INL/CON-23-73727-Revision-0

Bayesian Inference with Latent Hamiltonian Neural Networks (L-HNNs)

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Changing the World's Energy Future

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Idaho National Laboratory

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17th US National Congress on Computational Mechanics

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Motivation

Variational inference

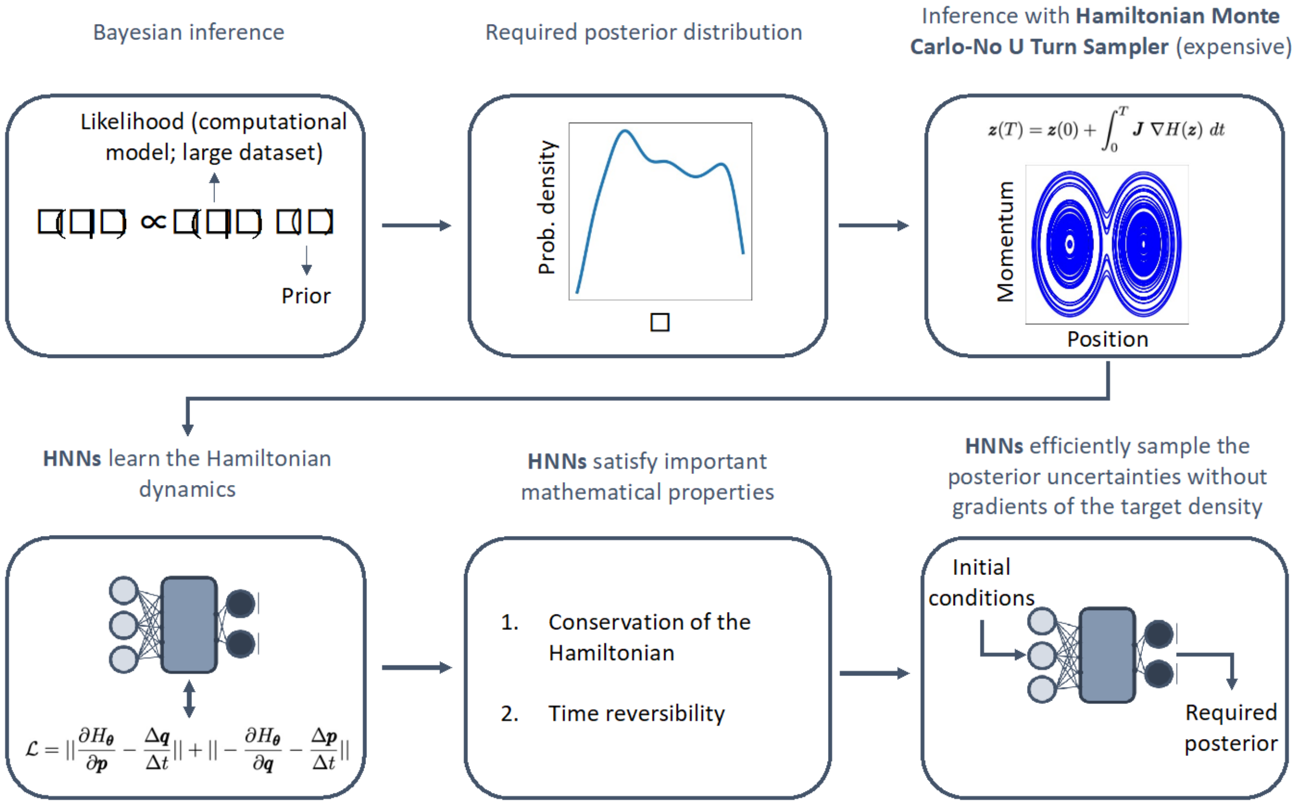
Markov-chain Monte Carlo

Particle-based inference (Stein variational gradient descent)

Normalizing flows

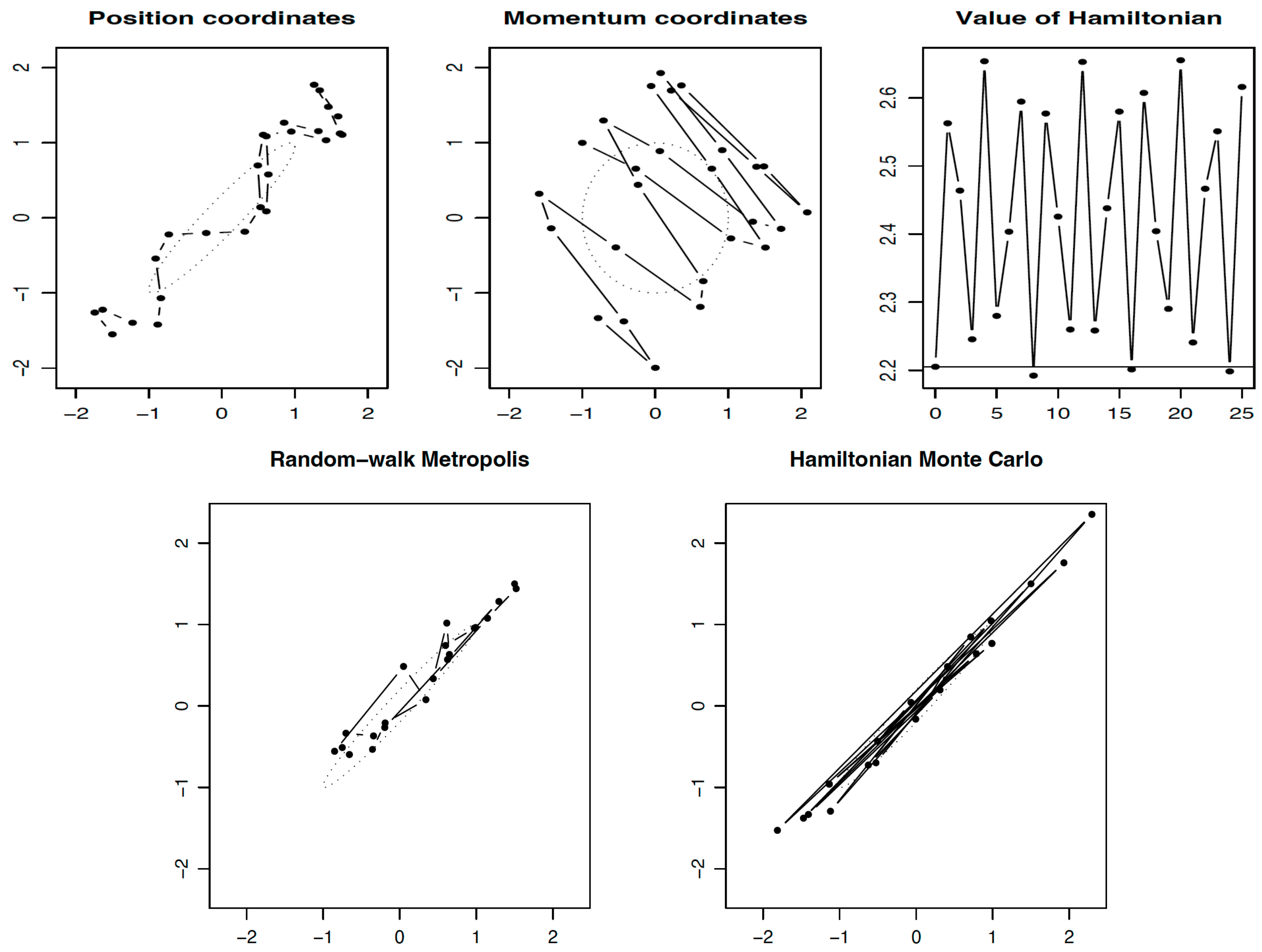
Least expensive	Moderately expensive	Very expensive
Random walk	**Langevin-based**	**Hamiltonian-based**
• No gradient information required • Poor scalability with dimensionality • Large correlations b/w samples	• Uses gradient information • Better scalability with dimensionality • Fairly large correlations b/w samples	• Uses gradient information • Best scalability with dimensionality • Small correlations b/w samples

Proposed contributions



- Use of Hamiltonian Neural Networks (HNNs) for Bayesian inference without needing numerous gradients of target posterior
- Introduction of latent variable outputs to HNNs (L-HNNs) for improved expressivity
- L-HNNs in No-U-Turn Sampling (NUTS) with an online error monitoring scheme

Background: Hamiltonian Monte Carlo



Credit: Neal (2013)

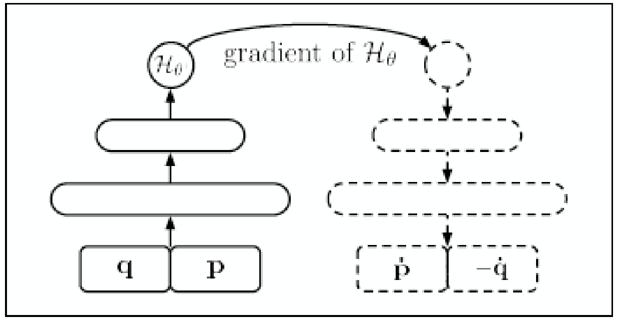
- Sampling is "similar" to MCMC: Random momenta, compute particle trajectory by solving the governing equation, Metropolis acceptance step
- positions **q** and momenta **p**:

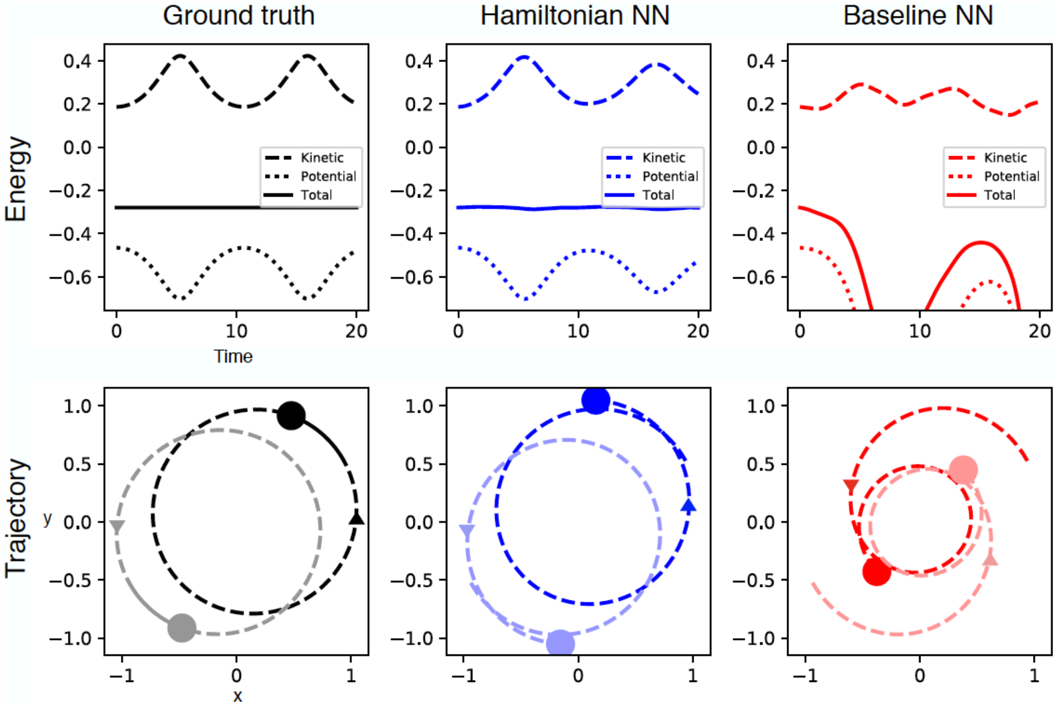
$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} \qquad \forall \quad i \in [1, \ldots, d].$$
$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}$$

- Hamiltonian (H) definition: Potential energy U(**q**) is dependent on the target posterior and Kinetic energy K(**p**) is based on "Canonical distribution"
- Exact numerical integration: all proposed samples accepted
- Better scalability than random-walk due to use of gradient information

Background: Hamiltonian Neural Networks (HNNs)

Hamiltonian NN





Credit: Greydanus et al. (2019)

- In forward pass, HNNs predict the Hamiltonian (H) and gradients of it are computed
- HNNs minimize the loss function:

$$\underset{\theta}{\operatorname{argmin}} \left\| \frac{d\mathbf{q}}{dt} - \frac{\partial \mathcal{H}_\theta}{\partial \mathbf{p}} \right\|^2 + \left\| \frac{d\mathbf{p}}{dt} + \frac{\partial \mathcal{H}_\theta}{\partial \mathbf{q}} \right\|^2$$

- Hamilton's equations:

$$\begin{aligned} \frac{dq_i}{dt} &= \frac{\partial H}{\partial p_i} \\ \frac{dp_i}{dt} &= -\frac{\partial H}{\partial q_i} \end{aligned} \qquad \forall \quad i \in [1, \ldots, d].$$

- Better performance than Neural Nets
- HNNs applied to classical mechanics problems
- Not used for Bayesian inference (to our knowledge)

Bayesian inference with HNNs

Leap frog integration with HNNs for solving: $\begin{aligned} \frac{dq_i}{dt} &= \frac{\partial H}{\partial p_i} \\ \frac{dp_i}{dt} &= -\frac{\partial H}{\partial q_i} \end{aligned} \quad \forall \quad i \in [1, \ldots, d].$

Hamiltonian Monte Carlo

Algorithm 3.3 HNNs in Hamiltonian Monte Carlo

```
Hamiltonian: H = U(q) + K(p); Samples: M; Starting sample: {q^0, p^0}; End time for trajectory: T; Steps: N; Dimensions: d
for i = 1 : M do
    p(0) ~ N(0, I_d)
    q(0) = q^{i-1}
    Compute {q*, p*} = {q(T), p(T)} with Algorithm 3.2
    α = min{1, exp(H({q^{i-1}, p^{i-1}}) − H({q*, p*}))}
    With probability α, set {q^i, p^i} ← {q*, p*}
end for
```

$$U(\boldsymbol{q}) \propto -\log\left[\mathcal{L}(\boldsymbol{q}|D)\ g(\boldsymbol{q})\right]$$

$$K(\boldsymbol{p}) \propto -\log[N(\boldsymbol{0}, \boldsymbol{I})]$$

Algorithm 3.2 Hamiltonian neural networks evaluation in leapfrog integration

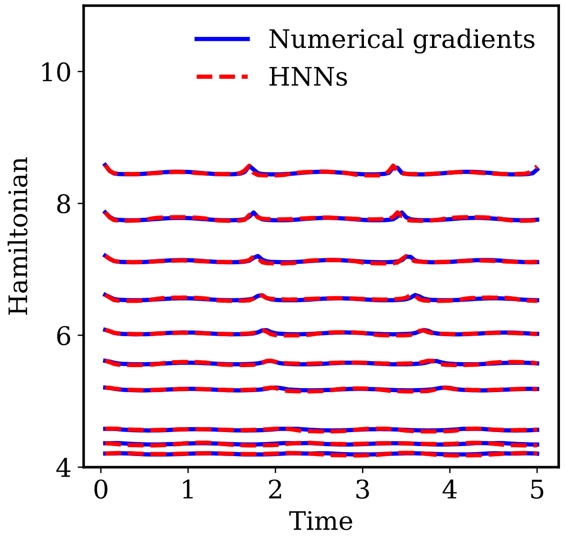
```
Hamiltonian: H; Initial conditions: z(0) = {q(0), p(0)}; Dimensions: d; Steps: N; End time: T
Δt = T/N
for j = 0 : N − 1 do
    t = j Δt
    Compute HNN output gradient ∂H_θ/∂q(t)
    for i = 1 : d do
        q_i(t + Δt) = q_i(t) + (Δt/m_i) p_i(t) − (Δt^2/2m_i) ∂H_θ/∂q_i(t)
    end for
    Compute HNN output gradient ∂H_θ/∂q(t+Δt)
    for i = 1 : d do
        p_i(t + Δt) = p_i(t) − (Δt/2) (∂H_θ/∂q_i(t) + ∂H_θ/∂q_i(t+Δt))
    end for
end for
```

Using HNNs (traditional: numerical gradients)

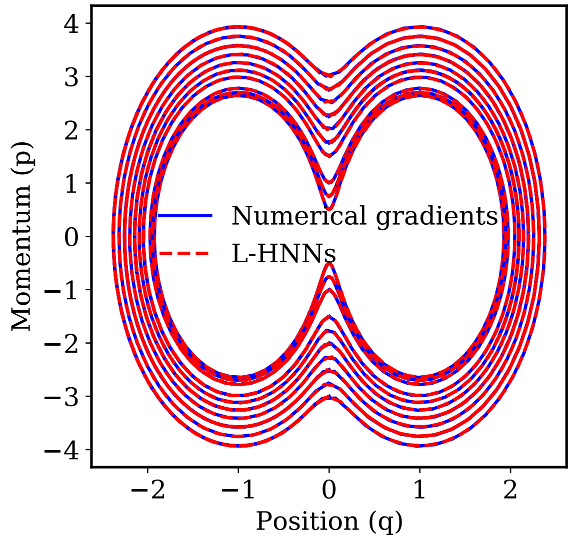
Bayesian inference with HNNs

1-D Gaussian mixture density

$$f(q) \propto 0.5 \ \exp\left(\frac{(q-1)^2}{2 \times 0.35^2}\right) + 0.5 \ \exp\left(\frac{(q+1)^2}{2 \times 0.35^2}\right)$$



Hamiltonian conservation for some initial ***q*-*p*** values

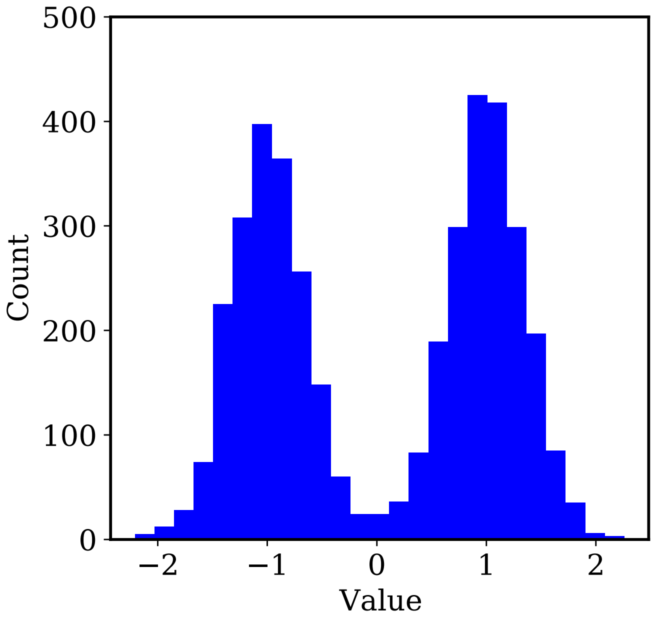


q*-*p phase space plots for some initial values

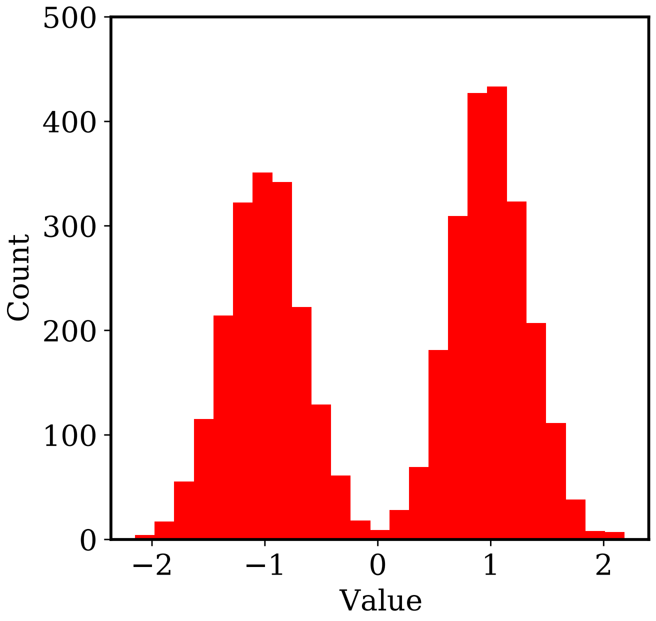
Bayesian inference with HNNs

1-D Gaussian mixture density

$$f(q) \propto 0.5 \ \exp\left(\frac{(q-1)^2}{2 \times 0.35^2}\right) + 0.5 \ \exp\left(\frac{(q+1)^2}{2 \times 0.35^2}\right)$$



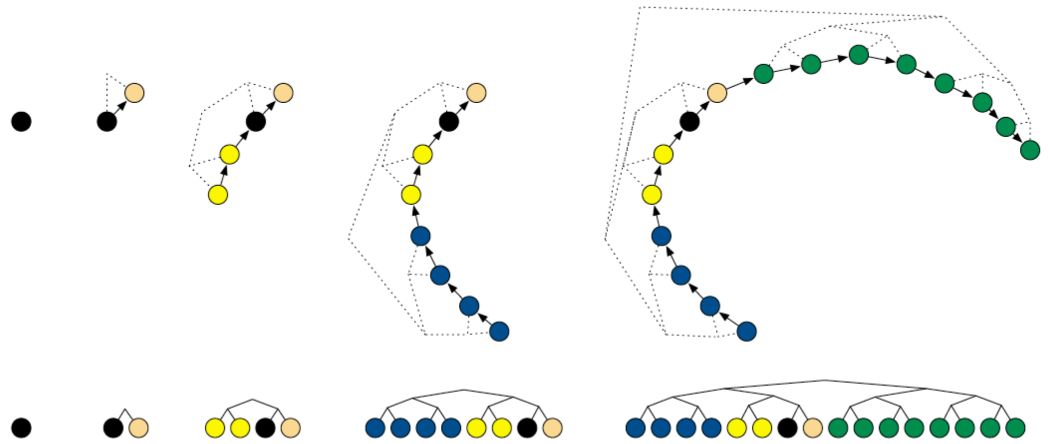
Samples using traditional HMC. 500,000 posterior gradients



Samples using HNNs in HMC. 8,000 posterior gradients

Background: No-U-Turn Sampling (NUTS)

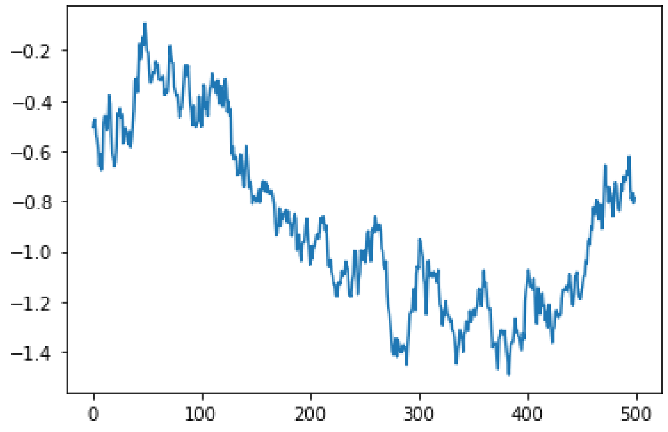
Theory



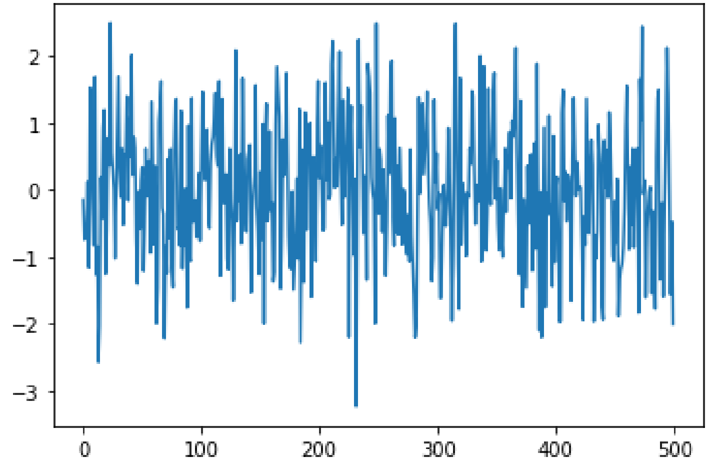
Credit: Hoffman and Gelman (2013)

- Successive binary trees with doubling length either in positive or negative direction
- "Slice sampling" to select **q-p** states that satisfy stationarity
- Tree building terminated when a u-turn is made (correlations between samples are small)
- Also terminated when integration errors are large when simulating the Hamiltonian dynamics

Practice (a high-dimensional posterior)



HMC with an end time of 5 units

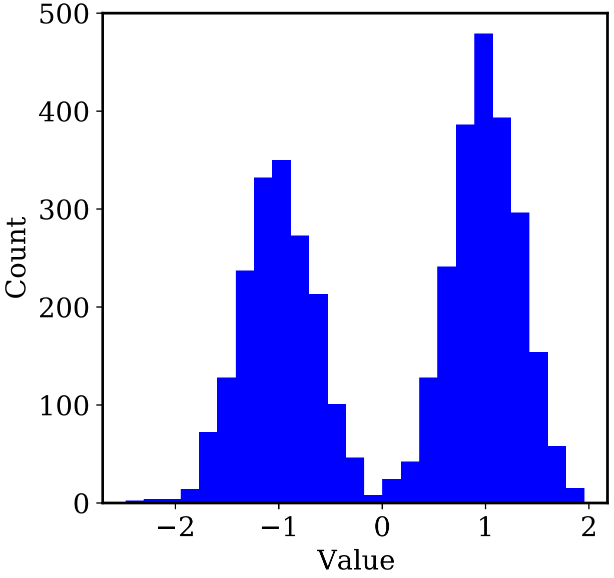


NUTS

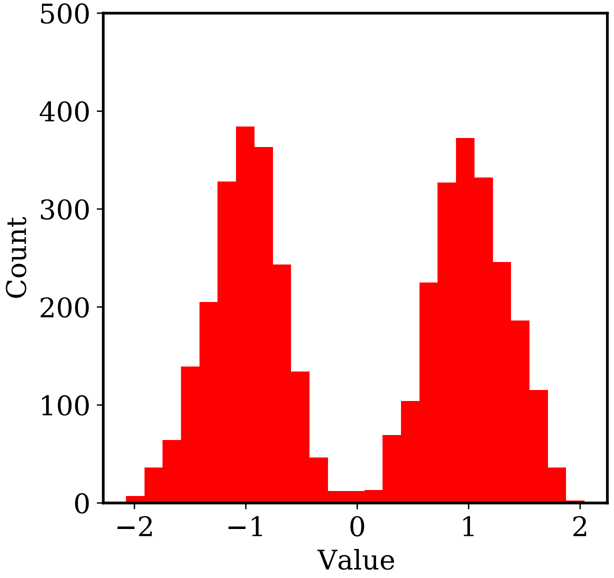
HNNs in NUTS

1-D Gaussian mixture density

$$f(q) \propto 0.5\ \exp\left(\frac{(q-1)^2}{2\times 0.35^2}\right) + 0.5\ \exp\left(\frac{(q+1)^2}{2\times 0.35^2}\right)$$



Samples using traditional NUTS



Samples using HNNs in NUTS

ESS: effective sample size to measure sampling quality

	ESS per gradient of target density
HNNs in HMC	$4.59E-3$
Traditional HMC	$8.42E-5$
HNNs in NUTS	$4.83E-3$
Traditional NUTS	$4.4E-4$

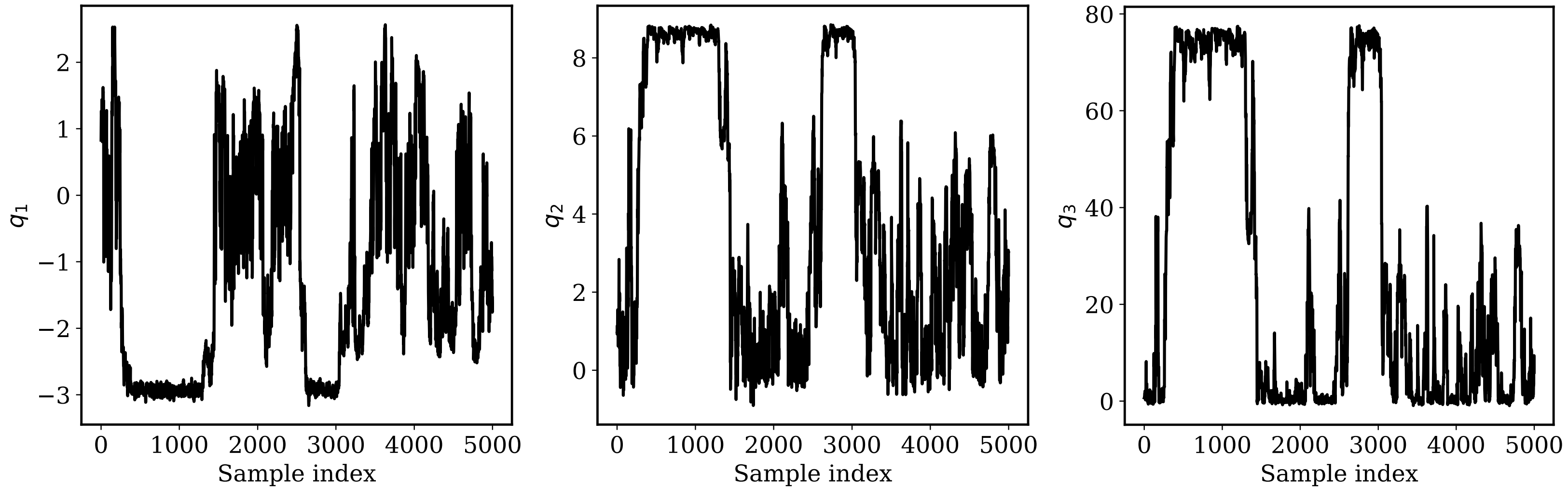
490,000 HNN gradients

91,000 HNN gradients

HNNs in NUTS: sampling degeneracy problem

3-D Rosenbrock density

$$f(\boldsymbol{q}) \propto \exp\left(-\sum_{i=1}^{N-1}\left[100(q_{i+1}-q_i^2)^2+(1-q_i)^2\right]/20\right)$$



Dimension 1 Dimension 2 Dimension 3

- In the tails, HNNs may have little to no training data
- Therefore, integration errors when simulating Hamiltonian dynamics using HNNs can be large
- As a result, NUTS prematurely terminates the tree building procedure
- Many sample clusters in regions of low density: sampling degeneracy problem

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HNNs in NUTS with online error monitoring

Integration error in the original NUTS (H: Hamiltonian; u: slice value; Δ_{max}: threshold [1000])

$$\varepsilon \equiv H(\boldsymbol{z}) + \ln u > \Delta_{max}$$

Proposed online error monitoring

$$\varepsilon^{hnn} \leq \Delta^{hnn}_{max} \rightarrow \text{use leap frog with L-HNN gradients}$$

$$\varepsilon^{hnn} > \Delta^{hnn}_{max},\ \varepsilon^{lf} \leq \Delta^{lf}_{max} \rightarrow \text{use leap frog with posterior gradients for } N^{lf} \text{ samples}$$

$$\varepsilon^{hnn} > \Delta^{hnn}_{max},\ \varepsilon^{lf} > \Delta^{lf}_{max} \rightarrow \text{terminate tree building; move to next sample}$$

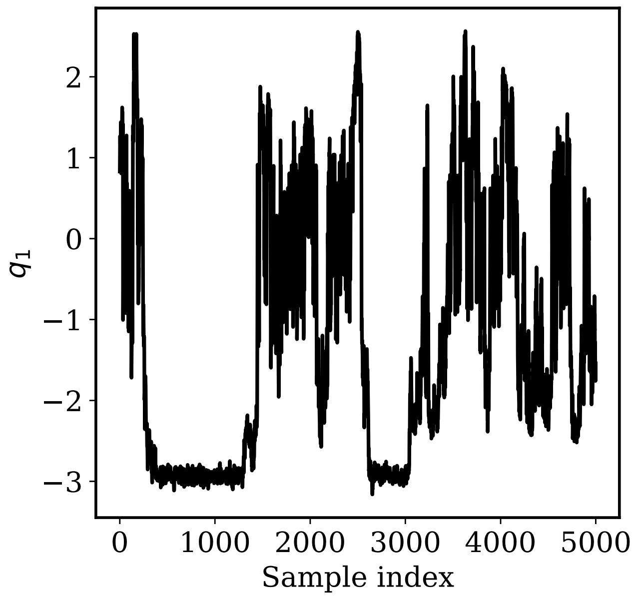
- Original NUTS terminates tree building when $\varepsilon > \Delta_{max}$
- Causes sampling degeneracy in the tails when using NUTS with HNNs
- Proposed online error monitoring:
  - $\Delta^{hnn}{}_{max}$: when using HNNs and $\Delta^{lf}{}_{max}$: when using posterior gradients
  - $\Delta^{hnn}{}_{max} \ll \Delta^{lf}{}_{max}$ (e.g., 10 and 1000)
  - Default use HNN gradients
  - Switch to posterior gradients for N_{lf} samples (e.g., 5-20) to bring sampler to high density regions
  - Then, HNN gradients take over

- Similar in concept to multifidelity modeling

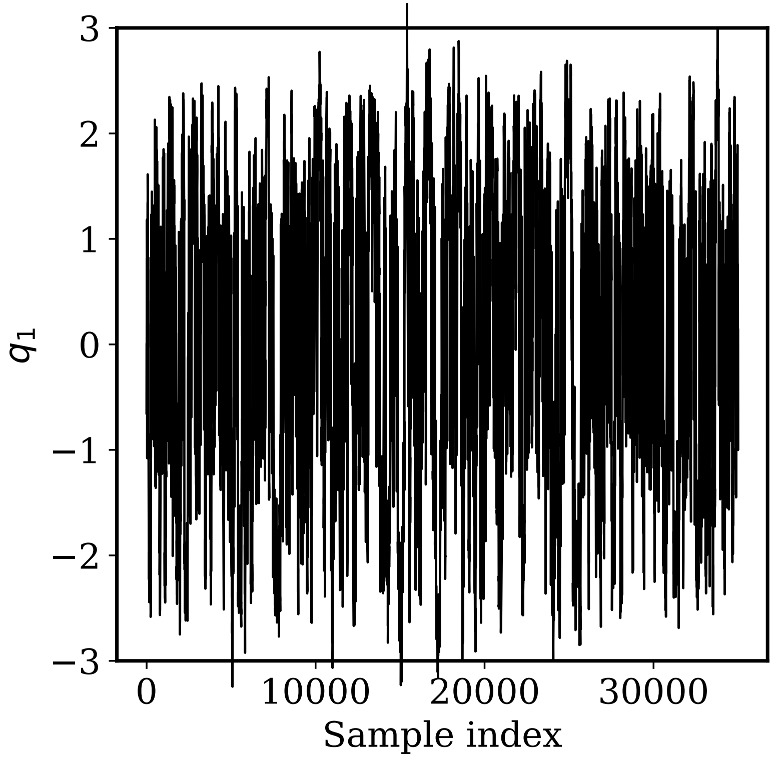
HNNs in NUTS with online error monitoring

3-D Rosenbrock density

$$f(\boldsymbol{q}) \propto \exp\left(-\sum_{i=1}^{N-1}\left[100(q_{i+1}-q_i^2)^2+(1-q_i)^2\right]/20\right)$$



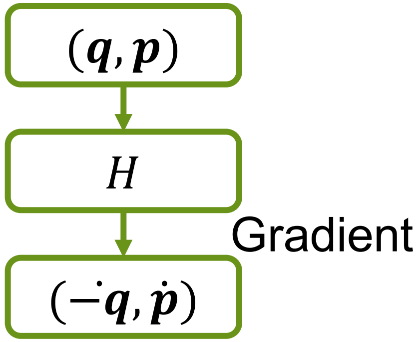
Naïve HNNs in NUTS



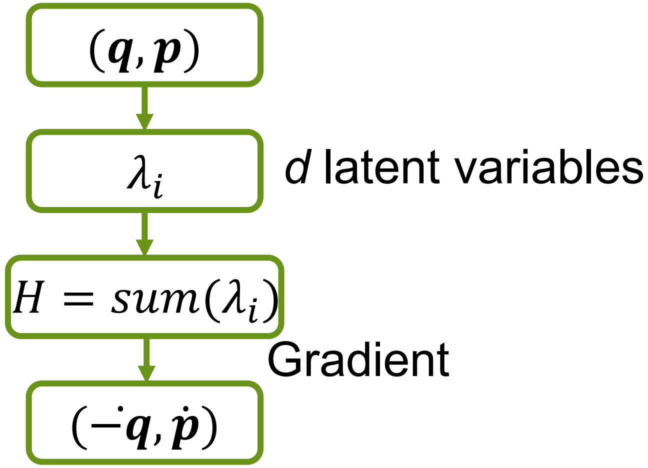
HNNs in NUTS with error monitoring (calls a few posterior gradients during the sampling)

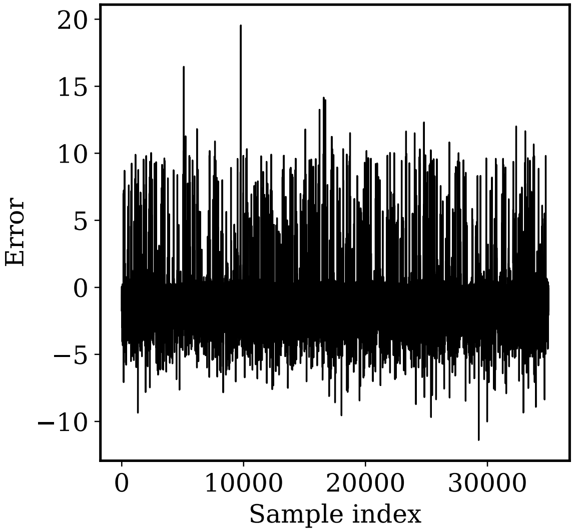
Latent output HNNs (L-HNNs)

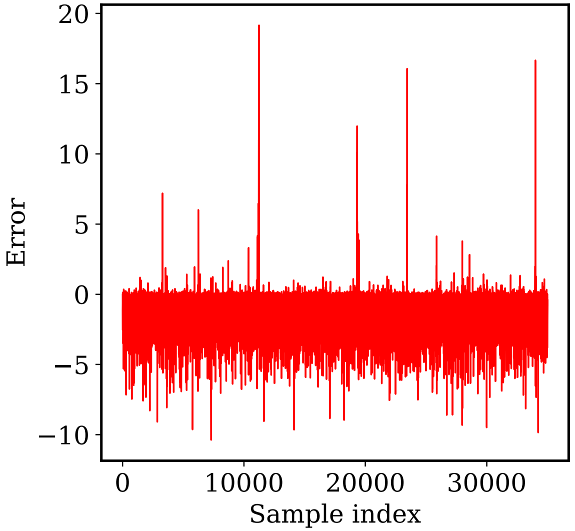
HNNs



L-HNNs





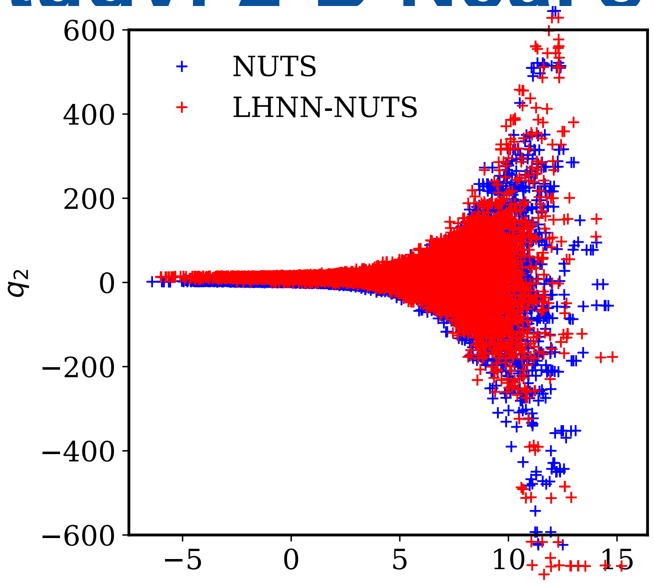


$$\varepsilon \equiv H(\boldsymbol{z}) + \ln u > \Delta_{max}$$

- 3-D Rosenbrock density
- HNNs and L-HNNs individually used in NUTS with online error monitoring
- HNNs and L-HNNs trained with the same training data
- HNNs: 4,706 samples used posterior gradients with ~1.5 Million posterior gradients during error monitoring
- L-HNNs: 180 samples used posterior gradients with ~0.064 Million posterior gradients during error monitoring

Method	ESS/gradient
Traditional NUTS	0.000128
HNNs in NUTS with online error monitoring	0.000824
L-HNNs in NUTS with online error monitoring	**0.00236**

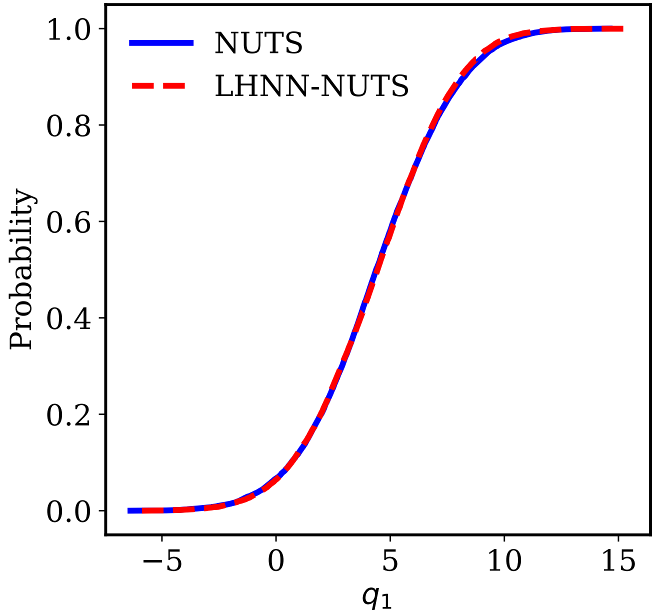
Case study: 2-D Neal's funnel density

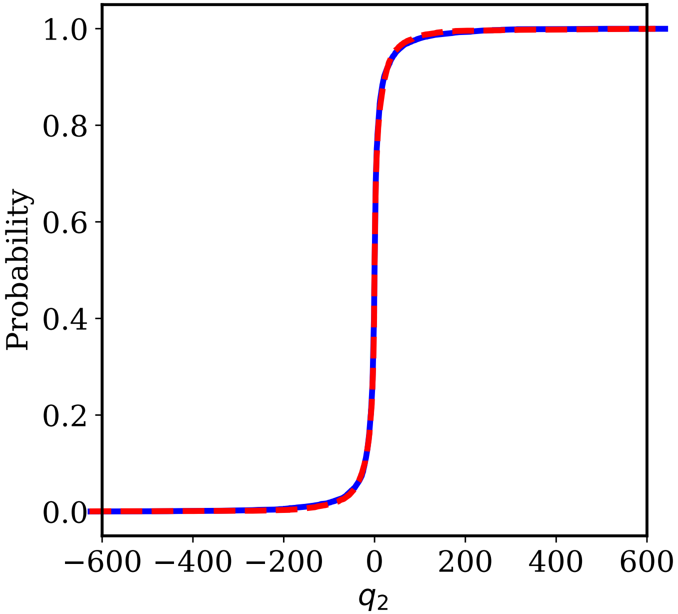


$$f(\boldsymbol{q}) \propto \begin{cases} q_1 = \mathcal{N}(0,\ 3) \\ q_2 = \mathcal{N}(0,\ \exp^{q_1}) \end{cases}$$

25,000 samples

Method	# gradients	ESS/gradient
Traditional NUTS	16.6 Mil	0.000052
L-HNNs in NUTS with online error monitoring (proposed)	**3.59 Mil**	**0.000234**





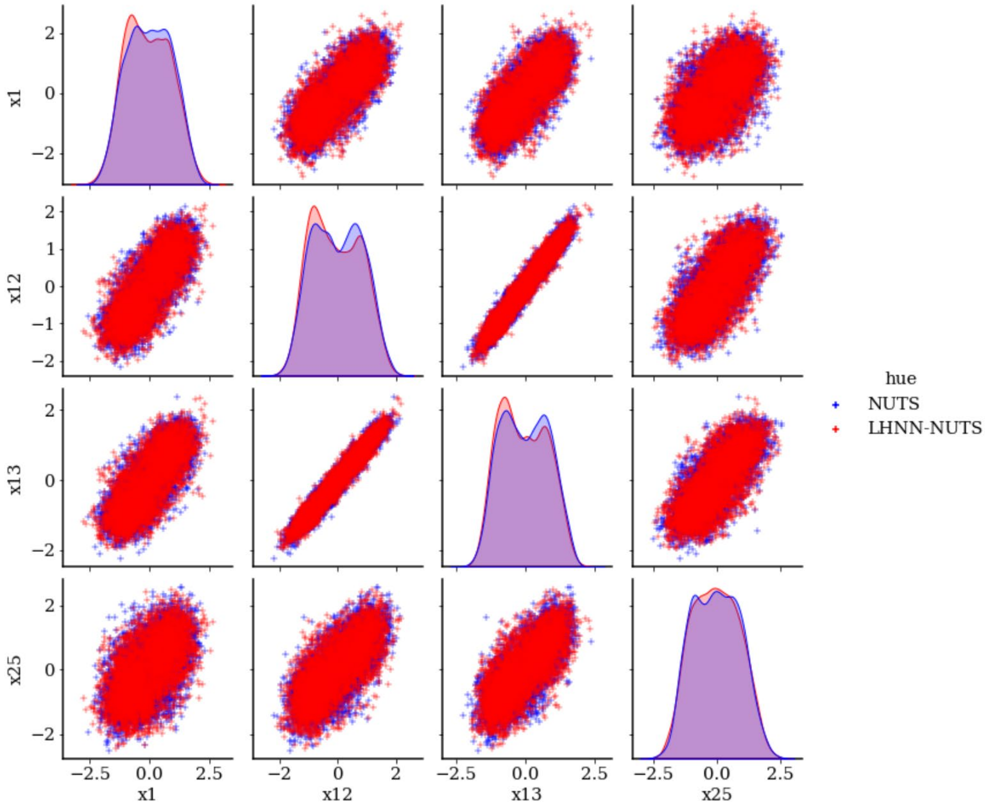
Case study: 25-D Allen-Cahn Equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - V'(u) + \sqrt{2}\eta$$

where, $V(u) = (1-u^2)^2$

$$\pi(\boldsymbol{u}) \propto \exp\left(-\int_0^1 \left(\frac{1}{2}\left(\frac{\partial u}{\partial x}\right)^2 + V(u(x))\right)dx\right)$$

$$\pi(\boldsymbol{u}) = \exp\left(-\sum_{i=0}^{d-1}\left(\frac{1}{2\Delta x}\big(u(i\Delta x+\Delta x) - u(i\Delta x)\big)^2 + \frac{\Delta x}{2}\Big(V\big(u(i\Delta x+\Delta x)\big) - V\big(u(i\Delta x)\big)\Big)\right)\right)$$



Method	# gradients	ESS/gradient
Traditional NUTS	0.681 Mil	0.00032
L-HNNs in NUTS with online error monitoring (proposed)	**0.097 Mil**	**0.00423**

Goodman and Weare (2010)

Case study: 50-D elliptic PDE

$$\frac{\partial}{\partial x}\left(k(x,y)\,\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(k(x,y)\,\frac{\partial u}{\partial y}\right) = f(x,y)$$

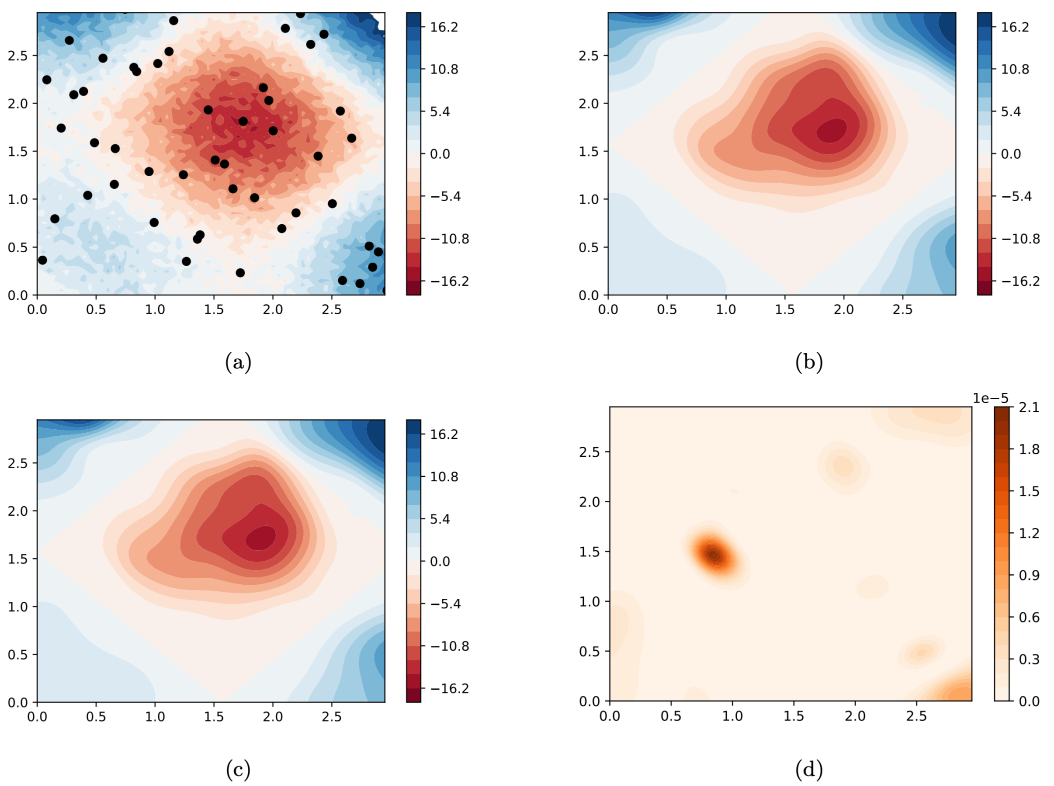
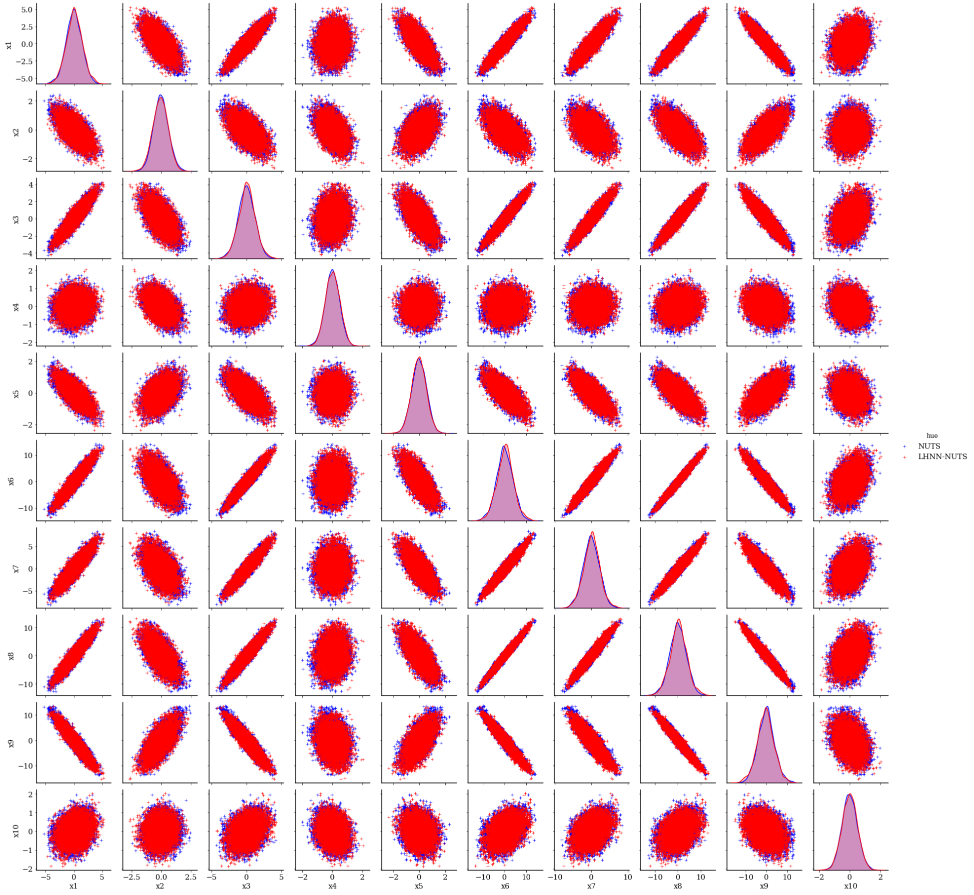


Figure 12: (a) The $f(x,y)$ field corrupted by a Gaussian noise and the points at which $f(x,y)$ is recorded for treating as experimental data. (b) and (c) The estimated mean $f(x,y)$ field after performing Bayesian inference using LHNN-NUTS and NUTS, respectively. (d) Mean squared error of the mean $f(x,y)$ field between LHNN-NUTS and NUTS.

Method	# gradients	ESS/gradient
Traditional NUTS	0.621 Mil	0.0065
L-HNNs in NUTS with online error monitoring (proposed)	**0.217 Mil**	**0.015**

Future work



100-D Gaussian with inverse Wishart covariance (NUTS: 5.61 Mil gradients; LHNN-NUTS: 1.46 Mil gradients)

- **Newer HNN-type architectures:** Physics-informed HNNs and SympNets
- **Sampling with physical constraints:** nuclear fuel model calibration. Spherical HMC with L-HNNs (Yifeng Che is leading this)
- **L-HNNs trained on Manifolds:** Riemannian HMC with L-HNNs; better ESS due to neutralizing bad posterior geometry
- **Active (or online) learning:** Proposed online error monitoring similar in concept; but no re-training of L-HNNs.

Thank you
(Som.Dhulipala@inl.gov)

Resources:

"Bayesian Inference with Latent Hamiltonian Neural Networks" *arXiV:2208.06120*

"Physics-Informed Machine Learning of Dynamical Systems for Efficient Bayesian Inference" *arXiv:2209.09349*