
A Revisit of Hamiltonian Monte Carlo Efficiency on Bayesian Neural Networks

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Abstract

Bayesian neural networks (BNNs) offer principled uncertainty quantification, yet sampling from their posteriors via Hamiltonian Monte Carlo (HMC) remains challenging. While recent work theoretically identified the efficiency degradation of ReLU-based networks, smooth unbounded activations (*e.g.*, GELU, Swish, Mish), which are prevalent in modern architectures, were assumed to be efficient due to their smoothness. In this work, we challenge this existing justification by deriving explicit local error formulas for the leapfrog integrator. Our analyses reveal that in addition to differentiability, third-order curvatures of the potential energy also have significant influences on the HMC efficiency of BNNs inference. Empirically, we found that even smooth unbounded activations may degrade sampling performance as severely as piecewise linear activations. Thus, optimally tuning the step size for these networks may require a comparable empirical step size scaling as their piecewise counterparts. This result sheds light on the implications for architecture design in Bayesian deep learning.

1 Introduction

Bayesian neural networks (BNNs) have emerged as an important research direction in recent years, offering principled uncertainty quantification in neural network predictions [Hernández-Lobato and Adams, 2015, Dhulipala et al., 2023, Liu et al., 2024, Papamarkou et al., 2024]. Unlike optimization-based approaches for neural networks, BNNs treat the parameters as random variables and infer a posterior distribution over the parameter space, allowing principled estimates of model confidence [Gal and Ghahramani, 2016, Wang et al., 2024] and robustness [Trinh et al., 2022]. However, sampling from the posterior of BNNs remains computationally challenging due to the high dimensionality of the parameter space and the non-convex nature of neural network loss landscapes.

Approximate posterior inference methods have been proposed to address this challenge. Variational inference [Blei et al., 2017, Ritter et al., 2018] offers computational scalability but suffers from variance underestimation [Blei et al., 2017, Giordano et al., 2018]. In contrast, Hamiltonian Monte Carlo (HMC) [Neal, 2011] provides a rigorous approach that asymptotically converges to the target distribution, offering more accurate uncertainty estimates. HMC leverages gradient information to generate distant, high-quality proposals in high-dimensional spaces, making it particularly suited for the parameter spaces of neural networks.

While theoretical analyses of HMC have been developed for various probabilistic models [Nishimura et al., 2020, Dinh et al., 2017, Mohasel Afshar and Domke, 2015], the theoretical understanding of HMC applied to BNNs remains overlooked. A recent work by Dinh et al. [2024] shows that BNNs with ReLU activations exhibit degraded sampling efficiency compared to those using smooth activation functions. This degradation stems from the non-differentiability of ReLU at zero, which introduces a qualitatively different type of discretization error. Consequently, ReLU-based BNNs require smaller step sizes and yield substantially lower acceptance rates than their smooth counterparts. However, this study does not account for other widely-used design choices in modern deep learning architectures [Vaswani et al., 2017, Dosovitskiy et al., 2021], most notably the class of smooth but unbounded activation functions. Recent state-of-the-art models [Grattafiori et al., 2024, Bai et al., 2023] increasingly employ this class of activation functions such as GELU [Hendrycks and Gimpel, 2016], Swish [Ramachandran et al., 2017], and Mish [Misra, 2019]. These functions are theoretically smooth everywhere, suggesting they should allow HMC to operate efficiently with the standard $O(\varepsilon^3)$ local error bounds [Neal, 2011, Betancourt et al., 2017]. Nevertheless, existing analyses typically treat the gradient magnitude as a static constant within the error bound, focusing primarily on tuning the step size ε to optimize efficiency, rather than accounting for the dynamic behaviour of the potential energy landscape.

To address this critical gap, we explicitly characterize how activation functions impact the error of the leapfrog integrator in HMC for BNNs. By deriving explicit local error formulas for both smooth and piecewise functions, we reveal that the energy function landscape, often treated as negligible coefficients in classical analyses [Dinh et al., 2017, Beskos et al., 2013], can become the primary source of HMC error. Furthermore, we demonstrate that sampling efficiency is driven by the complex interplay between this landscape, gradient stability, and smoothness. *Surprisingly, even smooth activation functions can be as ineffective as their piecewise counterparts (Figure 2).* These findings indicate that the choice of activation function is a crucial design hyperparameter that fundamentally dictates MCMC efficiency in BNNs.

Our contributions. In this work, we make the following contribution to the theoretical understanding of HMC with the leapfrog integrator for Bayesian neural networks inference:

- (1) We derive explicit constants in the leading order of local error formulas for HMC in BNNs, providing a theoretical analysis for smooth and piecewise activation regimes.
- (2) By analyzing these constants, we derive bounds and empirically verify that unbounded activation functions generate large third-order curvature, directly amplifying leapfrog local error. This severe degradation in sampling efficiency challenges the classical belief that simply having a smooth activation function guarantees effective HMC.
- (3) We empirically validate our theoretical framework on synthetic and real-world datasets, highlighting that even smooth activation functions might severely degenerate sampling performance.

Related works. Classical HMC analyses assume the potential energy function $U(\mathbf{q})$ is smooth. Under this assumption, the leapfrog integrator preserves volume, and the algorithm has well-established theoretical guarantees. Beskos et al. [2013] showed that HMC scales favourably with dimension and attains an optimal acceptance rate of 0.651 while it outperforms both MALA (0.574) and random-walk Metropolis (0.234). Betancourt et al. [2017] established conditions for geometric ergodicity, guaranteeing exponential convergence to the target distribution.

When the energy function is non-smooth, direct application of HMC is not straightforward. Non-smooth and discontinuous energy functions arise naturally in preference learning [Afshar et al., 2015], probabilistic programming [Lunn et al., 2009], phylogenetic tree inference [Dinh et al., 2017], and population sizes inference [Nishimura et al., 2020]. In such settings, the leapfrog integrator fails to conserve the Hamiltonian, and numerical modifications such as surrogate functions [Dinh et al., 2017] or variable mapping [Pakman and Paninski, 2013] are required to recover correctness.

The theoretical foundations of HMC for BNNs remained largely unaddressed until Dinh et al. [2024] established that piecewise affine activations (e.g., ReLU) suffer a degeneration of local error to $\Omega(\varepsilon)$ due to gradient jumps at surfaces of non-differentiability. However, their analysis primarily treats curvatures as static and neglects the empirical impacts of large curvature on the efficiency of HMC for BNNs with unbounded smooth activations.

2 Preliminaries

Bayesian Neural Networks. We consider a general feed-forward neural network represented by a function $f(\mathbf{x}; \mathbf{q})$, where the parameter vector $\mathbf{q}$ contains the flattened and concatenated weight matrices and bias vectors of all layers. The network is structured as a composition of M layers, that is, $f = f_M \circ f_{M-1} \circ \dots \circ f_1$. Here, each hidden layer $\{f_j\}_{j=1}^{M-1}$ applies a linear transformation followed by a point-wise non-linear activation function φ , and f_M linearly maps the last hidden representation to a d_y dimensional output space $\mathcal{Y} \subseteq \mathbb{R}^{d_y}$. Formally, given a d_i dimensional input $\mathbf{x} \in \mathbb{R}^{d_i}$ and let $d_0 = d_i$ and $d_M = d_y$, the network output is computed via the recursive equations:

$$\begin{aligned} z_0 &= \mathbf{x}, \\ z_j &= \varphi(\mathbf{W}_j z_{j-1} + \mathbf{b}_j), \quad \forall j = 1, \dots, M-1, \\ f(\mathbf{x}; \mathbf{q}) &= \mathbf{W}_M z_{M-1} + \mathbf{b}_M, \end{aligned}$$

where $\mathbf{W}_j \in \mathbb{R}^{d_j \times d_{j-1}}$ and $\mathbf{b}_j \in \mathbb{R}^{d_j}$ are the weight matrix and bias vector of the j^{th} layer, respectively.

Unlike optimization-based approaches that yield a single point estimate, BNNs treat parameters $\mathbf{q}$ as random variables and infer a posterior distribution over the parameters $\mathbf{q}$ conditioned on the observed dataset $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$. Here, x_i, y_i are the input and target value corresponding to the i^{th} observation, which are independently and identically sampled from an unknown distribution. Assuming that $\mathbf{q}$ belongs to a parameter space $\mathcal{Q}$, the posterior is defined following the Bayes' rule:

$$P(\mathbf{q} \mid \mathcal{D}) \propto \pi(\mathbf{q}) \prod_{i=1}^N \mathcal{L}(\mathbf{q} \mid \mathbf{x}_i, y_i), \quad (1)$$

where $\pi(\mathbf{q})$ is the prior density and $\mathcal{L}(\mathbf{q} \mid \mathbf{x}_i, y_i)$ is the likelihood function given a single data point. The posterior predictive distribution of target y^* at a new input $\mathbf{x}^*$ can be computed from the posterior expectation $P(y^* \mid \mathbf{x}^*, \mathcal{D}) = \int_{\mathbf{q} \in \mathcal{Q}} \mathcal{L}(\mathbf{q} \mid \mathbf{x}^*, y^*) P(\mathbf{q} \mid \mathcal{D}) d\mathbf{q}$. Computing this integral is generally intractable for complex neural networks; hence we can resort to Monte Carlo methods able to provide approximations $P(y^* \mid \mathbf{x}^*, \mathcal{D}) \approx \frac{1}{m} \sum_{i=1}^m \mathcal{L}(\mathbf{q}_i \mid \mathbf{x}^*, y^*)$ given a sample $\{\mathbf{q}_i\}$ suitably simulated from the posterior distribution $P(\mathbf{q} \mid \mathcal{D})$. HMC is a widely used simulation method due to the availability of the gradients of the neural networks and its efficiency in exploring the parameter space.

Hamiltonian Monte Carlo (HMC). HMC is a Markov chain Monte Carlo method that leverages gradient information to generate distant, high-quality proposals in high-dimensional settings (e.g., the parameter space of BNNs). To sample from a posterior distribution $P(\mathbf{q} \mid \mathcal{D})$, HMC augments the position $\mathbf{q} \in \mathbb{R}^d$ with an auxiliary momentum variable $\mathbf{p} \in \mathbb{R}^d$, typically drawn from a standard normal distribution for simplicity, $\mathbf{p} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$. This defines a joint canonical distribution:

$$P(\mathbf{q}, \mathbf{p}) \propto \exp(-H(\mathbf{q}, \mathbf{p})),$$

where $H(\mathbf{q}, \mathbf{p}) = U(\mathbf{q}) + K(\mathbf{p})$ with $U(\mathbf{q}) = -\log P(\mathbf{q} \mid \mathcal{D})$ and $K(\mathbf{p}) = \frac{1}{2} \|\mathbf{p}\|^2$. Here, $H(\mathbf{q}, \mathbf{p})$, $U(\mathbf{q})$, and $K(\mathbf{p})$ are the total energy (*Hamiltonian*), the potential energy, and the kinetic energy of the system, respectively. The system evolves according to Hamilton's equations:

$$\frac{d\mathbf{q}}{dt} = \frac{\partial H}{\partial \mathbf{p}} = \mathbf{p}, \quad \frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{q}} = -\nabla U(\mathbf{q}). \quad (2)$$

Because Hamiltonian dynamics are defined in continuous time, they must be discretised for practical implementation. The *leapfrog integrator* is the standard choice due to its reversibility and volume-preservation. Starting from the initial state $(\mathbf{q}_t, \mathbf{p}_t)$, the *leapfrog integrator* returns a new state $(\mathbf{q}_{t+\varepsilon}, \mathbf{p}_{t+\varepsilon})$ using the discrete steps:

$$\mathbf{p}_{t+\varepsilon/2} = \mathbf{p}_t - \frac{\varepsilon}{2} \nabla U(\mathbf{q}_t), \quad (3)$$

$$\mathbf{q}_{t+\varepsilon} = \mathbf{q}_t + \varepsilon \mathbf{p}_{t+\varepsilon/2}, \quad (4)$$

$$\mathbf{p}_{t+\varepsilon} = \mathbf{p}_{t+\varepsilon/2} - \frac{\varepsilon}{2} \nabla U(\mathbf{q}_{t+\varepsilon}). \quad (5)$$

HMC employs the above procedures to iteratively draw samples from the canonical distribution in two steps. In the first step, a momentum vector value $\mathbf{p}_i$ is sampled from $\mathcal{N}(\mathbf{0}, \mathbf{I})$, allowing the chain to explore different energy levels and discover the full parameter space. In the second step, given the current state $(\mathbf{q}_i, \mathbf{p}_i)$, HMC performs L leapfrog steps with step size ε to generate a new proposal

$(\mathbf{q}^*, \mathbf{p}^*)$. This proposal is accepted or rejected according to the Metropolis-Hastings criterion with probability $\alpha = \min\{1, \exp(-H(\mathbf{q}^*, \mathbf{p}^*) + H(\mathbf{q}_i, \mathbf{p}_i))\}$, resulting in a new state $(\mathbf{q}_{i+1}, \mathbf{p}_{i+1})$. This procedure allows HMC to suppress the random-walk behaviour of traditional sampling methods, offering a higher acceptance probability.

When the potential energy U is smooth, HMC has well-established theoretical properties that guarantee its correctness and efficiency, even with BNNs. In particular, the *local error* over a single step is of the order $O(\varepsilon^3)$. Since HMC is often tuned using a fixed traversal length $T = L\varepsilon$, the *global error* after L steps scales as $O(T\varepsilon^2)$ [Beskos et al., 2013].

Efficiency and Optimal Tuning of HMC. The practical performance of HMC depends critically on the step size ε and the trajectory length T . The efficiency of HMC is defined as

$$\text{eff}(\ell) = \ell \cdot \mathbb{E}[A(\mathbf{q}, \ell)], \quad (6)$$

where ℓ is a tunable scaling parameter for the step size (e.g., $\varepsilon = \ell d^{-1/4}$ in [Beskos et al., 2013]) and $\mathbb{E}[A(\mathbf{q}, \ell)]$ is the expected acceptance probability. Maximising this efficiency is equivalent to minimising the expected computational cost per accepted sample.

For a target distribution composed of $d \gg 1$ smooth i.i.d. components, Beskos et al. [2013] showed that the step size must scale as $\varepsilon = \mathcal{O}(d^{-1/4})$ to maintain an $\mathcal{O}(1)$ acceptance probability, and that efficiency is maximised at an optimal acceptance rate of approximately 0.651. In the high-dimensional limit, the expected acceptance probability satisfies

$$\lim_{d \rightarrow \infty} \mathbb{E}[A(\mathbf{q}, \ell)] = 2\Phi\left(-\frac{\ell^2 \sqrt{\Sigma}}{2}\right) =: a(\ell), \quad (7)$$

where Φ is the standard normal c.d.f. and Σ is a positive constant related to the leapfrog step size. Betancourt et al. [2017] subsequently relaxed the target to $a(\ell) \in [0.6, 0.9]$.

For BNNs with ReLU activations, Dinh et al. [2024] demonstrated that non-differentiability at the origin introduces a qualitatively different regime. Although HMC remains *correct*, provided that derivatives are defined consistently up to the second order and compatible with the chain rule, its *efficiency* degrades substantially: the local error grows from $O(\varepsilon^3)$ to $\Omega(\varepsilon)$. As a result, the step size must scale as $O(d^{-1/2})$, and the optimal acceptance rate reduces to approximately $[0.4, 0.75]$.

3 Errors of HMC for BNNs with Smooth Activations

3.1 Assumptions and Correctness

We formally state our assumption on the regularity of the loss function $\mathcal{L}(\mathbf{x}, y; \mathbf{q})$, which corresponds to the likelihood function:

Assumption 1 *The likelihood function $\mathcal{L}(\mathbf{q}|\mathbf{x}, y)$ is smooth (i.e., infinitely differentiable).*

This assumption is justified in practice by the widespread adoption of the Mean Squared Error loss for regression and the Cross-Entropy loss for classification. In addition, in our analysis, we assume that the activation function is smooth and well-defined up to the third order derivative. As a result, we only consider activation functions that belong to the $\mathbb{C}^3$ class, which is stated in the following assumption:

Assumption 2 *The function $\varphi \in C^3(\mathbb{R})$, i.e. φ is at least three times continuously differentiable.*

We note that this assumption is realistic and covers a vast number of activation functions in practice, including Sigmoid, Tanh, GeLU [Hendrycks and Gimpel, 2016], Swish [Ramachandran et al., 2017], Mish [Misra, 2019]. Under the above assumptions, following [Dinh et al., 2024], we can conclude that the leapfrog HMC applied to neural networks with smooth activation functions is correct, as the integrator remains reversible and volume-preserving. Traditional analyses of smooth Hamiltonian systems establish that the local error of the leapfrog integrator is of order $O(\varepsilon^3)$ [Neal, 2011, Betancourt et al., 2017]. These analyses treat the gradient’s magnitude as a fixed, static constant within the error bound, rather than a dynamic factor, and focus on how to tune the step size ε to attain the optimal efficiency. In addition, these analyses do not characterise how the local error depends on the neural network architecture, which could be attributed to activation functions. Next, we derive the explicit formula to reveal this dependency.

3.2 Explicit Local Error Formula

We consider an HMC sampler for BNNs with smooth activation functions to derive an explicit formula for the local error of a single leapfrog step. To give a demonstration of our result, we first consider a simple case where the particle moves following a single leapfrog update. The particle starts at $(\mathbf{q}_0, \mathbf{p}_0)$ and ends at $(\mathbf{q}_1, \mathbf{p}_1)$. Along the linear path from $\mathbf{q}_0$ to $\mathbf{q}_1 = \mathbf{q}_0 + \varepsilon \mathbf{p}_{1/2}$, the surface is smooth. The local error is $\Delta H = H(\mathbf{q}_1, \mathbf{p}_1) - H(\mathbf{q}_0, \mathbf{p}_0) = \Delta U + \Delta K$, where $\Delta U = U(\mathbf{q}_1) - U(\mathbf{q}_0)$ and $\Delta K = K(\mathbf{p}_1) - K(\mathbf{p}_0)$. Then, we derive an explicit formula of local error in Theorem 1.

Theorem 1 (Single-step local error) *Consider a single leapfrog step starting at $(\mathbf{q}_0, \mathbf{p}_0)$ and ending at $(\mathbf{q}_1, \mathbf{p}_1)$. There exists $\xi \in (0, \varepsilon)$ such that the local approximation error of a single leapfrog step is given by:*

$$\Delta H = \underbrace{\frac{\varepsilon^2}{8} \left(\|\nabla U(\mathbf{q}_1)\|^2 - \|\nabla U(\mathbf{q}_0)\|^2 \right)}_{\text{gradient norm difference}} - \underbrace{\frac{\varepsilon^3}{12} \langle \nabla^3 U(\mathbf{q}_0 + \xi \mathbf{p}_{1/2}), \mathbf{p}_{1/2} \otimes \mathbf{p}_{1/2} \otimes \mathbf{p}_{1/2} \rangle}_{\text{third-order curvature}}, \quad (8)$$

where $\otimes$ is the tensor product and, $(\mathbf{u} \otimes \mathbf{v} \otimes \mathbf{w})_{ijk} = \mathbf{u}_i \mathbf{v}_j \mathbf{w}_k, \forall \mathbf{u}, \mathbf{v}, \mathbf{w} \in \mathbb{R}^d$. We denote $\langle \mathbf{T}, \mathbf{v} \otimes \mathbf{v} \otimes \mathbf{v} \rangle := \sum_{i,j,k=1}^d \mathbf{T}_{ijk} \mathbf{v}_i \mathbf{v}_j \mathbf{v}_k$ as the tensor contraction.

Theorem 1 identifies two distinct sources by which the activation function influences the local error of HMC for BNNs (1) **Gradient stability**: The activation function directly controls the difference in gradient norms over a single leapfrog step; (2) **Energy function geometry**: The local error depends on the third-order derivatives of the potential energy U with respect to the network parameters, which in turn is affected by the activation function's output and the chain rule. Due to differences in the energy landscapes of neural networks with various activation functions, we hypothesize that the local error, which governs HMC efficiency, is primarily driven by third-order curvature. Our experiment in Section 5 verify this claim. Proofs are provided in the Appendix.

Example 1 (Regression). Consider a single-hidden-layer BNN with one neuron. The model parameters are $w, v \in \mathbb{R}$. The network output is given by $z = v\varphi(wx)$, where $\varphi \in C^3(\mathbb{R})$ is the activation function. Given a standard Gaussian prior $\mathcal{N}(0, 1)$ assigned independently on w, v and a squared error loss $(y - z)^2$, the potential energy function is $U(w, v) = \frac{1}{2}(w^2 + v^2) + (y - z)^2$. We can derive a local upper bound for the curvature:

$$\begin{aligned} \|\nabla^3 U(\mathbf{q})\|_\infty &\leq 6v^2 |x|^3 \|\varphi'\|_\infty \|\varphi''\|_\infty \\ &\quad + 2|v| |x|^3 |y - z| \|\varphi'''\|_\infty + 4|v|x^2 \|\varphi'\|_\infty^2 + 2x^2 \|\varphi''\|_\infty |y - 2z| + 4|x| |\varphi(u)| \|\varphi'\|_\infty, \end{aligned}$$

where $u = wx$ is the pre-activations. From the above inequality, the HMC efficiency is governed by the following elements: (1) **Data**: x, y ; (2) **Parameter state**: w (indirectly) and v (directly); (3) **Activation gradients**: $\|\varphi'\|_\infty, \|\varphi''\|_\infty, \|\varphi'''\|_\infty$, which are bounded for most popular smooth activation functions; (4) **Activation output**: $\varphi(u)$. Unbounded activations may let the activation output $\varphi \rightarrow \infty$, leading to an uncontrollable local error. Interestingly, in Section 5, we show that Softplus achieves a sampling efficiency comparable to GeLU despite having a significantly lower third-order derivative magnitude like Sigmoid ($\|\varphi'''\|_\infty = 0.125$). This observation confirms that smoothness is necessary but insufficient to guarantee HMC performance. Instead, the error characterized in Theorem 1 is fundamentally governed by the interplay between data, parameter state, and activation output. Full derivations are provided in the Appendix.

Example 2 (Binary Classification). We consider a binary classification problem with a one-hidden-layer BNN having a single neuron. In that case, we denote $w \in \mathbb{R}^d$ and $v \in \mathbb{R}$ as input-to-hidden and hidden-to-output weights, respectively. Let $u = wx$ be the pre-activation, the predictive function is given by $f(x; w) = \sigma(v\varphi(wx))$, where $\varphi \in C^3(\mathbb{R})$ is the activation function, σ is the sigmoid function. Given a standard Gaussian prior $\mathcal{N}(0, 1)$ assigned on w, v and a cross entropy loss $-\left[y \log p + (1 - y) \log(1 - p)\right]$, the potential energy function is $U(w, v) = \frac{1}{2}(w^2 + v^2) - y(v\varphi(wx)) + \log(1 + e^{v\varphi(wx)})$. Given the location of the network $\mathbf{q} = [w, v]$, the upper bound for

the third-order curvature is given as:

$$\begin{aligned} \|\nabla^3 U(\mathbf{q})\|_\infty &\leq C(|v|^3 \|\varphi'\|_\infty^3 |x|^3 + v^2 \|\varphi'\|_\infty \|\varphi''\|_\infty |x|^3 + |v| \|\varphi'''\|_\infty |x|^3 + |\varphi(u)|^3 \\ &\quad + |v| |x| \|\varphi'\|_\infty \varphi(u)^2 + |x| \|\varphi'\|_\infty |\varphi(u)| + v^2 x^2 |\varphi(u)| \|\varphi'\|_\infty^2 \\ &\quad + |v| x^2 (\|\varphi'\|_\infty^2 + |\varphi(u)| \|\varphi''\|_\infty) + x^2 \|\varphi''\|_\infty), \end{aligned}$$

where C is a universal constant. As in the regression example, the third-order curvature for classification remains dependent on the *data*, the *parameter state*, the *activation gradients*, and the *activation output*. More importantly, the degree of $\varphi(u)$ in the previous inequality is of order three, suggesting that the activation output is more influential in the classification problem. This phenomenon is evidenced by the degeneration of Softplus observed in Section 5. This example highlights how the boundedness of the activation function helps govern the local error of the leapfrog integrator in classification tasks. Detailed proofs are provided in the Appendix.

3.3 Global Error over a Full Trajectory

Using Theorem 1 on the error of a single leapfrog step, we extend our results to cover the error of a full trajectory. Corollary 1 below states our finding.

Corollary 1 (Global Error) *Under Assumption 1 and Assumption 2, there exists $\xi_l \in (0, \varepsilon)$ for each l^{th} step such that the accumulated error after L leapfrog steps with step size ε is given as:*

$$\Delta H_L = \frac{\varepsilon^2}{8} \left(\|\nabla U(\mathbf{q}_L)\|^2 - \|\nabla U(\mathbf{q}_0)\|^2 \right) - \frac{\varepsilon^3}{12} \sum_{l=0}^{L-1} \langle \nabla^3 U(\mathbf{q}_l + \xi_l \mathbf{p}_{l+\frac{1}{2}}), \mathbf{p}_{l+\frac{1}{2}} \otimes \mathbf{p}_{l+\frac{1}{2}} \otimes \mathbf{p}_{l+\frac{1}{2}} \rangle$$

where $\mathbf{p}_{l+\frac{1}{2}} = \mathbf{p}_l - \frac{\varepsilon}{2} \nabla U(\mathbf{q}_l)$ is the momentum at the half step of l^{th} step.

Remark. The gradient norm terms $\|\nabla U(\mathbf{q}_l)\|^2$ telescope across steps, leaving only boundary differences. In contrast, third-order terms accumulate additively; this is why unbounded activations cause progressively worse errors for longer trajectories.

According to Corollary 1, the efficiency of HMC, which is intrinsically linked to the acceptance rate α , is fundamentally governed by the global error ΔH_L . When $|\Delta H_L|$ is large, proposals are frequently rejected, causing the efficiency $\text{eff}(\ell) = \ell \cdot \mathbb{E}[A(\mathbf{q}, \ell)]$ in eq. (7) to degrade. In Section 5, we empirically demonstrate that smooth activation functions, particularly unbounded ones like Swish, can exhibit significantly large third-order curvature. Consequently, mathematically smooth functions suffer from poor sampling efficiency, potentially performing no better than piecewise linear counterparts. These results suggest that existing theoretical frameworks are insufficient to fully characterize the challenges of sampling from the posteriors of deep neural networks.

4 Errors of HMC for BNNs with Piecewise smooth Activations

Building on our previous derivation for smooth activations, we now relax these smoothness constraints and turn our attention to the piecewise smooth activation functions. These functions remain continuous but non-differentiable at specific points. By accounting for these functions, we extend our error analysis to cover a range of widely used activation functions in deep learning.

4.1 Assumptions and correctness

We relax the Assumption 2 with the following weaker assumption to cover the piecewise activations with a single point of non-differentiability at the origin:

Assumption 3 (Piecewise smooth function) *The activation function φ is piecewise smooth at the origin if and only if: (1) $\varphi \in C^0(\mathbb{R})$ (continuous everywhere); (2) $\varphi \in C^\infty(\mathbb{R} \setminus \{0\})$ (smooth everywhere except at 0); (3) $\varphi \notin C^1(\mathbb{R})$ (first-order derivative is not continuous at 0)*

This assumption is satisfied by most activations such as ReLU and LeakyReLU with $\alpha \neq 1$. Under these conditions, the HMC leapfrog integrator for BNNs works correctly regardless of the derivative's value at 0, so long as that value remains consistently defined. In addition, the potential energy function

$U(\mathbf{q})$ is smooth almost everywhere on $\mathcal{Q}$, but exhibits jump discontinuities in its first derivative across a collection of surfaces in the parameter space. Lemma 3.2 in [Dinh et al. \[2024\]](#) characterises the geometry of these surfaces. Briefly, this surface $\mathcal{S}$ is the union of many smooth surfaces $\mathcal{S}_i$ such that $\mathcal{S}_i = \{\mathbf{q} : g_i(\mathbf{q}) = 0\}$ for any analytic function g_i , that is, $\mathcal{S} = \bigcup_{i \in \mathcal{I}} \mathcal{S}_i$.

As the particle traverses the parameter space following the leapfrog integrator, discontinuities are encountered whenever the trajectory crosses a surface in $\mathcal{S}$, corresponding to a change in the activation state of a neuron. Specifically, for a single leapfrog step of size ε , the linear path $\mathbf{q}(t) = \mathbf{q}_0 + t\mathbf{p}_{1/2}$ for $t \in [0, \varepsilon]$ intersects a finite number of surfaces $\mathcal{S}_1, \mathcal{S}_2, \dots, \mathcal{S}_k$ at points $\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_k$. These crossings occur at discrete times $0 < \varepsilon_1 < \varepsilon_2 < \dots < \varepsilon_k < \varepsilon$. Consequently, the path segments within the open intervals $(\varepsilon_i, \varepsilon_{i+1})$ are contained within smooth regions of U . At each intersection point $\mathbf{z}_i$, we denote by $\nabla U^-(\mathbf{z}_i)$ and $\nabla U^+(\mathbf{z}_i)$ the left and right limit of the gradient at $\mathbf{z}_i$ from the two smooth regions, respectively.

4.2 Explicit Local Error Formula

Next, we establish the explicit local error formula for BNNs utilising piecewise activations. Unlike the smooth case, the energy function here contains "kinks" that result in a discontinuous gradient. Due to these discontinuities, expressing ΔU through a single trapezoidal rule over a full interval $(0, \varepsilon)$ is no longer valid. To resolve this, we decompose the trajectory into finite subintervals where the surface of the energy function is locally smooth, so the trapezoidal approximation remains mathematically applicable. In particular, we consider a particle that crosses many surfaces of non-differentiability at $\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_k$ at time $\varepsilon_1, \varepsilon_2, \dots, \varepsilon_k$. We apply the path integral on each interval $(\varepsilon_i, \varepsilon_{i+1})$ to derive the following theorem:

Theorem 2 *Consider a single leapfrog step starting at $(\mathbf{q}_0, \mathbf{p}_0)$ and ending at $(\mathbf{q}_1, \mathbf{p}_1)$ that crosses the surfaces of non-differentiability at $\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_k$ at time $\varepsilon_1, \varepsilon_2, \dots, \varepsilon_k$. Let $\mathbf{z}_0 = \mathbf{q}_0$, $\mathbf{z}_{k+1} = \mathbf{q}_1$, $\varepsilon_0 = 0$, $\varepsilon_{k+1} = \varepsilon$. The local approximation error is given by:*

$$\begin{aligned} \Delta H = & \mathbf{p}_{1/2} \cdot \sum_{i=0}^k \frac{\Delta \varepsilon_i}{2} (\nabla U^-(\mathbf{z}_{i+1}) + \nabla U^+(\mathbf{z}_i)) - \frac{\varepsilon}{2} \mathbf{p}_{1/2} \cdot (\nabla U(\mathbf{q}_0) + \nabla U(\mathbf{q}_1)) \\ & + \frac{\varepsilon^2}{8} (\|\nabla U(\mathbf{q}_1)\|^2 - \|\nabla U(\mathbf{q}_0)\|^2) - \sum_{i=0}^k \frac{\Delta \varepsilon_i^3}{12} \langle \nabla^3 U(\mathbf{q}_0 + \xi_i \mathbf{p}_{1/2}), \mathbf{p}_{1/2} \otimes \mathbf{p}_{1/2} \otimes \mathbf{p}_{1/2} \rangle, \end{aligned}$$

where $\Delta \varepsilon_i = \varepsilon_{i+1} - \varepsilon_i$, and $\xi_i \in (\varepsilon_i, \varepsilon_{i+1})$ is an unknown time.

Compared to the local error of HMC for BNNs with smooth functions, Theorem 2 states that the local error in HMC for BNNs with non-smooth activations includes an additional term proportional to the gradient jump at each point of non-differentiability. This error is explicitly associated with the time that particles spend at the smooth region $\Delta \varepsilon$, which is proportional to ε , and the frequency of surface crossings. Specifically, as the linear path intersects more non-differentiable surfaces, the cumulative local error of the leapfrog step increases. As a result, the sampling efficiency of HMC becomes significantly harder to regulate in this regime, as the energy conservation depends on the discrete geometry of the energy landscape. Detailed proofs are provided in the Appendix.

5 Simulations

5.1 Experiments on Toy Datasets

Datasets. We consider two synthetic datasets to isolate the effect of activation functions from confounding factors. Following [\[Dinh et al., 2024\]](#), we generate $N = 100$ samples with inputs $x_i \sim \text{Uniform}(0, 4)$ and targets $y_i = \cos(2x_i) + \varepsilon_i$, where $\varepsilon_i \sim \mathcal{N}(0, 0.01)$ for regression. For classification, we use the `make_moons` dataset from `sklearn`, which is a two-dimensional binary classification dataset. We generate the training samples with 300 training and 100 test samples at a noise level of 0.1. Visualization of these datasets is given in the Appendix.

Effects of the third-order curvature for the smooth activation functions. To investigate the impact of third-order curvature on sampling efficiency, we conduct HMC inference using a standard leapfrog integrator on both regression and classification dataset. We use a fixed step size $\varepsilon = 0.002$

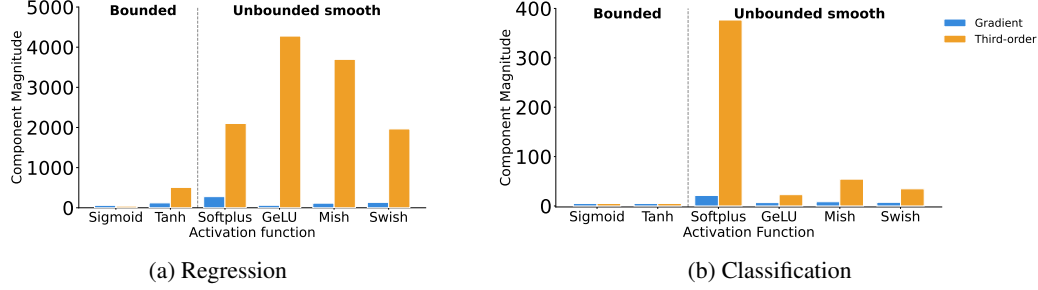


Figure 1: Decomposition of the error factors contributing to the local error of the leapfrog integrator. The third-order curvature strongly influences the error, leading to a degradation in sampling efficiency.

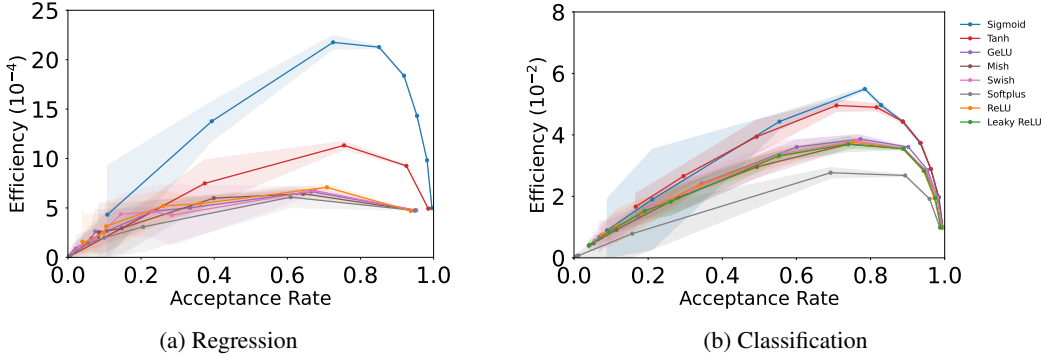


Figure 2: Efficiency of HMC with respect to acceptance rate on BNNs with different activation functions. On both synthetic regression and classification datasets, HMC inference on BNNs with bounded and smooth activations is more efficient than with unbounded or non-smooth counterparts.

with $L = 100$ leapfrog steps for regression, and $\varepsilon = 0.05$ with $L = 20$ steps for classification. We generate 3,000 samples, discarding the initial 1,000 for burn-in. To isolate the third-order contribution, we calculate its value by subtracting the gradient stability term, $\frac{\varepsilon^2}{8} (\|\nabla U(\mathbf{q}_L)\|^2 - \|\nabla U(\mathbf{q}_0)\|^2)$, from the total energy error ΔH . We use these settings for BNNs with a diverse set of smooth activation functions. We plot the averaged magnitudes over generated samples of different terms in Figure 1. We observe that curvature dynamics predominantly govern the local error for both regression and classification tasks. For regression, Sigmoid, characterized by its bounded nature and gradual slope, exhibits a minimal curvature term, resulting in a lower error than all the other activations tested. Notably, while Tanh is bounded, it incurs a higher error than Sigmoid due to its larger infinity norms of gradients and broader output range (*i.e.*, $(-1, 1)$), which will accumulate along the path. Interestingly, despite having the lowest $\|\varphi'''\|_\infty = 0.096$, Softplus exhibits a huge error due to its natural unboundedness, highlighting the effect of the unbounded activation functions on the approximation accuracy of the leapfrog integrator. Finally, unbounded activations, including GeLU, Swish, and Mish, trigger an explosion in local error that severely degrades HMC performance due to the unboundedness of the activation output. We observe the same trend for classification, except Softplus, which exhibits the highest error among unbounded activations. These empirical results provide strong validation for our theoretical derivation in Theorem 1, confirming that we cannot ignore the network gradient for efficiency analysis of HMC. Details on activation analyses are provided in the Appendix.

HMC efficiency vs. acceptance rate. We investigate HMC sampling efficiency as a function of step size ε and acceptance rate $\alpha(\varepsilon)$, using single-hidden-layer BNNs with 50 hidden units (as described above). Following Dinh et al. [2024], we fix the trajectory length $T = L\varepsilon$ and vary the step size, adjusting the number of leapfrog steps $L = \lceil T/\varepsilon \rceil$ accordingly. This protocol isolates the effect of step-size choice on sampling efficiency while maintaining constant total integration time. For regression, we set $T = 0.1$ and vary $\varepsilon \in \{0.0005, 0.001, \dots, 0.004\}$. For classification, we set $T = 0.2$ and vary $\varepsilon \in \{0.01, 0.02, \dots, 0.10\}$. For each configuration, we run HMC five times independently, generating 3000 samples per run and discarding the first 1000 as burn-in. Following

Beskos et al. [2013], we measure sampling efficiency as $\text{eff}(\varepsilon) = \varepsilon \cdot \alpha(\varepsilon)$, where $\alpha(\varepsilon)$ is the empirical Metropolis-Hastings acceptance rate at step size ε . This metric captures the trade-off between proposal distance (favored by large ε) and acceptance probability (favored by small ε). We report the mean efficiency curve across the five independent runs for each activation function.

As illustrated in Figure 2, several analytic BNN architectures exhibit an unexpected performance profile, with sampling efficiencies matching those of ReLU-based networks. While bounded activations like Sigmoid and Tanh remain significantly more efficient, surpassing other models by 3 to 4 times, their unbounded counterparts suffer from severe degradation. Our results provide a broader generalization of the findings by Dinh et al. [2024]. Specifically, we demonstrate that a comprehensive characterization of sampling performance must account for the boundedness of the activation functions, as this property directly influences the curvature term derived in our analysis. Furthermore, these results are consistent with the activation function error order observed in Figure 1. Finally, we observe that the optimal acceptance rates for Tanh and the unbounded activations are around 0.8. Despite exceeding the traditional optimal rate 0.651, this value remains consistent with the recommended range $[0.6, 0.9]$ proposed by Betancourt et al. [2017].

Effects of network architecture. We also examine how parameter dimensionality and network depth affect sampling. While acceptance rates generally decay as dimensionality increases, networks with unbounded activation functions show significantly lower acceptance rates than those with bounded ones (see Appendix D).

5.2 Experiments on Real-world Dataset

To investigate whether our theoretical findings hold on a real-world environment, we conduct an experiment using the TMDb movie dataset. This dataset provides comprehensive metadata for approximately 5,000 films, including financial metrics (e.g., budget, revenue), creative attributes (e.g., full cast and crew listings), and audience engagement markers (e.g., user ratings). Our primary objective is to predict the averaged_vote using five features as independent variables: budget, popularity, revenue, runtime, and vote count. In this experiment, we employ HMC with a fixed trajectory length $T = 0.005$ while varying the step size ε across the range $\{5 \times 10^{-5}, 2.5 \times 10^{-4}, \dots, 1.25 \times 10^{-3}\}$. Details are provided in the Appendix.

Following Section 5.1, we plot the efficiency as a function of the acceptance rate in Figure 3. The results demonstrate that BNNs utilizing the Sigmoid activation function achieve the highest efficiency, which directly aligns with our previous toy dataset simulations. Conversely, unbounded activations consistently exhibit lower efficiency compared to Sigmoid. Interestingly, the Tanh activation function shows a severe degradation in performance, falling to levels on par with unbounded activations. This phenomenon likely occurs because the influence of *activation gradients* is amplified within the complexities of a real-world data environment.

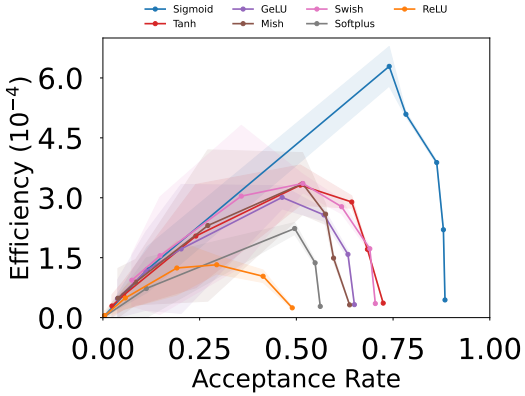


Figure 3: Efficiency of HMC with respect to acceptance rate on BNNs with different activations on TMDb Movie dataset. Sigmoid is more efficient than its counterparts.

6 Conclusion

We derived explicit local error formulas of the leapfrog integrator with HMC with smooth and non-smooth activation functions applied to Bayesian neural networks. Our analyses identify two error sources: gradient norm dynamics and third-order curvature, which are ignored in previous studies. Contrary to the classical assumption that smoothness guarantees HMC efficiency, we show that the boundedness of activation functions largely contributes to the efficiency of the HMC algorithm with BNNs. Extensive simulations on toy and real-world datasets verify our theoretical findings.

While the provided results establish a theoretical foundation, our current analysis and experiments are limited to shallow-layer networks. Deeper architectures introduce residual connections, layer normalization, and depth-dependent gradient dynamics that may alter the relative contributions of the two error sources. Extending our explicit error formulas to these complex settings represents a natural next step. Furthermore, our analysis considers only the simplified case of an identity mass matrix, which could be generalized by pre-conditioning matrices such as the Fisher Information Matrix in RMHMC [Girolami and Calderhead, 2011]. Another promising direction is to investigate adaptive samplers like NUTS [Hoffman et al., 2014], which may partially compensate for activation-induced curvature by shortening trajectories automatically; quantifying this interaction remains an important open question. We leave these extensions to future work.

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A Additional Proofs

A.1 Proof of Theorem 1

We consider a general case where a particle start at $(\mathbf{q}_0, \mathbf{p}_0)$ and end at $(\mathbf{q}_1, \mathbf{p}_1)$ after a single update step. The state $(\mathbf{q}_1, \mathbf{p}_1)$ is given as follows:

$$\mathbf{p}_{1/2} = \mathbf{p}_0 - \frac{\varepsilon}{2} \nabla U(\mathbf{q}_0) \quad (9)$$

$$\mathbf{q}_1 = \mathbf{q}_0 + \varepsilon \mathbf{p}_{1/2} \quad (10)$$

$$\mathbf{p}_1 = \mathbf{p}_{1/2} - \frac{\varepsilon}{2} \nabla U(\mathbf{q}_1) \quad (11)$$

Change in the kinetic energy. The difference in the kinetic energy is given by:

$$\begin{aligned} \Delta K &= K(\mathbf{p}_1) - K(\mathbf{p}_0) \\ &= \frac{1}{2} (\|\mathbf{p}_1\|^2 - \|\mathbf{p}_0\|^2) \\ &= \frac{1}{2} \left(\left\| \mathbf{p}_0 - \frac{\varepsilon}{2} \nabla U(\mathbf{q}_0) - \frac{\varepsilon}{2} \nabla U(\mathbf{q}_1) \right\|^2 - \|\mathbf{p}_0\|^2 \right) \\ &= \frac{1}{2} \left(\|\mathbf{p}_0\|^2 + \frac{\varepsilon^2}{4} \|\nabla U(\mathbf{q}_0)\|^2 + \frac{\varepsilon^2}{4} \|\nabla U(\mathbf{q}_1)\|^2 - \varepsilon \mathbf{p}_0 \cdot \nabla U(\mathbf{q}_0) - \varepsilon \mathbf{p}_0 \cdot \nabla U(\mathbf{q}_1) + \frac{\varepsilon^2}{2} \nabla U(\mathbf{q}_0) \cdot \nabla U(\mathbf{q}_1) - \|\mathbf{p}_0\|^2 \right) \\ &= -\frac{\varepsilon}{2} \mathbf{p}_0 \cdot (\nabla U(\mathbf{q}_0) + \nabla U(\mathbf{q}_1)) + \frac{\varepsilon^2}{4} \left(\frac{1}{2} \|\nabla U(\mathbf{q}_0)\|^2 + \frac{1}{2} \|\nabla U(\mathbf{q}_1)\|^2 + \nabla U(\mathbf{q}_0) \cdot \nabla U(\mathbf{q}_1) \right) \end{aligned}$$

The second to the third equation is from eq.(9) and eq.(11). Calculation of the first term:

$$\begin{aligned} & -\frac{\varepsilon}{2} \mathbf{p}_0 \cdot (\nabla U(\mathbf{q}_0) + \nabla U(\mathbf{q}_1)) \\ &= -\frac{\varepsilon}{2} \left(\mathbf{p}_{1/2} + \frac{\varepsilon}{2} \nabla U(\mathbf{q}_0) \right) \cdot (\nabla U(\mathbf{q}_0) + \nabla U(\mathbf{q}_1)) \\ &= -\frac{\varepsilon}{2} \mathbf{p}_{1/2} \cdot (\nabla U(\mathbf{q}_0) + \nabla U(\mathbf{q}_1)) - \frac{\varepsilon^2}{4} \left(\|\nabla U(\mathbf{q}_0)\|^2 + \nabla U(\mathbf{q}_0) \cdot \nabla U(\mathbf{q}_1) \right) \end{aligned}$$

Substituting it into ΔK , we have:

$$\Delta K = -\frac{\varepsilon}{2} \mathbf{p}_{1/2} \cdot (\nabla U(\mathbf{q}_0) + \nabla U(\mathbf{q}_1)) + \frac{\varepsilon^2}{8} \left(\|\nabla U(\mathbf{q}_1)\|^2 - \|\nabla U(\mathbf{q}_0)\|^2 \right) \quad (12)$$

Change in the potential energy. For a single step from $(\mathbf{q}_0, \mathbf{p}_0)$ to $(\mathbf{q}_1, \mathbf{p}_1)$ with smooth activation function, we have:

$$\Delta U = U(\mathbf{q}_1) - U(\mathbf{q}_0) = \int_0^\varepsilon \frac{\partial U}{\partial \mathbf{q}}(\mathbf{q}_0 + t\mathbf{p}_{1/2}) \cdot \mathbf{p}_{1/2} dt \quad (13)$$

We use the Trapezoidal rule as follow:

$$\int_a^b f(t) dt \approx \frac{(b-a)}{2} [f(b) + f(a)] - \frac{(b-a)^3}{12N^2} f''(\xi) \quad (14)$$

Following the above rule with $a = 0$, $b = \varepsilon$, $N = 1$ and the function $f(t) = \nabla U(\mathbf{q}_0 + t\mathbf{p}_{1/2}) \cdot \mathbf{p}_{1/2}$, we can express ΔU as:

$$\Delta U = \frac{\varepsilon}{2} \mathbf{p}_{1/2} \cdot (\nabla U(\mathbf{q}_0) + \nabla U(\mathbf{q}_1)) - \frac{\varepsilon^3}{12} \frac{d^2}{dt^2} (\nabla U(\mathbf{q}_0 + t\mathbf{p}_{1/2}) \cdot \mathbf{p}_{1/2}) \Big|_{t=\xi}, \quad (15)$$

The first derivative $f'(t)$ of $f(t)$ is given by:

$$\begin{aligned} f'(t) &= \frac{d}{dt} (\nabla U(\mathbf{q}_0 + t\mathbf{p}_{1/2}) \cdot \mathbf{p}_{1/2}) \\ &= \frac{d}{dt} (\nabla U(\mathbf{q}_0 + t\mathbf{p}_{1/2})) \cdot \mathbf{p}_{1/2} \\ &= (\nabla^2 U(\mathbf{q}_0 + t\mathbf{p}_{1/2}) \cdot \mathbf{p}_{1/2}) \cdot \mathbf{p}_{1/2} \end{aligned} \quad (16)$$

We derive the second derivative $f''(t)$ of $f(t)$ using chain rule:

$$\begin{aligned}
f''(t) &= \frac{d}{dt} (\nabla^2 U(\mathbf{q}_0 + t\mathbf{p}_{1/2}) \cdot \mathbf{p}_{1/2}) \cdot \mathbf{p}_{1/2} \\
&= ((\nabla^3 U(\mathbf{q}_0 + t\mathbf{p}_{1/2}) \cdot \mathbf{p}_{1/2}) \cdot \mathbf{p}_{1/2}) \cdot \mathbf{p}_{1/2} \\
&= \sum_{i,j,k} \frac{\partial^3 U}{\partial q_i \partial q_j \partial q_k} (\mathbf{q}_0 + t\mathbf{p}_{1/2}) \cdot (\mathbf{p}_{1/2})_i \cdot (\mathbf{p}_{1/2})_j \cdot (\mathbf{p}_{1/2})_k \\
&= \langle \nabla^3 U(\mathbf{q}_0 + t\mathbf{p}_{1/2}), \mathbf{p}_{1/2} \otimes \mathbf{p}_{1/2} \otimes \mathbf{p}_{1/2} \rangle
\end{aligned} \tag{17}$$

And then we have the change of ΔU :

$$\Delta U = \frac{\varepsilon}{2} \mathbf{p}_{1/2} \cdot (\nabla U(\mathbf{q}_0) + \nabla U(\mathbf{q}_1)) - \frac{\varepsilon^3}{12} \langle \nabla^3 U(\mathbf{q}_0 + \xi \mathbf{p}_{1/2}), \mathbf{p}_{1/2} \otimes \mathbf{p}_{1/2} \otimes \mathbf{p}_{1/2} \rangle \tag{18}$$

From eq.(12) and eq.(18), we have the local error $\Delta H = H(\mathbf{q}_1) - H(\mathbf{q}_0) = \Delta U + \Delta K$:

$$\Delta H = \frac{\varepsilon^2}{8} \left(\|\nabla U(\mathbf{q}_1)\|^2 - \|\nabla U(\mathbf{q}_0)\|^2 \right) - \frac{\varepsilon^3}{12} \langle \nabla^3 U(\mathbf{q}_0 + \xi \mathbf{p}_{1/2}), \mathbf{p}_{1/2} \otimes \mathbf{p}_{1/2} \otimes \mathbf{p}_{1/2} \rangle \tag{19}$$

A.2 Proof of Regression Example

We consider a single layer with one hidden neuron BNNs with:

- Parameters: $w, v \in \mathbb{R}$
- Activation function: $\varphi : \mathbb{R} \rightarrow \mathbb{R}$ (smooth, C^3)
- Network output: $z = v\varphi(wx)$
- Data point: (x, y) with $x \in \mathbb{R}, y \in \mathbb{R}$
- Prior: $\pi(w), \pi(v) \sim \mathcal{N}(0, 1)$
- Residual: $r = y - z$
- Loss: Squared error $(y - z)^2$
- Potential energy: $U(w, v) = \frac{1}{2}(w^2 + v^2) + (y - z)^2$

Let $u = wx$ be the pre-activation, we pre-compute some reused facts:

$$\begin{aligned}
\frac{\partial \varphi}{\partial w} &= x\varphi'; & \frac{\partial \varphi}{\partial v} &= 0; \\
\frac{\partial z}{\partial w} &= vx\varphi'; & \frac{\partial z}{\partial v} &= \varphi; \\
\frac{\partial r}{\partial w} &= -vx\varphi'; & \frac{\partial r}{\partial v} &= -\varphi
\end{aligned}$$

Note that for simplicity, we write φ instead of $\varphi(u)$. We derive the first-order derivative with respect to w and v :

$$\begin{aligned}
\frac{\partial U}{\partial w} &= w - 2rvx\varphi' \\
\frac{\partial U}{\partial v} &= v - 2r\varphi
\end{aligned}$$

We can derive the second derivatives as follows:

$$\begin{aligned}
\frac{\partial^2 U}{\partial w \partial w} &= 1 - 2vx \left[\frac{\partial r}{\partial w} \varphi' + rx \varphi'' \right] = 1 + 2v^2 x^2 (\varphi')^2 - 2rvx^2 \varphi'' \\
\frac{\partial^2 U}{\partial v \partial v} &= 1 - 2\varphi \frac{\partial r}{\partial v} = 1 + 2\varphi^2 \\
\frac{\partial^2 U}{\partial w \partial v} &= -2x\varphi'(r - v\varphi) = -2x\varphi'(y - 2z).
\end{aligned}$$

The third-order derivative is given as:

$$\begin{aligned}\frac{\partial^3 U}{\partial v \partial v \partial v} &= 0. \\ \frac{\partial^3 U}{\partial w \partial w \partial w} &= 6v^2 x^3 \varphi' \varphi'' - 2vx^3(y-z)\varphi''' \\ \frac{\partial^3 U}{\partial w \partial w \partial v} &= 4vx^2(\varphi')^2 - 2x^2\varphi''(y-2z) \\ \frac{\partial^3 U}{\partial w \partial v \partial v} &= 4x\varphi\varphi'\end{aligned}$$

Using triangle inequality, we have:

$$\begin{aligned}\|\nabla^3 U(\mathbf{q})\|_\infty &\leq \left| \frac{\partial^3 U}{\partial w \partial w \partial w} \right| + \left| \frac{\partial^3 U}{\partial w \partial w \partial v} \right| + \left| \frac{\partial^3 U}{\partial w \partial v \partial v} \right| \leq 6v^2 |x|^3 \|\varphi'\|_\infty \|\varphi''\|_\infty \\ &\quad + 2|v| |x|^3 |y-z| \|\varphi'''\|_\infty + 4|v|x^2 \|\varphi'\|_\infty^2 + 2x^2 \|\varphi''\|_\infty |y-2z| + 4|x| |\varphi| \|\varphi'\|_\infty.\end{aligned}$$

A.3 Proof of Classification Example

We consider a hidden layer Bayesian Neural Network with a single hidden unit with:

- Parameter: $w, v \in \mathbb{R}$
- Activation function: $\varphi : \mathbb{R} \rightarrow \mathbb{R}$ (smooth, C^3)
- Predictive function: $p = f(x; w) = \sigma(v\varphi(wx))$
- Data point: (x, y) with $x \in \mathbb{R}, y \in \mathbb{R}$
- Prior: $\pi(w), \pi(v) \sim \mathcal{N}(0, 1)$
- Negative log likelihood (cross-entropy loss): $-[y \log p + (1-y) \log(1-p)]$
- Potential energy: $U(w, v) = \frac{1}{2}(w^2 + v^2) - y(v\varphi(wx)) + \log(1 + e^{v\varphi(wx)})$.

Let $u = wx$, $z = v\varphi(wx)$, $p = \sigma(z)$ and $q = (1-p)$. Again, to shorten the notations, we write φ instead of $\varphi(u)$. We pre-compute some repeatedly used facts:

$$\begin{aligned}\frac{\partial U}{\partial z} &= p - y; \quad \frac{\partial \sigma(z)}{\partial z} = \sigma(z)(1 - \sigma(z)) = pq \\ \frac{\partial z}{\partial w} &= v\varphi'x; \quad \frac{\partial z}{\partial v} = \varphi \\ \frac{\partial p}{\partial w} &= pqv\varphi'x; \quad \frac{\partial p}{\partial v} = pq\varphi \\ \frac{\partial(pq)}{\partial z} &= \frac{\partial(\sigma(z)(1 - \sigma(z)))}{\partial z} = pq(1 - 2p) \\ \frac{\partial(pq)}{\partial w} &= pq(1 - 2p)v\varphi'x; \quad \frac{\partial(pq)}{\partial v} = pq(1 - 2p)\varphi.\end{aligned}$$

We have the first order derivative of U w.r.t. w and v is:

$$\begin{aligned}\frac{\partial U}{\partial w} &= (p - y) \cdot v\varphi'x + w, \\ \frac{\partial U}{\partial v} &= (p - y) \cdot \varphi + v.\end{aligned}$$

For the second order derivative, we have:

$$\begin{aligned}\frac{\partial^2 U}{\partial w \partial w} &= pqv^2(\varphi')^2x^2 + (p - y)v\varphi''x^2 + 1 \\ \frac{\partial^2 U}{\partial v \partial v} &= pq\varphi^2 + 1 \\ \frac{\partial^2 U}{\partial w \partial v} &= pqv\varphi\varphi'x + (p - y)\varphi'x.\end{aligned}$$

Applying the chain rule, we derive the third-order derivative *w.r.t.* w as:

$$\begin{aligned}\frac{\partial^3 U}{\partial w \partial w \partial w} &= pq(1-2p)v^3(\varphi')^3 x^3 + 3pqv^2\varphi'\varphi''x^3 + (p-y)v\varphi'''x^3 \\ \frac{\partial^3 U}{\partial v \partial v \partial v} &= pq(1-2p)\varphi^3 \\ \frac{\partial^3 U}{\partial w \partial v \partial v} &= pq(1-2p)vx\varphi'\varphi^2 + 2pqx\varphi\varphi' \\ \frac{\partial^3 U}{\partial w \partial w \partial v} &= pq(1-2p)v^2x^2\varphi(\varphi')^2 + 2pqvx^2(\varphi')^2 + pqvx^2\varphi\varphi'' + (p-y)x^2\varphi''.\end{aligned}$$

The upper-bound for the infinite-norm of the third-order curvature is given as:

$$\begin{aligned}\|\nabla^3 U(\mathbf{q})\|_\infty &\leq \left| \frac{\partial^3 U}{\partial w^3} \right| + \left| \frac{\partial^3 U}{\partial w \partial w \partial v} \right| + \left| \frac{\partial^3 U}{\partial w \partial v \partial v} \right| + \left| \frac{\partial^3 U}{\partial v^3} \right| \leq C(|v|^3 \|\varphi'\|_\infty^3 |x|^3 \\ &\quad + v^2 \|\varphi'\|_\infty \|\varphi''\|_\infty |x|^3 + |v| \|\varphi'''\|_\infty |x|^3 + |\varphi|^3 + |v| |x| \|\varphi'\|_\infty \varphi^2 + |x| \|\varphi'\|_\infty |\varphi| \\ &\quad + v^2 x^2 |\varphi| \|\varphi'\|_\infty^2 + |v| x^2 (\|\varphi'\|_\infty^2 + |\varphi| \|\varphi''\|_\infty) + x^2 \|\varphi''\|_\infty)\end{aligned}$$

where C is a universal constant.

A.4 Proof of Corollary 1

We extend this result for a longer trajectory containing L leapfrog steps. In particular, the particle starts from the initial point $(\mathbf{q}_0, \mathbf{p}_0)$ arrives at transition states $\{(\mathbf{q}_1, \mathbf{p}_1), (\mathbf{q}_2, \mathbf{p}_2), \dots, (\mathbf{q}_{L-1}, \mathbf{p}_{L-1})\}$ and ends at $(\mathbf{q}_L, \mathbf{p}_L)$.

$$\begin{aligned}\Delta H &= \Delta H_1 + \Delta H_2 + \dots + \Delta H_L \\ &= \frac{\varepsilon^2}{8} \sum_{l=0}^{L-1} \left(\|\nabla U(\mathbf{q}_{l+1})\|^2 - \|\nabla U(\mathbf{q}_l)\|^2 \right) - \frac{\varepsilon^3}{12} \sum_{l=0}^{L-1} \langle \nabla^3 U(\mathbf{q}_l + \xi_l \mathbf{p}_{l+\frac{1}{2}}), \mathbf{p}_{l+\frac{1}{2}} \otimes \mathbf{p}_{l+\frac{1}{2}} \otimes \mathbf{p}_{l+\frac{1}{2}} \rangle \\ &= \frac{\varepsilon^2}{8} \left(\|\nabla U(\mathbf{q}_L)\|^2 - \|\nabla U(\mathbf{q}_0)\|^2 \right) - \frac{\varepsilon^3}{12} \sum_{l=0}^{L-1} \langle \nabla^3 U(\mathbf{q}_l + \xi_l \mathbf{p}_{l+\frac{1}{2}}), \mathbf{p}_{l+\frac{1}{2}} \otimes \mathbf{p}_{l+\frac{1}{2}} \otimes \mathbf{p}_{l+\frac{1}{2}} \rangle.\end{aligned}$$

A.5 Proof of Theorem 2

Consider a leapfrog step starting at $(\mathbf{q}_0, \mathbf{p}_0)$ and ending at $(\mathbf{q}_1, \mathbf{p}_1)$ and crosses the surfaces of non-differentiability at $\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_k$ at time $\varepsilon_1, \varepsilon_2, \dots, \varepsilon_k$

Change in the kinetic energy.

$$\Delta K = -\frac{\varepsilon}{2} \mathbf{p}_{1/2} \cdot (\nabla U(\mathbf{q}_0) + \nabla U(\mathbf{q}_1)) + \frac{\varepsilon^2}{8} \left(\|\nabla U(\mathbf{q}_1)\|^2 - \|\nabla U(\mathbf{q}_0)\|^2 \right).$$

Change in the potential energy.

$$\begin{aligned}\Delta U &= \sum_{i=0}^k \int_{\varepsilon_i}^{\varepsilon_{i+1}} \nabla U(\mathbf{q}_0 + t\mathbf{p}_{1/2}) \cdot \mathbf{p}_{1/2} dt \\ &= \sum_{i=0}^k \left[\frac{\varepsilon_{i+1} - \varepsilon_i}{2} (\nabla U^+(\mathbf{z}_i) + \nabla U^-(\mathbf{z}_{i+1})) \cdot \mathbf{p}_{1/2} - \frac{(\varepsilon_{i+1} - \varepsilon_i)^3}{12} \langle \nabla^3 U(\mathbf{q}_0 + \xi_i \mathbf{p}_{1/2}), \mathbf{p}_{1/2} \otimes \mathbf{p}_{1/2} \otimes \mathbf{p}_{1/2} \rangle \right] \\ &= \sum_{i=0}^k \left[\frac{\Delta \varepsilon_i}{2} (\nabla U^+(\mathbf{z}_i) + \nabla U^-(\mathbf{z}_{i+1})) \cdot \mathbf{p}_{1/2} - \frac{(\Delta \varepsilon_i)^3}{12} \langle \nabla^3 U(\mathbf{q}_0 + \xi_i \mathbf{p}_{1/2}), \mathbf{p}_{1/2} \otimes \mathbf{p}_{1/2} \otimes \mathbf{p}_{1/2} \rangle \right]\end{aligned}$$

Activation	Formula $\varphi(u)$	Third-Order Derivative $\varphi'''(u)$
Sigmoid (σ)	$\frac{1}{1 + e^{-u}}$	$\sigma(1 - \sigma)[1 - 6\sigma(1 - \sigma)]$
Tanh	$\frac{e^u - e^{-u}}{e^u + e^{-u}}$	$2(1 - \tanh^2)(3 \tanh^2 - 1)$
Softplus	$\log(1 + e^u)$	$\sigma(1 - \sigma)(1 - 2\sigma)$
GELU	$u \cdot \Phi(u)$	$\phi(u)(u^3 - 4u)$
Swish	$u \cdot \sigma(u)$	$3\sigma(1 - \sigma)[1 - 2\sigma] + u\sigma(1 - \sigma)[1 - 6\sigma(1 - \sigma)]$
Mish	$u \cdot \omega(u)$	$\sigma(1 - \omega^2) [u (6\sigma^2\omega(\omega + 1) - 6\sigma\omega - 3\sigma + 1) + 3(1 - \sigma(2\omega + 1))]$

Table 1: Activation functions and their third-order derivatives in compact form. We omitted u as the input of σ , $\tanh$ and ω to shorten the notation.

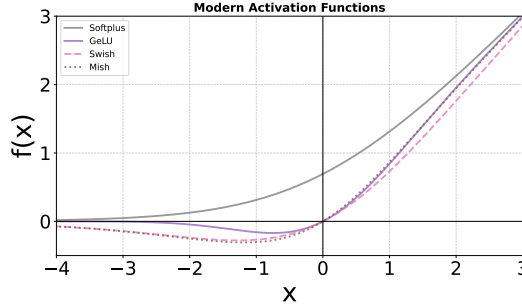


Figure 4: Visualization of different activation functions. Softplus is a pointwise upperbound for GeLU, Swish and Mish.

Adding these two terms, we have:

$$\begin{aligned}
\Delta H = & \mathbf{p}_{1/2} \cdot \sum_{i=0}^k \frac{\Delta \varepsilon_i}{2} (\nabla U^-(\mathbf{z}_{i+1}) + \nabla U^+(\mathbf{z}_i)) - \frac{\varepsilon}{2} \mathbf{p}_{1/2} \cdot (\nabla U(\mathbf{q}_0) + \nabla U(\mathbf{q}_1)) \\
& + \frac{\varepsilon^2}{8} (\|\nabla U(\mathbf{q}_1)\|^2 - \|\nabla U(\mathbf{q}_0)\|^2) - \sum_{i=0}^k \frac{\Delta \varepsilon_i^3}{12} \langle \nabla^3 U(\mathbf{q}_0 + \xi_i \mathbf{p}_{1/2}), \mathbf{p}_{1/2} \otimes \mathbf{p}_{1/2} \otimes \mathbf{p}_{1/2} \rangle.
\end{aligned}$$

B Activation Analyses

Derivatives of activation functions. In this section, we analyze the smoothness of various activation functions by examining their higher-order derivatives. To simplify our notation, let σ denote the sigmoid function, Φ the cumulative distribution function (c.d.f.) of the standard Gaussian distribution, and $\omega(u) = \tanh(\ln(1 + e^u))$ the core component of the Mish activation. The explicit formulas for these functions and their respective third-order derivatives are summarized in Table 1, while their calculated infinite norms are provided in Table 2. Our results indicate a clear correlation between the magnitude of $\|\varphi'''\|_\infty$ and the accumulation of error along the integration trajectory. As illustrated in Figure 1, GeLU and Mish exhibit $\|\varphi'''\|_\infty$ values approximately double that of Swish. This increased value in the third-order derivative directly translates to higher discretization error within the HMC leapfrog integrator, underscoring the critical role of functional smoothness in sampling stability.

Comparison between Softplus, GeLU, Swish and Mish. We show that $\text{Softplus} > \max(0, u) \geq \text{GeLU}$, Swish and Mish since this order contributes to the error order in Figure 1. We first show that

Activation	$\ \varphi'(u)\ _\infty$	$\ \varphi''(u)\ _\infty$	$\ \varphi'''(u)\ _\infty$	Range of $\varphi(u)$
Sigmoid	0.250	0.0962	0.125	$(0, 1)$
Tanh	1.000	0.7699	2.000	$(-1, 1)$
Softplus	1.000	0.250	0.096	$(0, \infty)$
GELU	1.1289	0.5117	0.779	$[-0.17, \infty)$
Swish	1.0890	0.6051	0.308	$[-0.278, \infty)$
Mish	1.0998	0.4999	0.588	$[-0.308, \infty)$

Table 2: Infinity norms of first, second and third-order gradients of different activation functions and their corresponding output range.

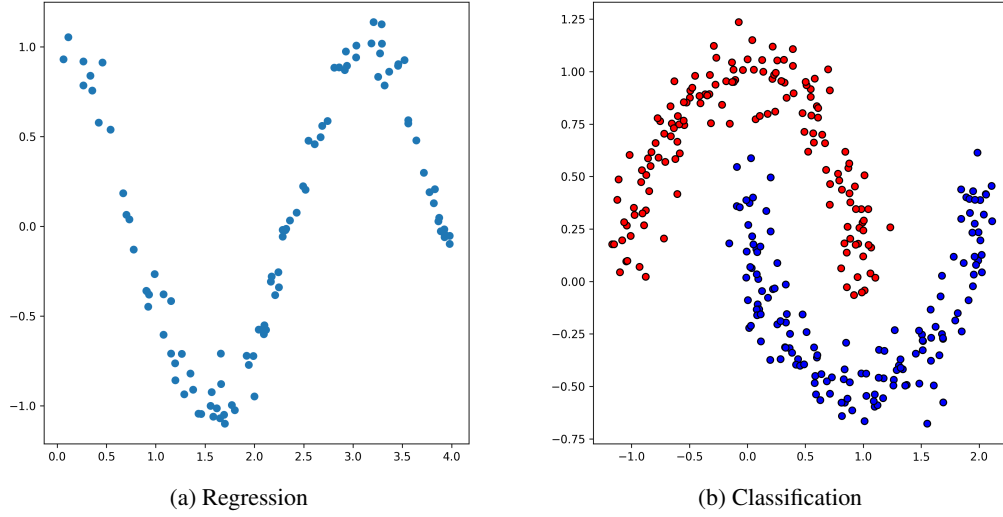


Figure 5: Visualization of synthetic regression and classification datasets.

Softplus $> \max(0, u)$. The Softplus function is given as:

$$\text{Softplus}(u) = \ln(1 + e^u) > \begin{cases} \ln(e^u) = u & u \geq 0, \\ \ln(1) = 0 & u < 0. \end{cases} \quad (20)$$

Next, we prove that $\max(0, u) \geq \text{GeLU}, \text{Swish}, \text{Mish}$. These three activation functions share the following structure:

$$f(u) = u \cdot g(u), \quad (21)$$

where $g(u)$ is a gating function. For Swish, GeLU and Mish, $g(u)$ is $\sigma(u)$ (sigmoid function), $\Phi(u)$ (Gaussian c.d.f.), and $\tanh(\ln(1 + e^u))$, respectively. Therefore, it is strictly bounded between 0 and 1. Consequently, $\max(0, u) \geq \text{GeLU}, \text{Swish}, \text{Mish}$. This result can combine with the classification example to explain the error behaviour of Softplus in Figure 1. We provide a visualization of activation function in Figure 4.

Activation	Regression		Classification	
	Gradient	Third-order	Gradient	Third-order
Sigmoid	0.05	2.47×10^{-6}	0.04	0.001
Tanh	121.52	507.11	0.05	0.03
Softplus	277.14	2099.58	21.28	376.59
GELU	61.83	4276.60	1.85	17.88
Swish	134.39	3696.57	3.52	49.31
Mish	114.57	1963.17	2.36	29.68

Table 3: Error decomposition of different activation functions.

C More details on experiment settings

C.1 Details on Toy Experiments

Visualization of synthetic datasets. We visualize both synthetic datasets for regression and classification used in our simulations in Figure 5.

Network configuration. Both tasks employ a single-hidden-layer Bayesian feed-forward neural network with 50 hidden units. In summary, the total parameter count is $d = 151$ for regression and $d = 252$ for classification. We consider the distribution of network parameters are fully independent, and place an isotropic Normal prior on each parameter, that is, $\pi(q) = \mathcal{N}(0, 1)$. The loss functions are mean squared error and binary cross-entropy for regression and classification, respectively. To examine the efficiency of HMC for BNNs with different activation functions, we investigate eight activation functions spanning three categories: *bounded smooth* (Sigmoid, Tanh), *unbounded smooth* (GELU, Swish, Mish, Softplus), and *piecewise* (ReLU, LeakyReLU). This selection covers the most commonly used activations in modern architectures, including transformers [Vaswani et al., 2017] and convolutional networks [He et al., 2016]. Crucially, unbounded smooth activations satisfy Assumption 2 yet exhibit unbounded activation growth, making them the main focus of our study. Our code is implemented by Jax [Bradbury et al., 2018]. The experiments for toy datasets run on Google Colab with 12GB T4 GPU, while experiments on TMDb dataset use a fraction of a H200 GPU with 18GB VRAM.

C.2 Details on Real Dataset Experiments

In this experiment, we used a neural network with a single hidden layer containing 50 hidden units. We ran HMC to generate 3,000 samples, discarding the first 1,000 samples for burn-in. For data preprocessing, we removed all rows with zero budget and zero revenue, and we applied z -normalization to the inputs. We randomly partitioned the dataset, using 80% for training and keeping 20% for testing. As a result, the training and testing sets contain 2,580 and 645 data points, respectively. We ran the experiment five times and averaged the results.

D More Experiment Results

Error Decomposition. In Table. 3, we provide the averaged values of each component in Figure 1. Clearly, the values for energy geometry dominate the gradient distance value, and strongly influence the efficiency of the HMC sampler.

Effects of dimensionality. This simulation investigates the impact of parameter space dimensionality d and network architecture on sampling performance. We consider two types of networks: (1) wide networks featuring 20, 50, 100, and 200 nodes; and (2) deep networks comprising 2, 3, and 4 hidden layers, with each layer containing 20 hidden nodes. Following [Dinh et al., 2024], we executed HMC with $L = 200$ and $\varepsilon = 0.001$ for each experiment. In Figure 6, we plot the acceptance rate against the total number of parameters. Generally, except for Sigmoid, the acceptance rate for

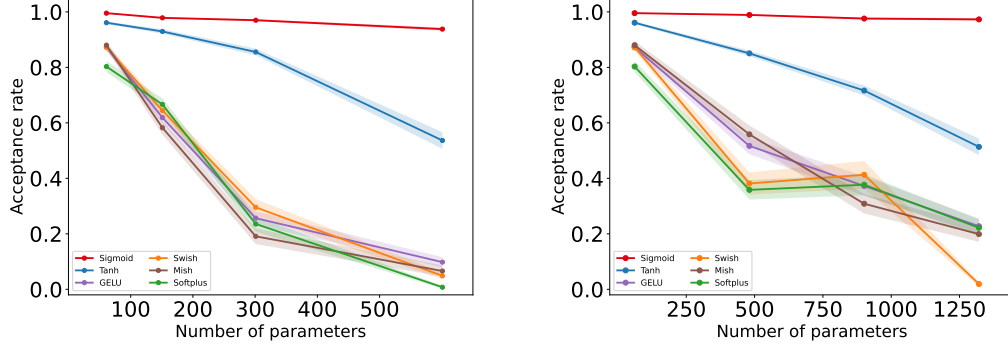


Figure 6: Acceptance rate of HMC with respect to the number of model parameters on wide (left) and deep (right) neural networks with different activation functions.

all models significantly decays as the sampling dimensionality increases. However, a consistent trend emerges: unbounded activation functions exhibit significantly lower acceptance rates than their bounded counterparts, leading to higher computational costs. Notably, even Tanh shows some degradation in acceptance rate compared to Sigmoid as the dimensionality grows. These simulations underscore the compound detrimental effect of the third-order curvature term, strongly aligning with our theoretical findings in Theorem 1 and the empirical evidence presented in Figure 1.

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