

LEARNING AT THE EDGE: TAILED-UNIFORM SAMPLING FOR ROBUST SIMULATION-BASED INFERENCE

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ABSTRACT

We introduce the TAILED-UNIFORM proposal distribution for generating training simulations in simulation-based inference. Instead of sampling parameters uniformly within bounded regions, we extend the distribution beyond prior boundaries with smooth Gaussian tails. This eliminates sharp discontinuities that cause neural posterior estimators to fail near parameter space boundaries. The method requires minimal hyperparameter tuning, with tail widths of 10–30% of the prior width proving robust across problems. We demonstrate these benefits on a synthetic Gaussian linear task and cosmological parameter inference from the matter power spectrum. We also find that TAILED-UNIFORM-trained models outperform UNIFORM ones near the boundaries across various training set sizes and dimensions of the parameter space. This advantage grows in higher dimensions, where boundaries dominate parameter space volume. All code is publicly available on Github ^a.

Subject headings: astrophysics, machine learning, deep learning, simulation-based inference, neural posterior estimation, Bayesian methods

1. INTRODUCTION

Today, researchers, among them astronomers, face a growing challenge, as many systems of interest (e.g., exoplanets, black hole binaries, or galaxy clusters) are not amenable to direct probing (Feigelson and Babu 2012; Dodelson and Schmidt 2020). Thus emerges a new class of problems known as “inverse problems,” in which the key goal is to identify the model parameters that generated some observed data. The key challenge is that almost all mathematical models of real-world phenomena are complex in that they demand high-dimensional parameter space. This makes it prohibitively expensive to compute the probability density (i.e., likelihood) for some observation.

Traditionally, sampling from arbitrarily complex distributions has been done using explicit likelihood inference, in which we write down an analytic likelihood that relates parameters to data and then use Markov Chain Monte Carlo (MCMC; Metropolis et al. 1953; Hastings 1970) to sample posteriors. By definition, the method requires evaluating the likelihood, which results in the cost of running the full forward simulation accumulating at each step in the chain. MCMC also presupposes that the model can be defined analytically, which is not the case for most complex models (Pretorius 2005; Campanelli et al. 2006). Even in cases where evaluating likelihood is possible, MCMC can get “stuck” in some local minima when the posterior has tricky geometry, involving multimodal distributions, strong parameter degeneracies, or highly anisotropic structure (Brooks et al. 2011).

Simulation-based inference (SBI) has emerged as a gold standard framework for tackling these challenges (Cran-

mer et al. 2020). Most exciting SBI methods today rely on neural density estimation (Papamakarios and Murray 2018; Greenberg et al. 2019; Lueckmann et al. 2017), which incorporates deep neural networks to learn the posterior distribution. Although these networks come in many flavors, such as neural likelihood estimation (NLE) and neural ratio estimation (NRE), we primarily focus on neural posterior estimation (NPE) in this paper. In the NPE paradigm, we use model simulations to learn approximate posteriors directly from the simulated training dataset, rather than evaluating the explicit likelihood, which has proven to be unknown or intractable. Trained on pairs of parameters and simulations, the model learns the mapping between observations and the corresponding parameters that generated them. The cost of training simulations is also “amortized” over time, allowing the neural network to be trained once and used to repeatedly infer new observations.

Despite these advances, current SBI methodologies face various scalability issues. The first and perhaps most prominent is that as the number of parameters increases, so does the computational cost of generating simulations in high-dimensional space. In high dimensions, the volume of parameter space expands exponentially that achieving adequate coverage requires an unacceptably large number of simulations.

The second shortcoming lies in the method by which we generate model realizations. Often, the de facto technique involves a UNIFORM sampling of some parameter combinations within some Latin hypercube (McKay et al. 2000) which has the advantage of covering the whole region of interest. However, the training distribution, sampled with this UNIFORM distribution, will exhibit a sharp discontinuity at the boundary, where

^a <https://github.com/chaipattira/tailed-uniform-sbi>

the prior density collapses to zero. Driven by stochastic gradient descent, our neural network can interpolate the internal regions at ease but falls short near those boundaries. But due to practical constraints, we must prioritize the center of the parameter space, resulting in undersampling on the outskirts. The absence of adequate support corrodes the posterior estimates at the boundaries. We also believe that such pathology will be exacerbated in higher dimensions by the “curse of dimensionality,” (Bellman and Kalaba 2003) according to which the volume fraction of parameter space close to boundaries scales exponentially.

A third related limitation arises from the standard workflow in large-scale simulation campaigns, like the CAMELS project (Cosmology and Astrophysics with MachinE Learning Simulations), where simulations are generated once with a fixed prior, published as public datasets, and then reused for inference across multiple studies (Villaescusa-Navarro et al. 2021, 2023). Any researcher who wants to perform inference with a prior that stretches beyond the initial simulation bounds will likely obtain lower posterior quality, as the emulator has never seen the training data in that region before. Without access to the original, prohibitively priced simulator, this rigidity imposes a systematic constraint on all future analyses.

To address these problems, we present a novel parameter sampling technique for simulation-based inference. In particular, we propose TAILED-UNIFORM, a hybrid proposal that combines UNIFORM cores with smooth Gaussian tails and show that empirically, neural nets trained with our proposal achieve superior performance near the boundary and maintain consistent posterior quality across the overall parameter space. We also validate TAILED-UNIFORM on both synthetic benchmarks and realistic cosmological inference tasks, revealing that TAILED-UNIFORM enables robust inference with competitive simulation budgets.

The remainder of this paper is organized as follows. Section 2 reviews the fundamentals of SBI and neural posterior estimation, then introduce the mathematical formulation of the TAILED-UNIFORM proposal. Our method is validated on a controlled Gaussian linear benchmark in Section 3, and sensitivity studies are conducted to investigate the effects of dimensionality, simulation budget, and tail width. In Section 4, we demonstrate practical utility on cosmological parameter inference from matter power spectra, showing how TAILED-UNIFORM mitigates boundary pathology along degenerate parameter directions. Lastly, we provide a summary of our findings in Section 5.

2. METHODS

This section lays the groundwork for our proposed sampling technique. We propose TAILED-UNIFORM and show that the boundary discontinuities that afflict conventional UNIFORM sampling are ameliorated by smooth Gaussian tails.

2.1. Simulation-based Inference

For clarity, we review the established methodology of SBI. We define a simulator as a function \mathcal{M} that aims to mimic a physical, possibly stochastic process; that is,

it maps some parameters $\boldsymbol{\theta} \in \Theta \subseteq \mathbb{R}^d$ to observable quantities $\mathbf{x} \in \mathcal{X} \subseteq \mathbb{R}^D$ (Cranmer et al. 2020).

To generate each data-parameter pair $(\boldsymbol{\theta}_i, \mathbf{x}_i)$, we: (1) sample parameters $\boldsymbol{\theta}_i \sim \tilde{\mathcal{P}}(\boldsymbol{\theta})$ from the proposal prior, (2) run the forward model $\mathbf{x}_i = \mathcal{M}(\boldsymbol{\theta}_i) + \boldsymbol{\epsilon}_i$ where $\boldsymbol{\epsilon}_i$ represents some systematic noise, and (3) store the resulting data-parameter pairs. We can then feed these into an inverse model to make inferences on some real data $\mathbf{x} = \mathbf{x}_0$.

Bayesian workflow The goal of SBI is to discern the posterior distribution, which constrains the space of possible parameters of interest given an observed data point \mathbf{x}_0 . In most cases, such posterior is not available in closed form, but because it is contingent upon the provided data, we can invoke Bayes’ theorem to write

$$\mathcal{P}(\boldsymbol{\theta} | \mathbf{x}_0) = \frac{\mathcal{P}(\mathbf{x}_0 | \boldsymbol{\theta}) \mathcal{P}(\boldsymbol{\theta})}{\mathcal{P}(\mathbf{x}_0)}. \quad (1)$$

Here, $\mathcal{P}(\mathbf{x}_0 | \boldsymbol{\theta})$ is the likelihood (the probability of the data given certain parameters), $\mathcal{P}(\boldsymbol{\theta})$ is the prior (the proxy for our initial belief regarding the true distribution of the parameters), and $\mathcal{P}(\mathbf{x}_0) = \int \mathcal{P}(\mathbf{x}_0 | \boldsymbol{\theta}) \mathcal{P}(\boldsymbol{\theta}) d\boldsymbol{\theta}$ is the evidence.

Neural posterior estimation (NPE) Our objective then is to construct a neural architecture $q_w(\boldsymbol{\theta} | \mathbf{x})$ with weights w that outputs a probability distribution over $\boldsymbol{\theta}$ which approximates mapping from observational data to full posterior distribution $\mathcal{P}(\boldsymbol{\theta} | \mathbf{x})$ (Papamakarios and Murray 2018; Greenberg et al. 2019). To train this network to accurately represent the conditional probability, we maximize the joint likelihood of our training data $\mathcal{D}_{\text{train}}$. This is akin to minimizing the negative log-probability loss

$$\mathcal{L}_{\text{NPE}} := -\mathbb{E}_{\mathcal{D}_{\text{train}}} \log q_w(\boldsymbol{\theta} | \mathbf{x}) \quad (2)$$

$$= -\mathbb{E}_{\mathcal{D}_{\text{train}}} \log \left[\frac{\mathcal{P}(\boldsymbol{\theta})}{\tilde{\mathcal{P}}(\boldsymbol{\theta})} q_w(\boldsymbol{\theta} | \mathbf{x}) \right], \quad (3)$$

where the expectation $\mathbb{E}_{\mathcal{D}_{\text{train}}}$ in the loss function is taken over all parameter-observation pairs $\{(\boldsymbol{\theta}_i, \mathbf{x}_i)\}_{i=1}^N$ in the training dataset.

If such training data exhibits sufficient diversity and the neural architecture possesses adequate coverage of the parameter space $\Theta \subset \mathbb{R}^d$, then minimization of \mathcal{L}_{NPE} over the network weights w will drive $q_w(\boldsymbol{\theta} | \mathbf{x})$ toward the true posterior distribution $\mathcal{P}(\boldsymbol{\theta} | \mathbf{x})$ (Hornik et al. 1989). As a result, we can sample at inference time by evaluating the log-density of simulated parameters beforehand during training.

Priors It is crucial to make clear the difference between proposal and assumed priors (Cranmer et al. 2020):

- The proposal prior $\tilde{\mathcal{P}}(\boldsymbol{\theta})$, by definition, is the empirical distribution of parameters $\boldsymbol{\theta}$ found in the training dataset $\mathcal{D}_{\text{train}}$. For one thing, it will depend on our sampling strategy, or a Latin hypercube $\mathcal{U}([\theta_{\min,1}, \theta_{\max,1}] \times \dots \times [\theta_{\min,d}, \theta_{\max,d}])$, used to create training simulations.
- On the other hand, our preconceived notion of the global parameter distribution is encoded in the assumed prior $\mathcal{P}(\boldsymbol{\theta})$, which, we should note, is an

experimental design choice. It reflects scientific understanding, theoretical constraints, or previous empirical knowledge about plausible parameter values. In cosmological inference, for example, we may adopt priors centered on values from landmark observational campaigns like the Planck satellite measurements (Aghanim et al. 2020).

Broadly speaking, we can choose the assumed and proposed priors to be identical. This alignment, however, is not always preferable. Take a scenario where we sample training simulations from a UNIFORM distribution $\tilde{\mathcal{P}}(\theta) = \mathcal{U}([\theta_{\min}, \theta_{\max}])$ to ensure adequate coverage, while our scientific understanding may instead motivate a Gaussian prior $\mathcal{P}(\theta) = \mathcal{N}(\mu, \Sigma)$. In such a case, the neural network can only learn to assign reasonable probability densities to regions where it has observed training examples, that is, $\tilde{\mathcal{P}}(\theta) > 0$. Furthermore, since we do not have any support in regions that lack training data, the neural output will tend to zero $q_w(\theta|\mathbf{x}) \approx 0$, leading to poor inference quality near the boundaries. In this paper, we consider the baseline in which the proposal prior is UNIFORM and the assumed prior is continuous everywhere.

2.2. The TAILED-UNIFORM Proposal

We will now describe the theoretical foundations of the TAILED-UNIFORM, our suggested proposal that offers a smooth, continuously differentiable density across \mathbb{R}^d . By assigning weights beyond the primary region of interest, we can alleviate the sharp discontinuities at the boundary.

One-dimension derivation Consider a one-dimensional ($d = 1$) case and define the probability density function as

$$\tilde{\mathcal{P}}_{\text{TAILED-UNIFORM}}(x; a, b, \sigma) = \begin{cases} A \cdot \mathcal{N}(a, \sigma^2), & x \leq a \\ B \cdot \mathcal{U}(a, b), & x \in [a, b] \\ A \cdot \mathcal{N}(b, \sigma^2), & x \geq b \end{cases} \quad (4)$$

where a and b define the boundaries of the UNIFORM core region, and σ controls the width of the Gaussian tails. We also impose continuity at the boundary to guarantee that our distribution is well-defined, which in turn establishes the values of the normalization constants.

Putting things together, we have

$$A = \frac{\sqrt{2\pi}\sigma^2}{\sqrt{2\pi}\sigma^2 + (b - a)} \text{ and } B = \frac{b - a}{\sqrt{2\pi}\sigma^2 + (b - a)}, \quad (5)$$

which ensures that the distribution integrates to unity across the entire domain, and the Gaussian tail matches the UNIFORM core at the left and right boundaries.

Generalizing to higher dimensions To generalize to a multivariate parameter space $\boldsymbol{\theta} \in \mathbb{R}^d$, we write it as a product of independent uni-variate TAILED-UNIFORM distributions

$$\tilde{\mathcal{P}}_{\text{TAILED-UNIFORM}}(\boldsymbol{\theta}; \mathbf{a}, \mathbf{b}, \boldsymbol{\sigma}) = \prod_{i=1}^d \tilde{\mathcal{P}}_{\text{TAILED-UNIFORM}}(\theta_i; a_i, b_i, \sigma_i), \quad (6)$$

where $\mathbf{a} = (a_1, \dots, a_d)$ and $\mathbf{b} = (b_1, \dots, b_d)$ define the hypercube boundaries, and $\boldsymbol{\sigma} = (\sigma_1, \dots, \sigma_d)$ controls the tail-widths in each dimension.

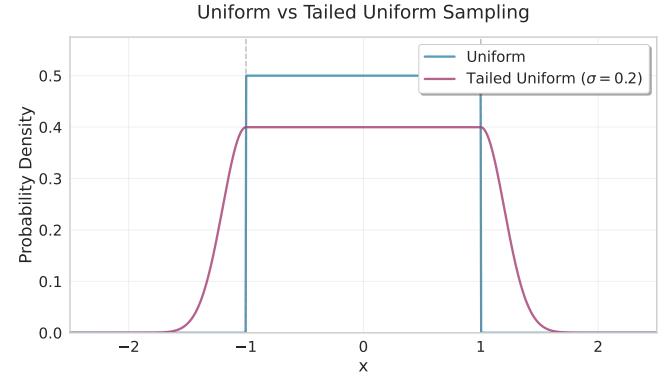


FIG. 1.— The standard UNIFORM distribution (blue) has constant probability density between -1 and 1 with zero probability outside this range. The TAILED-UNIFORM distribution (magenta) maintains a uniform density in the same central region $[-1, 1]$ but extends beyond these boundaries with Gaussian tails characterized by standard deviation $\sigma = 0.2$.

Here, the key hyperparameter is the tail width σ_i , which controls the balance between boundary smoothness and sampling efficiency. Smaller values of σ_i concentrate more samples within the target region $[a_i, b_i]$ but provide less smoothing at the boundaries. Larger values, on the other hand, provide better boundary smoothness but allocate more resources to regions far from the true posterior support. In practice, we recommend setting σ_i as about 10 – 40 percent of the box width; that is,

$$\sigma_i = \alpha \cdot (b_i - a_i), \quad (7)$$

where $\alpha \in [0.1, 0.4]$ (see Section 3.3 for more detail).

3. TOY PROBLEM

We first demonstrate the advantages of TAILED-UNIFORM sampling on a simple toy problem where analytical ground truth is available. This controlled setting allows us to isolate the effects of boundary pathology without confounding factors from complex simulators, providing clear intuition before tackling realistic scientific inference tasks in Section 4.

3.1. Gaussian Linear Task

We formulate a toy problem using the Gaussian Linear task from the simulation-based inference benchmark (**sbibm**) (Lueckmann et al. 2021).

Model As a proof-of-concept, we consider a simple, linear, 2-dimensional Gaussian simulator $\mathcal{M} : \mathbb{R}^2 \rightarrow \mathbb{R}^2$, which is defined as

$$\mathcal{M}(\boldsymbol{\theta}) = \mathbf{A}\boldsymbol{\theta} = \mathbf{I}_2\boldsymbol{\theta} = \boldsymbol{\theta} \quad (8)$$

with a standard Gaussian prior $\mathcal{N}(\mathbf{0}, \mathbf{I}_2)$ centered in the bounded parameter space $\boldsymbol{\theta} \in [-1, 1]^2$. We hence have a likelihood of the form

$$\mathcal{P}(\mathbf{x} | \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}; \boldsymbol{\theta}, \mathbf{I}_2) = \frac{1}{2\pi} \exp\left(-\frac{1}{2}\|\mathbf{x} - \boldsymbol{\theta}\|^2\right), \quad (9)$$

which implies that both the likelihood and prior are Gaussian.

Ground Truth We can leverage the aforementioned conjugate Gaussian-Gaussian structure to obtain a closed-form analytical posterior $\mathcal{P}(\boldsymbol{\theta} | \mathbf{x}) = \mathcal{N}\left(\frac{\mathbf{x}}{2}, \frac{\mathbf{I}_2}{2}\right)$, where the posterior covariance $\frac{\mathbf{I}_2}{2}$ results from $(\mathbf{I}_2^{-1} +$

$\mathbf{I}_2^{-1})^{-1} = \frac{\mathbf{I}_2}{2}$. This gives us reference posterior samples from which to evaluate performance.

Training Our goal is to investigate two distinct strategies for generating the training data:

1. Baseline (UNIFORM proposal): Training data is generated by sampling parameters uniformly across the 2-dimensional hypercube $\tilde{\mathcal{P}}_{\text{UNIFORM}} = \mathcal{U}([-1, 1]^2)$.
2. Proposed (TAILED-UNIFORM proposal): Training data is generated using our hybrid distribution $\tilde{\mathcal{P}}_{\text{TAILED-UNIFORM}}(\mathbf{a} = [-1, -1], \mathbf{b} = [1, 1], \boldsymbol{\sigma} = [0.2, 0.2])$, where the tail width $\sigma_i = 0.1 \times (b_i - a_i)$ represents 10% of each parameter range.

For both proposals, we generate $N = 6,000$ simulation pairs $\{(\boldsymbol{\theta}_i, \mathbf{x}_i)\}_{i=1}^N$ by: (1) sampling $\boldsymbol{\theta}_i$ from the respective proposal distribution, (2) running the forward simulator $\mathbf{x}_i = \mathcal{M}(\boldsymbol{\theta}_i) + \boldsymbol{\epsilon}_i$ with $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_2)$ and (3) training identical neural posterior estimators (NPE) on each dataset. Note again that the assumed prior in both cases is a Gaussian distribution centered at $(0, 0)$ with a standard deviation of $(0.2, 0.2)$. In what follows, we will associate UNIFORM and TAILED-UNIFORM to the NPE trained with these proposals (rather than the proposal itself).

Model Architectures We experiment with ensembles of neural density estimators comprising Masked Autoregressive Flows (MAF) (Papamakarios et al. 2018) and Masked Autoencoder for Distribution Estimation (MADE) (Germain et al. 2015) architectures, each featuring 16 hidden features and 5 coupling layers. Training uses a batch size of 64 and a learning rate of 5×10^{-5} . Our pipeline is built on the LtU-ILI (Learning the Universe—Implicit Likelihood Inference) framework (Ho et al. 2024), which offers standardized data handling and ensemble utilities for simulation-based inference. For this problem, we deliberately omit hyperparameter optimization, because the Gaussian Linear task, with its analytically tractable posterior and low dimensionality, is simple enough that most reasonable neural architectures converge to similar solutions. Note that we use hyperparameter optimization for more complex inference tasks (refer to Section 4).

3.2. Validation

Model validation aims to ascertain whether the approximate posteriors generated by our neural density estimators $q_w(\boldsymbol{\theta} | \mathbf{x}_0)$ will be “good enough” when faced with real unlabeled observational data \mathbf{x}_0 .

The bias-variance tradeoff One useful proxy for gauging the quality of our learned posterior is the degree to which it can concentrate probability mass around the true parameter $\boldsymbol{\theta}_{\text{true}}$. Practically worthless, for instance, will be a model that regurgitates the prior distribution, as it offers no additional insight whatsoever. After all, the goal of inference is to extract as much information as possible from the observed data \mathbf{x}_0 to narrow down the possible parameter values $\boldsymbol{\theta}$. Yet, if one only optimizes for the training set, the resulting model might end up overfitting and fail to generalize when exposed to new data.

Achieving the sweet spot between bias and variance (Gelman and Rubin 1992) is thus the characteristic of

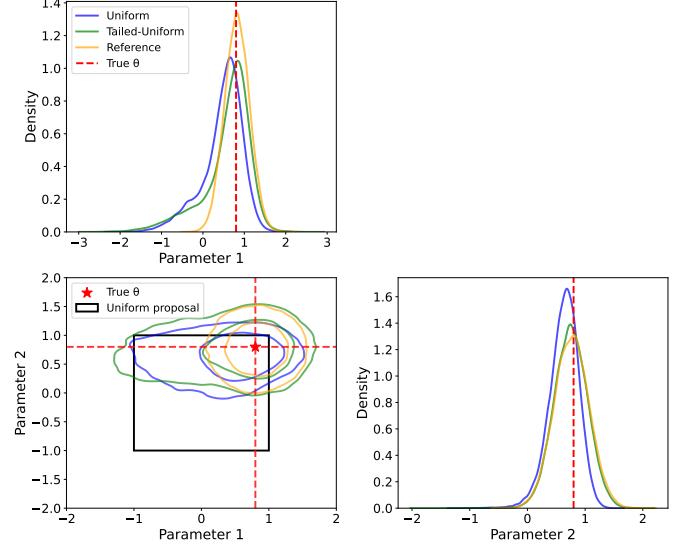


FIG. 2.— Corner plots comparing posterior estimation performance for the boundary test case. The TAILED-UNIFORM (green) demonstrates superior boundary behavior compared to the UNIFORM (blue), closely matching the MCMC reference (yellow). The red dashed line indicates the true parameter value.

a “good” model, as we want a model that is versatile enough to extract genuine information from observations (low bias) while remaining generalizable across different realizations of the data (low variance).

TABLE 1
POSTERIOR PERFORMANCE FOR $\boldsymbol{\theta}_{\text{TRUE}} = (0.8, 0.8)$.

Method	Parameter Estimates		C2ST
	θ_1	θ_2	
Analytical Reference	0.825 ± 0.301	0.763 ± 0.299	0.500
TAILED-UNIFORM	0.568 ± 0.590	0.777 ± 0.279	0.417
UNIFORM	0.469 ± 0.519	0.644 ± 0.286	0.329
C2ST Improvement			+27%

3.2.1. Single-Point Analysis

As a first pass, we select a test point $\boldsymbol{\theta}_{\text{true}} = (0.8, 0.8)$ near the boundary of parameter space, precisely where we anticipate the UNIFORM proposal to struggle most. We generate an observation $\mathbf{x}_0 = \mathcal{M}(\boldsymbol{\theta}_{\text{true}}) + \boldsymbol{\epsilon}$ for this test point, then draw $M = 40,000$ posterior samples from each method (analytic posterior, TAILED-UNIFORM, and UNIFORM). The goal is to assess how well each method constrains the parameters by examining the distribution and concentration of samples around the true value.

Quantitative Metrics To quantify the error between our learned posteriors and the true posterior, we employ the Classifier Two-Sample Test (C2ST) (Lopez-Paz and Oquab 2018), which is the most sensitive metric for evaluating distributional fidelity in SBI models (Lueckmann et al. 2021). The C2ST trains a logistic regression classifier to differentiate between samples from two distributions. If the two distributions are identical, the classifier can do no better than random guessing, yielding a score of 0.5 (zero distributional error). Conversely, scores that deviate from 0.5 signal that the classi-

fier can easily distinguish between the two distributions.

Figure 2 illustrates several instructive phenomena. First, we observe that some of the UNIFORM posterior (blue) leaks outside the proposal boundaries (indicated by the black square at $[-1, 1]^2$), despite being trained exclusively on simulations within this region. The observed leakage occurs because we use a Gaussian (assumed) prior, which is nonzero everywhere. Without gradient information at the boundaries, our flow-based density estimator cannot learn the correct density transitions near the cutoff, resulting in diffuse and poorly constrained samples.

Second, we see that by providing the network with training samples outside of the UNIFORM region (the extended Gaussian support beyond the black square), TAILED-UNIFORM learns a smooth, well-calibrated posterior that extends to boundary-adjacent test points. As a result, the TAILED-UNIFORM’s posterior samples closely resemble the true analytic posterior. This is further corroborated by the C2ST scores in Table 1: the UNIFORM score of 0.329 shows that a classifier can readily distinguish between its posterior samples and the reference, whereas TAILED-UNIFORM’s C2ST score of 0.417 indicates that its learned posterior is closer to the true posterior.

3.2.2. Spatial Performance Analysis

Next, we construct a test to measure TAILED-UNIFORM’s performance across the entire parameter space. And so, we discretize a uniform rectangular grid with $n = 20$ test locations along each dimension of the parameter space $[-1, 1]^2$, yielding a total of 400 evaluation points. We want to exhaustively sample areas of varying distances, ranging from the center of the priors, where traditional techniques work well, to points near the boundaries. As before, we generate observations for each test point, draw $M = 1000$ posterior samples from all three methods, and calculate pairwise C2ST scores at each test location.

Figure 3 shows how UNIFORM’s performance deteriorates as it drifts away from the central regions, as evidenced by the proliferation of blue patches near the boundary. In contrast, our TAILED-UNIFORM maintains more red and orange coloration (with C2ST scores around 0.44–0.49) across the parameter space.

Furthermore, we observe that the C2ST degradation pattern itself is rotationally invariant; that is, its performance depends only on the radial distance (no angular dependence). This spherical symmetry allows us to visualize the performance trends by binning the test points as a function of their distance from the center, as seen in Figure 4. We see that at further radial distances from the center of the prior, the UNIFORM-trained models significantly degrade in performance relative to the TAILED-UNIFORM.

3.3. Prior Hyper-Optimization

Our subsequent evaluations aim to answer three operational questions: the optimal tail width, whether additional training data can mitigate boundary pathology, and whether TAILED-UNIFORM’s advantages persist in higher dimensions.

3.3.1. Sensitivity to the Prior Tail Widths

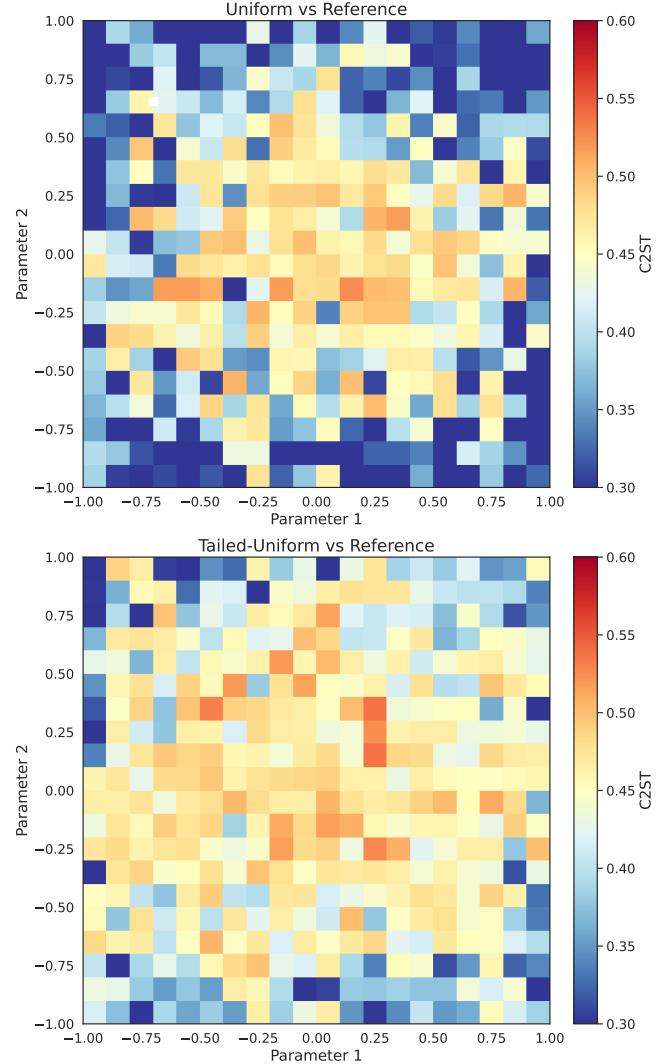


FIG. 3.— Spatial distribution of C2ST performance across the parameter space, with blue regions indicating poor distributional matching ($C2ST \ll 0.5$) and red/orange regions indicating good performance ($C2ST \approx 0.5$). **Top:** UNIFORM versus analytical reference, showing systematic boundary degradation with glaring blue regions near parameter space edges. **Bottom:** TAILED-UNIFORM versus reference, demonstrating consistent performance across the entire parameter space.

The tail width σ (Equation 7) represents a bias-variance tradeoff: narrower tails mitigate the boundary pathologies, while wider tails allocate more simulations outside the primary region of interest, thus decreasing constraining power. To assess the importance of the tails, we train one UNIFORM baseline and several TAILED-UNIFORM models, each with different σ values as fractions of prior width: $\alpha \in \{0.01, 0.05, 0.1, 0.2, 0.4\}$.

Figure 5 reveals that performance improves monotonically with tail width for the toy problem. At the prior boundary ($r = 1.0$), C2ST scores improve from 0.331 ($\sigma = 0.01$, equivalent to UNIFORM) to 0.465 ($\sigma = 0.4$, near-ideal), demonstrating the value of wider tails. As might be expected given its higher sample density in the core region, UNIFORM performs better close to the center of the prior. However, it is important to note that while UNIFORM achieves marginally superior performance near the center, this comes at the expense of

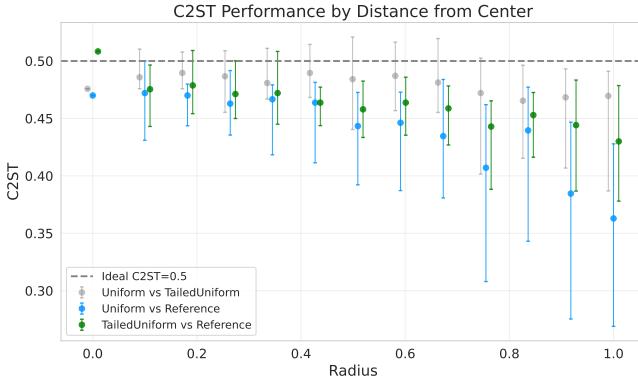


FIG. 4.— C2ST performance degradation as a function of distance from parameter space center. The blue curve reveals systematic deterioration of UNIFORM near boundaries, while the green curve demonstrates that TAILED-UNIFORM maintains consistent performance across all radii. The gray curve quantifies the increasing divergence between methods, with boundary regions showing substantial differences in posterior approximation quality. Values closer to 0.5 indicate better distributional matching. The error bars represent the 16th-84th percentile range of values at a fixed radius from the prior center.

significant degradation in performance near the boundaries. TAILED-UNIFORM, on the other hand, sacrifices a reasonably small amount of accuracy to maintain robust inference across the entire parameter space. The reassuring robustness indicates that even moderate tail samples suffice for learning smooth density transitions, which will prove insightful in higher dimensions. At $\sigma = 0.01$, TAILED-UNIFORM degenerates as anticipated toward UNIFORM behavior with characteristic boundary degradation, confirming that the tails themselves (not some arbitrary artifacts) are responsible for the observed improvements.

3.3.2. Sensitivity to the number of simulations

If insufficient data in the near-boundary regions causes degradation, just increasing the training set size could very well solve the problem. After all, neural networks are universal function approximators, so given enough training data, they should be able to learn complex mappings, including sharp transitions at parameter space boundaries. To interrogate this hypothesis, we conduct a study over various training set sizes, varying $N \in \{2000, 4000, 8000, 16000\}$ while holding all other hyperparameters fixed.

Empirically, we find in Figure 6 that increasing the number of simulations barely helps with the NPE’s performance, suggesting that the boundary degradation stems not from absence of data, but from an inbuilt discontinuous mapping that cannot be learned from samples within the prior alone. Since no amount of supplementary data can smooth a non-smooth function, the hard truncation at prior boundaries poses a fundamental learning barrier. In contrast, we see that every single TAILED-UNIFORM ($N = 2000$) outperforms even the largest UNIFORM ($N = 16000$) with 8 times more training data, demonstrating the impact of different proposals. One can achieve better posterior quality at a fraction of the computational cost just by sampling in a judicious manner.

3.3.3. Scaling to higher dimensions

While we have shown TAILED-UNIFORM to be effective in two dimensions, the critical question is whether this benefit transfers to higher-dimensional parameter spaces, which are necessary for the majority of astrophysical inference problems. By the curse of dimensionality, high-dimensional spaces become ever more sparse, as the volume of a d -dimensional hypercube grows exponentially while the number of samples remains fixed. Corners, edges, and boundary regions come to dominate the landscape.

We now examine the probability of obtaining samples near boundaries. For a d -dimensional hypercube $[0, 1]^d$, we define the interior region as the set of points at least a distance ε away from any boundary, which occupies a fraction $P_{\text{int}}^{\text{UNIFORM}}(d, \varepsilon) = (1 - 2\varepsilon)^d$ of the total volume. Complementarily, the probability that a UNIFORM ly-sampled point lies in the boundary shell (within ε of any face) grows exponentially as $P_{\text{bdry}}^{\text{UNIFORM}}(d, \varepsilon) = 1 - (1 - 2\varepsilon)^d$, which approaches unity at high dimensions.

The Tail Allocation Budget For TAILED-UNIFORM, samples extend beyond the hypercube boundaries into tail regions. With independent marginals, the probability that a sample lands inside the d -dimensional hypercube is the product

$$P_{\text{cube}}^{\text{TAILED-UNIFORM}}(d) = \prod_{i=1}^d B_i = B^d = \left(\frac{1}{1 + \alpha\sqrt{2\pi}} \right)^d, \quad (10)$$

assuming identical α across dimensions. This means the probability of sampling in the tail regions grows as $P_{\text{tail}}^{\text{TAILED-UNIFORM}}(d) = 1 - B^d$. By the same token, the probability of landing in the interior becomes $P_{\text{int}}^{\text{TAILED-UNIFORM}}(d, \varepsilon) = B^d \cdot (1 - 2\varepsilon)^d$, while the boundary shell captures $P_{\text{bdry}}^{\text{TAILED-UNIFORM}}(d, \varepsilon) = B^d [1 - (1 - 2\varepsilon)^d]$. Figure 8 summarizes these quantities for representative dimensions.

At first glance, it might seem that by bleeding samples into the tails, too many samples will wind up outside the region of interest, thus diminishing the overall performance of TAILED-UNIFORM. To test this suspicion, we evaluate NPE trained with UNIFORM and TAILED-UNIFORM proposals on a Gaussian linear inference task across $d \in \{4, 8, 16\}$ dimensions.

Boundary Dominance in Higher Dimensions: Figure 7 shows that while both methods degrade with increasing dimensionality, TAILED-UNIFORM regularly outperforms UNIFORM, with the performance gap widening at higher dimensions. This somewhat paradoxical finding suggests that the ratio of information gained from exterior support to cost of interior sample dilution remains favorable or even improves with dimension. Extra samples from TAILED-UNIFORM flow into the tail regions, surrounding the boundaries and offering regularization. Indeed, at $d = 16$, boundaries are so dominant that the marginal value of additional interior samples is low, as the network has ample interior coverage even when 99.99% of TAILED-UNIFORM samples lie outside the region of interest. Meanwhile, the marginal value of tail samples is high, as they are the only source of information near the boundary, which explains why TAILED-UNIFORM still achieves somewhat better C2ST scores

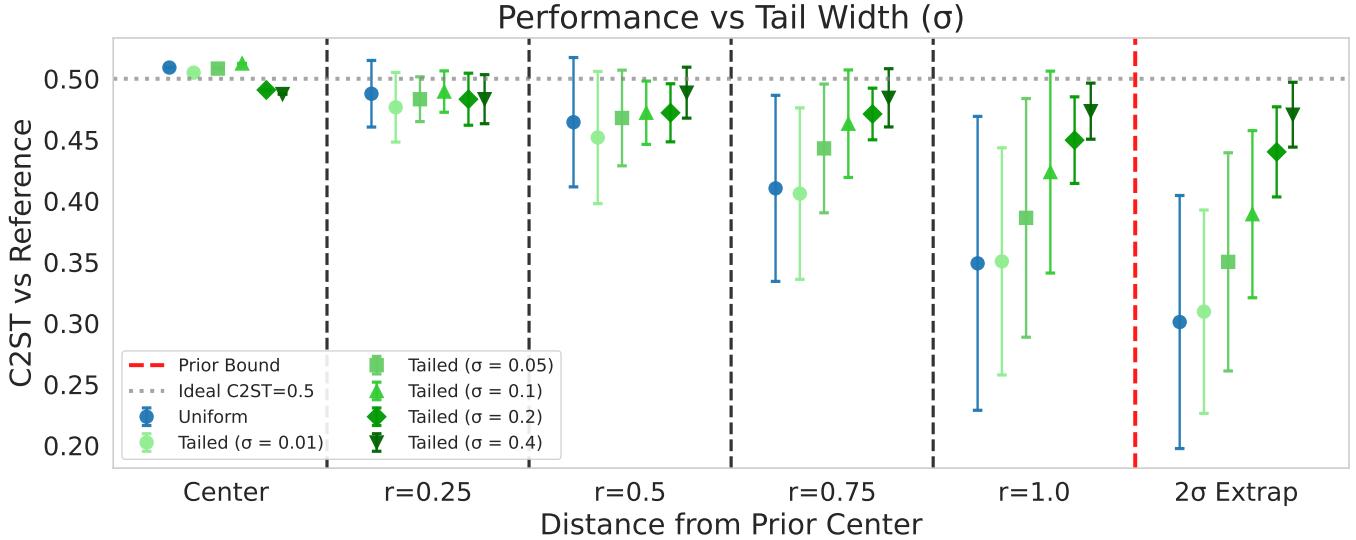


FIG. 5.— C2ST performance versus distance from center, stratified by tail width σ . The UNIFORM baseline (blue) exhibits systematic boundary degradation. The TAILED-UNIFORM’s with varying tail widths (shown in green; lighter shades for smaller σ values) exhibit robustness across a broad range of tail widths. Notably, performance becomes quite good for $\sigma \geq 0.2$. The error bars represent the 16th-84th percentile range of values at a fixed radius from the prior center.

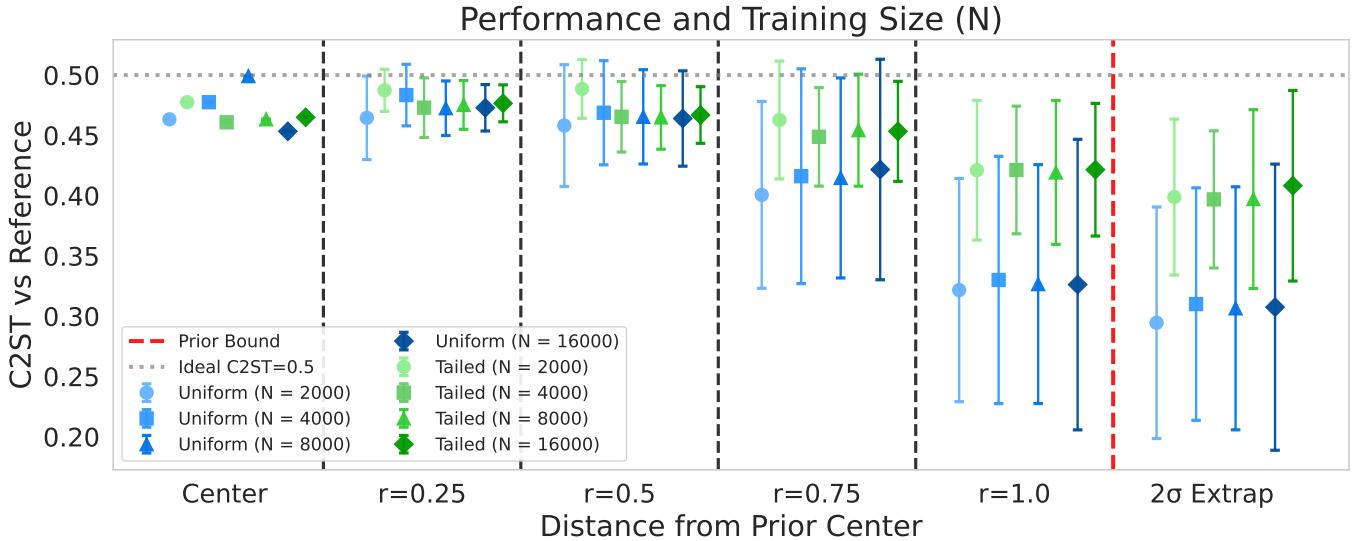


FIG. 6.— C2ST performance versus distance from parameter space center, stratified by training set size N (circles: 2000, squares: 4000, triangles: 8000, diamonds: 16000). Increasing N provides minimal benefit for both proposals. The error bars represent the 16th-84th percentile range of values at a fixed radius from the prior center.

than UNIFORM at the boundary and in the extrapolation regime (2σ beyond the prior boundary). We acknowledge that at very high dimensions, dilution effects will inevitably dominate, but these regimes are beyond the scope of most practical simulation-based inference tasks.

4. SCIENCE EXPERIMENT

Following the proof-of-concept-validation in Section 3, we show the practical utility of TAILED-UNIFORM by applying it to a realistic astrophysical inference problem.

4.1. Matter Power Spectrum

We demonstrate the versatility of the TAILED-UNIFORM proposal in a popular inference benchmark in cosmology: the inference of cosmological parameters

from the matter power spectrum (Dodelson and Schmidt 2020). To recreate the problem, we aim to predict the posterior distribution of two cosmological parameters $\theta = (\Omega_m, h)$ using the forward simulator $\mathcal{M} : \mathbb{R}^2 \rightarrow \mathbb{R}^{64}$ that maps a two-dimensional parameter vector to the power spectrum $\mathbf{P} \in \mathbb{R}^{64}$. Here, Ω_m is the matter density parameter that governs the growth rate of perturbations and h is the dimensionless Hubble parameter, which determines the physical scale of the horizon at matter-radiation equality.

In modern cosmology, the power spectrum $\mathbf{P}(k)$ measures the amplitude of density contrast fields $\delta(\mathbf{k})$ in Fourier space and is strictly dependent on the magnitude of the wave vector $k = |\mathbf{k}|$ (Dodelson and Schmidt 2020). This can be thought of as the ensemble average of all universes with the same cosmological parameters

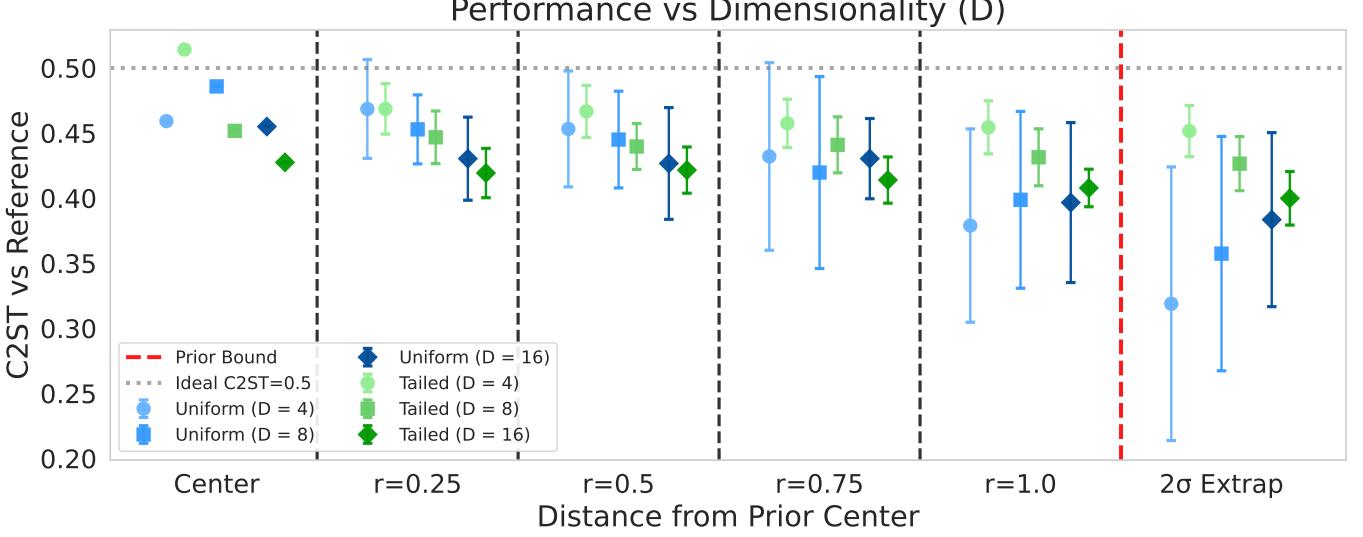


FIG. 7.— C2ST performance versus distance from parameter space center in different representative dimensions. TAILED-UNIFORM maintains superior performance with the advantage growing at higher dimensions, particularly near boundaries ($r \geq 0.75$) and in the extrapolation regime. The error bars represent the 16th-84th percentile range of values at a fixed radius from the prior center.

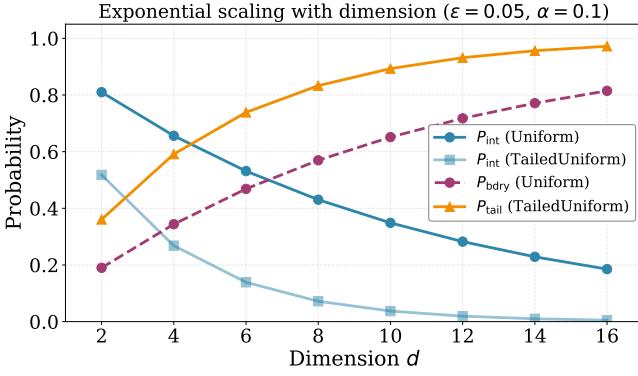


FIG. 8.— Exponential scaling of sample allocation with dimension for UNIFORM and TAILED-UNIFORM proposals ($\varepsilon = 0.05$, $\alpha = 0.1$). The probability of sampling in the interior region P_{int} (solid blue) decays exponentially for both methods, while the boundary region P_{bdry} (dashed purple) grows correspondingly for UNIFORM. For TAILED-UNIFORM, samples increasingly concentrate in the tail regions P_{tail} (solid orange), rising from 36% at $d = 2$ to 97% at $d = 16$. The crossing point around $d = 4$ marks where tail allocation exceeds interior allocation. Despite this apparent “waste,” we see that TAILED-UNIFORM maintains superior performance.

but different initial fluctuations. We also assume a flat Λ CDM cosmology with $w_0 = -1$, $w_a = 0$, and negligible neutrino masses $m_\nu = 0$, and fix the remaining cosmological parameters to Planck 2018 (Aghanim et al. 2020) values (the primordial scalar amplitude $A_s = 2.105 \times 10^{-9}$, the baryon density parameter $\Omega_b h^2 = 0.02242$, and the scalar spectral index $n_s = 0.9665$).

Model To circumvent the need to solve the perturbation equations numerically, we use the `syren-new` emulator (Sui et al. 2025), which leverages symbolic regression to produce a closed functional form for the theoretical power spectrum $\mathbf{P}_{\text{theory}}$ at negligible compute power. The power spectrum from `syren-new` is not the observed power spectrum per se, as our universe (armed with specific initial conditions) is merely one realization of some stochastic process. If we observe a sufficiently large volume, different regions within that volume will serve as independent samples of the same underlying pro-

cess (Baumann 2022). But since galaxy surveys cannot cover an infinite volume, the spatial average will not be exactly equal to the ensemble average.

For a comoving survey volume of $V = L^3$, the longest wavelength that fits in the box (i.e., the fundamental mode) is $k_f = |\mathbf{k}| = \frac{2\pi}{L}$, and by assuming the universe to be homogeneous and isotropic (i.e., rotationally invariant) on large scales (Dodelson and Schmidt 2020), we then find the number of modes inside a spherical shell at wavenumber k with thickness $\Delta k = k_f$ to be

$$N_k = \frac{4\pi k^2 \Delta k}{k_f^3} = \frac{L^3 k^2 k_f}{2\pi^2}. \quad (11)$$

This is called cosmic variance, which arises from the limited number of independent modes available in our finite observation volume (Dodelson and Schmidt 2020; Baumann 2022).

Together, we can construct an observation as

$$\mathbf{x}_i = \mathbf{P}(k | \boldsymbol{\theta}_i) = \underbrace{\mathbf{P}_{\text{theory}}(k | \boldsymbol{\theta}_i)}_{\text{syren_new emulator}} + \underbrace{\boldsymbol{\epsilon}_i}_{\text{cosmic noise}}, \quad (12)$$

where $\boldsymbol{\epsilon}_i \sim \mathcal{N}(\mathbf{0}, \text{diag}(\sigma_1^2, \dots, \sigma_{N_k}^2))$ represents the heteroskedastic (scale-dependent) cosmic noise with a variance $\sigma_k^2 = \frac{2\mathbf{P}_{\text{theory}}^2(k | \boldsymbol{\theta}_i)}{N_k}$.

Ground Truth As in Section 3, we have the luxury of direct sampling via MCMC (Brooks et al. 2011), as the forward model is explicit and the joint likelihood $\mathcal{P}(\mathbf{x} | \boldsymbol{\theta})$ can be evaluated point-wise. We choose a truncated Gaussian prior centered at the midpoint of $\Omega_m \in [0.24, 0.40]$ and $h \in [0.61, 0.73]$. Assuming independent Gaussian noise in each k -bin, we can write the log-likelihood as

$$\log \mathcal{P}(\mathbf{x} | \boldsymbol{\theta}) = -\frac{1}{2} \sum_{i=1}^N \left(\frac{\mathbf{x}_i - P_{\text{theory},i}(\boldsymbol{\theta})}{\sigma_i(\boldsymbol{\theta})} \right)^2 - \sum_{i=1}^N \log \sigma_i(\boldsymbol{\theta}), \quad (13)$$

where the first term quantifies the chi-squared misfit be-

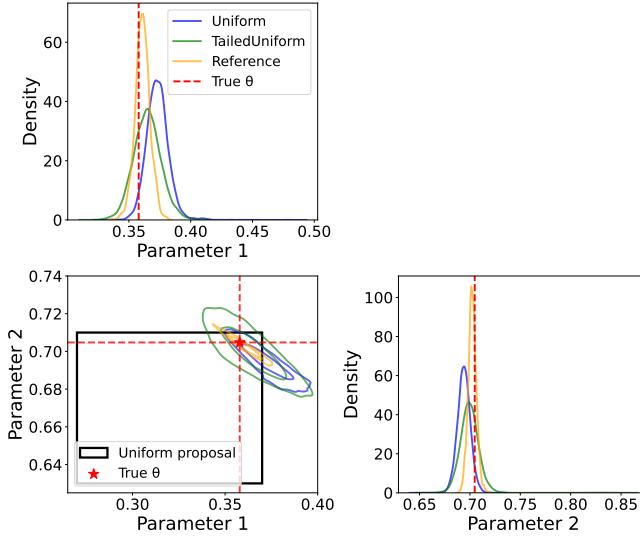


FIG. 9.— Corner plots comparing posterior estimation performance for test point $\theta_{\text{true}} = (0.358, 0.702)$. The TAILED-UNIFORM (green) closely matches the MCMC reference (yellow), maintaining tight concentration along the banana-shaped posterior. In contrast, the UNIFORM (blue) exhibits excessive spread, leaking probability mass into regions inconsistent with the data. The characteristic anti-correlation between Ω_m and h is visible in all methods, but only TAILED-UNIFORM accurately captures the posterior near the boundary.

tween theory and observation, and the second term accounts for the uncorrelated nature of the noise. Putting things together, the log posterior we aim to sample is $\log \mathcal{P}(\boldsymbol{\theta} | \mathbf{x} = \mathbf{x}_0) = \log \mathcal{P}(\mathbf{x}_0 | \boldsymbol{\theta}) + \log \mathcal{P}(\boldsymbol{\theta})$.

To sample the true posterior distribution, we run four MCMC walkers via the affine-invariant ensemble sampler in the `emcee` package (Foreman-Mackey et al. 2013), each generating 2000 samples after a burn-in period of 500 steps to ensure convergence. In total, we collect $4 \times 2000 = 8000$ posterior samples, which we treat as our ground truth.

Training and Model Architectures In this experiment, we choose a comoving box size of $L = 1000 h^{-1} \text{Mpc}$ and measure the power spectrum at $N = 64$ logarithmically spaced wavenumbers spanning from the fundamental mode $k_f = 2\pi/L$ to the Nyquist frequency $k_{\text{nyq}} = \pi N/L$, evaluated at the present epoch ($a = 1.0$). Recall again that we want to compare the performance of neural networks trained with two distinct proposals $\tilde{\mathcal{P}}_{\text{UNIFORM}}$ and $\tilde{\mathcal{P}}_{\text{TailedUNIFORM}}$, which by the relative complexity of the problem, will most likely be affected by our architectural choices. One could now proceed by trial and error: training dozens of models with different configurations and choosing the ones with the best log-probability. We advise against that method and instead choose to perform Bayesian optimization via the `Optuna` framework (Akiba et al. 2019) with a search space consisting of flow architecture (MAF or NSF), hidden features (4 to 64), number of transform layers (1 to 5), batch size (8 to 256), and learning rate (10^{-4} to 10^{-2}). Once the hyperparameter search concludes, we rank all trained networks by their validation log-probability and ensemble the top 10 performing models.

4.2. Validation

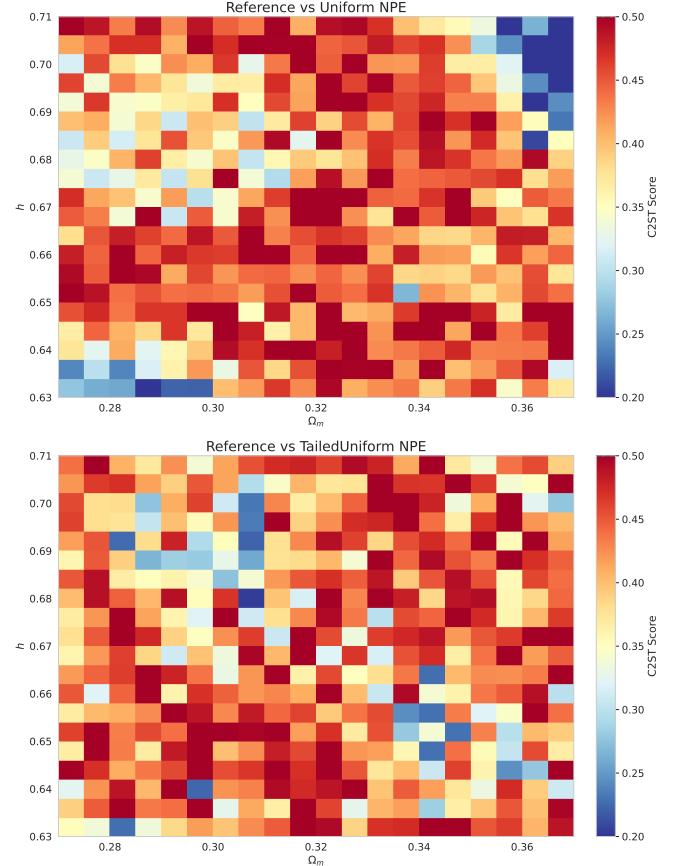


FIG. 10.— Spatial distribution of C2ST performance across the (Ω_m, h) parameter space, with darker blue regions indicating poor distributional matching ($\text{C2ST} \ll 0.5$) and orange-red regions indicating good performance ($\text{C2ST} \approx 0.5$). **Top:** UNIFORM versus MCMC reference, showing systematic degradation with blue patches near parameter space edges and corners. **Bottom:** TAILED-UNIFORM NPE versus reference, demonstrating consistent orange coloration across the parameter space.

To assess the performance of our competing proposals in this cosmological inference task, we adopt the same spatial evaluation framework as in Section 3. We should first discuss why Ω_m and h are given special consideration, which led us to select them as the inference parameter. There is a variety of factors, the most notable of which is the strong degeneracies between them.

Degeneracies Degeneracy refers to situations in which multiple parameters replicate the same observable. In our case, the matter power spectrum at small and intermediate scales is sensitive to the physical matter density, which happens to scale as $\Omega_m h$, rather than by Ω_m and h independently (Peacock and Dodds 1996). The two parameters are thereby anti-correlated.

As a result, the information embedded in our posterior will be weak along certain directions in the parameter space, where Ω_m trades off against h such that $\Omega_m h$ remains about constant, leading to the slanted banana-shaped contours (as also reflected in the posteriors' performance in Figure 10). Such geometric degeneracies in the power spectrum from different combinations of Ω_m and h , combined with the likelihood being non-linear, make this a challenging inference problem.

4.2.1. Single-Point Analysis

To study this phenomenon in detail, we first select a test point $\theta = (0.358, 0.702)$ positioned near the top-right boundary. We generate observations and draw $M = 8,000$ posterior samples from the MCMC reference, UNIFORM, and TAILED-UNIFORM.

TABLE 2
POSTERIOR PERFORMANCE FOR TEST POINT $\theta_{\text{TRUE}} = (0.358, 0.702)$

Method	Parameter Estimates		C2ST
	Ω_m	h	
MCMC Reference	0.361 ± 0.006	0.702 ± 0.004	0.500
TAILED-UNIFORM	0.365 ± 0.011	0.700 ± 0.011	0.405
Uniform	0.373 ± 0.009	0.694 ± 0.006	0.259
C2ST Improvement			+56%

Figure 9 shows that UNIFORM has notable dispersion along the degenerate direction. This leakage shows that when observations overlap boundary regions of the training distribution, UNIFORM has learned an inaccurate, spewed-out posterior and is unable to constrain parameters. The TAILED-UNIFORM, on the other hand, reproduces the banana-shaped contours of the MCMC reference, with samples tightly concentrated around the true parameter values. Table 2 quantifies these results. While all three methods recover similar point estimates for both parameters, the C2ST scores reveal substantial differences in posterior quality. The UNIFORM has a C2ST of only 0.395, while the TAILED-UNIFORM scores 0.452, which is very close to the ideal value of 0.5, showing a 14% increase in distributional fidelity. This improvement demonstrates that TAILED-UNIFORM can capture the full covariance structure of the banana-shaped posterior, more so along the degenerate direction.

4.2.2. Spatial Performance Analysis

As before, we discretize a UNIFORM rectangular grid with $n = 20$ test locations along each dimension, spanning $\Omega_m \in [0.27, 0.37]$ and $h \in [0.63, 0.71]$. For each of the 400 evaluation points, we generate observations, draw $M = 1000$ posterior samples from all three methods, and calculate pairwise C2ST scores.

Both methods achieve similar C2ST scores in Figure 10, but by eye inspection, TAILED-UNIFORM appears to provide reliable inference everywhere, whereas UNIFORM is only productive near the center. To connect the performance degradation trend to the underlying physics, we propose a different binning strategy. We first define the degeneracy direction as $d_1 = \Omega_m + h$, which describes movement along the banana-shaped posterior where the physical matter density $\Omega_m h$ varies slowly. Perpendicular to this, we define $d_2 = \Omega_m - h$, which captures variation across the degeneracy.

Figure 11 shows that boundary pathology is anisotropic, with the most severe manifestation along degenerate directions where posteriors are elongated into the prior boundaries. As a result, both approaches perform about the same (excluding statistical fluctuations) along the perpendicular direction d_2 . However, across the degeneracy direction d_1 , the UNIFORM performance sinks at both boundaries, with C2ST scores falling to 0.22–0.30. The UNIFORM is unable to learn the posterior

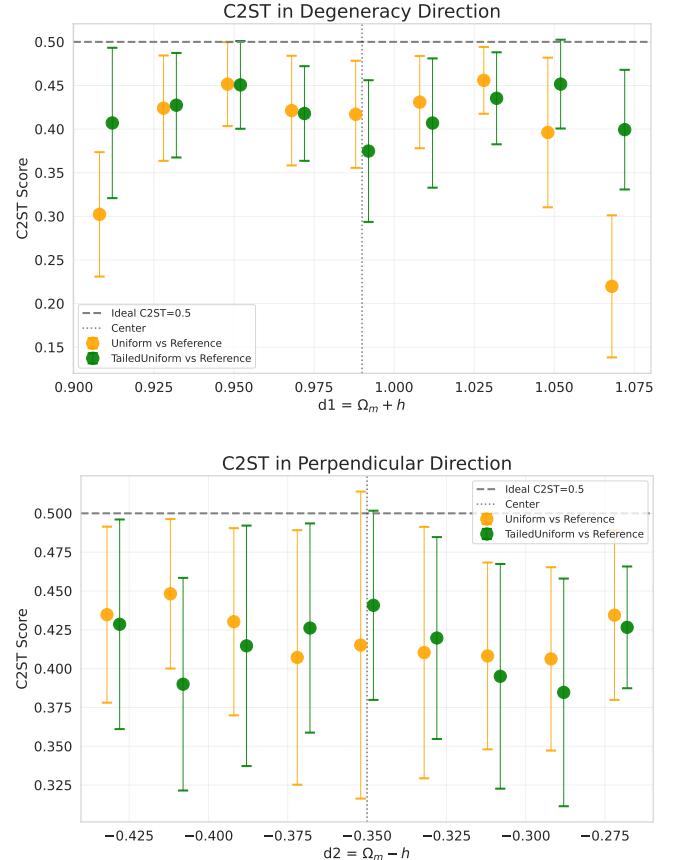


FIG. 11.— C2ST performance as a function of position along two orthogonal directions in parameter space. The error bars represent the 16th–84th percentile range of values at a fixed bin. **Top:** Along the degeneracy direction, the *Uniform* (yellow) exhibits performance degradation at the boundaries. The *TailedUniform* (green) maintains robust performance throughout. **Bottom:** Along the perpendicular direction, both methods perform similarly.

tails because the elongated banana-shaped posterior has spread into and beyond areas with sparse training coverage. By extending the simulation distribution beyond the prior boundaries, the TAILED-UNIFORM enables robust, unbiased inference across the full parameter space.

5. CONCLUSION

We have identified and addressed a fundamental limitation of neural posterior estimation: the boundary pathology caused by sharp discontinuities in UNIFORM proposal distributions, which systematically degrades posterior quality near parameter space boundaries and is exacerbated both in high-dimensional spaces and when parameter degeneracies extend posteriors toward prior edges. To resolve this limitation, we proposed the TAILED-UNIFORM proposal, a hybrid distribution that maintains UNIFORM density within the primary region of interest while extending smooth Gaussian tails beyond the boundaries, providing neural networks with the gradient information necessary to learn continuous density transitions.

In the two-dimensional Gaussian Linear benchmark, TAILED-UNIFORM maintains consistent performance ($\text{C2ST} \approx 0.44\text{--}0.49$) throughout the domain, while UNIFORM exhibits systematic degradation toward parameter space edges (C2ST scores falling below 0.35). We also

validated our method for inferring cosmological parameters (Ω_m, h) from matter power spectra. Empirically, TAILED-UNIFORM provides support along the Ω_m-h degeneracy, as elongated posteriors extend toward prior boundaries.

Perhaps most critically, our sensitivity studies demonstrate that the degradation of the original sampling strategy is structural rather than statistical: increasing training data yields negligible improvement for UNIFORM, whereas TAILED-UNIFORM with as few as $N = 2,000$ simulations consistently outperforms UNIFORM with eight times the training budget. This confirms that the problem lies in the discontinuous proposal itself rather than insufficient coverage. Our method also exhibits counter-intuitive scaling behavior in higher dimensions: despite allocating an increasingly large fraction of samples to tail regions as dimensionality grows (from 24% at $d = 2$ to 86% at $d = 16$), TAILED-UNIFORM maintains superior performance over UNIFORM sampling across all tested dimensions.

In conclusion, TAILED-UNIFORM gives neural posterior estimators the support they need to learn accurate

posteriors close to boundaries by expanding the training distribution beyond the primary region of interest with smooth Gaussian tails. Our method provides a parsimonious, computationally cheap modification to existing SBI workflows that results in significant improvements in posterior quality across inference tasks.

While we have demonstrated TAILED-UNIFORM’s effectiveness up to $d = 16$ dimensions, the scaling behavior at very high dimensions ($d \gtrsim 32$) remains unexplored. At high dimensionality, the dilution of interior samples may come to dominate over the benefits of boundary smoothing. Additionally, while we focused on neural posterior estimation (NPE), we maintain that TAILED-UNIFORM is architecture-invariant and can be used with neural likelihood estimation (NLE) and neural ratio estimation (NRE); comparative studies across these methodologies would further establish the universality of our approach.

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