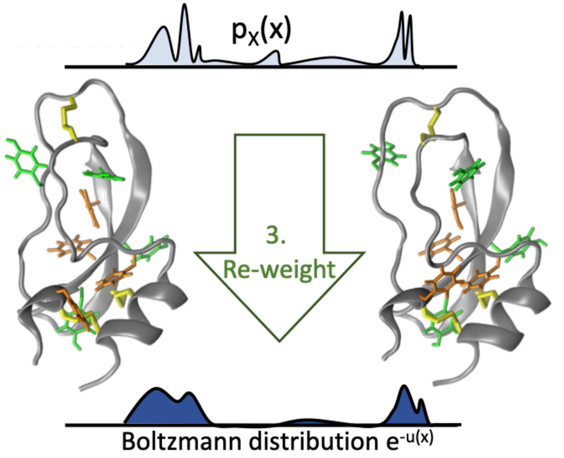
- M. S. Albergo, et al., Phys. Rev. D 100, 034515 (2019)
- K. A. Nicoli, et al., Phys. Rev. Lett. 126, 032001 (2021)
- P. deHaan, et al., arXiv: 2110.02673 @ ML4Pys workshop (2021)
- L. Vaitl et al., arXiv: 2206.09016 @ ICML (2022)
- A. Matthews et al., arXiv:2201.13117 @ ICML (2022)
- M. Caselle, et al., J. High Energ. Phys. 2022, 15 (2022)
- M. Gerdes, et al., SciPost Phys. 15, 238 (2023)
- A. Singha, et al., Phys. Rev. D 107, 014512 (2023)

Lattice Gauge Theories ($U(1), SU(N)$)

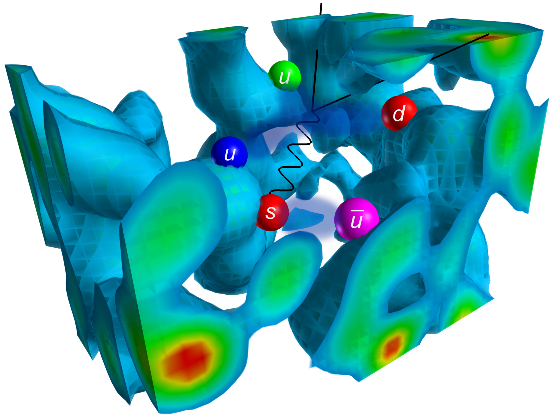
- G. Kanwar, et al., Phys. Rev. Lett. 125, 121601 (2020)
- S. Bacchio, et al., Phys. Rev. D 107, L051504 (2023)
- R. Abbott et al., Phys. Rev. D 106, 074506 (2022)
- M. S. Albergo, et al., Phys. Rev. D 106, 014514 (2022)
- R. Abbott, et al., arXiv:2305.02402 (2023)
- J. Finkenrath, arXiv: 2201.02216 (2022)

Sampling Multimodal Densities in QFT

- D.C. Hackett et al., arXiv:2107.00734 (2021)
- K. A. Nicoli, et al., arXiv: 2111.11303 @ LATTICE21 (2021)
- K. A. Nicoli, et al., Phys. Rev. D 108, 114501 (2023)
- B. Maté et al., TMLR 2835-8856 (2023)
- V. Kanaujia et al., arXiv:2401.15948 (2024)



(Image credits: F. Noé, et al., Science, eaaw1147 (2019))



(Image credits: Lattice QCD © Derek Leinweber/CSSM/University of Adelaide)

Scaling to Larger Lattices

- L. Del Debbio, et al., Phys. Rev. D 104, 094507 (2021)
- R. Abbott et al., Eur. Phys. J. A 59, 257 (2023)
- A. Faraz et al., arXiv:2308.08615 (2022)
- B. Maté et al., arXiv: 2401.00828 (2024)
- R. Abbott et al., arXiv: 2401.10874v1 (2024)
- J. Finkenrath, arXiv: 2402.12176 (2024)

Autoregressive Models in Stat. Mech.

- D. Wu et al., Phys. Rev. Lett. 122 (8), 080602 (2019)
- K. A. Nicoli, et al., Phys. Rev. E 101 (2), 023304 (2019)
- P. Bialas et al., Computer Physics Communications 281 (2022)
- P. Bialas et al., Phys. Rev. E 107 (1), 015303 (2023)

Interesting Readings

- **F. Noé, et al., Science, eaaw1147 (2019)**
- S. Chen, et al., Phys. Rev. D 107, 056001 (2022)
- B. Maté et al., arXiv: 2210.13772 (2022)
- L. Vaitl et al., MLST 3 (4), 045006 (2022)
- Caselle, M., et al., J. High Energ. Phys. 2024, 48 (2024)
- Cranmer K. et al., Nature Reviews Physics 5 (9), 526-535

And much more...

Preliminaries: LQFT and HMC

$$\langle \mathcal{O} \rangle_p = \int D[\phi]\, \mathcal{O}(\phi)\, p(\phi) \approx \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}(\phi_i)$$

The field configuration $\phi(x)$ is a **random variable** sampled with **MCMC** to estimate computed over a Boltzmann-like density:

$$p(\phi) = \frac{e^{-S(\phi)}}{Z} \longrightarrow Z = \int D[\phi] e^{-S(\phi)}$$

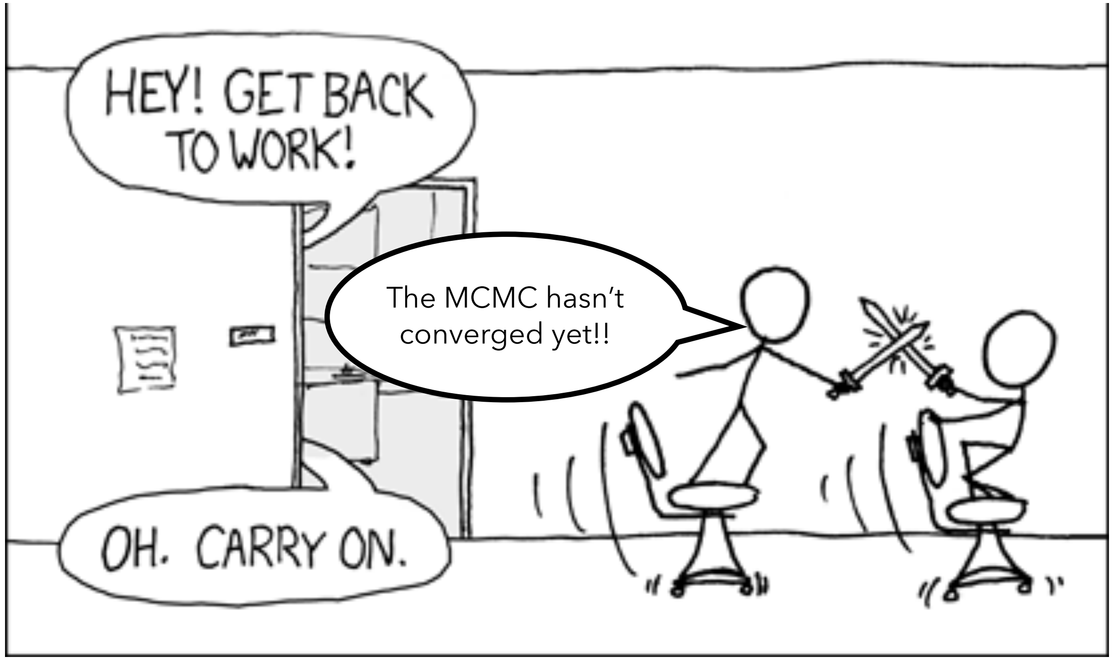
known in **closed form** up to a **numerically intractable** normalisation

HMC and its flaws

MCMC: sequentially proposes new sample and guarantees to eventually converge to a target density.

However MCMC algorithms come at a **cost**:

- 👎 **Sequential** $\Longrightarrow$ MCMC chains can't be parallelized.
- 👎 **Critical slowing down** $\Longrightarrow$ Phase transitions.
- 👎 Long-range autocorrelations $\Longrightarrow$ **large statistical errors.**
- 👎 The partition function Z **is unknown**.
- 👎 No direct estimation of **thermodynamic observables.**



(Adapted from:)

What about flow-based sampling?

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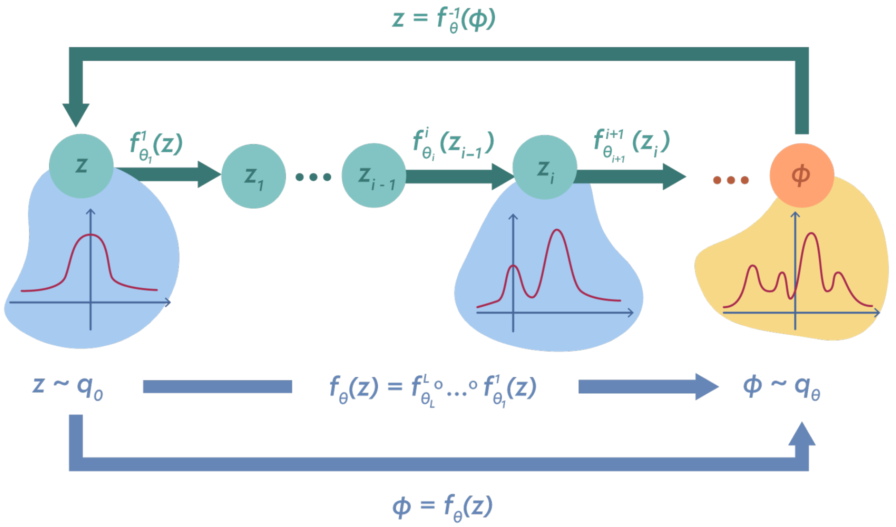
We use a parametric function f_θ (a **diffeomorphism**) to transform Gaussian samples $z \sim q_0$ into physical configurations $\phi \sim q_\theta$

$$f_\theta : \; z \in \mathcal{Z} \sim q_z \to x = f_\theta(z) \in \mathcal{X} \sim q_\theta \, .$$

The parametric function needs to fulfill certain criteria:

- Bijective transformation $\phi = f_\theta(z)$
- Invertible and differentiable
- Tractable Jacobian



What’s flow-based sampling?

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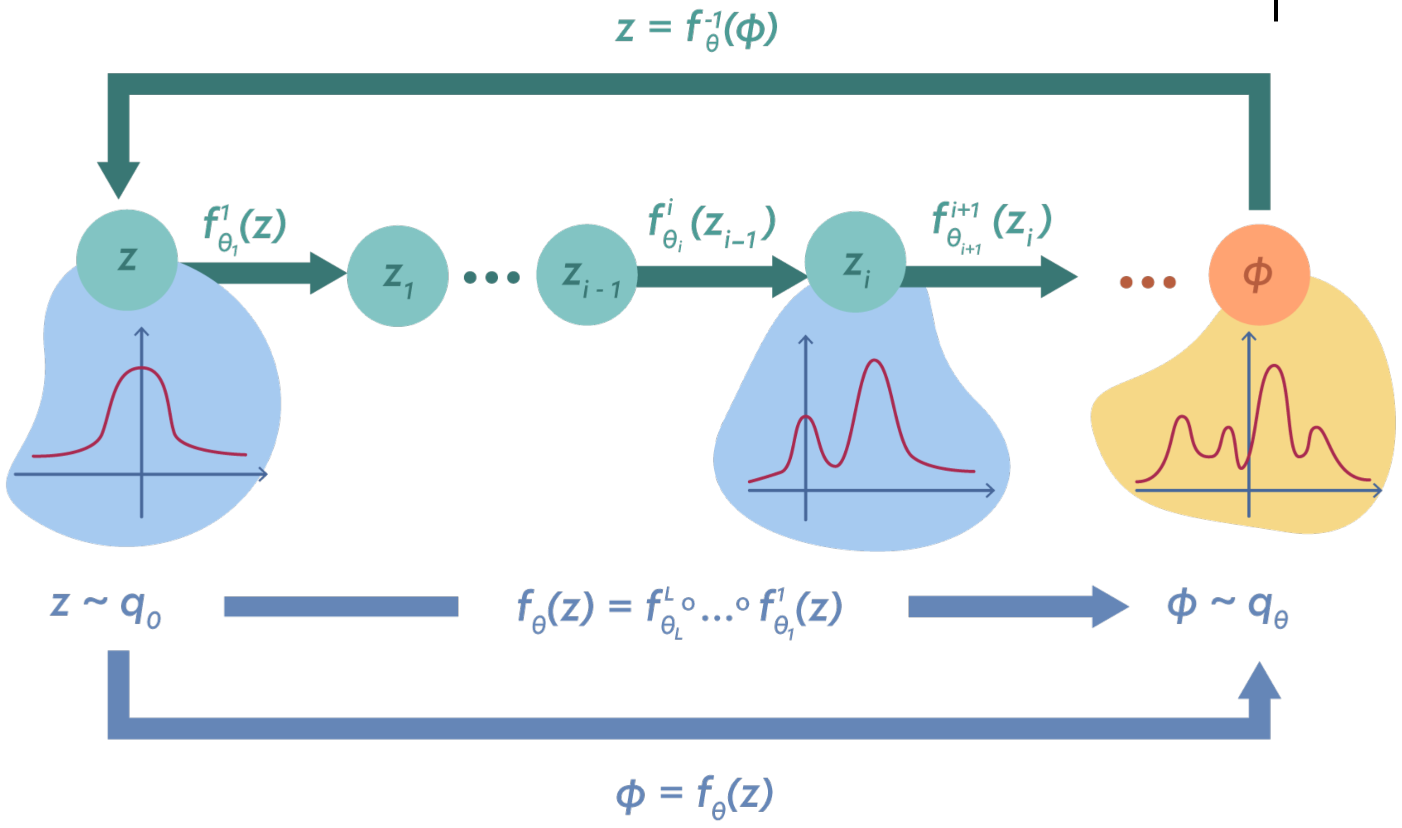
The likelihood of q_θ can be computed exactly: $q_\theta(\phi) = q_0(f_\theta^{-1}(\phi)) \left| \det \left(\frac{\partial f_\theta}{\partial z} \right) \right|^{-1}$



How do we train a generative model?

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Often the variational density q_θ is trained by minimizing the **Reverse-KL** divergence:

$$KL(q_\theta || p) = \int D[\phi] q_\theta(\phi) \ln \frac{q_\theta(\phi)}{p(\phi)} \equiv \mathbb{E}_{q_\theta}\left[\ln \frac{q_\theta(\phi)}{p(\phi)}\right]$$

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since we know the target $p(\phi)$ is a Boltzmann distribution $p(\phi) = Z^{-1} \exp\{-S(\phi)\}$

$$KL(q_\theta || p) = \mathbb{E}_{q_\theta}\left[\ln \frac{q_\theta(\phi)}{p(\phi)}\right] = \mathbb{E}_{q_\theta}\left[\ln q_\theta(\phi) + S(\phi) + \ln Z\right]$$

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since we know the target $p(\phi)$ is a Boltzmann distribution $p(\phi) = Z^{-1} \exp\{-S(\phi)\}$

$$\nabla_\theta KL(q_\theta || p) = \mathbb{E}_{q_\theta}\left[\nabla_\theta \ln q_\theta(\phi) + \nabla_\theta S(\phi) + \cancel{\ln Z}\right]$$

How do we train a generative model?

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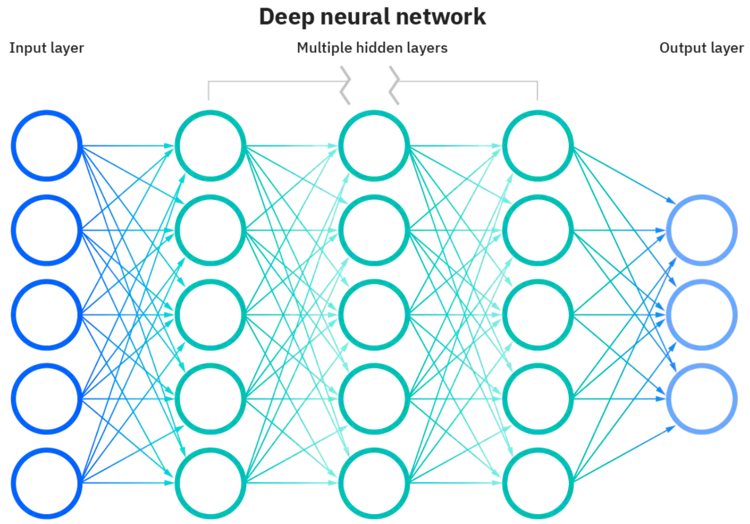
$$\nabla_\theta KL(q_\theta || p) = \mathbb{E}_{q_\theta}\left[\nabla_\theta \ln q_\theta(\phi) + \nabla_\theta S(\phi) + \cancel{\ln Z}\right]$$

Training can be performed **by self-sampling** from the model we are training!

How do we train a generative model?

Sample $\hat{\phi} \sim q_\theta \approx p$

$p(\phi)$



(Image credits: Kavlakoglu, www.ibm.com)

$q_\theta(\phi)$

Minimize the reverse-KL

How do we train a generative model?

$$p(\phi) \overset{?}{=} q_\theta(\phi)$$

🤔

How do we train a generative model?

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$$p(\phi) = q_\theta(\phi)$$

😭

How do we train a generative model?

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$$p(\phi) = q_\theta(\phi)$$

$$p(\phi) \approx q_\theta(\phi)$$

Neural Importance Sampling (NIS)

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$$p(\phi) \approx q_\theta \sim \phi_i \qquad \text{with} \qquad p(\phi) = \frac{\exp\{-S(\phi)\}}{Z}$$

$$Z = \int D[\phi]\, \exp\{-S(\phi)\} = \int D[\phi]\, q_\theta(\phi)\, \tilde{w}(\phi) \quad \text{where} \quad \tilde{w}(\phi) = \frac{\exp\{-S(\phi)\}}{q_\theta(\phi)}$$

Neural Importance Sampling (NIS)

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Neural Importance Sampling (NIS)

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$$Z \overset{\text{MC}}{\approx} \hat{Z} = \frac{1}{N} \sum_{i=1}^{N} \tilde{w}(\phi_i) \qquad \phi_i \sim q_\theta$$

Neural Importance Sampling (NIS)

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$$Z \overset{\text{MC}}{\approx} \hat{Z} = \frac{1}{N} \sum_{i=1}^{N} \tilde{w}(\phi_i) \qquad \phi_i \sim q_\theta \longrightarrow \hat{F} = -T \ln \hat{Z} \; ⚠$$

Nicoli+, Phys. Rev. Lett. (2021)

Asymptotically Unbiased Estimators

$$\langle \mathcal{O} \rangle_p = \langle w \mathcal{O} \rangle_{q_\theta} \overset{\text{MC}}{\approx} \frac{1}{N} \sum_{i=1}^{N} w(\phi_i)\mathcal{O}(\phi_i) \quad \phi_i \sim q_\theta$$

Asymptotically Unbiased Estimators

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$$\langle \mathcal{O} \rangle_p = \langle w \mathcal{O} \rangle_{q_\theta} \overset{\text{MC}}{\approx} \frac{1}{N} \sum_{i=1}^{N} w(\phi_i) \mathcal{O}(\phi_i) \quad \phi_i \sim q_\theta$$

$$w(\phi) = \frac{p(\phi)}{q_\theta(\phi)}$$

Asymptotically Unbiased Estimators

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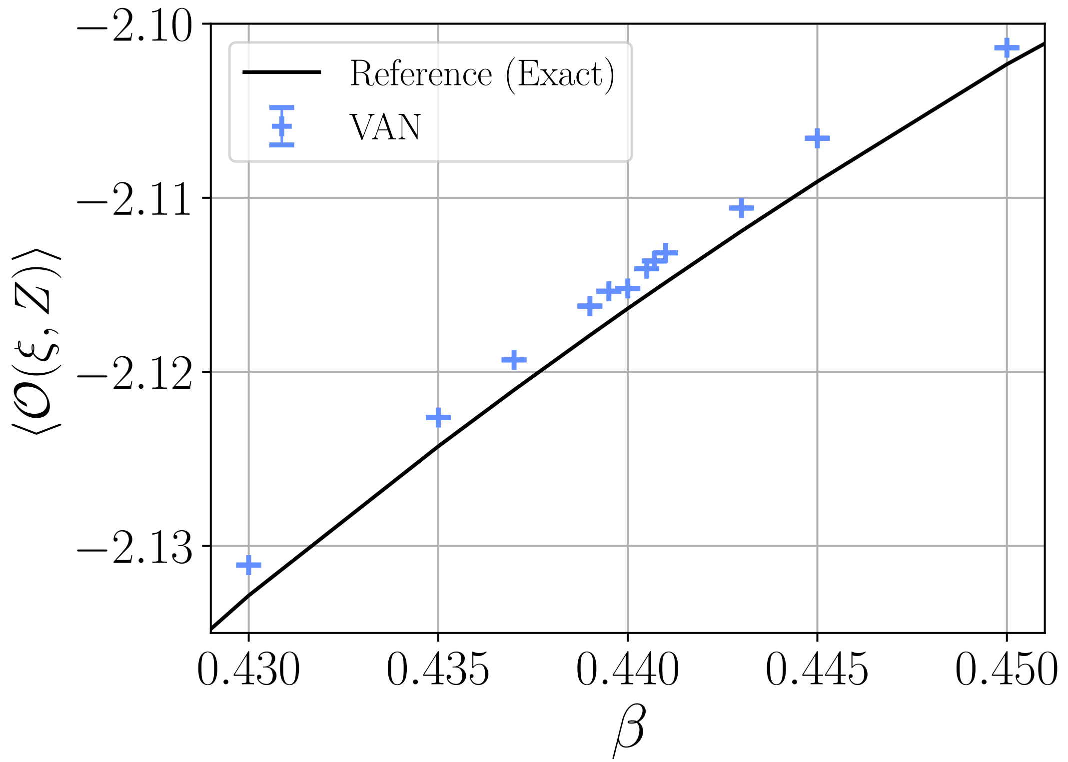
$$\langle \mathcal{O} \rangle_p = \langle w \mathcal{O} \rangle_{q_\theta} \overset{\mathrm{MC}}{\approx} \frac{1}{N} \sum_{i=1}^{N} w(\phi_i) \mathcal{O}(\phi_i) \qquad \phi_i \sim q_\theta$$

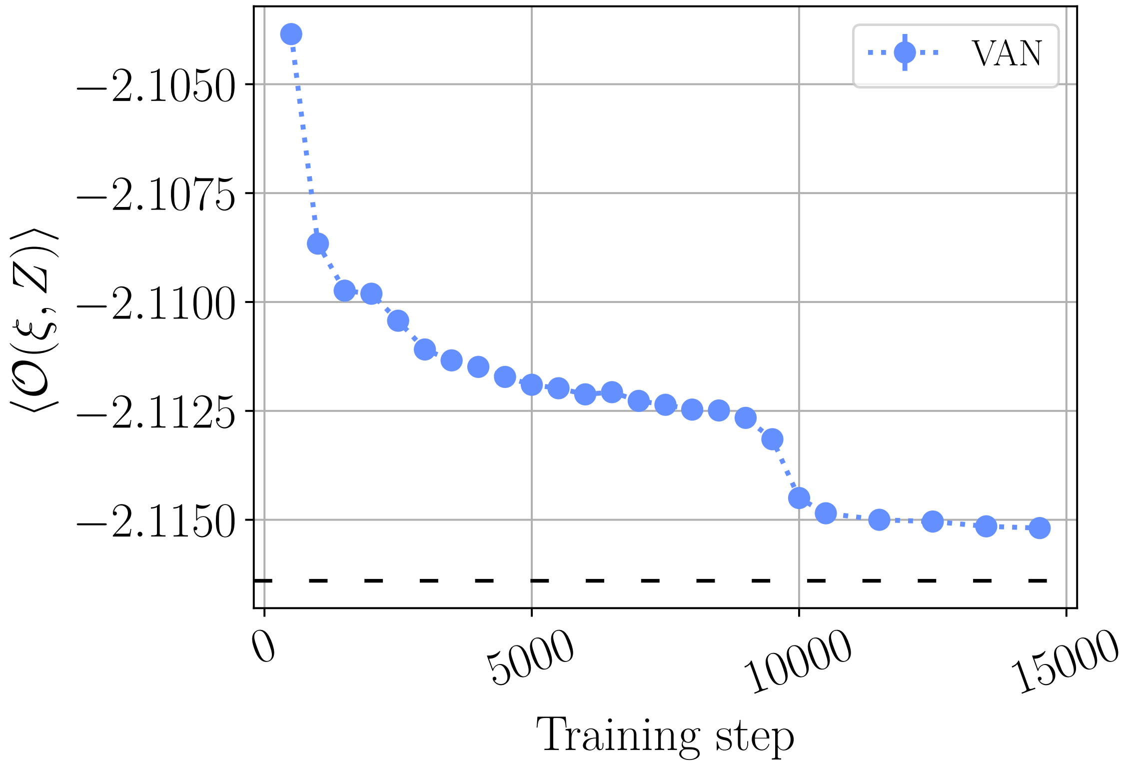
$$w(\phi) = \frac{p(\phi)}{q_\theta(\phi)}$$

The 2D Ising Model

$$H(\xi) = -J \sum_{<i,j>} \xi_i \xi_j \qquad p(\xi) = \frac{e^{-\beta H(\xi)}}{Z}$$

$$\langle \mathcal{O} \rangle_{q_\theta} \neq \langle \mathcal{O} \rangle_p$$



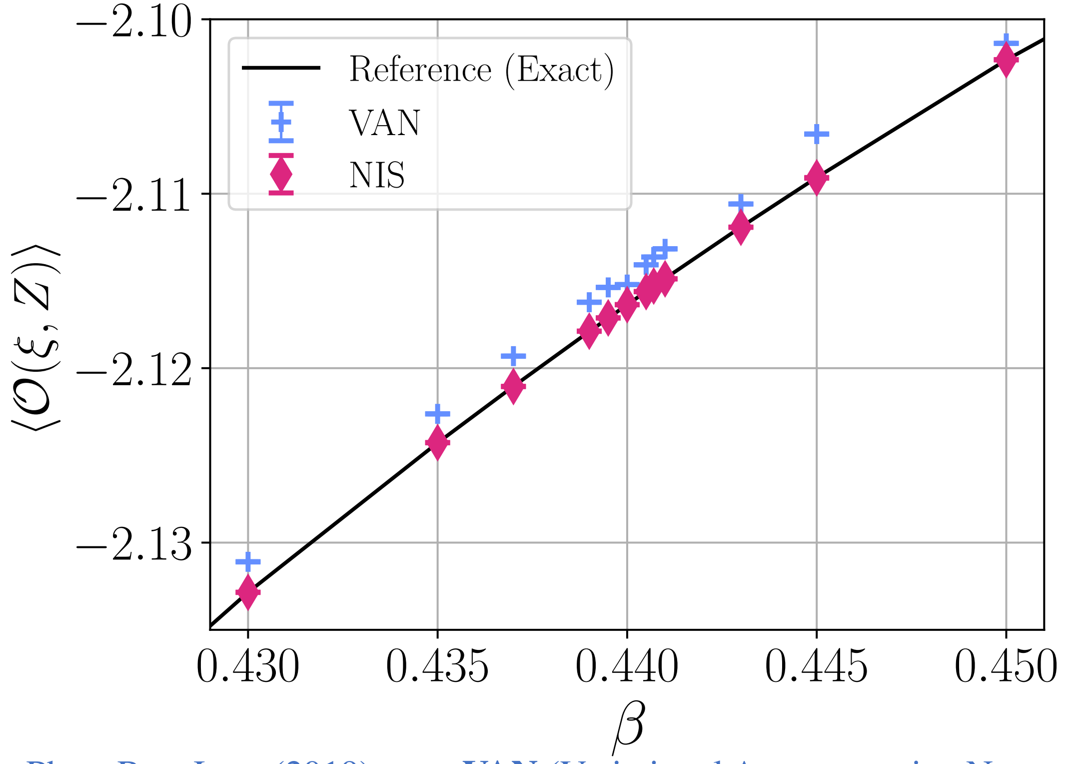


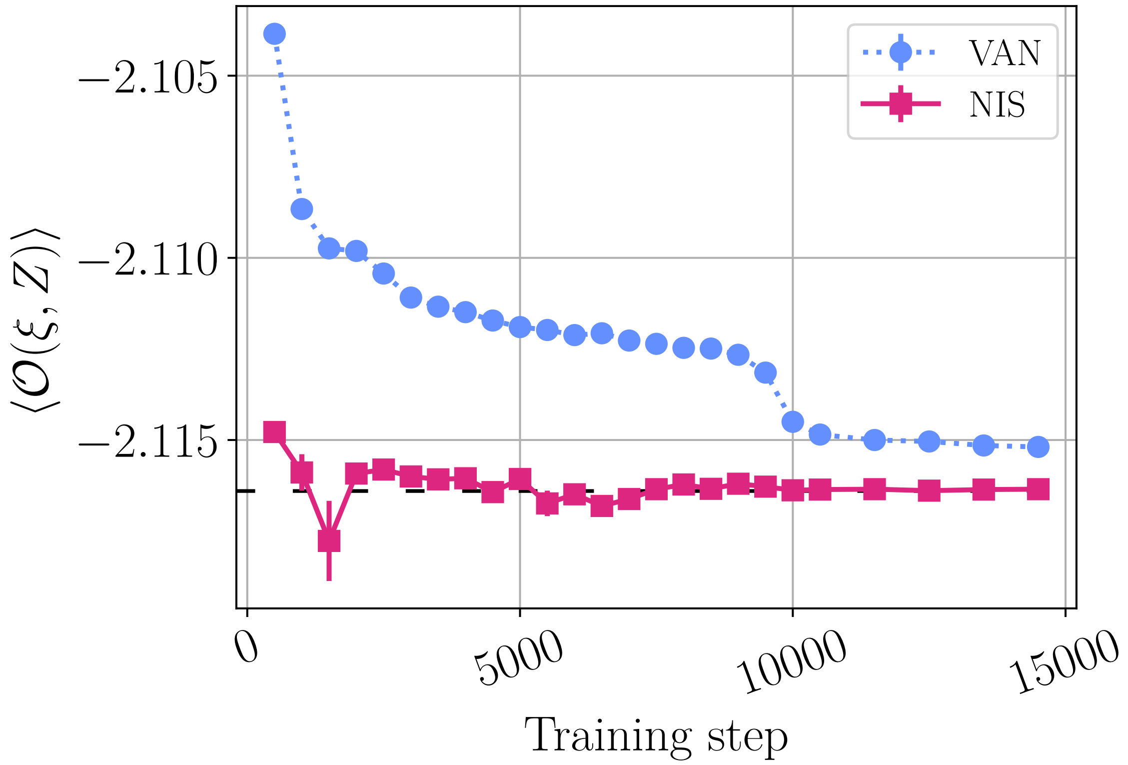
Wu+, Phys. Rev. Lett. (2019) $\Longrightarrow$ **VAN** (Variational Autoregressive Network)

The 2D Ising Model

$$H(\xi) = -J \sum_{<i,j>} \xi_i \xi_j \qquad p(\xi) = \frac{e^{-\beta H(\xi)}}{Z}$$

$$\langle \mathcal{O} \rangle_{q_\theta} \longrightarrow \langle w \mathcal{O} \rangle_{q_\theta}$$





Wu+, Phys. Rev. Lett. (2019) $\Longrightarrow$ **VAN** (Variational Autoregressive Network)
Nicoli+, Phys. Rev. E (2020) $\Longrightarrow$ **NIS** (Neural Importance Sampling)

Real Scalar ϕ^4-Theory in (1+1) D

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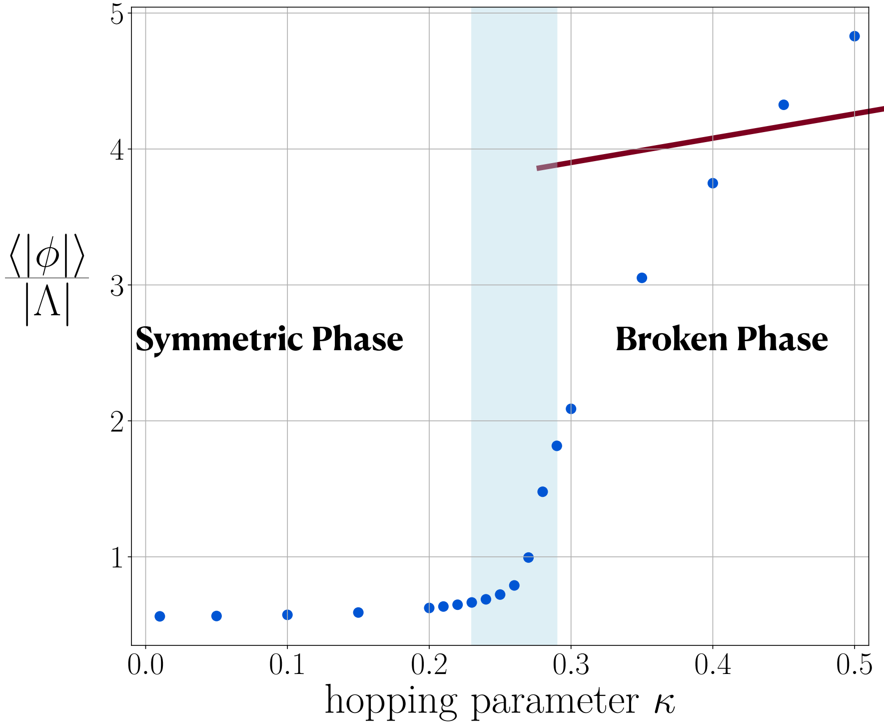
$$S(\phi) = \sum_{x\in\Lambda} \left\{ -2\kappa \sum_{\mu=1}^{d} \phi(x)\phi(x+\hat{\mu}) + (1-2\lambda)\phi(x)^2 + \lambda\phi(x)^4 \right\}$$



PHASE TRANSITION

Real Scalar ϕ^4-Theory in (1+1) D

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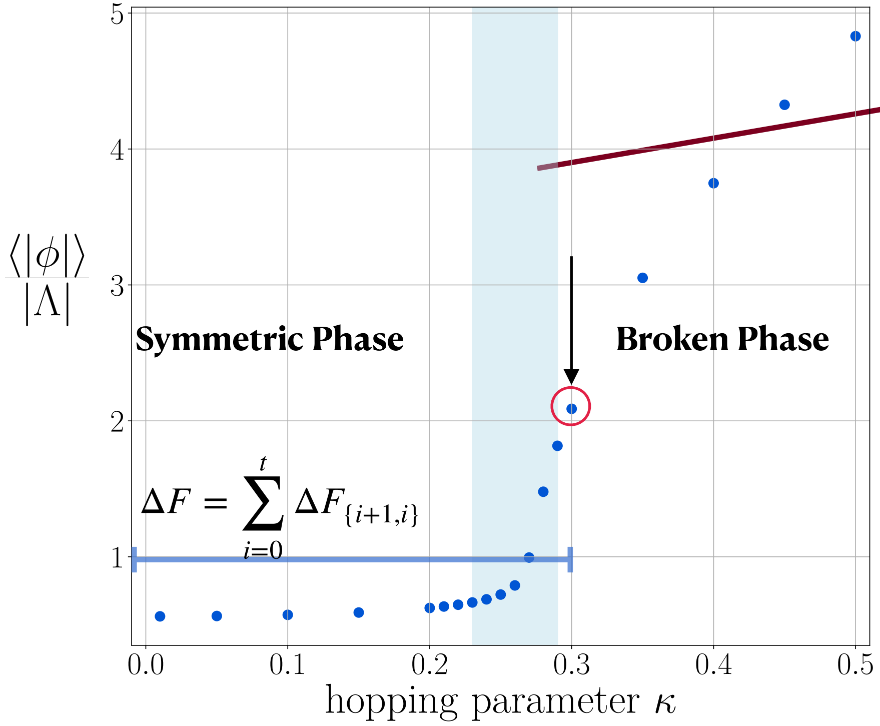
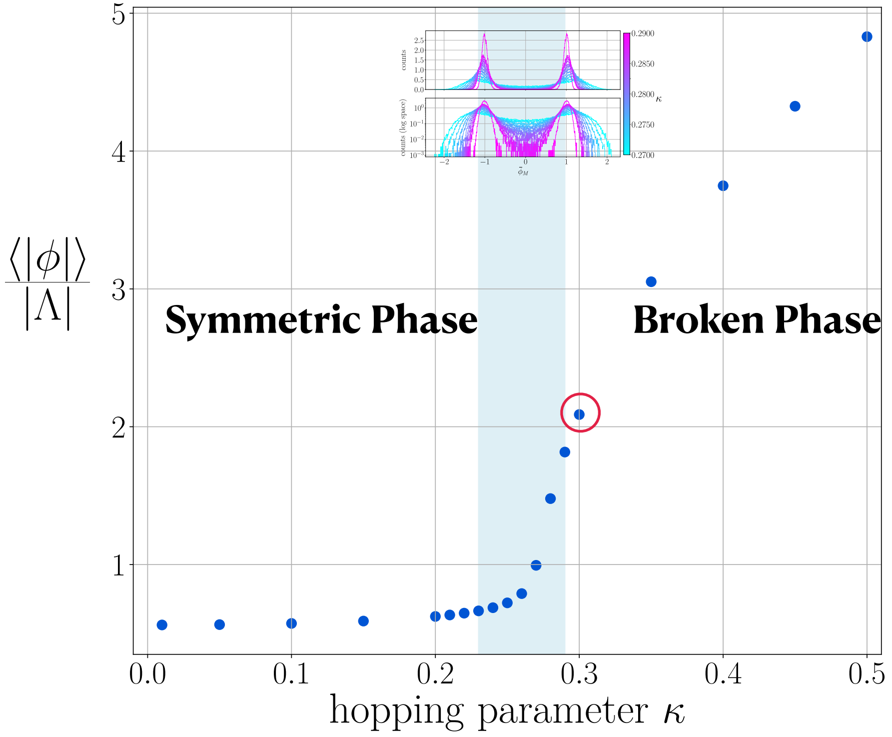


PHASE TRANSITION

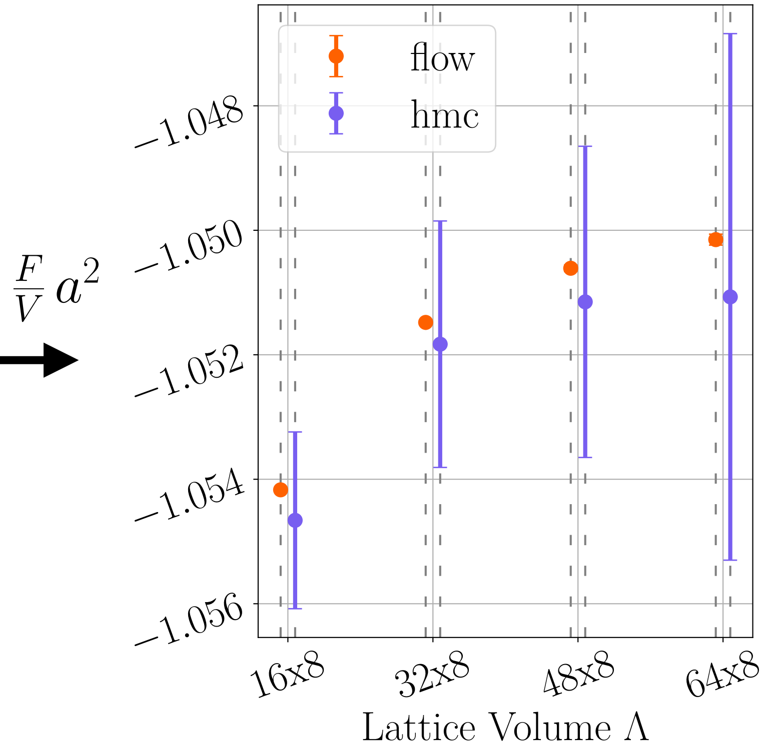
- $\Delta F = F_t - F_0 = -T \ln Z_t / Z_0$
- F_0 is needed to compute F_{target}
- Integration through phase space (MCMC)
- Intermediate steps $\Delta F_{\{i+1,i\}} = -T \ln \frac{Z_{i+1}}{Z_i}$

Real Scalar ϕ^4-Theory in (1+1) D

$$S(\phi) = \sum_{x\in\Lambda} \left\{ -2\kappa \sum_{\mu=1}^{d} \phi(x)\phi(x+\hat{\mu}) + (1-2\lambda)\phi(x)^2 + \lambda\phi(x)^4 \right\}$$



Nicoli+, Phys. Rev. Lett. (2021)



Real Scalar ϕ^4-Theory in (1+1) D

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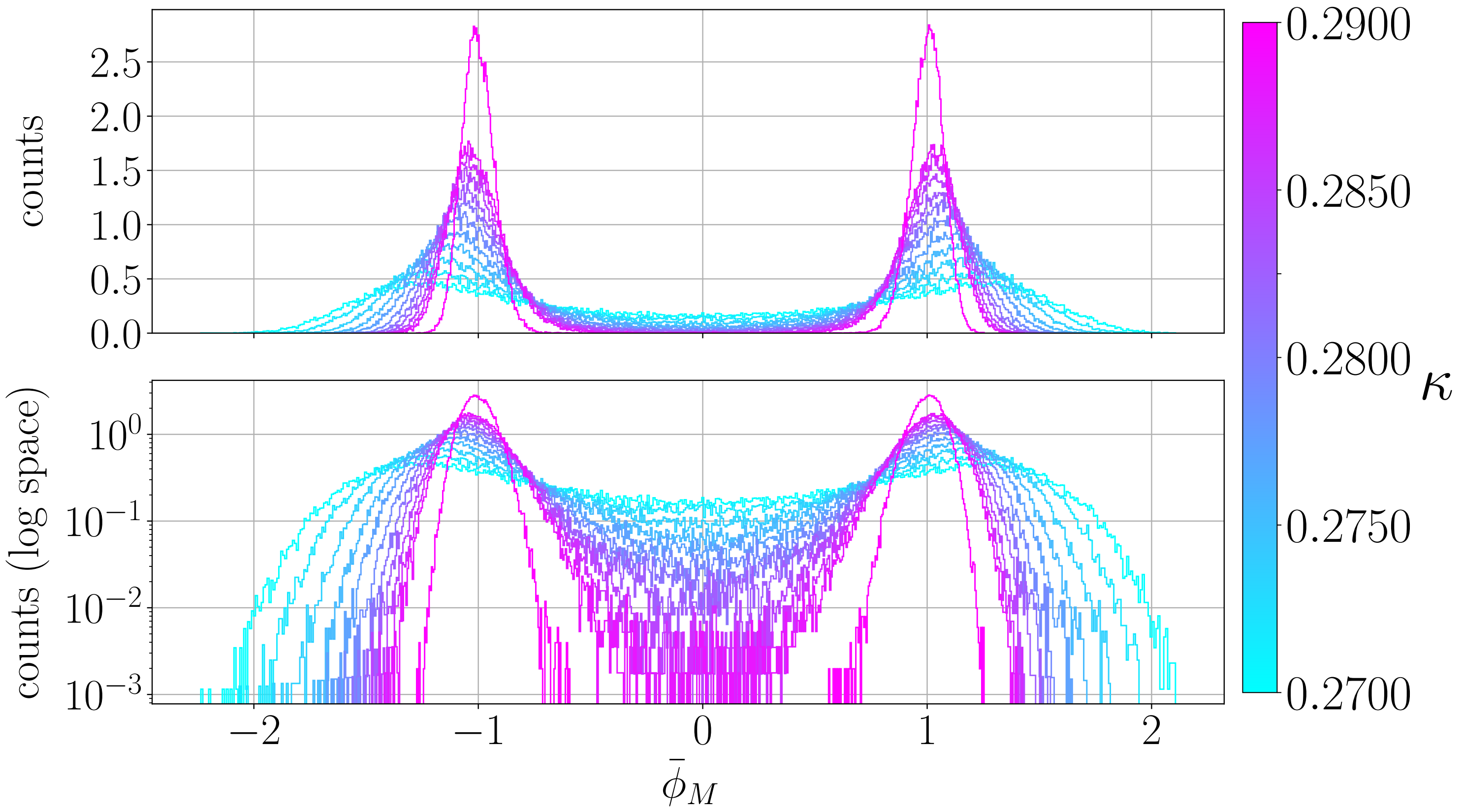
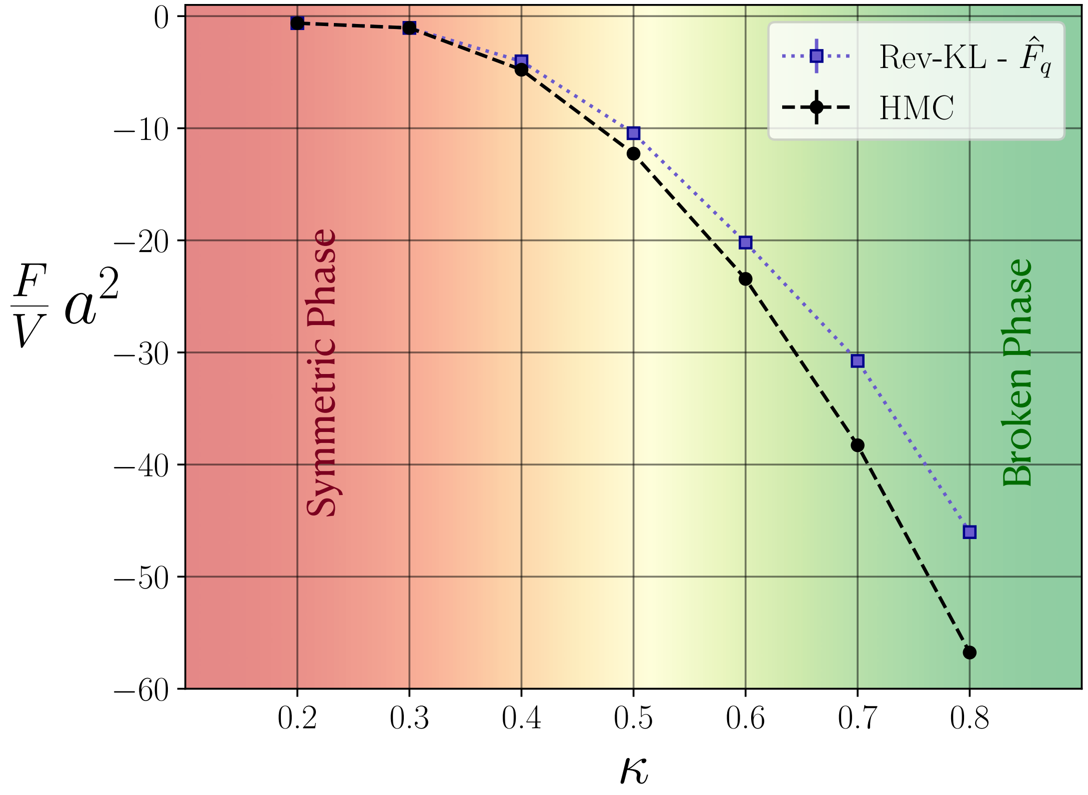


Nicoli+, Phys. Rev. D (2023)

Real Scalar ϕ^4-Theory in (1+1) D



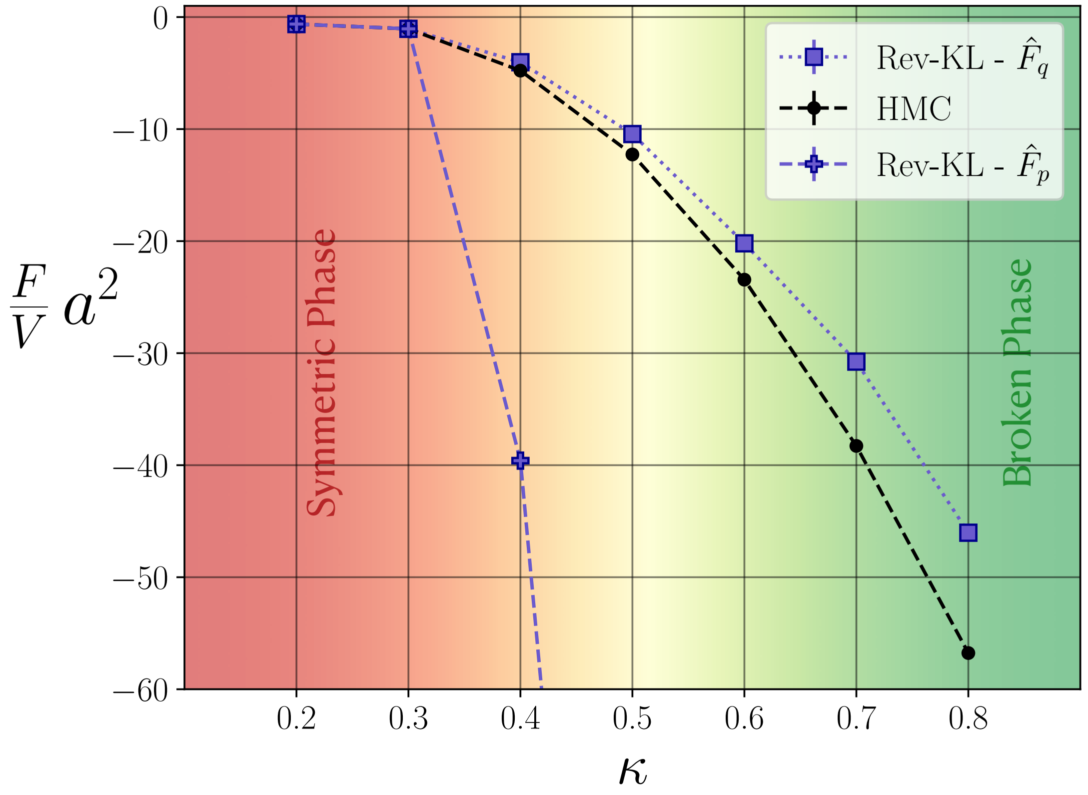
$$Z = \mathbb{E}_{\phi\sim q_\theta}\left[\frac{e^{-S(\phi)}}{q_\theta(\phi)}\right] \approx \frac{1}{N}\sum_{i=1}^{N}\frac{e^{-S(\phi_i)}}{q_\theta(\phi_i)} \equiv \hat{Z}_{q_\theta}$$

$\phi_i \sim q_\theta$

$$\hat{F}_q = -T\log(\hat{Z}_{q_\theta})$$

Nicoli+, Phys. Rev. D (2023)

Real Scalar ϕ^4-Theory in (1+1) D



Nicoli+, Phys. Rev. D (2023)

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$\phi_i \sim q_\theta$

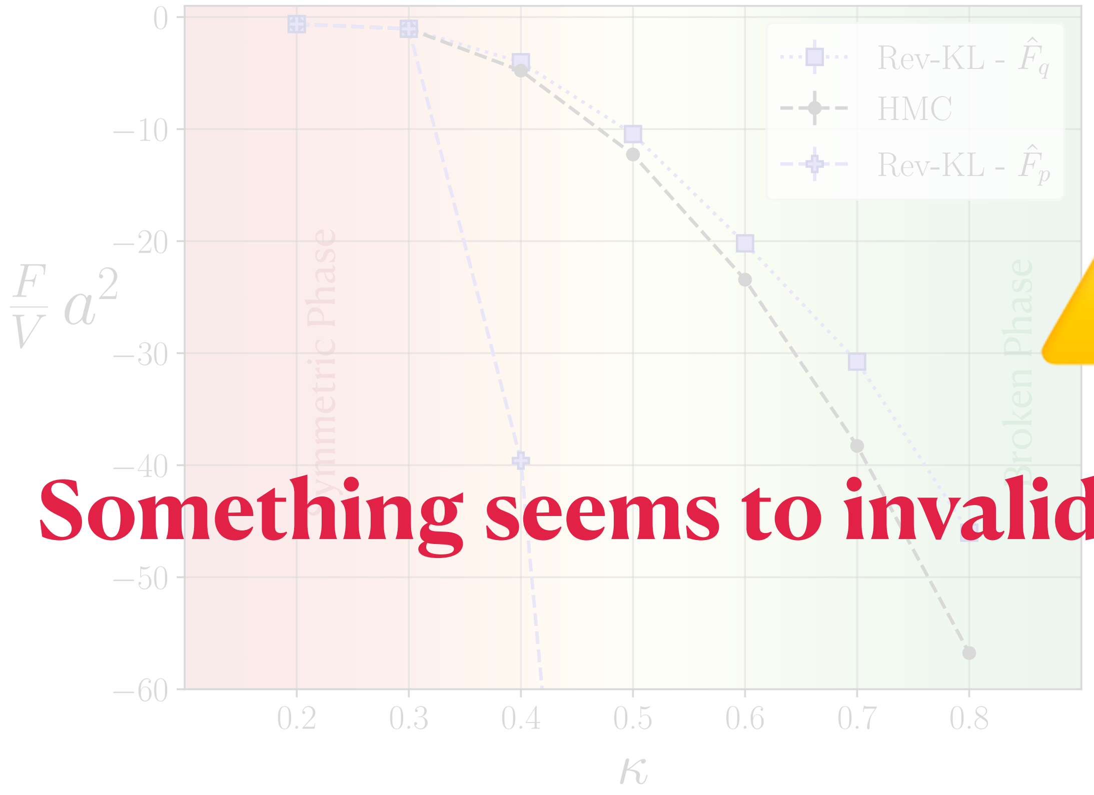
$$\hat{F}_q = -T\log(\hat{Z}_{q_\theta})$$

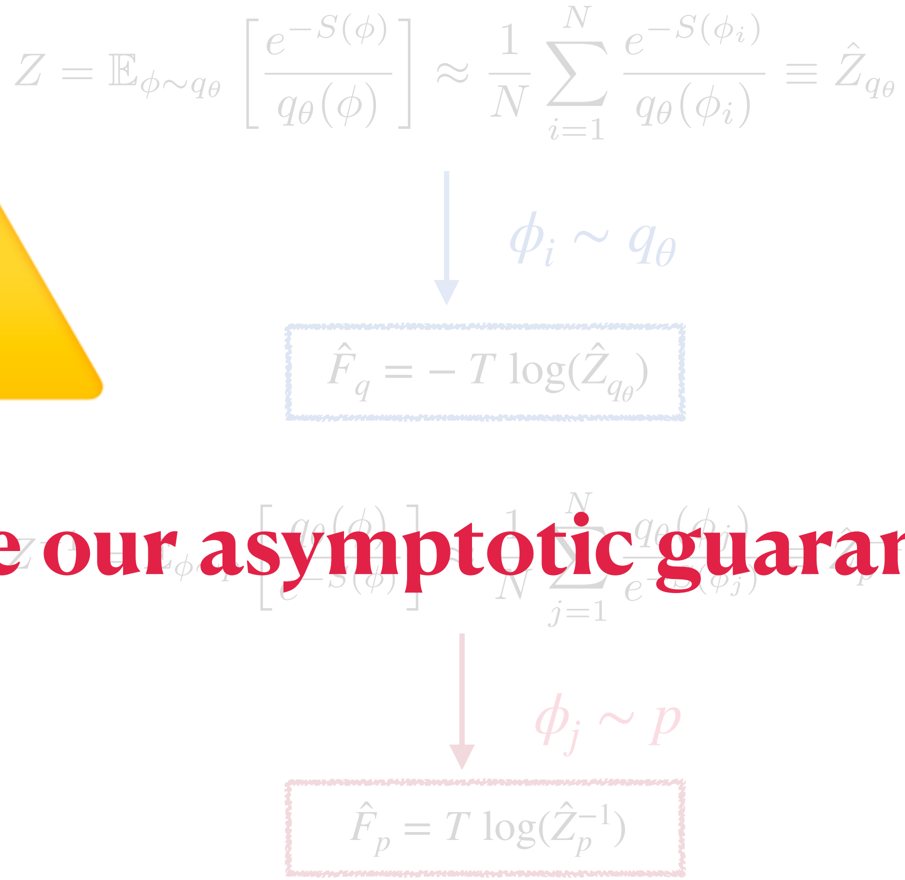
$$Z^{-1} = \mathbb{E}_{\phi \sim p}\left[\frac{q_\theta(\phi)}{e^{-S(\phi)}}\right] \approx \frac{1}{N}\sum_{j=1}^{N}\frac{q_\theta(\phi_j)}{e^{-S(\phi_j)}} \equiv \hat{Z}_p^{-1}$$

$\phi_j \sim p$

$$\hat{F}_p = T\log(\hat{Z}_p^{-1})$$

Real Scalar ϕ^4-Theory in (1+1) D





Something seems to invalidate our asymptotic guarantees!

Nicoli+, Phys. Rev. D (2023)

What’s going wrong then?

Reverse-KL Div.

$$KL_R(q_\theta || p) = \int D[\phi] q_\theta(\phi) \ln \frac{q_\theta(\phi)}{p(\phi)}$$

What's going wrong then?

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Reverse-KL Div.

$$KL_R(q_\theta || p) = \int D[\phi] q_\theta(\phi) \ln \frac{q_\theta(\phi)}{p(\phi)}$$

Forward-KL Div.

$$KL_F(p || q_\theta) = \int D[\phi] p(\phi) \ln \frac{p(\phi)}{q_\theta(\phi)}$$

What's going wrong then?

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Reverse-KL Div.

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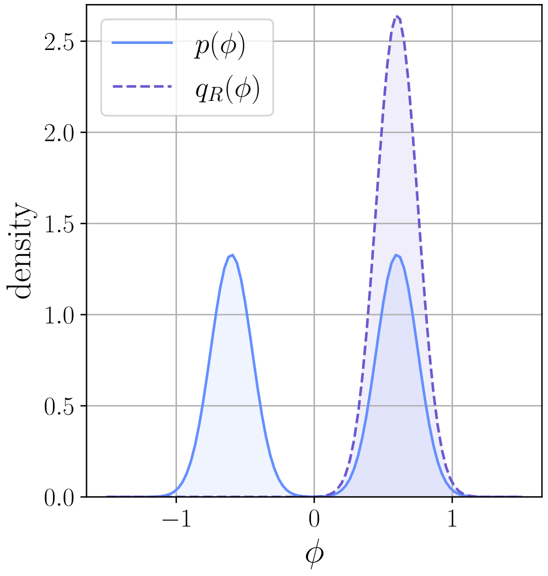
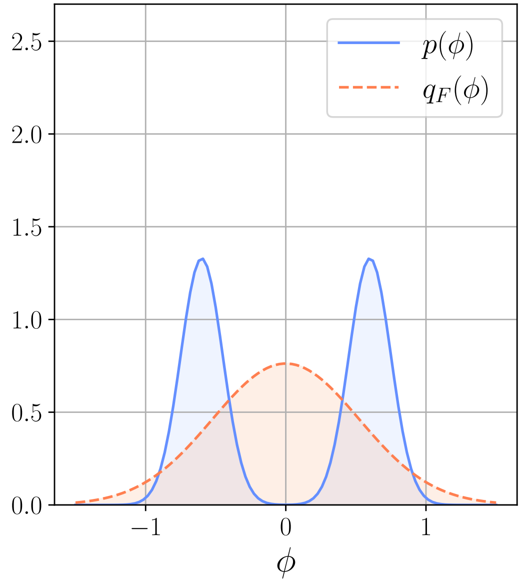


- Self-Sampling (efficient).
- No need for training data.
- Mode-dropping.

Forward-KL Div.

$$KL_F(p||q_\theta) = \int D[\phi] p(\phi) \ln \frac{p(\phi)}{q_\theta(\phi)}$$



- Maximum Likelihood.
- Requires training data.
- Fake modes.

What's going wrong then?

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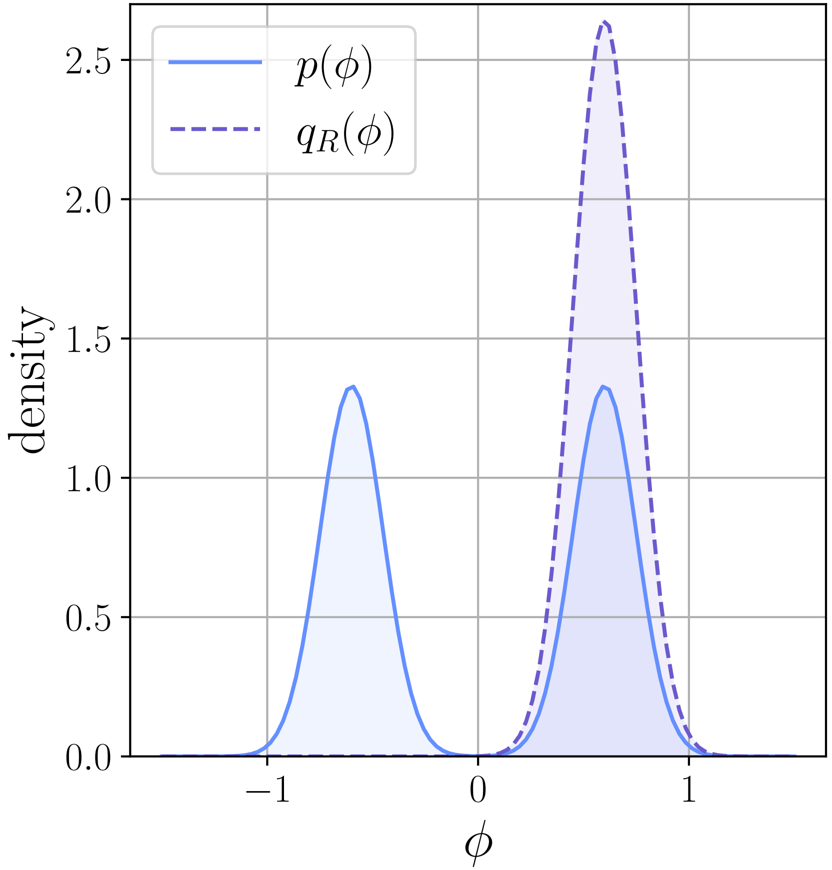

$$\mathrm{ESR} = \frac{\mathrm{ESS}}{N} = \frac{1}{\mathbb{E}_{q_\theta}\left[w^2\right]}$$

Where $\quad w = \dfrac{p(\phi)}{q_\theta(\phi)}$

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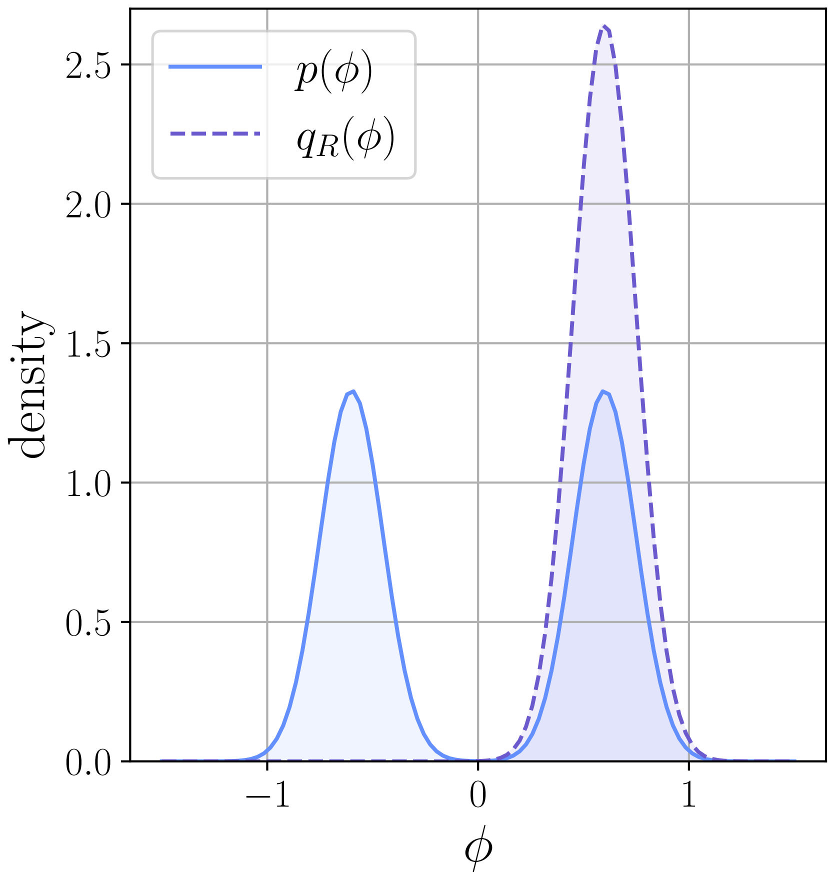

ESR is not a good metric!

$$\mathrm{ESR} = \frac{\mathrm{ESS}}{N} = \frac{1}{\mathbb{E}_{q_\theta}\left[w^2\right]}$$

Where $$w = \frac{p(\phi)}{q_\theta(\phi)}$$

The model is **blind** with respect to one (or more) of the modes of the target density.

The effect of mode-dropping

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<u>Definition.</u> *The effective support of the variational density q_θ <u>relative</u> to p*

$$\widetilde{\mathrm{supp}}_{p,\epsilon}(q_\theta) = \{\phi \in \mathrm{supp}(q_\theta);\ q_\theta(\phi) > \epsilon p(\phi)\}$$

for a given numerical threshold ϵ. The mode dropping set is then given by

$$\mathcal{S} := \mathrm{supp}(p) \setminus \widetilde{\mathrm{supp}}_{p,\epsilon}(q_\theta)$$

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The effect of mode-dropping

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if the flow is **effectively mode-dropping**, the importance-weighted estimator, with a finite number of samples N, will miss a contribution from the mass $\int_{\mathcal{S}} p(\phi)d\phi$ with approximately the probability $1 - \epsilon N \int_{\mathcal{S}} p(\phi)d\phi$.

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The effect of mode-dropping

Definition. *We define the effective sampler distribution*

$$\widetilde{q}_\theta(\phi) = \begin{cases} q_\theta(\phi)/\zeta & \text{if } \phi \in \widetilde{\text{supp}}_{p,\epsilon}(q_\theta) \\ 0 & \text{otherwise,} \end{cases} \qquad \textit{where} \qquad \zeta = \int_{\widetilde{supp}_{p,\epsilon}} \mathcal{D}[\phi] q_\theta(\phi) \leq 1$$

is the multiplicative renormalization factor necessary to guarantee the normalization of $\widetilde{q}_\theta(\phi)$.

The effect of mode-dropping

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It follows that the importance-weighted estimator misses the contribution from the mode-dropping set $\mathcal{S}$

$$\hat{\mathcal{O}} \equiv \frac{1}{N} \sum_{i=1}^{N} \frac{p(\phi_i)}{q_\theta(\phi_i)} \mathcal{O}(\phi_i) \approx \mathbb{E}_{\phi \sim \widetilde{q}_\theta} \left[\frac{p(\phi)}{q_\theta(\phi)} \mathcal{O}(\phi) \right] \equiv \bar{\mathcal{O}}$$

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the typical values of the estimator $\hat{\mathcal{O}} \approx \bar{\mathcal{O}}$ can be **significantly different** from the true expectation value! 👎

The mode-dropping estimator

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When q_θ has **full effective support** on the domain of p

$$w^* = \mathbb{E}_{q_\theta}\left[\frac{p(\phi)}{q_\theta(\phi)}\right] = \int_{\mathrm{supp}(q_\theta)} q_\theta(\phi)\frac{p(\phi)}{q_\theta(\phi)}\,\mathcal{D}[\phi] = \int_{\mathrm{supp}(q_\theta)} p(\phi)\,\mathcal{D}[\phi] = 1\,.$$

The mode-dropping estimator

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however if q_θ is **effectively mode-dropping** this expectation value becomes

$$\bar{w} \equiv \frac{1}{Z}\mathbb{E}_{\phi\sim\tilde{q}_\theta}\left[\frac{e^{-S(\phi)}}{q_\theta(\phi)}\right] \quad \in (0,1]$$

The mode-dropping estimator

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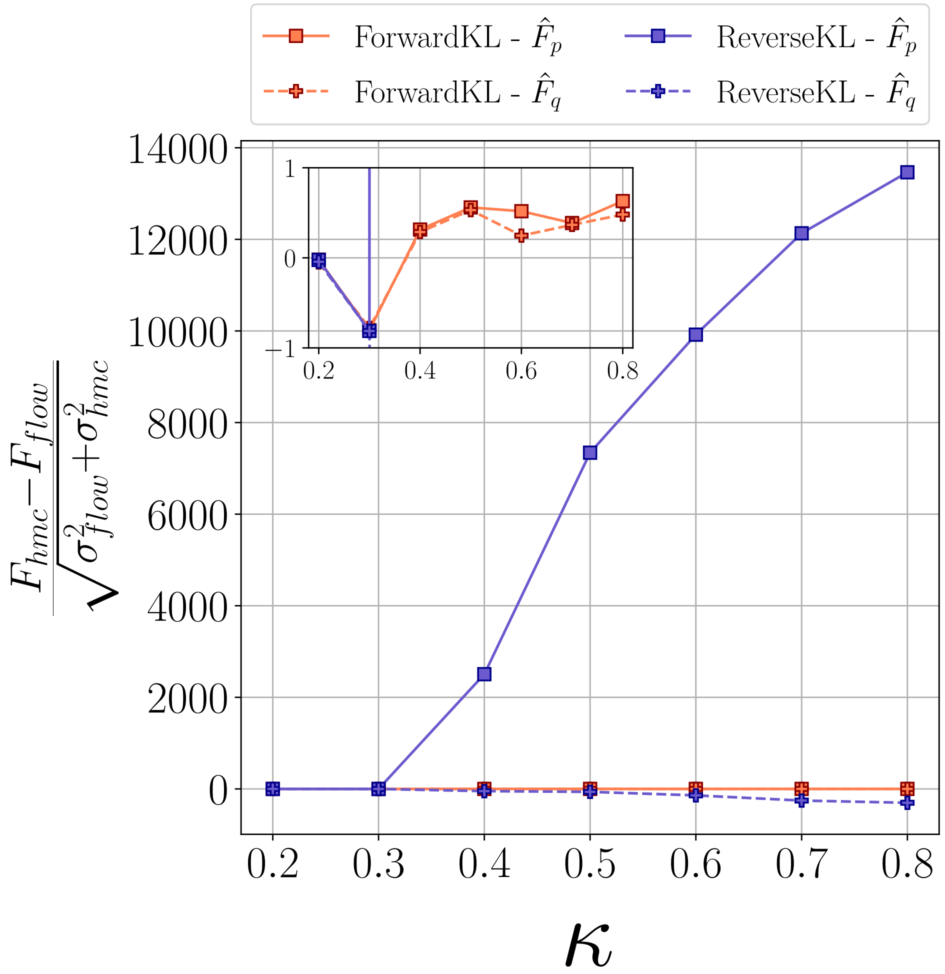
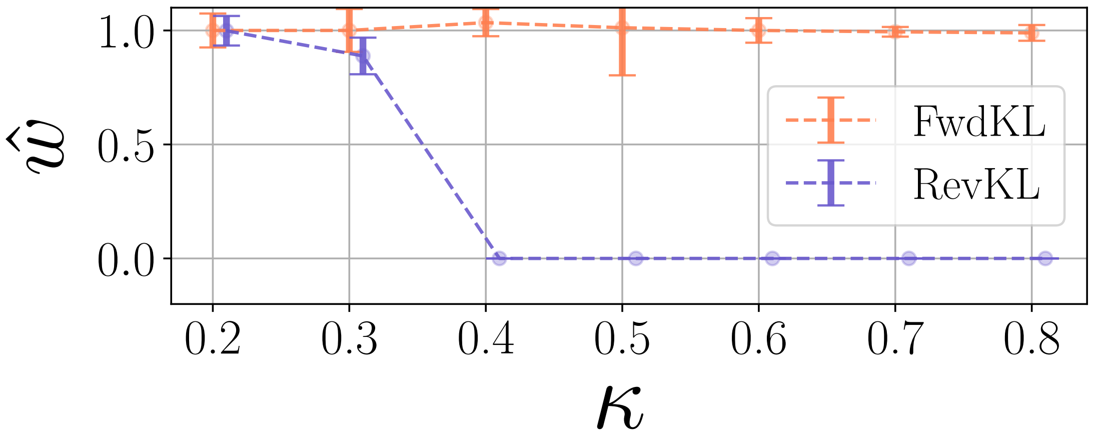
for which we can get the corresponding Monte Carlo estimator, i.e., the **mode-dropping estimator**

$$\bar{w} \approx \frac{1}{\hat{Z}_p}\left(\frac{1}{N}\sum_{i=1}^{N}\frac{e^{-S(\phi_i)}}{q_\theta(\phi_i)}\right) = \left(\frac{1}{N}\sum_{j=1}^{N}\frac{q_\theta(\phi_j)}{e^{-S(\phi_j)}}\right)\left(\frac{1}{N}\sum_{i=1}^{N}\frac{e^{-S(\phi_i)}}{q_\theta(\phi_i)}\right) \equiv \hat{w}$$

Estimation of Mode Dropping Across Criticality



$$\Lambda = 64 \times 8, \lambda = 0.022$$



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Summary and Conclusions

i) **Asymptotically unbiased samplers** can be constructed from trained DGMs (NIS or NMCMC).

ii) **Direct** estimation of the **partition function** and **thermodynamic observables**.

iii) Sampling from DGMs is **embarrassingly parallelizable** $\neq$ MCMC (**sequential**).

iv) Training with **forward-KL** leads to better models though requires training samples.

v) Derivation of **mode-dropping estimator** to reliably assess the goodness of the model.

vi) **Mitigation** of mode-dropping using different **objectives** (FWD-KL) or **stochastic** approaches (SNFs).

Thank you for your attention!