Amortized Bayesian Workflow

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Abstract

Bayesian inference often faces a trade-off between computational speed and sampling accuracy. We propose an adaptive workflow that integrates rapid amortized inference with gold-standard MCMC techniques to achieve a favorable combination of both speed and accuracy when performing inference on many observed datasets. Our approach uses principled diagnostics to guide the choice of inference method for each dataset, moving along the Pareto front from fast amortized sampling via generative neural networks to slower but guaranteed-accurate MCMC when needed. By reusing computations across steps, our workflow synergizes amortized and MCMC-based inference. We demonstrate the effectiveness of this integrated approach on several synthetic and real-world problems with tens of thousands of datasets, showing efficiency gains while maintaining high posterior quality.

1 Introduction

In many statistical modeling applications, from finance to biology and neuroscience, we often aim to infer unknown parameters θ from observables y modeled as a joint distribution $p(\theta, y)$ (e.g., Raulo et al., 2023; Seaton et al., 2023; George et al., 2022; Landmeyer et al., 2020; Chen et al., 2019; Malén et al., 2022; Schneider et al., 2018; Tsilifis & Ghosh, 2022). The posterior $p(\theta \mid y)$ is the statistically optimal solution to this inverse problem, and there are different computational approaches to approximate this target distribution.

Markov chain Monte Carlo (MCMC) methods constitute the most popular family of posterior sampling algorithms and still remain the gold standard for modern Bayesian inference due to their theoretical guarantees and powerful diagnostics (Gelman et al., 2013; 2020). MCMC methods yield autocorrelated draws conditional on a fixed dataset y_{obs}. As a consequence, the probabilistic model has to be re-fit for each new dataset, which involves repeating the entire MCMC procedure from scratch. Modern implementations equip MCMC with state-of-the-art extensions, for example, through Hamiltonian dynamics (HMC; Neal, 2011), by minimizing the required tuning by users (NUTS; Hoffman & Gelman, 2014), or by parallelizing thousands of chains on GPU hardware (ChEES-HMC; Hoffman et al., 2021). The well-established *Bayesian workflow* (Gelman et al., 2020) leverages these tools in an iterative process of model specification, fitting, evaluation, and revision. While powerful, this approach becomes computationally burdensome when applied independently to large collections of datasets.

Differently, *amortized Bayesian inference* (ABI) aims to learn a direct mapping from observables y to the corresponding posterior $p(\theta \mid y)$, using flexible function approximators such as deep neural networks (Cranmer et al., 2020; Radev et al., 2020; Greenberg et al., 2019; Papamakarios et al., 2021; Wildberger et al., 2023; Sharrock et al., 2024; Zammit-Mangion et al., 2025). Amortized inference typically follows a two-stage approach: (i) a training stage, where neural networks learn to distill information from the probabilistic model based on simulated examples of observations and parameters $(\theta, y) \sim p(\theta)\, p(y \mid \theta)$; and (ii) an inference stage where the neural networks approximate the posterior distribution for an unseen dataset y_{obs} in near-instant time without repeating the training stage. In other words: The upfront training cost is *amortized* by negligible inference cost on arbitrary amounts of unseen test data. Owing to its reliance on simulated data, amortized inference in this form overlaps with *simulation-based inference* (Cranmer et al., 2020), which originated from posterior computations for models with intractable likelihood.

However, amortized inference lacks the powerful diagnostics and gold-standard guarantees associated with MCMC samplers in the standard Bayesian workflow (Gelman et al., 2020). Yet, applying a standard workflow

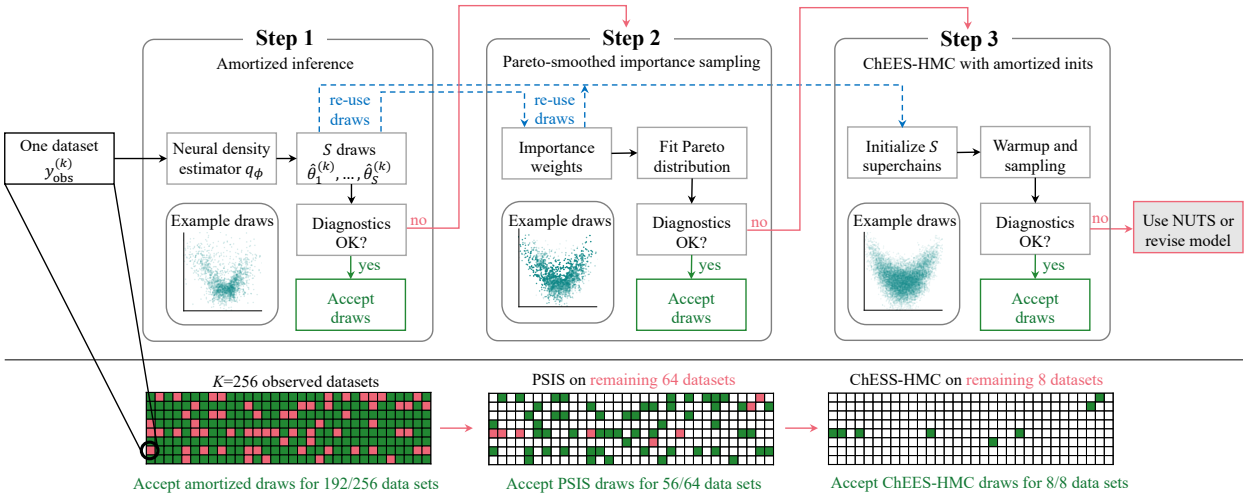

Figure 2: Our adaptive workflow leverages near-instant amortized posterior sampling when possible and gradually resorts to slower—but more accurate—sampling algorithms. As indicated by the blue dashed arrows, we reuse the S draws from the amortized posterior in Step 1 for the subsequent steps in the form of PSIS proposals (Step 2) and initial values in ChEES-HMC (Step 3).

is computationally prohibitive at scale. In modern Bayesian computation, MCMC and ABI occupy different ends of a Pareto frontier (see Figure 1): the former provides reliable accuracy at high cost, while the latter offers near-instant inference speed with limited per-dataset reliability (Hermans et al., 2022; Schmitt et al., 2023; Lueckmann et al., 2021).

In this paper, we propose an adaptive workflow that consistently yields high-quality posterior draws while remaining computationally efficient. Our proposed workflow *moves along the Pareto front*, enabling fast-and-accurate inference when possible, and slow-but-guaranteed-accurate inference when necessary (see Figure 1). It combines the strengths of ABI and MCMC by incorporating diagnostic checks to guide inference decisions and reuse computations wherever possible. The resulting *amortized Bayesian workflow* therefore offers a principled, scalable, and diagnostic-driven approach for efficient posterior inference on many observed datasets; see Figure 2 for a conceptual overview.

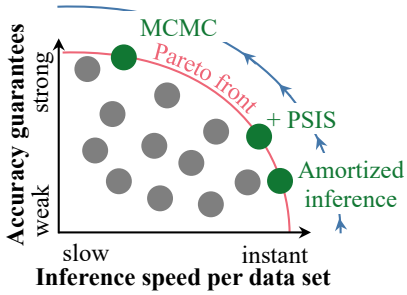

Figure 1: Our workflow adaptively moves along the Pareto front and reuses previous computations.

2 Integrating amortized inference into the Bayesian workflow

Our adaptive workflow starts with neural network training to enable subsequent amortized inference on a large number of unseen datasets—typically well into tens of thousands. This training phase is conceptually identical to standalone amortized inference training (e.g., Radev et al., 2020; Cranmer et al., 2020). For the inference phase, however, we develop a principled control flow that guides the analysis. Based on state-of-the-art diagnostics that are tailored to each step along the workflow, we propose decision criteria to select the appropriate inference algorithm for each observed dataset. In order to optimize the overall efficiency, our workflow contains mechanisms to reuse previous computations along the way.

2.1 Training phase: simulation-based optimization

In ABI, we train an amortized estimator q_ϕ which is parameterized by neural network weights ϕ. This optimization objective is formalized as minimizing the Kullback–Leibler (KL) divergence between the true posterior $p(\theta \mid y)$ and the learned approximation $q_\phi(\theta \mid y)$ (Papamakarios & Murray, 2016; Greenberg et al.,

2019; Radev et al., 2020):

$$\phi = \arg\min_{\phi} \mathbb{E}_{p(y)} \left[\mathrm{KL} \left(p(\theta \,|\, y) \,\|\, q_\phi(\theta \,|\, y) \right] = \arg\min_{\phi} \mathbb{E}_{p(\theta)} \mathbb{E}_{p(y \,|\, \theta)} \left[-\log q_\phi(\theta \,|\, y) \right] . \tag{1}$$

Since most Bayesian models are generative by design, we can readily simulate M synthetic tuples of parameters and corresponding observations from the joint probabilistic model,

$$(\theta^{(m)}, y^{(m)}) \sim p(\theta, y) \quad \Leftrightarrow \quad \theta^{(m)} \sim p(\theta), \; y^{(m)} \sim p(y \,|\, \theta) \;\; \text{for } m = 1, \ldots, M, \tag{2}$$

which results in the training set $\{(\theta^{(m)}, y^{(m)})\}_{m=1}^{M}$ for optimizing Eq. 1. Throughout this paper, we use coupling-based normalizing flows (Durkan et al., 2019; Papamakarios et al., 2021) as a flexible conditional density estimator q_ϕ. However, our proposed workflow is agnostic to the specific choice of neural network architecture used for amortization, as long as the model supports efficient sampling (see Section 2.2.1) and density evaluations (see Section 2.2.2).

Diagnostics. Since the neural network training algorithm hinges on simulated data, we cannot evaluate the amortized posterior approximator on real data just yet. However, we can easily simulate a synthetic *test set* $\{(\theta_\star^{(j)}, y^{(j)})\}_{j=1}^{J}$ of size J from the joint model via Eq. 2. In this *closed-world* setting, we know which "true" parameter vector $\theta_\star^{(j)}$ generated each simulated test dataset $y^{(j)}$. A key diagnostic for evaluating the amortized posterior estimator is *simulation-based calibration checking* (SBC; Talts et al., 2018; Säilynoja et al., 2022; Modrák et al., 2023). Formally, SBC involves defining a test quantity $f : \Theta \times Y \to \mathbb{R}$ (e.g., marginal projections θ or the log likelihood $p(y \,|\, \theta)$), computing this statistic for the true data-generating parameter $\theta_\star^{(j)}$, and comparing it to the empirical distribution of the same statistic computed from amortized posterior draws given $y^{(j)}$ (Modrák et al., 2023). The rank of the true statistic within the posterior draws should be uniformly distributed if the amortized posterior estimator is well-calibrated. A complementary diagnostic to SBC is the parameter recovery check, where parameter estimates are compared against known ground-truth parameters (Radev et al., 2020; 2023). We refer to Appendix A for details.

Training phase: If simulation-based calibration checking and parameter recovery diagnostics pass, proceed to Step 1. Otherwise, tune the training hyperparameters (e.g., simulation budget, training epochs, learning rate, or neural network architecture) and re-train the amortized network.

2.2 Inference phase: posterior approximation on observed datasets

Once the amortized estimator is capable of yielding sufficiently accurate posterior draws in closed-world settings (i.e., in-distribution), we use the pre-trained neural network to achieve rapid amortized posterior inference on a total of K observed datasets $\{y_{\text{obs}}^{(k)}\}_{k=1}^{K}$. Recall that a given pre-trained amortized neural approximator may be perfectly suitable for some real datasets while it is utterly untrustworthy for others. Therefore, we want to assess on a per-dataset basis whether the amortized posterior draws are trustworthy and should be accepted, or whether we should proceed to a slower algorithm with stronger accuracy guarantees. The diagnostics in the inference phase are evaluated conditionally on each observed dataset, with the ultimate goal of determining whether the set of current posterior draws is acceptable for that specific dataset.

2.2.1 Step 1: Amortized posterior draws

We want to exploit the rapid sampling capabilities of the amortized posterior approximator q_ϕ as much as possible, as long as the sampled posteriors are reliable according to a set of principled diagnostics. Therefore, the natural first step for each observed dataset $y_{\text{obs}}^{(k)}$ is to query the amortized posterior and sample S posterior draws $\hat{\theta}_1^{(k)}, \ldots, \hat{\theta}_S^{(k)} \sim q_\phi(\theta \,|\, y^{(k)})$ in near-instant time (see Figure 2, first panel).

Diagnostics. Like other neural network based approaches, amortized inference may yield unfaithful results under distribution shifts (Schmitt et al., 2023; Ward et al., 2022; Huang et al., 2023). To address this, we directly quantify whether an observed dataset y_{obs} is *atypical* under the data-generating process $p(\theta, y)$. We first compute a low-dimensional summary statistic $s(y) \in \mathbb{R}^d$ for each dataset.[1] The summary statistics

[1]The summary statistic can be either learned by the amortized estimator q_ϕ or be based on domain knowledge.

from the training dataset $\{y^{(m)}\}_{m=1}^{M}$ are used to define a Mahalanobis distance. We compute this metric for each training dataset $y^{(m)}$ to establish a frequentist sampling distribution under the null hypothesis (i.e., of in-distribution datasets). Given a new dataset y_{obs}, we can now simply compare its empirical Mahalanobis distance to a predefined percentile threshold (e.g., 95^{th}) of the sampling distribution (see Figure 3). In a nutshell, this is a sampling-based hypothesis test for distributional typicality, similar in spirit to the kernel-based test proposed by Schmitt et al. (2023). Since the amortized approximator has no guarantees nor known error bounds for data outside of the typical set of the joint model (Elsemüller et al., 2024; Schmitt et al., 2023; Frazier et al., 2024; Elsemüller et al., 2025), we propagate such atypical datasets to Step 2.

Alternative diagnostics. In addition to the proposed OOD test, more sophisticated data-conditional diagnostics can further assess the accuracy of amortized posterior draws for individual datasets. Examples include posterior simulation-based calibration checking (posterior SBC; Säilynoja et al., 2025) or the local classifier two-sample test (L-C2ST; Linhart et al., 2023), to name a few. These diagnostics each offer distinct advantages and limitations, but typically require substantially more computation than the OOD test; we refer to Appendix B for a detailed discussion. By default, we recommend the OOD test for its simplicity, efficiency, and suitability as a first-line diagnostic.

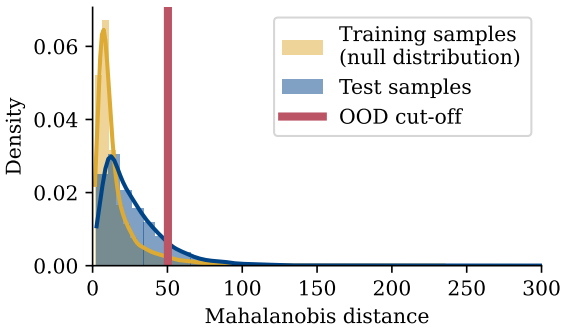

Figure 3: Illustration of our sampling-based hypothesis test that flags atypical datasets.

Step 1: If the observed dataset passes the OOD test (i.e., Mahalanobis distance is below the threshold), accept the amortized draws; otherwise, proceed to Step 2.

2.2.2 Step 2: Pareto-smoothed importance sampling

In this step, we use a Pareto-smoothed sampling importance sampling (PSIS) scheme (Vehtari et al., 2024) to improve the quality of the amortized posterior draws of datasets which have previously been rejected (see Figure 2, second panel). Based on the amortized posterior draws from Step 1, PSIS computes importance weights $w_s^{(k)} = p(y^{(k)} \mid \hat{\theta}_s)\, p(\hat{\theta}_s)/q_\phi(\hat{\theta}_s \mid y^{(k)})$ for each observed dataset $y^{(k)}$ (as in default importance sampling). Then, PSIS fits a generalized Pareto distribution, which in turn is used to smooth the tail of the weight distribution (Vehtari et al., 2024). Finally, these smoothed importance weights are used for computing posterior expectations and for improving the posterior draws with the sampling importance resampling (SIR) scheme (Rubin, 1988). While the utility of standard importance sampling for improving neural posterior draws has previously been investigated (Dax et al., 2023), we specifically use the PSIS algorithm, which is self-diagnosing (see **Diagnostics** below) and therefore better suited for a principled workflow. Further details of PSIS are provided in Appendix A.

Diagnostics. We use the Pareto-$\hat{k}$ diagnostic to gauge the fidelity of the PSIS-refined posterior draws. According to established guidelines (Vehtari et al., 2024; Yao et al., 2018), Pareto-$\hat{k} \leq 0.7$ indicates good results, whereas $\hat{k} > 0.7$ implies that the draws should be rejected and the respective datasets proceed to Step 3.

Note. The posterior estimator in ABI is typically mass-covering since it optimizes the *forward* KL divergence in Eq. 1. When the neural network training is insufficient (e.g., small simulation budget or poorly optimized network), this may lead to overdispersed posteriors. Fortunately, this tends to err in the right direction, and PSIS can generally mitigate overdispersed *mass-covering* draws in low to moderate dimensions (Dhaka et al., 2021). In contrast, variational inference typically optimizes the *reverse* KL divergence (Rezende & Mohamed, 2015), which implies *mode-seeking* behavior that is less favorable for importance sampling.

Step 2: If Pareto-$\hat{k} \leq 0.7$, accept the importance sampling results; otherwise, proceed to Step 3.

2.2.3 Step 3: Many-chains MCMC with amortized initializations

If PSIS does not yield satisfactory samples, we resort to an MCMC sampling scheme as a safe fall-back option. In our amortized workflow, the MCMC step is augmented by reusing computations from the previous steps as initialization values. In principle, this step can incorporate any MCMC algorithm suited to the problem at hand. Examples include slice sampling for models with non-differentiable likelihoods (Neal, 2003), or HMC (Neal, 2011) samplers when gradients are available.

In this work, we use the ChEES-HMC algorithm (Hoffman et al., 2021) as an instantiation of MCMC. Most notably, ChEES-HMC supports the execution of thousands of parallel chains on a GPU for high-throughput sampling (Sountsov et al., 2024). Amortized posterior draws from previous steps provide a natural and convenient choice for initializing MCMC chains to accelerate convergence (Figure 4). This approach is conceptually similar to using methods like parallel quasi-Newton variational inference (i.e., *Pathfinder*; Zhang et al., 2022) to obtain initial values for MCMC chains. However, the amortized initial values are drawn in parallel in near-instant time, while Pathfinder requires re-fitting the variational approximation for each new observed dataset. For the purpose of ChEES-HMC initializations with multimodal posterior distributions, it is again desirable that the amortized posterior draws are typically mass-covering (cf. Step 2). See Appendix A for additional details on the ChEES-HMC algorithm.

Diagnostics. In this last step, we use the nested $\widehat{R}$ diagnostic (Margossian et al., 2024), which is specifically designed to assess the convergence of the *many-but-short* MCMC chains.[2] If the diagnostics in this step indicate unreliable inference, we recommend resorting to the overarching Bayesian workflow (Gelman et al., 2020) and addressing the computational issues that even persist when using the (ChEES-)HMC algorithm. This could involve increasing the number of warmup iterations, using the established NUTS-HMC algorithm (Hoffman & Gelman, 2014; Carpenter et al., 2017), or revising the Bayesian model specification and parametrization.

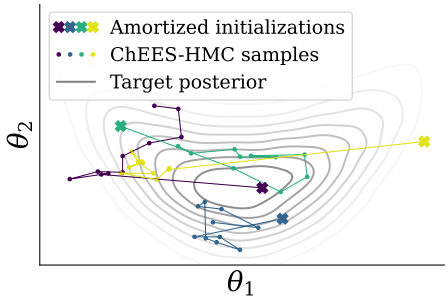

Figure 4: We initialize many ChEES-HMC chains with amortized draws.

Step 3: If (nested) $\widehat{R}$ is below the convergence threshold (e.g., 1.01), accept the MCMC draws. Otherwise, increase warm-up or revise the model according to the standard Bayesian workflow.

2.3 Related work

Both simulation-based inference and amortized inference have seen rapid progress over the past decade (Zammit-Mangion et al., 2025; Cranmer et al., 2020; Lavin et al., 2021), driven by the need to perform Bayesian inference in complex models with intractable likelihoods (e.g., Dingeldein et al., 2024; Wehenkel et al., 2024; Zhou et al., 2024; Ghaderi-Kangavari et al., 2023; von Krause et al., 2022; Bieringer et al., 2021; Radev et al., 2021). These advances have been fueled by modern generative modeling, such as normalizing flows (Papamakarios et al., 2021; Radev et al., 2020; Greenberg et al., 2019), transformers (Müller et al., 2022; Chang et al., 2025; Whittle et al., 2025), diffusion models (Song et al., 2021; Sharrock et al., 2024; Linhart et al., 2024; Geffner et al., 2023; Gloeckler et al., 2024), consistency models (Song et al., 2023; Schmitt et al., 2024b), and flow matching (Lipman et al., 2023; Wildberger et al., 2023).

To address the potential systematic errors of (amortized) neural posteriors, several works propose corrections using importance reweighting schemes (Dax et al., 2023; Starostin et al., 2025), augmented training objectives (Delaunoy et al., 2022; Mishra et al., 2025; Orozco et al., 2025; Schmitt et al., 2024a), or post-hoc corrections (Siahkoohi et al., 2023). Simultaneously, hybrid approaches that combine density estimators with MCMC have gained traction (Salimans et al., 2015; Hoffman et al., 2019; Gabrié et al., 2022; Midgley et al., 2022; Arbel et al., 2021; Cabezas et al., 2024; Grenioux et al., 2023). These include using variational approximations or learned flows as preconditioners for MCMC (Hoffman et al., 2019; Cabezas & Nemeth, 2023), adaptive

[2] In more conventional settings involving long MCMC chains, the standard $\widehat{R}$ diagnostics (Vehtari et al., 2021) can be applied.

proposal mechanisms (Parno & Marzouk, 2018; Gabrié et al., 2022), and initialization strategies to accelerate convergence or improve diagnostics (Zhang et al., 2022; Wang et al., 2023; Starostin et al., 2025).

Our proposed workflow builds on these lines of work by integrating amortized inference, likelihood-based correction, and many-chain MCMC into a unified, diagnostic-driven pipeline. It dynamically adapts the inference strategy to the dataset at hand, improving robustness without retraining. This modular design provides a practical foundation for principled amortized inference across diverse data regimes.

3 Experiments

In this section, we empirically evaluate the effectiveness of our proposed amortized Bayesian workflow across various synthetic and real-world problems. We also examine how reusing amortized posterior draws in subsequent steps can improve the downstream sampling performance. The source code to reproduce all experiments is available in the supplementary material.

3.1 Procedure

Training settings. For each problem, we begin by training the amortized posterior approximator on simulated parameter-observation pairs (i.e., simulation-based training). We verify that the model performance is satisfactory in a closed-world setting, as diagnosed by simulation-based calibration and parameter recovery checking (see Section 2.1). Details on diagnostic results, simulation budgets, and training hyperparameters are provided in Appendix C.

Inference settings. For the out-of-distribution diagnostics in Step 1, we use the $1 - \alpha = 95\%$ percentile as the rejection threshold. We compute Mahalanobis distances in the summary statistics using 10,000 training simulations. We draw 2,000 posterior samples from the amortized posterior q_ϕ at Step 1. In Step 2, we correct the amortized draws using PSIS, rejecting draws if Pareto-$\hat{k} > 0.7$. Step 3 uses ChEES-HMC with convergence determined by nested $\widehat{R} < 1.01$. We run 2048 chains in parallel (16 superchains, each with 128 subchains), with 200 warmup steps and *a single sampling step*, for a total of 2048 posterior draws.

Evaluation metrics. To assess the quality of posterior draws from our workflow, we compare them to reference posterior draws using two evaluation metrics: the 1-Wasserstein distance (W1) and the mean marginal total variation distance (MMTV). The W1 distance quantifies the overall discrepancy between full joint distributions. MMTV measures the lack of overlap between marginal distributions and takes value in the range $[0, 1]$; for example, an MMTV value of 0.2 implies that, on average, the approximate posterior draws and reference draws share an 80% overlap for their marginal distributions. For both metrics, lower values indicate better posterior approximation quality. As a rule of thumb, MMTV values below 0.2 indicate good posterior approximation fidelity (Acerbi, 2020; Li et al., 2025).

3.2 Applications

We apply the proposed workflow to four posterior inference problems, including both simulated benchmarks and real-world experimental datasets. These case studies were chosen to reflect a range of commonly encountered statistical inference scenarios, including classical distributional parameter estimation and analyses of large-scale datasets arising in psychology and cognitive modeling. We describe each problem briefly below, with further details provided in Appendix C.

Generalized extreme value distribution (GEV). We consider parameter inference for the generalized extreme value (GEV) distribution, which models the maxima of samples from a distribution family. Each observation y_i is modeled as:

$$y_i \sim \text{GEV}(\mu, \sigma, \xi), \tag{3}$$

where $\mu \in \mathbb{R}$ is the location, $\sigma \in \mathbb{R}_{>0}$ is the scale, and $\xi \in \mathbb{R}$ is the shape parameter. We follow the prior specification from Caprani (2021). For each dataset, we collect $N = 65$ i.i.d. observations and infer the posterior distribution over the parameter vector $\theta = (\mu, \sigma, \xi)$. We generate a total of $K = 1000$ test datasets

by deliberately simulating from a model with a 2× wider prior distribution to emulate out-of-distribution settings in real applications (see Appendix C for details).

Bernoulli GLM. The Bernoulli generalized linear model (GLM) is a classical model with binary outcomes, included in the SBI benchmark suite (Lueckmann et al., 2021). Each observation $y_i \in \{0, 1\}$ is modeled as:

$$y_i \sim \text{Bernoulli}(\sigma(v_i^\top \theta)), \tag{4}$$

where $v_i \in \mathbb{R}^{10}$ is a fixed input vector, $\theta \in \mathbb{R}^{10}$ is the parameter vector, and $\sigma(\cdot)$ denotes the logistic function. We generate $K = 10,000$ in-distribution test datasets by sampling parameters from the model prior and simulating corresponding observations $\{y_i\}_{i=1}^{100}$ (Lueckmann et al., 2021).

Psychometric curve fitting. Psychometric functions are widely used in perceptual and cognitive science to characterize the relationship between stimulus intensity and the probability of a specific response (Wichmann & Hill, 2001). We use the overdispersed hierarchical model from Schütt et al. (2016), where the number of correct trials y_i at stimuli level x_i is modeled as:

$$y_i \sim \text{Binomial}(n_i, p_i), \quad p_i \sim \text{Beta}\left(\left(\frac{1}{\eta^2} - 1\right)\bar{p}_i,\ \left(\frac{1}{\eta^2} - 1\right)(1 - \bar{p}_i)\right), \tag{5}$$

where n_i is the number of trials, $\eta \in [0, 1]$ controls overdispersion, and $\bar{p}_i = \psi(x_i; m, w, \lambda, \gamma)$ is the expected success probability given by the psychometric function $\psi(x; m, w, \lambda, \gamma) = \gamma + (1 - \lambda - \gamma)\, S(x; m, w)$, where S is a sigmoid function (e.g., cumulative normal), m is the threshold, w is the width, λ is the lapse rate for infinitely high stimulus levels, and γ is the guess rate for infinitely low stimulus levels. In total, the model parameters are $\theta = (m, w, \lambda, \gamma, \eta)$. Our empirical evaluation uses 8,526 mouse behavioral datasets from the International Brain Laboratory public database (The International Brain Laboratory et al., 2021).

Decision model. The drift-diffusion model (DDM) is a popular evidence accumulation model for psychological models of human decision making (Ratcliff & McKoon, 2008). It describes a two-choice decision task as a stochastic process in which noisy evidence accumulates over time until it reaches one of the decision boundaries. The evolution of the decision variable $z(t)$ is modeled as

$$\mathrm{d}z(t) = v\,\mathrm{d}t + \sigma\,\mathrm{d}W(t), \tag{6}$$

where v is the drift rate (the average rate of evidence accumulation), σ is the noise scale, and $W(t)$ denotes a standard Wiener process. A decision is made when $z(t)$ reaches either a positive or negative boundary, typically placed symmetrically at $\pm a$, where a is the boundary separation. The model also includes a non-decision time parameter τ, capturing processes that are not part of the decision process. We adopt the model specification from von Krause et al. (2022), which extends the standard DDM to incorporate experimental condition effects via six parameters: $\theta = (v_1, v_2, a_1, a_2, \tau_c, \tau_n)$. The test datasets consist of 15,000 participants from the online implicit association test (IAT) database (Xu et al., 2014; von Krause et al., 2022), providing a large-scale, real-world benchmark for Bayesian inference in cognitive modeling.

3.3 Main Results

Table 1 summarizes the performance of the proposed amortized Bayesian workflow across the four problems described in Section 3.2. Step 1 (ABI) exhibits extremely low time per accepted dataset (TPA), with most of the cost incurred as a one-time expense during the training phase—including prior simulation, model training, and diagnostic evaluation. Once trained, ABI incurs negligible marginal cost ($\ll$ 1sec) when applied to a new dataset. Datasets flagged as out-of-distribution in Step 1 are forwarded to Step 2 for correction via PSIS. PSIS is highly effective, successfully correcting most rejected amortized draws and substantially reducing the number of datasets requiring full MCMC. Only a small subset of datasets progresses to Step 3, where ChEES-HMC is used for high-fidelity sampling. As the most computationally expensive component, ChEES-HMC is applied selectively, allowing the workflow to retain both accuracy and efficiency. Overall, the amortized workflow completes inference for nearly all datasets.[3] Compared to using ChEES-HMC for all

[3]A small number of datasets with particularly difficult properties require extended MCMC runs to converge.

Table 1: Summary of our amortized Bayesian workflow across four problems. For each step, we report the number of accepted datasets, wall-clock time (minutes), and **t**ime **p**er **a**ccepted dataset (TPA) in seconds. The time for Step 1 includes training, inference, and diagnostics for the amortized model. "Workflow total" aggregates the results of our method across all steps. As a baseline reference, "Baseline workflow total" is an estimate of the total required runtime for ChEES-HMC on all datasets.

Problem	Step	Accepted datasets	Time (min)	TPA (s)
GEV	Step 1: Amortized inference	523/1000	3	0.4
	Step 2: Amortized + PSIS	357/477	0.8	0.1
	Step 3: ChEES-HMC w/ inits	87/120	11	7
	Workflow total (ours)	967/1000	15	0.9
	Baseline workflow total	—	85	—
Bernoulli GLM	Step 1: Amortized inference	9519/10000	1	0.007
	Step 2: Amortized + PSIS	425/481	0.4	0.06
	Step 3: ChEES-HMC w/ inits	56/56	4	4
	Workflow total (ours)	10000/10000	5	0.03
	Baseline workflow total	—	688	—
Psychometric curve	Step 1: Amortized inference	7213/8526	7	0.06
	Step 2: Amortized + PSIS	1215/1313	4	0.2
	Step 3: ChEES-HMC w/ inits	69/98	26	22
	Workflow total (ours)	8497/8526	37	0.3
	Baseline workflow total	—	2217	—
Decision model	Step 1: Amortized inference	13498/15000	86	0.4
	Step 2: Amortized + PSIS	827/1502	47	3
	Step 3: ChEES-HMC w/ inits	554/675	526	57
	Workflow total (ours)	14879/15000	659	3
	Baseline workflow total	—	11594	—

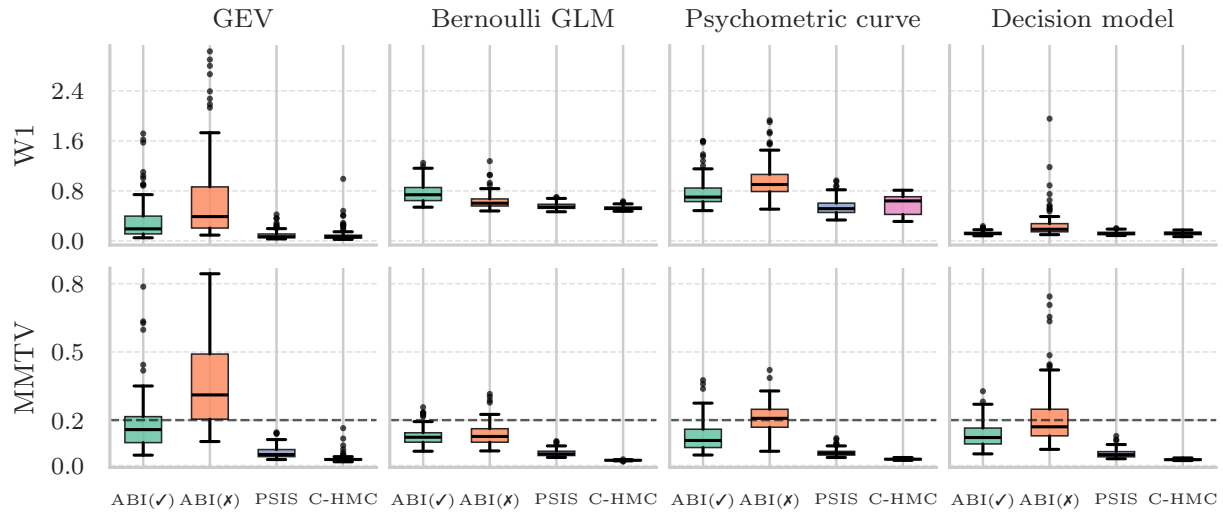

Figure 5: Evaluation of posterior draws across four problems based on two metrics: W1 distance (top row) and MMTV distance (bottom row). Lower values indicate better posterior approximation. ABI(✓) and ABI(✗) denote accepted and rejected draws, respectively, from amortized Bayesian inference in Step 1. PSIS denotes importance-weighted draws accepted in Step 2, and C-HMC denotes draws accepted via ChEES-HMC in Step 3.

datasets, our workflow achieves substantial computational savings—approximately over 5×, 120×, 60×, and 15× faster for the GEV, Bernoulli GLM, psychometric curve, and decision model tasks, respectively.

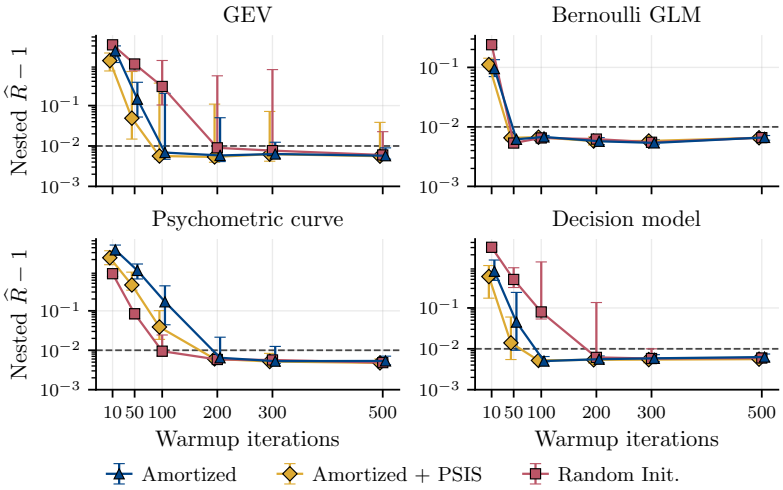

Figure 6: Using amortized posterior draws as initializations for ChEES-HMC reduces the required warmup in the GEV and decision model tasks. We show median±IQR across 20 test datasets in Step 3.

Figure 5 presents the quality of posterior draws using the W1 distance (top row) and MMTV distance (bottom row), comparing draws from each step of the workflow against reference posteriors obtained via well-tuned NUTS. Rejected amortized draws (ABI✗) exhibit markedly worse performance than accepted ones (ABI✓), confirming the effectiveness of the OOD diagnostics.[4] PSIS-corrected draws offer accuracy comparable to ChEES-HMC samples, with only a slight decrease in quality. While amortized draws accepted in Step 1 are less accurate than those produced by PSIS or ChEES-HMC, they still provide high-quality approximations across the majority of datasets, as implied by the W1 and MMTV metrics. These results demonstrate that the proposed workflow not only scales efficiently but also consistently produces high-quality posterior estimates.

3.4 Advantage of amortized initializations for MCMC

One major goal of our workflow is to minimize reliance on expensive MCMC by maximizing the reuse of computations. Even when ABI and the PSIS refinement fail to yield acceptable posterior draws after Step 2, we can still leverage the amortized outputs to accelerate MCMC in Step 3.

To evaluate whether amortized posterior estimates remain useful in such cases, we test their effectiveness as initializations for ChEES-HMC chains. We conduct experiments on 20 randomly selected test datasets that progress to Step 3 of the workflow. This indicates that both the amortized posterior draws and their Pareto-smoothed refinement are deemed unacceptable, as quantified by Pareto-$\hat{k} > 0.7$ in Step 2. We compare three initialization methods for ChEES-HMC chains: (1) amortized posterior draws, (2) PSIS-refined amortized draws, and (3) a random initialization scheme similar to Stan (Carpenter et al., 2017). We run the chains for varying numbers of warmup iterations, followed by a single sampling iteration. As described in Section 2, we use the nested $\widehat{R}$ value to gauge whether the chains converged appropriately during the warmup stage, as quantified by the common $\widehat{R} - 1$ threshold of 0.01 (Vehtari et al., 2021).

Figure 6 shows that amortized posterior draws (and their PSIS-refined counterparts) can significantly reduce the required number of warmup iterations to achieve ChEES-HMC chain convergence, *even though the draws themselves have previously been flagged as unacceptable*. For the GEV problem and the decision model, chains initialized with amortized draws converge faster than those using random initialization. In the Bernoulli GLM, all methods perform similarly. For the psychometric curve model, random initialization leads to faster convergence for the early stage, but amortized draws still reach the convergence threshold at a similar speed at iteration 200, indicating competitive performance. These findings are particularly relevant in the many-short-chains regime, where computational cost is dominated by the warmup phase. For instance, with 2048 parallel chains, every single post-warmup step yields 2048 posterior samples, leading to enormous efficiency gains from shorter warmup.

[4]For the Bernoulli GLM, the rejected amortized draws appear of good quality because the test datasets are drawn directly from the same prior used during training (i.e., in-distribution).

Overall, these results demonstrate that amortized inference may provide suitable initializations for ChEES-HMC. However, the added benefit of initializing chains with PSIS-refined amortized draws (Step 2) instead of raw amortized draws (Step 1) remains unclear. While PSIS often accelerates convergence, it occasionally degrades worst-case performance (see upper error bounds for GEV task in Figure 6). We further study the impact of initialization for the popular NUTS sampler (Hoffman & Gelman, 2014), with similar results: amortized initializations reduce the required warmup in most cases (see Appendix D).

4 Discussion

We presented an adaptive Bayesian workflow to combine the rapid speed of amortized inference with the undisputed sampling quality of MCMC. Our amortized workflow enables a fundamental shift in the scale and feasibility of Bayesian inference. Applying traditional MCMC (e.g., ChEES-HMC) within a standard Bayesian workflow to every dataset independently would require approximately 10 days of GPU computation across our experimental suite. In contrast, our amortized workflow completes inference in half a day, achieving speedups ranging from over 5× to 120× depending on the problem. Crucially, high-quality posterior draws are retained through a cascade of diagnostics and selective escalation to PSIS and MCMC. In conclusion, our workflow efficiently uses resources by (i) applying fast amortized inference when the results are accurate; (ii) refining draws with PSIS when possible; and (iii) amortized initializations of slower but accurate MCMC chains when needed.

Modularity and practical flexibility. A key strength of the proposed workflow lies in its modular structure, which allows practitioners to tailor each component to the specific constraints and objectives of their application. For example, the choice of MCMC sampler in Step 3 is fully interchangeable: alternative algorithms such as slice sampling, ensemble samplers (e.g., `emcee`; Foreman-Mackey et al., 2013), or NUTS can be substituted if the model is non-differentiable, multimodal, or requires richer exploration. In settings where GPU resources are limited, launching many parallel MCMC chains on CPUs offers a practical alternative, making the workflow more accessible for a broader range of users.

In cases where preliminary analysis or low-latency decision-making is essential (e.g., real-time experimental pipelines) or where likelihood evaluations are computationally expensive, the workflow can operate in a lightweight mode using amortized inference with out-of-distribution rejection alone (i.e., Step 1 in our workflow). Conversely, in high-stakes applications where accuracy is paramount, analysts can route all amortized draws through PSIS and, if needed, proceed to full MCMC to guarantee statistical robustness.

Limitations and future directions. Training amortized models requires upfront investment in optimization and simulation. In our experiments, we found that default neural network hyperparameter settings, such as normalizing flow architectures, summary network configurations, and optimizer settings, generally yield good performance. However, in more challenging cases, such as the GEV problem, adjustments may be necessary, guided by training-phase diagnostics. The simulation burden can be exacerbated in high-dimensional or weakly identifiable models, where neural estimators may struggle to approximate complex inverse maps. Alternative amortized inference approaches (see, e.g., Mittal et al., 2025) could be explored in future work to complement simulation-based amortized inference in such scenarios. Moreover, while our diagnostic for the amortized posterior draws in Step 1 is effective and highly efficient in practice, it remains an imperfect proxy for the true posterior approximation error and can occasionally result in the acceptance of poor-quality amortized draws (cf. Figure 5). Future work could explore even more expressive discrepancy measures tailored to the task at hand.

More broadly, the workflow supports a compelling vision of training amortized models once and reusing them across tasks or studies—a strategy well suited to applications ranging from psychology to computational biology, among others. In such settings, our layered diagnostics and selective escalation are crucial for maintaining reliability and efficiency. This positions the workflow as a practical bridge between amortized inference and traditional Bayesian rigor, enabling scalable yet trustworthy inference.

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This appendix provides additional details and analyses to complement the main text, included in the following sections:

- Background, Appendix A
- Inference phase: Step 1 diagnostics, Appendix B
- Experiment details, Appendix C
- Amortized initialization for NUTS, Appendix D

A Background

In this section, we give a brief review of simulation-based calibration checking, parameter recovery checking, Pareto-smoothed importance sampling, and ChEES-HMC algorithm.

Simulation-based calibration checking. Simulation-based calibration (SBC; Talts et al., 2018; Modrák et al., 2023) is a principled technique for assessing the calibration of posterior distributions estimated by Bayesian inference procedures, particularly useful in simulation-based amortized inference settings. SBC is based on the idea that if the posterior $p(\theta \mid y)$ is correctly specified, then the rank of the true parameter $\theta_\star$ among posterior draws should follow a uniform distribution. Formally, SBC defines a test statistic $f : \Theta \times Y \to \mathbb{R}$ (e.g., a component of θ, or the log-likelihood $p(y \mid \theta)$). For each simulated dataset $y^{(j)}$ generated from the joint model $p(\theta, y)$, the test statistic is evaluated at the ground-truth parameter $\theta_\star^{(j)}$ and compared to the same statistic evaluated over posterior samples $\{\theta_s^{(j)}\} \sim q_\phi(\theta \mid y^{(j)})$. The rank of $f(\theta_\star^{(j)}, y^{(j)})$ among $\{f(\theta_s^{(j)}, y^{(j)})\}$ is recorded. Repeating this process for all simulated datasets yields a distribution of rank statistics, which should be uniform under well-calibrated inference. Deviations from uniformity signal systematic bias (e.g., over/under-dispersion) in the posterior approximation. We use the graphical-based approach proposed by Säilynoja et al. (2022) to assess the uniformity of the rank statistics in SBC. This method provides visual diagnostics for identifying systematic biases or miscalibrations in the posterior approximation by plotting the empirical cumulative distribution function (ECDF) and confidence bands. Examples of SBC checking results using this approach are provided in Appendix C.

Parameter recovery checking. Parameter recovery is a complementary diagnostic to SBC and provides a direct visualization of posterior approximation in recovering true generative parameters (Radev et al., 2020; 2023). The idea is to simulate a collection of datasets $\{y^{(j)}\}$ along with their corresponding ground-truth parameters $\{\theta_\star^{(j)}\}$ from the joint model, and assess whether the posterior distributions $q_\phi(\theta \mid y^{(j)})$ effectively recover these known values. In our workflow, we compare the posterior median extracted from each posterior to the corresponding ground-truth values, along with the median absolute deviation to indicate uncertainty. These comparisons are visualized using scatter plots, with correlation coefficients quantifying the strength of recovery. While not a direct measure of posterior calibration or correctness, parameter recovery provides important practical insight into whether the learned inverse mapping from y to θ is effective. Examples of parameter recovery checking results using this approach are provided in Appendix C.

Pareto-smoothed importance sampling. Pareto-smoothed importance sampling (PSIS; Vehtari et al., 2024) is a robust method for improving the stability and reliability of importance sampling (IS) estimates. Given a target distribution $p(y \mid \theta)\, p(\theta)$ and a proposal distribution $q_\phi(\theta)$, with samples $\hat{\theta}_s \sim q_\phi(\theta)$, PSIS stabilizes the raw importance weights $w_s = p(y \mid \hat{\theta}_s)\, p(\hat{\theta}_s)/q_\phi(\hat{\theta}_s \mid y)$ by modeling the tail behavior of the importance weights. Specifically, the distribution of extreme importance weights can be approximated by a generalized Pareto distribution:

$$p(t \mid u, \sigma, k) = \begin{cases} \frac{1}{\sigma}\left(1 + k\left(\frac{t-u}{\sigma}\right)\right)^{-\frac{1}{k}-1}, & k \neq 0 \\ \frac{1}{\sigma}\exp\left(\frac{t-u}{\sigma}\right), & k = 0, \end{cases} \tag{7}$$

where k is the shape parameter, u is the location parameter and σ is the scale parameter. The number of finite fractional moments of the importance weight distribution depends on k: a generalized Pareto distribution

has $1/k$ finite moments when $k > 0$. To stabilize the importance sampling estimate, the extreme importance weights are replaced with well-spaced order statistics drawn from the fitted generalized Pareto distribution, leading to a more stable and efficient IS estimator. The estimated shape parameter $\hat{k}$ serves as a diagnostic for the reliability of the importance sampling estimate. For moderate sample size ($S > 2000$), $\hat{k} < 0.7$ indicates good reliability.

ChEES-HMC algorithm. The ChEES-HMC algorithm (Hoffman et al., 2021) is a massively parallel and adaptive extension of Hamiltonian Monte Carlo (HMC) designed to leverage single-instruction multiple-data (SIMD) hardware accelerators such as GPUs. This enables rapid generation of posterior draws following an initial warm-up phase. During warm-up, ChEES-HMC adaptively tunes the trajectory length T and step size ϵ by maximizing the "Change in the Estimator of the Expected Square" (ChEES), a heuristic that serves as a proxy for reducing autocorrelation in the second moments of the Markov chain. ChEES-HMC is particularly suitable for our amortized workflow, as we can easily generate a large number of good starting points (amortized draws) to launch many short MCMC chains. For our experiments, we used ChEES-HMC to run 2048 parallel chains, organized into 16 superchains with 128 subchains each. This configuration is essential for computing the nested $\widehat{R}$ diagnostic (Margossian et al., 2024), which assesses convergence across a large number of short chains.

B Inference phase: Step 1 diagnostics

In this section, we provide details on the out-of-distribution (OOD) checking procedure used to detect atypical datasets in Step 1 of the workflow. We also discuss potential additional diagnostics that can be used to assess the quality of amortized inference beyond the default check.

B.1 Testing for atypicality in Step 1

Inspired by an out-of-distribution checking method for amortized inference under model misspecification (Schmitt et al., 2023), we use a sampling-based hypothesis test to flag atypical datasets where the trustworthiness of amortized inference might be impeded.

Concretely, let $\{y^{(m)}\}_{m=1}^{M}$ denote the training datasets used during simulation-based amortization, and let $h_\psi(y)$ denote a low-dimensional summary statistic (e.g., learned or handcrafted) that maps a dataset y into a feature space $\mathbb{R}^d$. We compute the summary statistics $s^{(m)} = h_\psi(y^{(m)})$ for all training datasets and use them to estimate the empirical mean μ_s and covariance Σ_s in the summary space. Then, for any dataset y, its Mahalanobis distance to the training set is:

$$D_M(y) = \sqrt{(h_\psi(y) - \mu_s)^\top \Sigma_s^{-1} (h_\psi(y) - \mu_s)}. \tag{8}$$

To form a null distribution of typical distances, we compute $\{D_M(y^{(m)})\}_{m=1}^{M}$ for all training datasets. Given a new observed dataset y_{obs}, we then compute its Mahalanobis distance $D_M(y_{\text{obs}})$ and compare it to the empirical distribution of training distances.

We define the out-of-distribution rejection rule as:

$$\text{Reject}_{\text{OOD}}(y_{\text{obs}}) = \mathbb{I}\left\{ D_M(y_{\text{obs}}) > \text{Quantile}_\alpha\left(\{D_M(y^{(m)})\}_{m=1}^{M} \right) \right\}, \tag{9}$$

where α is typically set to 95% to flag the top 5% most atypical datasets under the training distribution. The type-I error rate $(1 - \alpha)$ of this test can be set relatively high to obtain a conservative test that will flag many datasets for detailed investigation in further steps of our workflow.

Note. In the applications of this paper, we perform the above test in the learnt summary space, that is, h_ψ is a summary neural network that learns a low-dimensional representation of the data (see Appendix C for details).[5]

[5]Except for Bernoulli GLM problem, the sufficient summary statistics is known without the need for learning.

B.2 Additional diagnostics

In addition to OOD tests for identifying atypical datasets, data-conditional diagnostics can gauge the reliability of amortized posterior inferences for specific datasets. Examples for such data-conditional diagnostics include posterior simulation-based calibration checking (posterior SBC; Säilynoja et al., 2025) and the local classifier two-sample test (L-C2ST; Linhart et al., 2023). These diagnostics each offer distinct advantages and limitations.

Posterior SBC is conceptually straightforward and offers necessary conditions for the accuracy of amortized posterior samples by assessing consistency. However, it requires additional simulations for each test dataset and requires training the amortized estimator on inputs that effectively double the size of the original observations. L-C2ST, which trains classifiers to distinguish between $q_\phi(\theta \mid y)\, p(y)$ and the joint distribution $p(\theta, y)$, provides theoretically sufficient and necessary conditions for amortized inference accuracy. In practice, however, its effectiveness can be very sensitive to several factors, including classifier design choices (e.g., data pre-processing and optimization strategies), classifier calibration, and the relative sizes of the simulation budgets allocated to classifier training and amortized estimator training.

The choice to apply these additional diagnostics depends on context-specific factors, including the number of observed datasets, the relative computational cost of simulations versus likelihood evaluations,[6] and the dimensionality of the observations. Ultimately, whether amortized posterior draws are deemed acceptable hinges on the accuracy requirements of the specific application. By default, we recommend the OOD test for its simplicity, efficiency, and suitability as a first-line diagnostic.

C Experiment details

In this section, we provide additional experimental details omitted from the main text for brevity.

Evaluation metrics. To assess the quality of posterior approximations produced by each step of the workflow, we compare them against reference posterior draws obtained via a well-tuned No-U-Turn Sampler (NUTS). Specifically, we precomputed NUTS-based posterior samples for a subset of 5000 test datasets, which serve as a ground-truth reference for evaluation.[7] We then evaluate the 1-Wasserstein distance (W1) and the mean marginal total variation (MMTV) distance on up to 100 datasets from each inference step: Step 1 (amortized inference), Step 2 (amortized + PSIS), and Step 3 (ChEES-HMC with amortized initializations). These metrics are reported in the main text (Figure 5).

Neural network architecture for amortized inference. For all experiments, we use a coupling-based normalizing flow implemented in BayesFlow (Radev et al., 2023). The flow consists of 6 transformation layers, each comprising an invertible normalization, two affine coupling transformations, and a random permutation between elements. Before entering the coupling flow network as conditioning variables, the observed dataset y is encoded into a lower-dimensional summary statistic $h_\psi(y)$ via a summary network h_ψ. This summary network is implemented either as a DeepSet architecture (Zaheer et al., 2017) or a SetTransformer (Lee et al., 2019), depending on the problem setting. Both architectures are designed to handle permutation-invariant data structures. For the Bernoulli GLM, we bypass the summary network and directly use the known 10-dimensional sufficient statistics (Lueckmann et al., 2021). The specific choice of summary network for each application is described in the respective problem descriptions below.

Training-phase optimization. For all problems, the neural network is optimized via the AdamW optimizer (Loshchilov & Hutter, 2019) with weight decay of 10^{-3} and a cosine decay learning rate schedule (initial learning rate of 2.5×10^{-4}, a warmup target of 5×10^{-4}, $\alpha = 0$) as implemented in Keras (Chollet et al., 2015). A global gradient clip norm of 1.5 is applied. Training is performed with a batch size of 512 for 300

[6] For example, if likelihood evaluations are cheap, it is often worthwhile to process to Step 2, where Pareto-smoothed importance sampling can offer more informative and powerful diagnostics.

[7] For the generalized extreme value distribution problem, 1000 reference datasets were used, corresponding to the total number of test datasets.

epochs,[8] with cosine decay steps set to the product of batch size and epochs. A held-out validation set is used to monitor optimization and select the best-performing model checkpoint.

Space transformation. Following standard practice in Bayesian computation (e.g., PyMC; Oriol et al., 2023, Stan; Carpenter et al., 2017), we transform parameters to an *unconstrained* space for inference. The amortized neural approximator is trained to estimate parameters in this unconstrained space. PSIS operates independently of the parameterization and thus remains unaffected by this transformation. ChEES-HMC also performs inference in the unconstrained space. All evaluation metrics (W1 and MMTV distances) are computed in this space. However, parameter recovery and simulation-based calibration plots are shown in the original constrained space for better interpretability.

Computing infrastructure and software. For all applications, the full workflow—including amortized training, inference, diagnostics, Pareto-smoothed importance sampling, and ChEES-HMC sampling—was conducted on a single NVIDIA V100 GPU (32GB), 8 cores of an AMD EPYC 7452 processor, and 8-16GB RAM. For runtime details across experiments, refer to Table 1 in the main text. The core code base was built using BayesFlow (Radev et al., 2023) (MIT license), PyMC (Oriol et al., 2023) (Apache-2.0 license), ArviZ (Kumar et al., 2019) (Apache-2.0 license) and JAX (Bradbury et al., 2018) (Apache-2.0 license). We used the implementation of ChEES-HMC provided by TensorFlow Probability (Dillon et al., 2017) (Apache-2.0 license).

Below, we provide details for each problem to complement the main text.

C.1 Generalized extreme value distribution

Problem description. Following Caprani (2021), the prior distribution for the parameters of the generalized extreme value distribution (GEV) is defined as:

$$\begin{aligned} \mu &\sim \mathcal{N}(3.8, 0.04) \\ \sigma &\sim \text{Half-Normal}(0, 0.09) \\ \xi &\sim \text{Truncated-Normal}(0, 0.04) \text{ with bounds } [-0.6, 0.6]. \end{aligned} \tag{10}$$

Simulation budgets. We use 10,000 simulated parameter–observation pairs for training the amortized approximator, 1000 for validation, and 200 for training-phase diagnostics, including parameter recovery and simulation-based calibration.

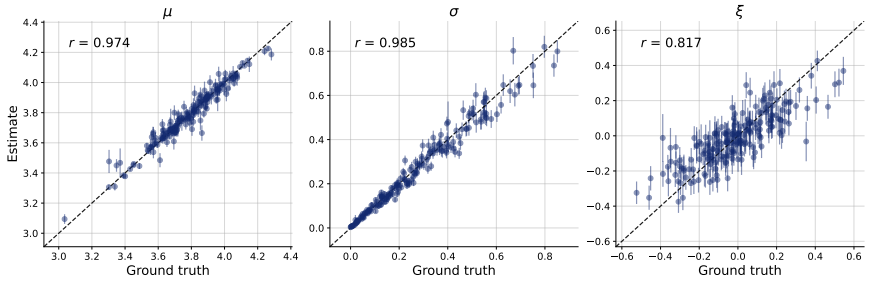
Summary network. We use a DeepSet as the summary network. The dimensionality of the learned summary statistics is 16. The DeepSet has a depth of 1, uses a *mish* activation, max inner pooling layers, 64 units in the equivariant and invariant modules, and 5% dropout.

Training-phase diagnostics. The closed-world diagnostics (parameter recovery and simulation-based calibration checking) in Figure 7 indicate that the neural network training has successfully converged to an acceptable posterior approximator within the scope of the training set.

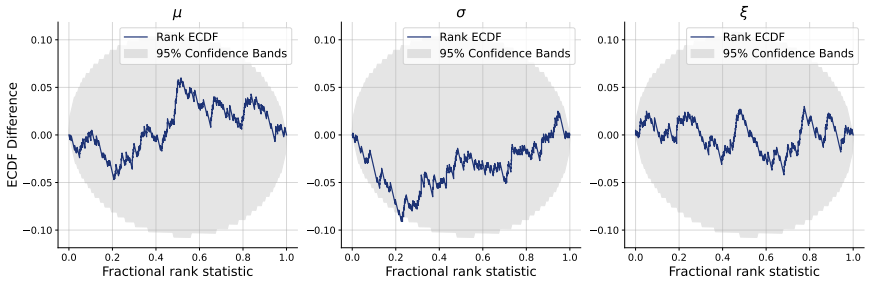
Test datasets. In order to emulate distribution shifts that arise in real-world applications while preserving the controlled experimental environment, we simulate the "observed" datasets from a joint model whose prior is 2× wider (i.e., with 4× the variance) than the model used during training. More specifically, the prior is specified as:

$$\begin{aligned} \mu &\sim \mathcal{N}(3.8, 0.16) \\ \sigma &\sim \text{Half-Normal}(0, 0.36) \\ \xi &\sim \text{Truncated-Normal}(0, 0.16) \text{ with bounds } [-1.2, 1.2]. \end{aligned} \tag{11}$$

[8] For Bernoulli GLM, we only train for 100 epochs.



(a) Parameter recovery checking.



(b) Simulation-based calibration checking.

Figure 7: Training-phase diagnostics for the GEV problem. The parameter recovery is strong for the parameters μ, σ, and good for the shape parameter ξ. Simulation-based calibration checking indicates good calibration for all parameters. Parameter recovery and simulation-based calibration checking indicate acceptable convergence of the amortized posterior estimator.

C.2 Bernoulli GLM

Problem description. Following Lueckmann et al. (2021), we set the prior for θ as:

$$\theta \sim \mathcal{N}\left(0, \begin{bmatrix} 2 & 0 \\ 0 & (F^\top F)^{-1} \end{bmatrix}\right), \tag{12}$$

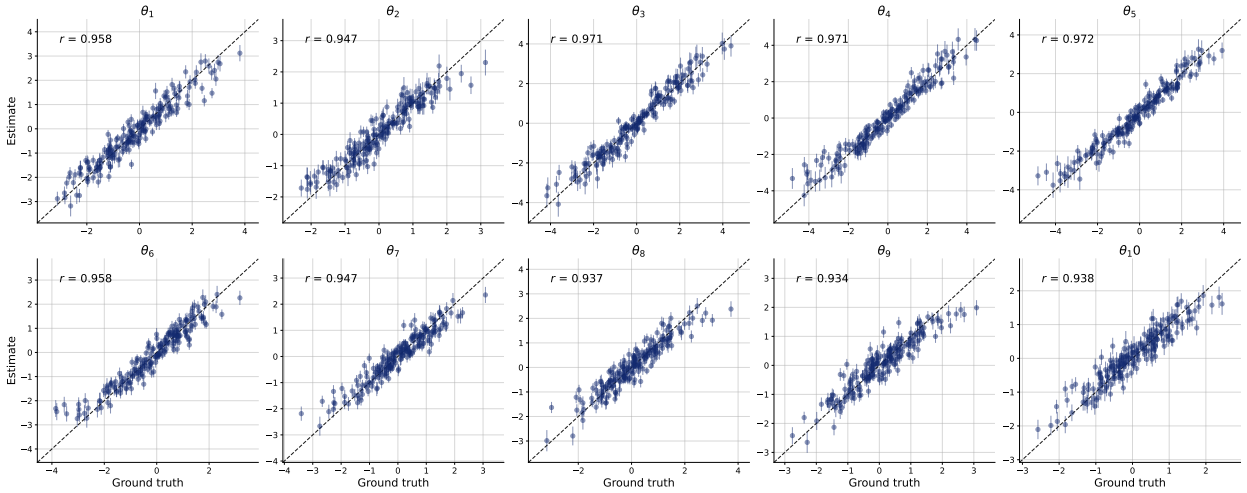
where the matrix F is defined such that $F_{i,i-2} = 1$, $F_{i,i-1} = -2$, $F_{i,i} = 1 + \sqrt{\frac{i-1}{9}}$, and $F_{i,j} = 0$ otherwise, for $1 \leq i, j \leq 9$. The task duration is set to $T = 100$, with fixed input vectors $\{v_i\}_{i=1}^{100}$, where each $v_i \in \mathbb{R}^{10}$. Corresponding observations are denoted by $\{y_i\}_{i=1}^{100}$. Further details can be found in Lueckmann et al. (2021); Gonçalves et al. (2020).

Simulation budgets. We use 10,000 simulated parameter–observation pairs for training the amortized approximator, 1000 for validation, and 200 for training-phase diagnostics, including parameter recovery and simulation-based calibration.

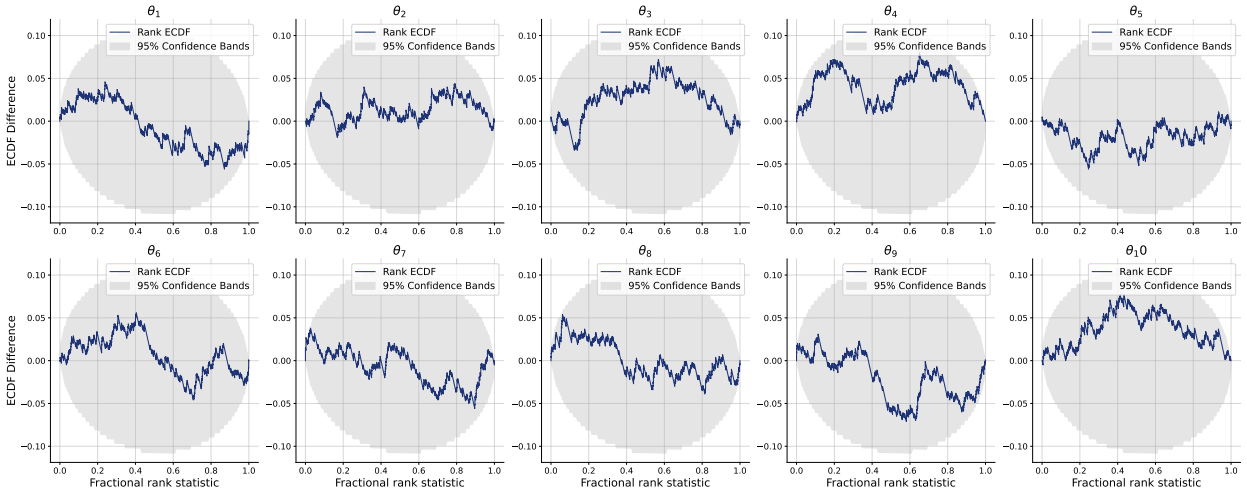
Summary network. For Bernoulli GLM, the 10-dimensional sufficient summary statistic for each dataset can be computed as $Vy^\top$ where $y = [y_1, \cdots, y_{100}]$ and $V = [v_1, \cdots, v_{100}]$. We therefore use this summary statistic for amortized training directly without relying on a separate summary neural network.

Training-phase diagnostics. The closed-world diagnostics (parameter recovery and simulation-based calibration checking) in Figure 8 indicate that the neural network training has successfully converged to an acceptable posterior approximator within the scope of the training set.

Test datasets. We generate $K = 10{,}000$ in-distribution test datasets by sampling parameters from the model prior and simulating corresponding observations $\{y_i\}_{i=1}^{100}$ from the Bernoulli distribution.



(a) Parameter recovery checking.



(b) Simulation-based calibration checking.

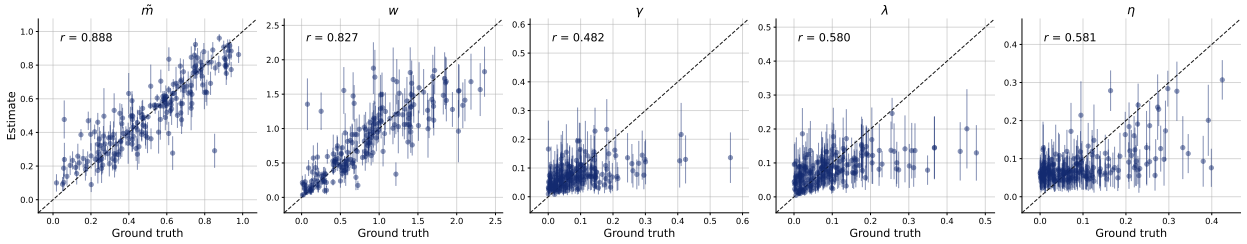
Figure 8: Training-phase diagnostics for the Bernoulli GLM problem. The parameter recovery is strong for all parameters. Simulation-based calibration checking indicates good calibration for all parameters. Parameter recovery and simulation-based calibration checking indicate acceptable convergence of the amortized posterior estimator.

C.3 Psychometric curve fitting

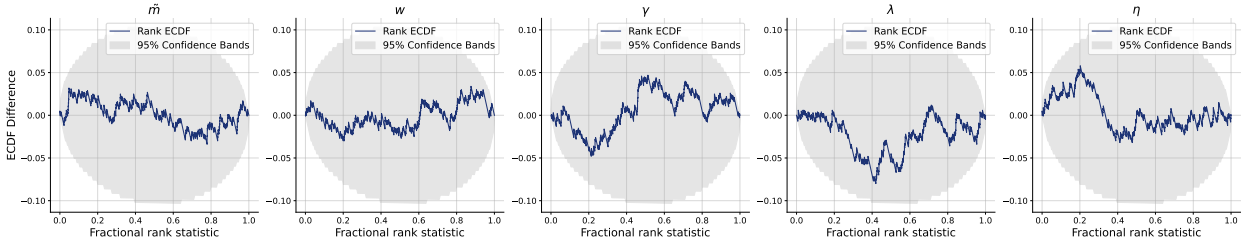
Problem description. We adopt an overdispersed psychometric model (Schütt et al., 2016) with the error function (erf) as the sigmoid function in the psychometric function:

$$\psi(x; m, w, \lambda, \gamma) = \gamma + (1 - \lambda - \gamma)\ \mathrm{erf}(x; m, w), \tag{13}$$

where m is the threshold, w is the width, λ is the lapse rate, and γ is the guess rate.



(a) Parameter recovery checking.



(b) Simulation-based calibration checking.

Figure 9: Training-phase diagnostics for the psychometric curve fitting problem. Recovery is good for $\tilde{m}$ and w, while the other parameters exhibit weaker recoverability. Simulation-based calibration checking indicates excellent calibration for all parameters. Parameter recovery and simulation-based calibration checking indicate acceptable convergence of the amortized posterior estimator.

The full probabilistic model is defined as follows:

$$
\begin{aligned}
\tilde{m} &\sim \text{Beta}(2, 2), \\
w &\sim \text{Half-Normal}(0, 1), \\
\lambda, \gamma, \eta &\sim \text{Beta}(1, 10), \\
m &= 2\tilde{m} - 1, \\
\bar{p}_i &= \psi(x_i; m, w, \lambda, \gamma), \\
p_i &\sim \text{Beta}\left(\left(\frac{1}{\eta^2} - 1\right)\bar{p}_i,\ \left(\frac{1}{\eta^2} - 1\right)(1 - \bar{p}_i)\right), \\
y_i &\sim \text{Binomial}(n_i, p_i),
\end{aligned}
\tag{14}
$$

where n_i denotes the number of trials, and x_i is the stimulus level. Stimuli are presented at nine fixed levels: $x_i \in \{-100.0,\ -25.0,\ -12.5,\ -6.25,\ 0.0,\ 6.25,\ 12.5,\ 25.0,\ 100.0\}$ and each value is further normalized by dividing by 100.

Simulation budgets. We use 50,000 simulated parameter–observation pairs for training the amortized approximator, 1000 for validation, and 200 for training-phase diagnostics, including parameter recovery and simulation-based calibration.

Summary network. We use a DeepSet as the summary network, which maps the input dataset to a 16-dimensional summary statistic. The DeepSet has a depth of 2, uses a *gelu* activation, mean inner pooling layers, 64 units in the equivariant and invariant modules, and 5% dropout.

Training-phase diagnostics. The closed-world diagnostics (parameter recovery and simulation-based calibration checking) in Figure 9 indicate that the neural network training has successfully converged to an acceptable posterior approximator within the scope of the training set.

Test datasets. Our empirical evaluation uses 8,526 mouse behavioral datasets from the International Brain Laboratory public database (The International Brain Laboratory et al., 2021). We retrieve the data using

the provided API with the argument `task="biasedChoiceWorld"`, which corresponds to behavioral data collected after the mice have completed training. Each dataset is processed into an observation tensor of shape $(9, 3)$, where each row contains the number of correct trials y_i, the total number of trials n_i, and the stimulus level x_i.

C.4 Decision model

Problem description. Following von Krause et al. (2022), we specify the prior distributions for the drift-diffusion model parameters as:

$$\begin{aligned} v_1, v_2 &\sim \text{Gamma}(2, 1), \\ a_1, a_2 &\sim \text{Gamma}(6, 0.15), \\ \tau_c &\sim \text{Gamma}(3, 0.15), \\ \tau_n &\sim \text{Gamma}(3, 0.5), \end{aligned} \tag{15}$$

where all Gamma distributions use the shape–scale parametrization.[9] We implement the drift-diffusion model likelihood using the `hssm` package (Fengler et al., 2025) and PyMC.

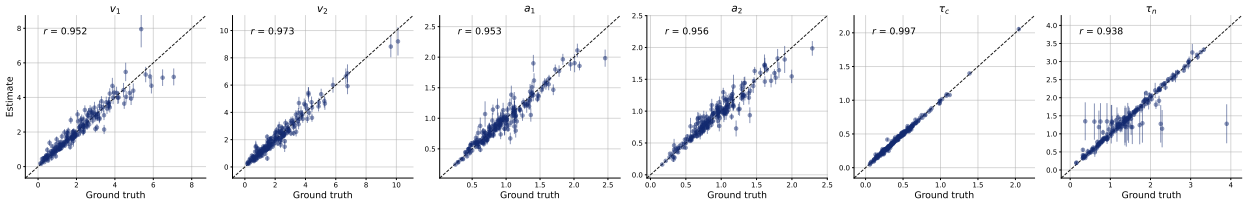
Simulation budgets. We use 100,000 simulated parameter–observation pairs for training the amortized approximator, 1000 for validation, and 200 for training-phase diagnostics, including parameter recovery and simulation-based calibration.

Summary network. We use a SetTransformer as the summary network, which maps the input dataset to a 16-dimensional summary statistic. The SetTransformer has two set attention blocks, followed by a pooling multi-head attention block and a fully connected output layer. Each multilayer perceptron (MLP) in the set blocks has two hidden layers of width 128, with *gelu* activation and 5% dropout.

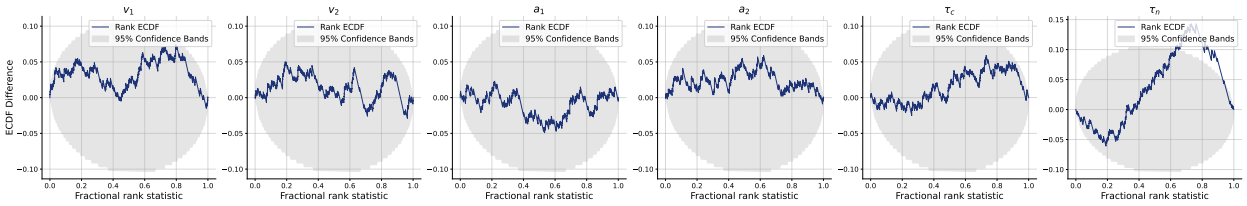
Training-phase diagnostics. The closed-world diagnostics (parameter recovery and simulation-based calibration checking) in Figure 10 indicate that the neural network training has successfully converged to an acceptable posterior approximator within the scope of the training set.

Test datasets. The test datasets consist of 15,000 participants pre-processed from the online implicit association test (IAT) database (Xu et al., 2014; von Krause et al., 2022). Each test dataset is a tensor of shape $(120, 4)$, where each row corresponds to a single trial and contains the response time, missing data mask, experiment condition type, and stimulus type.

[9] The prior distributions for the boundary separation parameters a_1 and a_2 differ slightly from those in von Krause et al. (2022) due to a different parametrization of boundary separation.



(a) Parameter recovery checking.



(b) Simulation-based calibration checking.

Figure 10: Training-phase diagnostics for the decision model. Parameter recovery is strong for all parameters. Simulation-based calibration checking indicates good calibration for all parameters except τ_n, which shows mild deviations, suggesting occasional overestimation by the amortized estimator for this parameter. Parameter recovery and simulation-based calibration checking indicate acceptable convergence of the amortized posterior estimator.

D Amortized initialization for NUTS

In addition to ChEES-HMC, we evaluate the effectiveness of amortized posterior draws as initializations for the NUTS sampler. The experimental settings mirror those used for ChEES-HMC (Section 3.4), except that we launch only four chains, which is the typical configuration for NUTS. As shown in Figure 11, amortized initializations reduce the number of required warm-up iterations for both the GEV problem and the decision model. For the psychometric curve and Bernoulli GLM problems, all three initialization methods (amortized, PSIS-refined, and random) yield similar convergence behavior according to $\hat{R}$ diagnostic.

Notably, NUTS generally requires fewer warm-up iterations than ChEES-HMC across the evaluated problems, suggesting that while amortized initializations are still beneficial, the relative gain is more pronounced for ChEES-HMC, which runs many short chains in parallel.

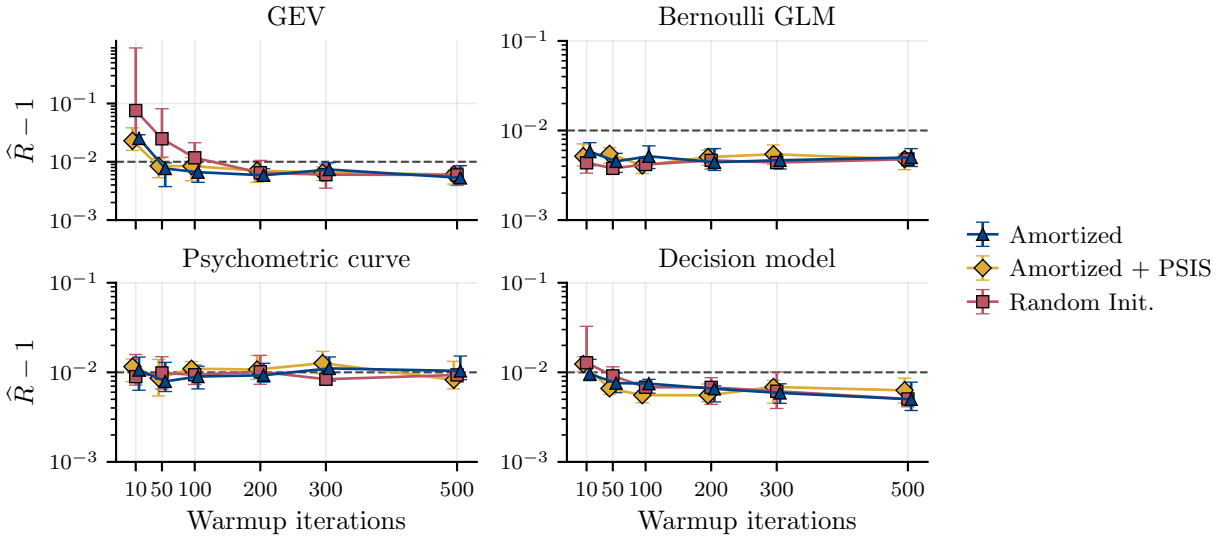


Figure 11: The effect of initialization for NUTS. The figure shows median±IQR across 20 test datasets. Using amortized posterior draws as initializations for ChEES-HMC reduces the required warmup in the GEV and decision model tasks.