Model-Informed Flows for Bayesian Inference

Joohwan Ko, Justin Domke

Manning College of Information and Computer Sciences University of Massachusetts Amherst {joohwanko,domke}@cs.umass.edu

Abstract

Variational inference often struggles with the posterior geometry exhibited by complex hierarchical Bayesian models. Recent advances in flow-based variational families and Variationally Inferred Parameters (VIP) each address aspects of this challenge, but their formal relationship is unexplored. Here, we prove that the combination of VIP and a full-rank Gaussian can be represented exactly as a forward autoregressive flow augmented with a translation term and input from the model's prior. Guided by this theoretical insight, we introduce the Model-Informed Flow (MIF) architecture, which adds the necessary translation mechanism, prior information, and hierarchical ordering. Empirically, MIF delivers tighter posterior approximations and matches or exceeds state-of-the-art performance across a suite of hierarchical and non-hierarchical benchmarks.

1 Introduction

Inference remains challenging for many complex Bayesian models. Variational Inference (VI) casts posterior approximation as minimization of the Kullback-Leibler divergence between a tractable approximating distribution and the true posterior [9, 25, 23]. Recent advances have focused on increasing the expressiveness of variational families. Flow-based models, which apply a sequence of invertible transformations to a simple base distribution, have shown particular promise [34, 36, 28].

Variationally Inferred Parameters (VIP) [19] address a key challenge in VI: The posteriors of hierarchical Bayesian models often exhibit pronounced curvature or "funnel-like" geometry [7, 24] that standard families like Gaussians cannot capture. VIP builds on insights from non-centered parameterization (NCP) in Markov chain Monte Carlo (MCMC) [35], adaptively learning the optimal degree of non-centering for each latent variable during the VI optimization process.

Our preliminary investigations reveal a striking observation: When VIP is combined with full-rank Gaussian variational families, it achieves performance comparable to state-of-the-art methods from recent evaluation [10] (See Tables 1 and 3). Since VIP and flow-based models both excel at navigating posterior geometry, might they be manifestations of a common principle? In particular, can a flow-based distribution encapsulate the benefits of VIP?

Our core theoretical result, formalized in Theorem 4, shows that every full-rank VIP transformation can be represented exactly as a forward autoregressive flow (FAF), provided that the flow (i) respects the topological order of the latent variables, (ii) augments the usual affine mapping with a new "translation" term, and (iii) receives the model's prior mean and scale functions as additional inputs.

Guided by these principles, we introduce the Model-Informed Flow (MIF), a forward autoregressive architecture that includes the necessary translation term and incorporates the distributional form of the model's prior. Across a range of benchmark models, MIF compares well to state-of-the-art VI methods. We also perform targeted ablations to verify the predicted implications and practical consequences of our theory.

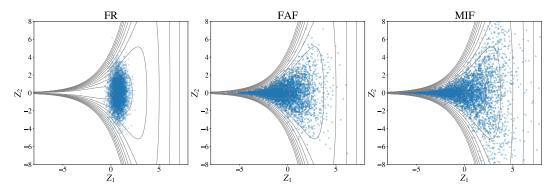


Figure 1: "Funnel"-type distributions commonly arise in hierarchical model. This figure shows the funnel distribution (gray contours) approximated with 5000 samples from three families (blue points): A Full-Rank Gaussian (FR) is very poor (KL-divergence of 1.86 nats). A standard Forward Autoregressive Flow (FAF) is much better (0.38 nats) but still imperfect. Our proposed model-informed flow (MIF) achieves a KL-divergence of effectively 0.

2 Preliminaries

2.1 Variational Inference

In Bayesian inference, given a model p(z,x), the goal is to approximate the posterior distribution p(z|x) given observed data x. Direct computation of this posterior is typically intractable, so variational inference (VI) introduces a tractable family $q_w(z)$ and minimises the Kullback–Leibler (KL) divergence from $q_w(z)$ to the true posterior. The marginal likelihood then decomposes as

$$\log p(x) = \underbrace{\mathbb{E}_{q_w(z)} \left[\log \frac{p(z,x)}{q_w(z)} \right]}_{\text{ELBO} \left[q_w(z) \parallel p(z,x) \right]} + \underbrace{\text{KL} \left[q_w(z) \parallel p(z|x) \right]}_{\text{divergence}}.$$
 (2.1)

Since $\log p(x)$ is constant with respect to the variational parameters w, maximising the ELBO in (2.1) is equivalent to minimising the KL divergence between q_w and the posterior.

2.2 Hierarchical Bayesian Models

Hierarchical Bayesian models are common in domains such as ecology [12, 43, 38] and epidemiology [16, 37, 29]. Following Gorinova et al. [19], we consider a hierarchical model in which each latent variable z_i is conditionally Gaussian with a mean and variance that are arbitrary function of parent variables, while the observed data x_j is generated from an arbitrary likelihood $p(x_j|\pi(x_j))$. In particular, the likelihood for x_j may depend on one or more latent variables through its parent set $\pi(x_j)$. Formally, write

$$z_i \sim \mathcal{N}\Big(f_i\big(\pi(z_i)\big), g_i\big(\pi(z_i)\big)\Big), \quad x_j \sim p\big(x_j|\pi(x_j)\big),$$
 (2.2)

where $\pi(\cdot)$ denotes the set of parent variables. Throughout, $\pi(\cdot)$ may include both observed and latent variables; that is, a variable can be conditioned on any subset of the remaining variables permitted by the model graph. In practice, the functions f_i and g_i (which return the mean and standard deviation of z_i , respectively) often arise directly from a probabilistic programming system, encoding how the mean and variance of each latent variable depend on its parent variables.

The joint density corresponding to Eq 2.2 is

$$p(z,x) = \prod_{i=1} \mathcal{N}\left(z_i | f_i(\pi(z_i)), g_i(\pi(z_i))\right) \times \prod_{j=1} p(x_j | \pi(x_j)).$$
 (2.3)

Example. As a concrete instance of Equation (2.2), consider the model

$$z_1 \sim \mathcal{N}(0,1), \qquad z_2 \sim \mathcal{N}(\alpha z_1, \exp(\beta z_1)),$$

$$x_1 \mid z_1, z_2 \sim \text{Poisson}(\exp(z_1 + \frac{1}{2}z_2)), \qquad x_2 \mid z_2, x_1 \sim \text{Binomial}(n = x_1, p = \sigma(z_2)),$$

where $\sigma(u) = \frac{1}{1+\exp(-u)}$. To cast this as an instance of Equation (2.2), define the parent sets $\pi(z_1) = \emptyset$, $\pi(z_2) = \{z_1\}$, $\pi(x_1) = \{z_1, z_2\}$, $\pi(x_2) = \{z_2, x_1\}$,

and the functions

$$f_1(\emptyset) = 0$$
, $g_1(\emptyset) = 1$, $f_2(z_1) = \alpha z_1$, $g_2(z_1) = \exp(\beta z_1)$.

In Equation (2.2), we make no assumptions about the distributional form of the observed variables x_i , so $p(x_1|\pi(x_1)) = \operatorname{Poisson}\left(\exp\left(z_1 + \frac{1}{2}z_2\right)\right)$ and $p(x_2|\pi(x_2)) = \operatorname{Binomial}(n = x_1, p = \sigma(z_2))$ can be arbitrary.

2.3 Non-Centered Parameterization

Hierarchical models often exhibit difficult curvature and "funnel-like" geometries. These are a challenge for both sampling and variational inference approaches [7, 24, 22]. A common strategy in MCMC to alleviate these issues is the *non-centered parameterization* (NCP) [35]. To illustrate, consider two latent variables z_1 and z_2 having prior of

$$z_1 \sim \mathcal{N}(\mu, \sigma), \quad z_2 \sim \mathcal{N}(0, \exp(z_1/2)).$$
 (2.4)

In the standard (centered) parameterization, the goal is to approximate p(z|x). However, the nonlinear dependence of z_2 on z_1 can yield a sharply funnel-shaped joint posterior. As illustrated in Figure 1 (left panel), a full-rank Gaussian struggles to capture this funnel structure.

The non-centered approach introduces auxiliary variables $\epsilon = (\epsilon_1, \epsilon_2) \sim \mathcal{N}(0, I)$ and defines a transformation $z = T_{\text{NCP}}(\epsilon)$ that recovers (z_1, z_2) via

$$z_1 = \mu + \sigma \epsilon_1, \quad z_2 = \exp\left(\frac{z_1}{2}\right) \epsilon_2.$$
 (2.5)

Instead of p(z,x), inference is done on $p(\epsilon,x)$ where $p(\epsilon) = \mathcal{N}(0,I)$ and $p(x|\epsilon) = p(x|z = T_{\text{NCP}}(\epsilon))$. The intuition is that if x is relatively uninformative, then $p(\epsilon|x)$ will be close to a standard Gaussian, even when p(z|x) might have a funnel-type geometry.

2.4 Variationally Inferred Parameters

While NCP helps alleviate pathologies in hierarchical models, it is not ideal for every latent variable. Non-centering can prevent funnel-shaped geometries in cases with limited data, but when data is highly informative, a centered formulation may be better. *Variationally Inferred Parameters* (VIP) addresses this trade-off by learning a partial non-centered parameterization for each variable [19].

VIP reparameterizes $z \in \mathbb{R}^D$ by introducing an auxiliary variable $\tilde{z} = (\tilde{z}_1, \dots, \tilde{z}_D)$, and by defining a parameter $\lambda_i \in [0,1]$ per dimension. Rather than drawing z_i directly from its prior, VIP samples

$$\tilde{z}_{i} \sim \mathcal{N}\left(\lambda_{i} f_{i}\left(\pi\left(z_{i}\right)\right), g_{i}\left(\pi\left(z_{i}\right)\right)^{\lambda_{i}}\right),$$
(2.6)

then recovers z_i via VIP transformation, T_{VIP} , as in Definition 1. Note that λ_i interpolates between the centered ($\lambda_i = 1$) and fully non-centered ($\lambda_i = 0$) extremes.

Definition 1 (VIP Transformation). For a fixed ordering of latent variables $z=(z_1,\ldots,z_D)$, and auxiliary variables $\tilde{z}=(\tilde{z}_1,\ldots,\tilde{z}_D)$, let $\lambda_i\in[0,1]$ be the partial non-centering parameter for each coordinate i, and $f_i(\pi(z_i))$ and $g_i(\pi(z_i))$ be continuous functions that return the mean and standard deviation of z_i (respectively) based on the parent nodes $\pi(z_i)$. Then, the VIP transformation $z=T_{\mathrm{VIP}}(\tilde{z})$ is defined coordinate-wise by

$$z_{i} = f_{i}(\pi(z_{i})) + g_{i}(\pi(z_{i}))^{1-\lambda_{i}} \Big(\tilde{z}_{i} - \lambda_{i} f_{i}(\pi(z_{i}))\Big),$$
(2.7)

for i = 1, ..., D.

Substituting $T_{\rm VIP}$ into the joint distribution (Equation (2.3)) yields a partially non-centered representation

$$p_{\text{VIP}}(\tilde{z}, x) = \prod_{i=1} \mathcal{N}\left(\tilde{z}_i | \lambda_i f_i(\pi(z_i)), g_i(\pi(z_i))^{\lambda_i}\right) \times \prod_{i=1} p(x_i | \pi(x_i)). \tag{2.8}$$

VIP then learns a variational distribution $q_w(\tilde{z})$ by minimizing $\mathrm{KL}\left(q_w(\tilde{z}) \| p_{\mathrm{VIP}}(\tilde{z} \mid x)\right)$, optimizing both the variational parameters w and the partiality parameters λ .

2.5 Equivalence of VIP in Model vs Variational Spaces

VIP applies T_{VIP} , in the *model space*. However, there is a straightforward analog in the *variational space*. Suppose $q_w(\tilde{z})$ is any distribution over the non-centered latent variables \tilde{z} . We define a new distribution $q_{w,\text{VIP}}(z)$ by letting

$$z = T_{\text{VIP}}(\tilde{z}, x) \quad \text{with} \quad \tilde{z} \sim q_w(\tilde{z}).$$
 (2.9)

In other words, $q_{w,\rm VIP}$ is the distribution induced on z by applying the VIP transformation $T_{\rm VIP}$ to samples from q_w . Concretely, its density follows from the change-of-variables formula

$$q_{w,\text{VIP}}(z) = q_w \left(T_{\text{VIP}}^{-1}(z, x) \right) \left| \det \nabla_{\tilde{z}} T_{\text{VIP}}(\tilde{z}, x) \right|^{-1}. \tag{2.10}$$

Since the KL divergence is invariant under such invertible transformations [11], we have that

$$KL\left(q_{w,\text{VIP}}(z)\|p(z|x)\right) = KL\left(q_{w}(\tilde{z})\|p_{\text{VIP}}(\tilde{z}|x)\right). \tag{2.11}$$

Thus, optimizing $\min_{w,\lambda} \mathrm{KL}\left(q_{w,\mathrm{VIP}}(z) \middle| p(z|x)\right)$ with the posterior fixed is equivalent to reparameterizing the posterior as in 2.4. In this paper, we choose a Gaussian distribution for $q_w(\tilde{z})$ following the original framework [19]. In practice, we can choose any base family $q_w(\tilde{z})$ and still reap the benefits of partial non-centering. For more details please refer to Algorithm 2 in the Appendix B.

2.6 Forward Autoregressive Flows

Flows offer a powerful way to extend the expressiveness of variational families, thereby reducing the KL divergence between the variational approximation and the true posterior [36, 28, 2, 1]. In flows, a simple base distribution is gradually transformed into a more complex one through a sequence of invertible mappings. One such transformation is the forward autoregressive flow.

Definition 2. A forward autoregressive flow (FAF) is an invertible transformation $z = T_{\text{FAF}}(\epsilon)$, which maps a base random variable $\epsilon = (\epsilon_1, \dots, \epsilon_D) \sim p_{\epsilon}$ to the target variable $z = (z_1, \dots, z_D)$ via an autoregressive transformation

$$z_i = m_i(z_{1:i-1}) + s_i(z_{1:i-1}) \epsilon_i, \quad i = 1, \dots, D,$$
 (2.12)

where p_{ϵ} is a base distribution, m_i is a shift function and s_i is a scaling function. Furthermore, an *affine* forward autoregressive flow is one in which m_i and $\log s_i$ are affine functions.

In practice, the scaling function is often parameterized in terms of $\log s_i$ and subsequently recovered using the exponential function, which ensures positivity; however, alternative nonlinear functions can also be used. Also, multiple layers of the transformation can be composed to build more flexible variational families.

3 Model-Informed Flows: Bridging VIP and Autoregressive Flows

We return to our central question: Can a flow-based distribution encapsulate the benefits of VIP? The VIP process, when applied in the variational space, involves two key stages: first, sampling an auxiliary variable \tilde{z} from a base variational distribution $q_w(\tilde{z})$, and second, transforming \tilde{z} into the latent variable z using the VIP transformation, T_{VIP} .

The original VIP framework [19] primarily considers $q_w(\tilde{z})$ to be a mean-field Gaussian (i.e., with a diagonal covariance matrix). Our investigation extends this by considering $q_w(\tilde{z})$ as a full-rank Gaussian.

We first establish that a full-rank Gaussian is a special case of FAF. A full-rank Gaussian variational distribution $\tilde{z} \sim \mathcal{N}(\mu, LL^{\top})$ is generated by an affine transformation T_A , applied to a standard normal variable $\epsilon \sim \mathcal{N}(0, I)$

$$\tilde{z} = T_A(\epsilon) = \mu + L \epsilon, \tag{3.1}$$

where $\mu \in \mathbb{R}^D$ is the mean vector and $L \in \mathbb{R}^{D \times D}$ is a lower-triangular Cholesky factor of the covariance matrix. This affine transformation, T_A , can be replicated by an affine FAF by defining the shift and scale functions of the FAF (recall Definition 2) as

$$m_i(\tilde{z}_{1:i-1}) = \mu_i + L_{i,1:i-1} L_{1:i-1,1:i-1}^{-1} (\tilde{z}_{1:i-1} - \mu_{1:i-1}), \quad \log s_i(\tilde{z}_{1:i-1}) = \log L_{ii},$$
 (3.2)

(see Lemma 7 in Appendix C). Thus, a full-rank Gaussian distribution can be viewed as a specific instance of an affine FAF.

While a standard affine FAF can represent the initial transformation T_A (generating \tilde{z} from ϵ), it cannot, by itself, fully represent the composite transformation $T_{\text{VIP}} \circ T_A$ that yields z. To see why, observe that the composite transformation reduces to

$$z_{i} = f_{i}(\pi(z_{i})) + g_{i}(\pi(z_{i}))^{1-\lambda_{i}} \left(\mu_{i} + \sum_{j=1}^{i-1} L_{ij}\epsilon_{j} + L_{ii}\epsilon_{i} - \lambda_{i}f_{i}(\pi(z_{i}))\right).$$
(3.3)

If we attempt to cast this composite transformation into the standard affine FAF form from Equation (2.12) the terms would need to be

$$m_i(z_{1:i-1}) \stackrel{?}{=} f_i(\pi(z_i)) + g_i(\pi(z_i))^{1-\lambda_i} \Big(\mu_i + \sum_{j=1}^{i-1} L_{ij}\epsilon_j - \lambda_i f_i(\pi(z_i))\Big),$$
 (3.4)

$$\log s_i(z_{1:i-1}) \stackrel{?}{=} \log g_i(\pi(z_i))^{1-\lambda_i} + \log L_{ii}. \tag{3.5}$$

In principle, sufficiently powerful networks in the FAF could represent these forms. However, they could not be captured in an affine FAF due to dependence on ϵ and prior functions. In addition, Equation (3.4) contains the product $g_i(\pi(z_i))$ $f_i(\pi(z_i))$, which induces quadratic dependence on z that an affine mapping cannot represent. These nonlinearities may be difficult to capture even with an FAF that uses, e.g., multi-layer perceptrons. To remedy this, we introduce a generalized flow.

Definition 3. A generalized forward autoregressive flow (GFAF) is an invertible transformation $z = T_{\text{GFAF}}(\epsilon)$, which maps a base random variable $\epsilon = (\epsilon_1, \dots, \epsilon_D) \sim p_{\epsilon}$ to the target variable $z = (z_1, \dots, z_D)$ via an autoregressive transformation

$$z_i = m_i(z_{1:i-1}) + s_i(z_{1:i-1}) \left(\epsilon_i - t_i(\epsilon_{1:i-1}, z_{1:i-1}) \right), \quad i = 1, \dots, D,$$
(3.6)

where p_{ϵ} is a base distribution, m_i is a shift function, s_i is a scaling function, and t_i is a translation function. Furthermore, an *affine* generalized forward autoregressive flow is one in which m_i , $\log s_i$, and t_i are affine functions.

Our main theoretical result, stated in Theorem 4, demonstrates how the composite transformation $T = T_{\text{VIP}} \circ T_A$ (a full-rank Gaussian transformation followed by the VIP transformation) can be exactly represented by such a generalized forward autoregressive flow.

Theorem 4. Let $T = T_{VIP} \circ T_A$ where T_{VIP} is the VIP transformation (Definition 1) and T_A is the affine transformation from full-rank Gaussian. If f_i and $\log g_i$ in the hierarchical Bayesian model (Equation (2.2)) are arbitrary continuous functions, and the parent nodes $\pi(z_i)$ are a subset of the preceding variables $z_{1:i-1}$ (respecting the causal dependency structure of the model), then T can be represented as an affine generalized forward autoregressive flow with

$$m_i(z_{1:i-1}) = f_i(\pi(z_i)),$$
 (3.7)

$$\log s_i(z_{1:i-1}) = \log L_{ii} + (1 - \lambda_i) \log g_i(\pi(z_i)), \tag{3.8}$$

$$t_i(\epsilon_{1:i-1}, z_{1:i-1}) = \frac{1}{L_{ii}} \left(\lambda_i f_i(\pi(z_i)) - \mu_i - L_{i,1:i-1} \epsilon_{1:i-1} \right)$$
(3.9)

Theorem 4 therefore demonstrates that GFAF, by leveraging its novel translation term t_i (which depends on past noise $\epsilon_{1:i-1}$) and by incorporating the model's prior functions, can replicate the full-rank VIP mechanism.

3.1 Model-Informed Flows

Building on the previous ideas, we introduce a simple generalization of FAFs designed to capture the VIP mechanism even if the conditioning networks are affine.

Definition 5. A *Model-Informed Flow* (MIF) is an invertible transformation $z = T_{\text{MIF}}(\epsilon)$, which maps a base random variable $\epsilon = (\epsilon_1, \dots, \epsilon_D) \sim p_{\epsilon}$ to the target variable $z = (z_1, \dots, z_D)$ via an autoregressive transformation

$$z_i = m_i(u_i) + s_i(u_i)(\epsilon_i - t_i(\epsilon_{1:i-1}, u_i)), \quad i = 1, \dots, D,$$
 (3.10)

$$u_i = [z_{1:i-1}, f_i(\pi(z_i)), g_i(\pi(z_i))]$$
 (3.11)

Algorithm 1 Model-Informed Flow (MIF)

```
Input: \epsilon = (\epsilon_1, \dots, \epsilon_D), prior functions f_1, \dots, f_D and g_1, \dots, g_D (or their logs for scale)
                                              ▶ Process in a pre-defined topological order of latent variables
 1: for i = 1 to D do
          u_i \leftarrow [z_{1:i-1}, f_i(\pi(z_i)), \log g_i(\pi(z_i))] \triangleright Construct input incorporating prior information
          m_i \leftarrow NN_m(u_i)
 3:
                                                                             ▶ Neural network for the shift function
          \log s_i \leftarrow NN_s(u_i)
 4:
                                                                       Neural network for the log-scale function
          t_i \leftarrow \text{NN}_t([u_i, \epsilon_{1:i-1}])
                                                  \triangleright Neural network for the translation term with \epsilon_{1:i-1} inputs
 5:
         z_i \leftarrow m_i + \exp(\log s_i) \cdot \left(\epsilon_i - t_i\right)
                                                                      ▶ Generalized autoregressive transformation
 7: end for
 8: return z = (z_1, ..., z_D)
```

where p_{ϵ} is a base distribution, m_i is a shift function, s_i is a scaling function, and t_i is a translation term. Furthermore, an *Affine* Model-Informed Flow is one in which m_i , $\log s_i$, and t_i are affine functions.

Algorithm 1 presents the pseudocode for implementing MIF, highlighting in blue the components that extend a standard forward autoregressive flow; omitting these reduces MIF to such a standard FAF. The key architectural differences are, first, MIF employs conditioning networks not only for the shift m_i and log-scale $\log s_i$ but also for the translation term t_i , with the latter explicitly taking previous noise variables $\epsilon_{1:i-1}$ as inputs, as motivated by Theorem 4. Second, MIF is designed to incorporate the model's prior functions f_i and $\log g_i$ as additional inputs to these conditioning networks, providing them with valuable, explicit structural guidance from the target model. Third, the generation process in MIF (the loop over i) must adhere to a pre-defined topological order of the latent variables consistent with the hierarchical Bayesian model.

Before moving on to experiments, we discuss two practical issues.

3.2 Incorporating Prior Information through f_i and $\log g_i$

Our preliminary experiments revealed that omitting explicit prior function inputs $(f_i, \log g_i)$ from MIF often minimally impacted performance. This occurs when these priors are affine, as the target generalized forward autoregressive flow (GFAF) representing full-rank VIP (per Theorem 4) then simplifies to an *affine* GFAF. An MIF, even without these explicit prior inputs, can learn to reproduce this affine GFAF if its own conditioning functions for m_i , $\log s_i$, and t_i possess at least affine capacity. This is shown in the following corollary.

Corollary 6. Let $T = T_{\text{VIP}} \circ T_A$ where T_{VIP} is the VIP transformation (see Definition 1) and T_A is the affine transformation from full-rank Gaussian. If f_i and $\log g_i$ in the hierarchical Bayesian model (see Equation (2.2)) are affine functions, then T can be represented as an affine generalized forward autoregressive flow.

This corollary shows that when the prior functions are affine, affine MIFs have enough capacity to learn them even if they are not provided, meaning there is no impact on the optimal KL-divergence. Still, in practice providing f_i and $\log g_i$ is helpful in practice to accelerate convergence and reduce training complexity. We suspect the same pattern holds more generally—if a MIF is trained with high-capacity networks, it may be able to learn to represent the prior functions if not provided, at some extra training cost.

3.3 The Necessity of Conditioning on Previously Generated Latent Variables

Inverse Autoregressive Flows (IAFs) [28] represent an important class of normalizing flows, lauded for the computational efficiency of their sampling process. Unlike FAFs, conditioning networks of IAFs depend solely on the base noise variables $\epsilon_{1:i-1}$, allowing parallel computation of all z_i :

$$z_i = m_i(\epsilon_{1:i-1}) + s_i(\epsilon_{1:i-1})\epsilon_i, \quad i = 1, \dots, D.$$
 (3.12)

This structure makes it challenging to accurately represent the VIP mechanism. To capture VIP, an IAF's conditioning networks would need to replicate target forms that intrinsically depend on previously generated latent variables $z_{1:i-1}$ via the model's prior functions $(f_i(\pi(z_i)))$ and $g_i(\pi(z_i))$.

Table 1: Negative ELBOs (-ELBO) for hierarchical benchmark models using mean-field Gaussian (MF), mean-field Gaussian with VIP (MF-VIP), full-rank Gaussian (FR), and full-rank Gaussian with VIP (FR-VIP). Lower values indicate tighter posterior approximations.

Model	MF	MF-VIP	FR	FR-VIP
8Schools	34.80	31.89	33.85	31.86
Credit	548.65	533.90	535.88	525.02
Funnel	1.86	0.00	1.86	0.00
Radon	1267.99	1215.17	1220.73	1213.52
Movielens	870.93	850.49	856.11	844.51
IRT	823.15	822.58	817.38	816.64

Specifically, they would need to satisfy

$$m_i(\epsilon_{1:i-1}) \stackrel{?}{=} f_i(\pi(z_i)) + g_i(\pi(z_i))^{1-\lambda_i} \Big(\mu_i + \sum_{i=1}^{i-1} L_{ij}\epsilon_j - \lambda_i f_i(\pi(z_i))\Big),$$
 (3.13)

$$\log s_i(\epsilon_{1:i-1}) \stackrel{?}{=} (1 - \lambda_i) \log g_i(\pi(z_i)) + \log L_{ii}, \tag{3.14}$$

where z_i (and thus $\pi(z_i)$) on the right-hand side are themselves complex functions of $\epsilon_{1:i-1}$. Asking $m_i(\epsilon_{1:i-1})$ and $s_i(\epsilon_{1:i-1})$ to represent this transformation is challenging as it essentially requires the network to reproduce the entire process that produced $z_{1:i-1}$ in previous steps.

Particularly, an IAF with *affine* conditioning networks for m_i , $\log s_i$ (and a term like t_i , if added) cannot capture the VIP transformation, since $z_{1:i-1}$ and $\epsilon_{1:i-1}$ have a complex non-linear relationship. This limitation underscores the advantage of forward autoregressive structures. We show in our experiments (e.g., results related to Figure 2) that IAFs require substantially greater model capacity to approach the effectiveness of MIF in representing VIP.

4 Related Work

Early flow-based generative models—including MADE [18], Real NVP [15], Glow [27], and Masked Autoregressive Flow [34]—established that autoregressive masking, coupling transforms, and invertible 1×1 convolutions enable tractable likelihoods with strong high-dimensional density estimation. Normalizing flows were subsequently adapted for variational inference, first as post-hoc enrichments of diagonal Gaussians [36] and later as architectures that scale in latent dimensionality, most notably Inverse Autoregressive Flow (IAF) [28]. These developments demonstrated that flexible, invertible parameterizations can substantially tighten the ELBO without sacrificing computational efficiency.

For hierarchical Bayesian models, *Variationally Inferred Parameters* (VIP) introduced gradient-based partial non-centering to alleviate the funnel geometry typical of deep hierarchies [19]. Building on VIP's idea of injecting model structure into the variational family, hybrids such as Automatic Structured Variational Inference (ASVI) [3], Cascading Flows [4], and Embedded-Model Flows (EMF) [41] couple model-aware parameterizations with flow flexibility. Our *Model-Informed Flow* continues this line by proving that full-rank VIP can be represented in a forward autoregressive flow augmented with translation and prior inputs, yielding a compact yet expressive variational family for hierarchical models.

5 Experiments

5.1 Experimental Setup

To validate our theoretical results, we evaluate on six different hierarchical Bayesian models: 8Schools, German Credit, Funnel, Radon, Movielens, and IRT. These models exhibit varying degrees of funnel-like posterior geometries, making them ideal testbeds for examining the benefits of VIP-inspired flow designs. For our final comprehensive benchmark experiments, we also include more models such as Seeds, Sonar, and Ionosphere.

Table 2: Negative ELBOs (—ELBO) for ablation study comparing affine Model-Informed Flow (MIF) against variations and baselines across hierarchical models. MIF includes z-conditioning, translation term, prior info, and correct order. Please refer to Appendix D for more details of variants of MIF. Lower values indicate tighter posterior approximations.

Model	FR-VIP	MIF	$\begin{array}{c} \text{MIF} \\ (\epsilon\text{-cond}) \end{array}$		MIF (w/o Prior)	MIF (w/o Order)	IAF
8Schools	31.86	31.74	32.04	31.86	31.83	33.83	32.22
Credit	525.02	520.72	523.92	525.87	522.75	534.63	523.85
Funnel	0.00	0.01	0.38	0.38	0.38	1.86	0.37
Radon	1213.52	1213.11	1215.11	1214.31	1213.45	1259.13	1215.23
Movielens	844.51	842.91	844.01	846.66	843.59	854.10	844.23
IRT	816.64	815.49	815.70	815.74	815.53	815.58	815.66

For all experiments, we utilize the Adam optimizer [26] and initialize all learnable parameters from a standard Gaussian distribution with a standard deviation of 0.1. For our Model-Informed Flow (MIF) evaluations, distinct configurations are used: the experiments in Section 5.3 primarily consider a single-layer *affine* MIF to clearly assess its structural components. In subsequent experiments, including the network expressiveness analysis and comprehensive benchmarks, MIF's conditioning networks are implemented as multi-layer perceptrons with ReLU activation functions to explore the impact of increased representational capacity via hidden units.

We perform 100,000 optimization iterations, using 256 Monte Carlo samples to approximate the ELBO during training. After training, the final ELBO is evaluated using 100,000 fresh samples for reliable estimation. For each model configuration, we report the best ELBO achieved after exploring six learning rates (logarithmically spaced from 10^{-1} to 10^{-6}). Additional details regarding the benchmark models, specific variational family configurations, training time comparison, and MLP architectures are provided in Appendix D. Our implementation is available at https://github.com/joohwanko/Model-Informed-Flow

5.2 Preliminary Observations: Full-Rank VIP Outperforms Baselines

Prior work on VIP focused exclusively on mean-field Gaussian approximations [19]. To assess whether the advantages of VIP extend to richer variational families, we apply VIP to a full-rank Gaussian setting and compare four configurations—MF, MF-VIP, FR, and FR-VIP—across six canonical hierarchical models. As shown in Table 1, FR-VIP achieves the lowest negative ELBO in every case, outperforming both its non-VIP counterpart and mean-field VIP, and achieving performance comparable to more complex state-of-the-art methods (cf. Table 3). These results highlight the power of combining full-rank with VIP and motivate our design of VIP-inspired low architectures.

5.3 Impact of Design Components

In this section, we empirically validate the contribution of MIF's distinct design elements through a targeted ablation study, with results presented in Table 2. We compare the affine MIF against variants that individually alter or remove its key theoretically-motivated components: the ϵ -dependent translation term (t_i) , by evaluating MIF $(w/o\ t_i)$; the use of explicit prior information, by assessing MIF $(w/o\ Prior)$ which omits f_i , $\log g_i$ as inputs; and adherence to the hierarchical variable processing order, examined via MIF $(w/o\ Order)$. Additionally, we test an IAF-like variant, MIF $(\epsilon$ -cond), which conditions primarily on base noise $\epsilon_{1:i-1}$ instead of previously generated latents $z_{1:i-1}$, alongside relevant baselines like FR-VIP and a standard IAF. The consistent outcome is that deviating from the full MIF design by removing or altering these components generally degrades performance, underscoring their collective importance to its effectiveness.

5.4 Impact of Network Expressiveness

Recall from Section 3.3 that while IAFs face fundamental challenges in representing the VIP mechanism due to their conditioning solely on noise (ϵ) , it was posited that sufficient network expressiveness might partially overcome these limitations. We empirically investigate this by comparing our full

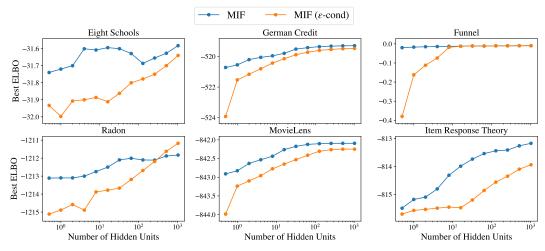


Figure 2: Best ELBO achieved by full MIF (blue) and the variant without latent-variable conditioning (orange) as a function of MLP hidden-unit count. Higher capacity allows the no-latent variant to close the gap, showing that sufficiently expressive networks can implicitly learn dependencies otherwise provided by explicit latent inputs.

MIF, which conditions on previously generated latents $z_{1:i-1}$, against MIF (ϵ -cond), an IAF-like variant where the conditioning networks primarily use $\epsilon_{1:i-1}$ instead of $z_{1:i-1}$.

Figure 2 illustrates the performance of MIF versus MIF (ϵ -cond) as the expressiveness of their conditioning networks (e.g., by increasing the number of hidden units) is varied. Across most benchmarked models, enhancing network capacity allows MIF (ϵ -cond) to substantially improve its ability to capture complex dependencies. Consequently, the performance gap between this IAF-like variant and the standard MIF significantly narrows with increased expressiveness, demonstrating that sufficiently powerful IAF-like architectures can indeed achieve strong results, in many cases closely approaching or nearly matching the performance of MIF, which itself may maintain a slight lead or offer benefits in parameter efficiency.

5.5 Comprehensive Evaluation on Hierarchical and Non-hierarchical Benchmarks

To assess its generality and competitive strength, we benchmark MIF with 1024 hidden units per conditioning network, denoted MIF($h=2^{10}$), against several leading variational inference methods. These baselines, primarily drawn from the recent benchmark by [10] and detailed with their acronyms in the caption of Table 3, provide a robust comparison. The evaluation spans the six previously discussed hierarchical models and three additional datasets (Seeds[†], Sonar[†], Ionosphere[†]) to test MIF's broad applicability. Results in the Table 3 show that MIF($h=2^{10}$) achieves the best or equal-best performance on most of the benchmarks. These strong results, obtained using just a single layer of our expressive MIF transformation, demonstrate that its theory-driven design effectively delivers state-of-the-art performance with notable architectural simplicity.

6 Discussion and Limitation

This paper introduces the Model-Informed Flow (MIF), a new architecture for variational inference designed for complex hierarchical Bayesian models. MIF originates from a connection between VIP and FAFs. A significant finding is that even a single-layer affine MIF can achieve surprisingly competitive performance against other methods. A limitation of MIF is its reliance on the FAF structure. Although FAFs may not inherently demand more floating-point operations (FLOPs) per sample than Inverse Autoregressive Flows (IAFs), with variational inference, IAFs are better suited for modern parallel computing environments. The VIP mechanism appears to be essentially sequential in nature. Thus, our research suggests a consideration for flows and VI: to capture difficult posterior geometry may require either sequential processing as in MIF or high-capacity conditioning networks.

Table 3: Negative ELBOs (—ELBO) for various VI methods on hierarchical and non-hierarchical benchmarks. Compared methods include: Gaussian Mean-Field (MF) [8], Gaussian Mixture Model VI (GMMVI) [6], Sequential Monte Carlo (SMC) [14], Annealed Flow Transport (AFT) [5], Flow Annealed IS Bootstrap (FAB) [32], Continual Repeated AFT (CRAFT) [31], and Uncorrected Hamiltonian Annealing (UHA) [42]. Lower values indicate tighter posterior approximations; † denotes results taken from [10].

Model	MF	GMMVI	SMC	AFT	FAB	CRAFT	UHA	$\mathrm{MIF}(h=2^{10})$
8Schools	34.80	31.70	31.80	31.81	31.79	31.90	33.09	31.78
German Credit	548.65	519.35	531.42	527.60	519.39	524.59	536.30	519.29
Funnel	1.86	0.01	0.29	0.30	0.01	0.02	0.38	0.00
Radon	1267.99	1213.67	1221.63	1236.42	1215.92	1229.77	1260.38	1211.83
Movielens	870.93	848.00	849.68	853.84	845.32	850.20	861.22	842.09
IRT	823.15	815.05	820.46	819.56	816.44	818.66	821.84	813.17
Seeds [†]	76.73	73.41	74.69	74.26	73.41	73.79	N/A	72.00
\mathtt{Sonar}^\dagger	137.67	108.72	111.35	110.67	108.59	115.61	N/A	108.85
${\tt Ionosphere}^{\dagger}$	123.41	111.83	114.75	113.27	111.67	112.38	N/A	111.85

7 Acknowledgement

This material is based upon work supported in part by the National Science Foundation under Grant No. 2045900.

References

- [1] A. Agrawal and J. Domke. Disentangling impact of capacity, objective, batchsize, estimators, and step-size on flow vi. *arXiv preprint arXiv:2412.08824*, 2024.
- [2] A. Agrawal, D. R. Sheldon, and J. Domke. Advances in black-box vi: Normalizing flows, importance weighting, and optimization. *Advances in Neural Information Processing Systems*, 33:17358–17369, 2020.
- [3] L. Ambrogioni, K. Lin, E. Fertig, S. Vikram, M. Hinne, D. Moore, and M. van Gerven. Automatic structured variational inference. In *International Conference on Artificial Intelligence and Statistics*, pages 676–684. PMLR, 2021.
- [4] L. Ambrogioni, G. Silvestri, and M. van Gerven. Automatic variational inference with cascading flows. In *International Conference on Machine Learning*, pages 254–263. PMLR, 2021.
- [5] M. Arbel, A. Matthews, and A. Doucet. Annealed flow transport monte carlo. In *International Conference on Machine Learning*, pages 318–330. PMLR, 2021.
- [6] O. Arenz, P. Dahlinger, Z. Ye, M. Volpp, and G. Neumann. A unified perspective on natural gradient variational inference with gaussian mixture models. *arXiv* preprint arXiv:2209.11533, 2022.
- [7] M. Betancourt and M. Girolami. Hamiltonian monte carlo for hierarchical models. *Current trends in Bayesian methodology with applications*, 79(30):2–4, 2015.
- [8] C. M. Bishop and N. M. Nasrabadi. *Pattern recognition and machine learning*, volume 4. Springer, 2006.
- [9] D. M. Blei, A. Kucukelbir, and J. D. McAuliffe. Variational inference: A review for statisticians. *Journal of the American Statistical Association*, 112(518):859–877, 2017.
- [10] D. Blessing, X. Jia, J. Esslinger, F. Vargas, and G. Neumann. Beyond elbos: A large-scale evaluation of variational methods for sampling. *arXiv preprint arXiv:2406.07423*, 2024.
- [11] T. M. Cover and J. A. Thomas. *Elements of information theory*. Wiley-Interscience, 1991.
- [12] N. Cressie, C. A. Calder, J. S. Clark, J. M. Ver Hoef, and C. K. Wikle. Accounting for uncertainty in ecological analysis: the strengths and limitations of hierarchical statistical modeling. *Ecological Applications*, 19(3):553–570, 2009.
- [13] M. J. Crowder. Beta-binomial anova for proportions. Applied statistics, pages 34–37, 1978.
- [14] P. Del Moral, A. Doucet, and A. Jasra. Sequential monte carlo samplers. *Journal of the Royal Statistical Society Series B: Statistical Methodology*, 68(3):411–436, 2006.
- [15] L. Dinh, J. Sohl-Dickstein, and S. Bengio. Density estimation using real NVP. arXiv preprint arXiv:1605.08803, 2017.
- [16] F. Dominici, J. M. Samet, and S. L. Zeger. Combining evidence on air pollution and daily mortality from the 20 largest us cities: a hierarchical modelling strategy. *Journal of the Royal Statistical Society Series A: Statistics in Society*, 163(3):263–302, 2000.
- [17] A. Gelman and J. Hill. *Data analysis using regression and multilevel/hierarchical models*. Cambridge university press, 2007.
- [18] M. Germain, K. Gregor, I. Murray, and H. Larochelle. Made: Masked autoencoder for distribution estimation. In *International conference on machine learning*, pages 881–889. PMLR, 2015.
- [19] M. Gorinova, D. Moore, and M. Hoffman. Automatic reparameterisation of probabilistic programs. In *International Conference on Machine Learning*, pages 3648–3657. PMLR, 2020.
- [20] R. P. Gorman and T. J. Sejnowski. Analysis of hidden units in a layered network trained to classify sonar targets. *Neural networks*, 1(1):75–89, 1988.

- [21] F. M. Harper and J. A. Konstan. The movielens datasets: History and context. *Acm transactions on interactive intelligent systems (tiis)*, 5(4):1–19, 2015.
- [22] M. Hoffman, P. Sountsov, J. V. Dillon, I. Langmore, D. Tran, and S. Vasudevan. Neutralizing bad geometry in hamiltonian monte carlo using neural transport. arXiv preprint arXiv:1903.03704, 2019.
- [23] M. D. Hoffman, D. M. Blei, C. Wang, and J. Paisley. Stochastic variational inference. *Journal of Machine Learning Research*, 2013.
- [24] J. Ingraham and D. Marks. Variational inference for sparse and undirected models. In *International Conference on Machine Learning*, pages 1607–1616. PMLR, 2017.
- [25] M. I. Jordan, Z. Ghahramani, T. S. Jaakkola, and L. K. Saul. An introduction to variational methods for graphical models. *Machine learning*, 37:183–233, 1999.
- [26] D. P. Kingma. Adam: A method for stochastic optimization. arXiv preprint arXiv:1412.6980, 2014.
- [27] D. P. Kingma and P. Dhariwal. Glow: Generative flow with invertible 1x1 convolutions. *Advances in neural information processing systems*, 31, 2018.
- [28] D. P. Kingma, T. Salimans, R. Jozefowicz, X. Chen, I. Sutskever, and M. Welling. Improved variational inference with inverse autoregressive flow. *Advances in neural information processing systems*, 29, 2016.
- [29] A. B. Lawson. *Bayesian disease mapping: hierarchical modeling in spatial epidemiology*. Chapman and Hall/CRC, 2018.
- [30] F. M. Lord and M. R. Novick. Statistical theories of mental test scores. IAP, 2008.
- [31] A. Matthews, M. Arbel, D. J. Rezende, and A. Doucet. Continual repeated annealed flow transport monte carlo. In *International Conference on Machine Learning*, pages 15196–15219. PMLR, 2022.
- [32] L. I. Midgley, V. Stimper, G. N. Simm, B. Schölkopf, and J. M. Hernández-Lobato. Flow annealed importance sampling bootstrap. arXiv preprint arXiv:2208.01893, 2022.
- [33] R. M. Neal. Slice sampling. The annals of statistics, 31(3):705–767, 2003.
- [34] G. Papamakarios, T. Pavlakou, and I. Murray. Masked autoregressive flow for density estimation. *Advances in neural information processing systems*, 30, 2017.
- [35] O. Papaspiliopoulos, G. O. Roberts, and M. Sköld. A general framework for the parametrization of hierarchical models. *Statistical Science*, pages 59–73, 2007.
- [36] D. J. Rezende and S. Mohamed. Variational inference with normalizing flows. In *Proceedings* of the 32nd International Conference on Machine Learning (ICML), pages 1530–1538, 2015.
- [37] S. Richardson and N. Best. Bayesian hierarchical models in ecological studies of health-environment effects. *Environmetrics: The official journal of the International Environmetrics Society*, 14(2):129–147, 2003.
- [38] J. A. Royle and R. M. Dorazio. *Hierarchical modeling and inference in ecology: the analysis of data from populations, metapopulations and communities.* Elsevier, 2008.
- [39] D. B. Rubin. Estimation in parallel randomized experiments. *Journal of Educational Statistics*, 6(4):377–401, 1981.
- [40] V. G. Sigillito, S. P. Wing, L. V. Hutton, and K. B. Baker. Classification of radar returns from the ionosphere using neural networks. *Johns Hopkins APL Technical Digest*, 10(3):262–266, 1989.
- [41] G. Silvestri, E. Fertig, D. Moore, and L. Ambrogioni. Embedded-model flows: Combining the inductive biases of model-free deep learning and explicit probabilistic modeling. *arXiv* preprint *arXiv*:2110.06021, 2021.

- [42] A. Thin, N. Kotelevskii, A. Doucet, A. Durmus, E. Moulines, and M. Panov. Monte carlo variational auto-encoders. In *International Conference on Machine Learning*, pages 10247–10257. PMLR, 2021.
- [43] C. K. Wikle. Hierarchical bayesian models for predicting the spread of ecological processes. *Ecology*, 84(6):1382–1394, 2003.

NeurIPS Paper Checklist

1. Claims

Question: Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope?

Answer: [Yes]

Justification: Section 2 defines the scope of the paper and Section 3 gives evidence to the main claims.

Guidelines:

- The answer NA means that the abstract and introduction do not include the claims made in the paper.
- The abstract and/or introduction should clearly state the claims made, including the contributions made in the paper and important assumptions and limitations. A No or NA answer to this question will not be perceived well by the reviewers.
- The claims made should match theoretical and experimental results, and reflect how much the results can be expected to generalize to other settings.
- It is fine to include aspirational goals as motivation as long as it is clear that these goals
 are not attained by the paper.

2. Limitations

Question: Does the paper discuss the limitations of the work performed by the authors?

Answer: [Yes]

Justification: We state possible limitations of MIF compared to inverse autoregressive flows in terms of speed.

Guidelines:

- The answer NA means that the paper has no limitation while the answer No means that the paper has limitations, but those are not discussed in the paper.
- The authors are encouraged to create a separate "Limitations" section in their paper.
- The paper should point out any strong assumptions and how robust the results are to violations of these assumptions (e.g., independence assumptions, noiseless settings, model well-specification, asymptotic approximations only holding locally). The authors should reflect on how these assumptions might be violated in practice and what the implications would be.
- The authors should reflect on the scope of the claims made, e.g., if the approach was only tested on a few datasets or with a few runs. In general, empirical results often depend on implicit assumptions, which should be articulated.
- The authors should reflect on the factors that influence the performance of the approach. For example, a facial recognition algorithm may perform poorly when image resolution is low or images are taken in low lighting. Or a speech-to-text system might not be used reliably to provide closed captions for online lectures because it fails to handle technical jargon.
- The authors should discuss the computational efficiency of the proposed algorithms and how they scale with dataset size.
- If applicable, the authors should discuss possible limitations of their approach to address problems of privacy and fairness.
- While the authors might fear that complete honesty about limitations might be used by reviewers as grounds for rejection, a worse outcome might be that reviewers discover limitations that aren't acknowledged in the paper. The authors should use their best judgment and recognize that individual actions in favor of transparency play an important role in developing norms that preserve the integrity of the community. Reviewers will be specifically instructed to not penalize honesty concerning limitations.

3. Theory assumptions and proofs

Question: For each theoretical result, does the paper provide the full set of assumptions and a complete (and correct) proof?

Answer: [Yes]

Justification: See Section 3 and the corresponding proofs in the Appendix.

Guidelines:

- The answer NA means that the paper does not include theoretical results.
- All the theorems, formulas, and proofs in the paper should be numbered and cross-referenced.
- All assumptions should be clearly stated or referenced in the statement of any theorems.
- The proofs can either appear in the main paper or the supplemental material, but if they appear in the supplemental material, the authors are encouraged to provide a short proof sketch to provide intuition.
- Inversely, any informal proof provided in the core of the paper should be complemented by formal proofs provided in appendix or supplemental material.
- Theorems and Lemmas that the proof relies upon should be properly referenced.

4. Experimental result reproducibility

Question: Does the paper fully disclose all the information needed to reproduce the main experimental results of the paper to the extent that it affects the main claims and/or conclusions of the paper (regardless of whether the code and data are provided or not)?

Answer: [Yes]

Justification: We provide experimental details in the Experiments section.

Guidelines:

- The answer NA means that the paper does not include experiments.
- If the paper includes experiments, a No answer to this question will not be perceived well by the reviewers: Making the paper reproducible is important, regardless of whether the code and data are provided or not.
- If the contribution is a dataset and/or model, the authors should describe the steps taken to make their results reproducible or verifiable.
- Depending on the contribution, reproducibility can be accomplished in various ways. For example, if the contribution is a novel architecture, describing the architecture fully might suffice, or if the contribution is a specific model and empirical evaluation, it may be necessary to either make it possible for others to replicate the model with the same dataset, or provide access to the model. In general, releasing code and data is often one good way to accomplish this, but reproducibility can also be provided via detailed instructions for how to replicate the results, access to a hosted model (e.g., in the case of a large language model), releasing of a model checkpoint, or other means that are appropriate to the research performed.
- While NeurIPS does not require releasing code, the conference does require all submissions to provide some reasonable avenue for reproducibility, which may depend on the nature of the contribution. For example
 - (a) If the contribution is primarily a new algorithm, the paper should make it clear how to reproduce that algorithm.
- (b) If the contribution is primarily a new model architecture, the paper should describe the architecture clearly and fully.
- (c) If the contribution is a new model (e.g., a large language model), then there should either be a way to access this model for reproducing the results or a way to reproduce the model (e.g., with an open-source dataset or instructions for how to construct the dataset).
- (d) We recognize that reproducibility may be tricky in some cases, in which case authors are welcome to describe the particular way they provide for reproducibility. In the case of closed-source models, it may be that access to the model is limited in some way (e.g., to registered users), but it should be possible for other researchers to have some path to reproducing or verifying the results.

5. Open access to data and code

Question: Does the paper provide open access to the data and code, with sufficient instructions to faithfully reproduce the main experimental results, as described in supplemental material?

Answer: [Yes]

Justification: We will provide the code for the experiments in the Appendix.

Guidelines:

- The answer NA means that paper does not include experiments requiring code.
- Please see the NeurIPS code and data submission guidelines (https://nips.cc/public/guides/CodeSubmissionPolicy) for more details.
- While we encourage the release of code and data, we understand that this might not be possible, so "No" is an acceptable answer. Papers cannot be rejected simply for not including code, unless this is central to the contribution (e.g., for a new open-source benchmark).
- The instructions should contain the exact command and environment needed to run to reproduce the results. See the NeurIPS code and data submission guidelines (https://nips.cc/public/guides/CodeSubmissionPolicy) for more details.
- The authors should provide instructions on data access and preparation, including how
 to access the raw data, preprocessed data, intermediate data, and generated data, etc.
- The authors should provide scripts to reproduce all experimental results for the new proposed method and baselines. If only a subset of experiments are reproducible, they should state which ones are omitted from the script and why.
- At submission time, to preserve anonymity, the authors should release anonymized versions (if applicable).
- Providing as much information as possible in supplemental material (appended to the paper) is recommended, but including URLs to data and code is permitted.

6. Experimental setting/details

Question: Does the paper specify all the training and test details (e.g., data splits, hyper-parameters, how they were chosen, type of optimizer, etc.) necessary to understand the results?

Answer: [Yes]

Justification: Every details of experiments is in Experiments section and Appendix.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The experimental setting should be presented in the core of the paper to a level of detail that is necessary to appreciate the results and make sense of them.
- The full details can be provided either with the code, in appendix, or as supplemental material.

7. Experiment statistical significance

Question: Does the paper report error bars suitably and correctly defined or other appropriate information about the statistical significance of the experiments?

Answer: [No]

Justification: We do not provide error bars, but the experiment results show average values across different runs.

- The answer NA means that the paper does not include experiments.
- The authors should answer "Yes" if the results are accompanied by error bars, confidence intervals, or statistical significance tests, at least for the experiments that support the main claims of the paper.
- The factors of variability that the error bars are capturing should be clearly stated (for example, train/test split, initialization, random drawing of some parameter, or overall run with given experimental conditions).

- The method for calculating the error bars should be explained (closed form formula, call to a library function, bootstrap, etc.)
- The assumptions made should be given (e.g., Normally distributed errors).
- It should be clear whether the error bar is the standard deviation or the standard error
 of the mean.
- It is OK to report 1-sigma error bars, but one should state it. The authors should preferably report a 2-sigma error bar than state that they have a 96% CI, if the hypothesis of Normality of errors is not verified.
- For asymmetric distributions, the authors should be careful not to show in tables or figures symmetric error bars that would yield results that are out of range (e.g. negative error rates).
- If error bars are reported in tables or plots, The authors should explain in the text how they were calculated and reference the corresponding figures or tables in the text.

8. Experiments compute resources

Question: For each experiment, does the paper provide sufficient information on the computer resources (type of compute workers, memory, time of execution) needed to reproduce the experiments?

Answer: [Yes]

Justification: All of the experiment details are in the Appendix.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The paper should indicate the type of compute workers CPU or GPU, internal cluster, or cloud provider, including relevant memory and storage.
- The paper should provide the amount of compute required for each of the individual experimental runs as well as estimate the total compute.
- The paper should disclose whether the full research project required more compute than the experiments reported in the paper (e.g., preliminary or failed experiments that didn't make it into the paper).

9. Code of ethics

Question: Does the research conducted in the paper conform, in every respect, with the NeurIPS Code of Ethics https://neurips.cc/public/EthicsGuidelines?

Answer: [Yes]

Justification: We follow the NeurIPS Code of Ethics

Guidelines:

- The answer NA means that the authors have not reviewed the NeurIPS Code of Ethics.
- If the authors answer No, they should explain the special circumstances that require a
 deviation from the Code of Ethics.
- The authors should make sure to preserve anonymity (e.g., if there is a special consideration due to laws or regulations in their jurisdiction).

10. Broader impacts

Question: Does the paper discuss both potential positive societal impacts and negative societal impacts of the work performed?

Answer: [NA]

Justification: We did not state broader impacts since there are no significant impacts we anticipate that need to be described in the paper.

- The answer NA means that there is no societal impact of the work performed.
- If the authors answer NA or No, they should explain why their work has no societal impact or why the paper does not address societal impact.

- Examples of negative societal impacts include potential malicious or unintended uses (e.g., disinformation, generating fake profiles, surveillance), fairness considerations (e.g., deployment of technologies that could make decisions that unfairly impact specific groups), privacy considerations, and security considerations.
- The conference expects that many papers will be foundational research and not tied to particular applications, let alone deployments. However, if there is a direct path to any negative applications, the authors should point it out. For example, it is legitimate to point out that an improvement in the quality of generative models could be used to generate deepfakes for disinformation. On the other hand, it is not needed to point out that a generic algorithm for optimizing neural networks could enable people to train models that generate Deepfakes faster.
- The authors should consider possible harms that could arise when the technology is being used as intended and functioning correctly, harms that could arise when the technology is being used as intended but gives incorrect results, and harms following from (intentional or unintentional) misuse of the technology.
- If there are negative societal impacts, the authors could also discuss possible mitigation strategies (e.g., gated release of models, providing defenses in addition to attacks, mechanisms for monitoring misuse, mechanisms to monitor how a system learns from feedback over time, improving the efficiency and accessibility of ML).

11. Safeguards

Question: Does the paper describe safeguards that have been put in place for responsible release of data or models that have a high risk for misuse (e.g., pretrained language models, image generators, or scraped datasets)?

Answer: [NA]

Justification: The paper poses no such risks.

Guidelines:

- The answer NA means that the paper poses no such risks.
- Released models that have a high risk for misuse or dual-use should be released with
 necessary safeguards to allow for controlled use of the model, for example by requiring
 that users adhere to usage guidelines or restrictions to access the model or implementing
 safety filters.
- Datasets that have been scraped from the Internet could pose safety risks. The authors should describe how they avoided releasing unsafe images.
- We recognize that providing effective safeguards is challenging, and many papers do
 not require this, but we encourage authors to take this into account and make a best
 faith effort.

12. Licenses for existing assets

Question: Are the creators or original owners of assets (e.g., code, data, models), used in the paper, properly credited and are the license and terms of use explicitly mentioned and properly respected?

Answer: [NA]

Justification: The paper does not use existing assets.

- The answer NA means that the paper does not use existing assets.
- The authors should cite the original paper that produced the code package or dataset.
- The authors should state which version of the asset is used and, if possible, include a URL.
- The name of the license (e.g., CC-BY 4.0) should be included for each asset.
- For scraped data from a particular source (e.g., website), the copyright and terms of service of that source should be provided.
- If assets are released, the license, copyright information, and terms of use in the package should be provided. For popular datasets, paperswithcode.com/datasets has curated licenses for some datasets. Their licensing guide can help determine the license of a dataset.

- For existing datasets that are re-packaged, both the original license and the license of the derived asset (if it has changed) should be provided.
- If this information is not available online, the authors are encouraged to reach out to the asset's creators.

13. New assets

Question: Are new assets introduced in the paper well documented and is the documentation provided alongside the assets?

Answer: [NA]

Justification: The paper does not release new assets.

Guidelines:

- The answer NA means that the paper does not release new assets.
- Researchers should communicate the details of the dataset/code/model as part of their submissions via structured templates. This includes details about training, license, limitations, etc.
- The paper should discuss whether and how consent was obtained from people whose asset is used.
- At submission time, remember to anonymize your assets (if applicable). You can either create an anonymized URL or include an anonymized zip file.

14. Crowdsourcing and research with human subjects

Question: For crowdsourcing experiments and research with human subjects, does the paper include the full text of instructions given to participants and screenshots, if applicable, as well as details about compensation (if any)?

Answer: [NA]

Justification: The paper does not involve crowdsourcing nor research with human subjects. Guidelines:

- The answer NA means that the paper does not involve crowdsourcing nor research with human subjects.
- Including this information in the supplemental material is fine, but if the main contribution of the paper involves human subjects, then as much detail as possible should be included in the main paper.
- According to the NeurIPS Code of Ethics, workers involved in data collection, curation, or other labor should be paid at least the minimum wage in the country of the data collector.

15. Institutional review board (IRB) approvals or equivalent for research with human subjects

Question: Does the paper describe potential risks incurred by study participants, whether such risks were disclosed to the subjects, and whether Institutional Review Board (IRB) approvals (or an equivalent approval/review based on the requirements of your country or institution) were obtained?

Answer: [NA]

Justification: The paper does not involve crowdsourcing nor research with human subjects. Guidelines:

- The answer NA means that the paper does not involve crowdsourcing nor research with human subjects.
- Depending on the country in which research is conducted, IRB approval (or equivalent) may be required for any human subjects research. If you obtained IRB approval, you should clearly state this in the paper.
- We recognize that the procedures for this may vary significantly between institutions and locations, and we expect authors to adhere to the NeurIPS Code of Ethics and the guidelines for their institution.
- For initial submissions, do not include any information that would break anonymity (if applicable), such as the institution conducting the review.

16. Declaration of LLM usage

Question: Does the paper describe the usage of LLMs if it is an important, original, or non-standard component of the core methods in this research? Note that if the LLM is used only for writing, editing, or formatting purposes and does not impact the core methodology, scientific rigorousness, or originality of the research, declaration is not required.

Answer: [NA]

Justification: The core method development in this research does not involve LLMs as any important, original, or non-standard components.

- The answer NA means that the core method development in this research does not involve LLMs as any important, original, or non-standard components.
- Please refer to our LLM policy (https://neurips.cc/Conferences/2025/LLM) for what should or should not be described.

Supplementary Materials

A Acronyms and Notations

This section provides a summary of acronyms and mathematical notations frequently used throughout the paper to aid the reader.

Table 4: List of Acronyms

Acronym	Definition
CP	Centered Parameterization
ELBO	Evidence Lower Bound
FAF	Forward Autoregressive Flow
FR	Full-Rank (Gaussian)
GFAF	Generalized Forward Autoregressive Flow
IAF	Inverse Autoregressive Flow
KL	Kullback-Leibler (divergence)
MF	Mean-Field (Gaussian)
MIF	Model-Informed Flow
MLP	Multi-Layer Perceptron
NCP	Non-Centered Parameterization
VI	Variational Inference
VIP	Variationally Inferred Parameters

Table 5: List of Notations

Symbol	Definition
\overline{x}	Observed data
z	Latent variables, $z = (z_1, \dots, z_D)$
D	Dimensionality of the latent space
$\pi(z_i)$	Set of parent variables for z_i in a hierarchical model
$f_i(\cdot)$	Prior mean function for z_i , i.e., $z_i \sim \mathcal{N}(f_i(\pi(z_i)), \cdot)$
$g_i(\cdot)$	Prior standard deviation function for z_i , i.e., $z_i \sim \mathcal{N}(\cdot, g_i(\pi(z_i)))$
ϵ	Base noise variable, typically $\epsilon \sim \mathcal{N}(0, I)$
$T_{\text{NCP}}(\cdot)$	Non-Centered Parameterization transformation
$ ilde{z}$	Auxiliary base variable in VIP/NCP, $z = T(\tilde{z})$
λ_i	Partial non-centering parameter for z_i in VIP, $\lambda_i \in [0,1]$
$T_{\mathrm{VIP}}(\cdot)$	VIP transformation
$T_A(\cdot)$	Affine transformation, e.g., $\mu + L\epsilon$ for a Gaussian
$m_i(\cdot)$	Shift function for z_i in an autoregressive flow
$s_i(\cdot)$	Scale function for z_i in an autoregressive flow
$t_i(\cdot)$	Translation function for ϵ_i in GFAF/MIF
u_i	Input to conditioning networks in MIF: $[z_{1:i-1}, f_i(\pi(z_i)), g_i(\pi(z_i))]$

B Algorithm

Algorithm 2 details the procedure for generating a sample z from the variational distribution $q_{w, \rm VIP}(z)$ and then evaluating its corresponding log-density.

Algorithm 2 Sampling from and Evaluating $q_{w,VIP}(z)$

```
Input: Parameters w of the base distribution q_w(\tilde{z}); VIP parameters \lambda_1, \ldots, \lambda_D; model prior functions f_i(\cdot), g_i(\cdot), and parent dependencies \pi(\cdot); dimensionality D; a topological ordering for z_1, \ldots, z_D.
```

- 1: Sample $\tilde{z} \sim q_w(\tilde{z})$
- 2: $\log J \leftarrow 0$
- 3: **for** i = 1, ..., D **do**
- 4: $z_i \leftarrow f_i(\pi(z_i)) + g_i(\pi(z_i))^{1-\lambda_i} (\tilde{z}_i \lambda_i f_i(\pi(z_i)))$
- 5: $\log J \leftarrow \log J + (1 \lambda_i) \log g_i(\pi(z_i))$
- 6: end for
- 7: $\log q_{w,\text{VIP}}(z) \leftarrow \log q_w(\tilde{z}) \log J$
- 8: **return z**, $\log q_{w,\text{VIP}}(z)$

C Proof

Lemma 7. The affine transformation T_A from full-rank VI can be represented as an affine forward autoregressive flow with

$$m_i(z_{1:i-1}) = \mu_i + L_{i,1:i-1} L_{1:i-1,1:i-1}^{-1} \Big(z_{1:i-1} - \mu_{1:i-1} \Big),$$
$$\log s_i(z_{1:i-1}) = \log L_{ii}.$$

Proof. We begin by expressing the affine transformation $T_A(\epsilon) = \mu + L\epsilon$ in a coordinate-wise form:

$$z_i = \mu_i + L_{ii}\epsilon_i + \sum_{j=1}^{i-1} L_{ij}\epsilon_j, \quad i = 1, \dots, D.$$
 (C.1)

For any forward autoregressive flow to be equivalent to this transformation, we need to derive appropriate functions $m_i(\cdot)$ and $s_i(\cdot)$ such that $z_i = m_i(z_{1:i-1}) + s_i(z_{1:i-1})\epsilon_i$ for each i.

First, observe that for any $i \ge 1$, the variables $z_{1:i-1}$ depend only on $\epsilon_{1:i-1}$ due to the lower-triangular structure of L. Since $L_{1:i-1,1:i-1}$ is a lower-triangular submatrix with positive diagonal entries (as L is a Cholesky factor), it is invertible. Thus, we can solve for $\epsilon_{1:i-1}$ in terms of $z_{1:i-1}$:

$$\epsilon_{1:i-1} = L_{1:i-1,1:i-1}^{-1}(z_{1:i-1} - \mu_{1:i-1}).$$
 (C.2)

Now, substituting this expression into our original coordinate-wise equation:

$$z_i = \mu_i + L_{ii}\epsilon_i + \sum_{j=1}^{i-1} L_{ij}\epsilon_j \tag{C.3}$$

$$= \mu_i + L_{ii}\epsilon_i + L_{i:1:i-1}\epsilon_{1:i-1} \tag{C.4}$$

$$= \mu_i + L_{ii}\epsilon_i + L_{i,1:i-1}L_{1:i-1,1:i-1}^{-1}(z_{1:i-1} - \mu_{1:i-1})$$
 (C.5)

This naturally suggests defining:

$$m_i(z_{1:i-1}) = \mu_i + L_{i,1:i-1}L_{1:i-1,1:i-1}^{-1}(z_{1:i-1} - \mu_{1:i-1}),$$
 (C.6)

$$s_i(z_{1:i-1}) = L_{ii}.$$
 (C.7)

With these definitions, the forward autoregressive flow transformation becomes:

$$z_i = m_i(z_{1:i-1}) + s_i(z_{1:i-1})\epsilon_i, \tag{C.8}$$

which is identical to our coordinate-wise expansion of the affine transformation T_A . Since this holds for all $i=1,\ldots,D$, we have shown that the full-rank VI affine transformation can be exactly represented as a forward autoregressive flow with the specified shift and scale functions.

Note that $m_i(z_{1:i-1})$ is an affine function of $z_{1:i-1}$, and $s_i(z_{1:i-1})$ is a constant function, confirming that this is indeed an affine forward autoregressive flow.

Theorem 4. Let $T = T_{VIP} \circ T_A$ where T_{VIP} is the VIP transformation (Definition 1) and T_A is the affine transformation from full-rank Gaussian. If f_i and $\log g_i$ in the hierarchical Bayesian model (Equation (2.2)) are arbitrary continuous functions, and the parent nodes $\pi(z_i)$ are a subset of the preceding variables $z_{1:i-1}$ (respecting the causal dependency structure of the model), then T can be represented as an affine generalized forward autoregressive flow with

$$m_i(z_{1:i-1}) = f_i(\pi(z_i)),$$
 (3.7)

$$\log s_i(z_{1:i-1}) = \log L_{ii} + (1 - \lambda_i) \log g_i(\pi(z_i)), \tag{3.8}$$

$$t_i(\epsilon_{1:i-1}, z_{1:i-1}) = \frac{1}{L_{ii}} \left(\lambda_i f_i(\pi(z_i)) - \mu_i - L_{i,1:i-1} \epsilon_{1:i-1} \right)$$
(3.9)

Proof. The affine transformation T_A is defined as $T_A(\epsilon) = \mu + L\epsilon$, where μ is the mean vector and L is a lower-triangular matrix with positive diagonal elements. In coordinate form, this gives us

$$\tilde{z}_i = \mu_i + L_{ii}\epsilon_i + \sum_{j=1}^{i-1} L_{ij}\epsilon_j, \tag{C.9}$$

where \tilde{z}_i denotes the intermediate result after applying T_A but before applying T_{λ} .

Now, the VIP transformation T_{λ} is defined in Definition 1 as

$$z_{i} = f_{i}(\pi(z_{i})) + g_{i}(\pi(z_{i}))^{1-\lambda_{i}} (\tilde{z}_{i} - \lambda_{i} f_{i}(\pi(z_{i}))),$$
 (C.10)

where \tilde{z}_i is the output of T_A . Substituting, we get

$$z_i = f_i(\pi(z_i)) + g_i(\pi(z_i))^{1-\lambda_i} \left(\tilde{z}_i - \lambda_i f_i(\pi(z_i))\right)$$
(C.11)

$$= f_i(\pi(z_i)) + g_i(\pi(z_i))^{1-\lambda_i} \left(\mu_i + L_{ii}\epsilon_i + \sum_{j=1}^{i-1} L_{ij}\epsilon_j - \lambda_i f_i(\pi(z_i))\right)$$
(C.12)

From our assumption that $\pi(z_i) \subset z_{1:i-1}$, we know that $f_i(\pi(z_i))$ and $g_i(\pi(z_i))$ are functions of only the preceding variables $z_{1:i-1}$.

To express this in the form of a generalized forward autoregressive flow, we need functions m_i , s_i , and t_i such that:

$$z_i = m_i(z_{1:i-1}) + s_i(z_{1:i-1}) \left(\epsilon_i - t_i(\epsilon_{1:i-1}, z_{1:i-1}) \right)$$
(C.13)

Let's rearrange our expression for z_i to match this form:

$$z_{i} = f_{i}(\pi(z_{i})) + g_{i}(\pi(z_{i}))^{1-\lambda_{i}} \left(\mu_{i} + L_{ii}\epsilon_{i} + \sum_{j=1}^{i-1} L_{ij}\epsilon_{j} - \lambda_{i}f_{i}(\pi(z_{i}))\right)$$
(C.14)

$$= f_i(\pi(z_i)) + g_i(\pi(z_i))^{1-\lambda_i} L_{ii} \left(\epsilon_i - \frac{1}{L_{ii}} \left(-\mu_i - \sum_{j=1}^{i-1} L_{ij} \epsilon_j + \lambda_i f_i(\pi(z_i)) \right) \right)$$
 (C.15)

By identifying terms, we can define:

$$m_i(z_{1:i-1}) = f_i(\pi(z_i)),$$
 (C.16)

$$\log s_i(z_{1:i-1}) = \log L_{ii} + (1 - \lambda_i) \log g_i(\pi(z_i)), \tag{C.17}$$

$$t_i(\epsilon_{1:i-1}, z_{1:i-1}) = \frac{1}{L_{ii}} \left(\lambda_i f_i(\pi(z_i)) - \mu_i - L_{i,1:i-1} \epsilon_{1:i-1} \right)$$
 (C.18)

Thus, we have shown that the composite transformation $T = T_{\lambda} \circ T_{A}$ can be represented as a generalized forward autoregressive flow with the specified functions m_{i} , s_{i} , and t_{i} , which completes the proof.

Corollary 6. Let $T = T_{\text{VIP}} \circ T_A$ where T_{VIP} is the VIP transformation (see Definition 1) and T_A is the affine transformation from full-rank Gaussian. If f_i and $\log g_i$ in the hierarchical Bayesian model (see Equation (2.2)) are affine functions, then T can be represented as an affine generalized forward autoregressive flow.

Proof. This result follows directly from Theorem 4, which established that the composite transformation $T = T_{\rm VIP} \circ T_A$ can be represented as a generalized forward autoregressive flow with specific functions m_i , s_i , and t_i . We now show that when f_i and $\log g_i$ are affine functions, all components of this flow become affine, reducing it to a standard affine forward autoregressive flow.

Since f_i and $\log g_i$ are affine functions, we can express them as

$$f_i(z_{1:i-1}) = a_i + b_i^{\mathsf{T}} z_{1:i-1},$$
 (C.19)

$$\log g_i(z_{1:i-1}) = c_i + d_i^{\top} z_{1:i-1}, \tag{C.20}$$

where a_i , c_i are scalar constants and b_i , d_i are vectors of appropriate dimensions.

From Theorem 4, we have

$$m_i(z_{1:i-1}) = f_i(z_{1:i-1}) = a_i + b_i^{\mathsf{T}} z_{1:i-1},$$
 (C.21)

$$\log s_i(z_{1:i-1}) = \log L_{ii} + (1 - \lambda_i) \log g_i(z_{1:i-1})$$
(C.22)

$$= \log L_{ii} + (1 - \lambda_i)(c_i + d_i^{\top} z_{1:i-1}), \tag{C.23}$$

$$t_i(\epsilon_{1:i-1}, z_{1:i-1}) = \frac{1}{L_{ii}} \left(-\mu_i - L_{i,1:i-1} \epsilon_{1:i-1} + \lambda_i f_i(z_{1:i-1}) \right)$$
 (C.24)

$$= \frac{1}{L_{ii}} \left(-\mu_i - L_{i,1:i-1} \,\epsilon_{1:i-1} + \lambda_i (a_i + b_i^{\top} z_{1:i-1}) \right) \tag{C.25}$$

$$= \frac{1}{L_{ii}}(-\mu_i + \lambda_i a_i) - \frac{1}{L_{ii}}L_{i,1:i-1} \epsilon_{1:i-1} + \frac{\lambda_i}{L_{ii}}b_i^{\top} z_{1:i-1}$$
 (C.26)

Clearly, $m_i(z_{1:i-1})$ is an affine function of $z_{1:i-1}$, and $\log s_i(z_{1:i-1})$ is also an affine function of $z_{1:i-1}$. Furthermore, $t_i(\epsilon_{1:i-1}, z_{1:i-1})$ is an affine function of both $\epsilon_{1:i-1}$ and $z_{1:i-1}$.

Since m_i , $\log s_i$, and t_i are all affine functions of their respective inputs, this formulation constitutes an affine generalized forward autoregressive flow.

D **Experimental Details**

All experiments were run on a single server with an Intel Xeon Platinum 8352Y CPU (128 hardware threads at 2.20 GHz), 512 GiB of RAM. For each experiment (i.e., each training or evaluation run), we used one NVIDIA A100 (40 GiB) under CUDA 12.8.

D.1 Models

Eight Schools The Eight Schools model [39] estimates treatment effects θ_i for $N_{\text{schools}} = 8$ schools, $\begin{array}{ll} \mu \sim \mathcal{N}\left(0,5\right) & \log \tau \sim \mathcal{N}(0,5) \\ \theta_i \sim \mathcal{N}(\mu, \exp(\log \tau)) & y_i \sim \mathcal{N}(\theta_i, \sigma_i), \quad i = 1, \dots, N_{\text{schools}}. \end{array}$ Latent variables: $z = (\mu, \log \tau, \theta_1, \dots, \theta_{N_{\text{schools}}}).$ given observed effects y_i and known standard errors σ_i .

$$\mu \sim \mathcal{N}(0,5)$$
 $\log \tau \sim \mathcal{N}(0,5)$ (D.1)

$$\theta_i \sim \mathcal{N}(\mu, \exp(\log \tau))$$
 $y_i \sim \mathcal{N}(\theta_i, \sigma_i), \quad i = 1, \dots, N_{\text{schools}}.$ (D.2)

German Credit A logistic regression model [17] with $N_{\text{features}} = K$ predictors x_{nk} for N_{obs} individuals, predicting binary outcomes y_n . It uses hierarchical priors on coefficient scales τ_k .

$$\log \tau_0 \sim \mathcal{N}(0, 10) \tag{D.3}$$

$$\log \tau_k \sim \mathcal{N}(\log \tau_0, 1), \qquad k = 1, \dots, K \tag{D.4}$$

$$\beta_k \sim \mathcal{N}(0, \exp(\log \tau_k)), \qquad k = 1, \dots, K$$
 (D.5)

$$\eta_n = \sum_{k=1}^K \beta_k x_{nk}, \qquad n = 1, \dots, N_{\text{obs}}$$
 (D.6)

$$y_n \sim \text{Bernoulli}(1/(1 + \exp(-\eta_n))), \qquad n = 1, \dots, N_{\text{obs}}.$$
 (D.7)

Latent variables: $z = (\log \tau_0, \{\log \tau_k\}_{k=1}^K, \{\beta_k\}_{k=1}^K).$

Funnel Neal's Funnel distribution [33] in D = 10 dimensions for $\mathbf{x} = (x_1, \dots, x_D)$.

$$x_1 \sim \mathcal{N}(0,3) \tag{D.8}$$

$$x_k \sim \mathcal{N}(0, \exp(x_1/2)), \quad k = 2, \dots, D.$$
 (D.9)

All variables x_1, \ldots, x_D are latent. (The variance for x_1 is $3^2 = 9$; the variance for $x_k, k \ge 2$ is $\exp(x_1)$.)

Radon A hierarchical linear regression [17] modeling log-radon levels $\log r_i$ in N_{homes} homes. Data includes x_i (floor indicator for home j), u_k (uranium reading for county k), and c_i (county for home j). Priors are inferred from the provided code structure.

$$\mu_0 \sim \mathcal{N}(0,1) \tag{D.10}$$

$$a \sim \mathcal{N}(0,1) \tag{D.11}$$

$$b \sim \mathcal{N}(0,1) \tag{D.12}$$

$$\log \sigma_{m_k} \sim \mathcal{N}(0, 10), \qquad k = 1, \dots, N_{\text{counties}}$$
 (D.13)

$$\log \sigma_y \sim \mathcal{N}(0, 10) \tag{D.14}$$

$$m_k \sim \mathcal{N}(\mu_0 + a \cdot u_k, \exp(\log \sigma_{m_k})), \qquad k = 1, \dots, N_{\text{counties}}$$
 (D.15)

$$m_k \sim \mathcal{N}(\mu_0 + a \cdot u_k, \exp(\log \sigma_{m_k})),$$
 $k = 1, \dots, N_{\text{counties}}$ (D.15)
 $\log r_j \sim \mathcal{N}(m_{c_j} + b \cdot x_j, \exp(\log \sigma_y)),$ $j = 1, \dots, N_{\text{homes}}.$ (D.16)

Latent variables: $z = (\mu_0, a, b, \{\log \sigma_{m_k}\}_{k=1}^{N_{\text{counties}}}, \log \sigma_y, \{m_k\}_{k=1}^{N_{\text{counties}}}).$

Movielens The Movielens model [21] is a hierarchical logistic regression for predicting movie ratings. Each rating n is given by a user $u_n \in \{1, \dots, M\}$ for a movie described by a binary attribute vector $\mathbf{x}_n \in \{0,1\}^D$ (with D=18 attributes). The rating is $y_n \in \{0,1\}$.

Each user m has an attribute preference vector $Z_m = (Z_{m,1}, \dots, Z_{m,D}) \in \mathbb{R}^D$. The model is:

$$\mu_j \sim \mathcal{N}(0,1), \qquad j = 1, \dots, D$$
 (D.17)

$$\lambda_i \sim \mathcal{N}(0,1), \qquad j = 1, \dots, D$$
 (D.18)

$$Z_{m,j} \sim \mathcal{N}(\mu_j, \exp(\lambda_j)),$$
 $m = 1, \dots, M; j = 1, \dots, D$ (D.19)

$$y_n \sim \text{Bernoulli (sigmoid } (\mathbf{x}_n^\top Z_{u_n})), \qquad n = 1, \dots, N.$$
 (D.20)

Here, μ_j is the mean preference for attribute j across users, and λ_j is the log standard deviation of preferences for attribute j. Latent variables: $z = (\{\mu_j\}_{j=1}^D, \{\lambda_j\}_{j=1}^D, \{Z_{m,j}\}_{m=1,j=1}^{M,D})$.

IRT The Item Response Theory (IRT) two-parameter logistic (2PL) model [30] is used to model student responses to test items. Let N_S be the number of students, N_Q be the number of questions (items), and N_R be the total number of responses. For each response r, s_r is the student ID and q_r is the question ID.

$$\alpha_s \sim \mathcal{N}(0, 1), \qquad s = 1, \dots, N_S$$
 (D.21)

$$\mu_{\beta} \sim \mathcal{N}(0,1)$$
 (D.22)

$$\log \sigma_{\beta} \sim \mathcal{N}(0, 1) \tag{D.23}$$

$$\log \sigma_{\gamma} \sim \mathcal{N}(0, 1) \tag{D.24}$$

$$\beta_q \sim \mathcal{N}(\mu_\beta, \exp(\log \sigma_\beta)), \qquad q = 1, \dots, N_Q$$
 (D.25)

$$\log \gamma_q \sim \mathcal{N}(0, \exp(\log \sigma_\gamma)), \qquad q = 1, \dots, N_Q \qquad (D.26)$$

$$\operatorname{logit}_{r} = \exp(\log \gamma_{q_r}) \alpha_{s_r} + \beta_{q_r}, \qquad r = 1, \dots, N_R$$
 (D.27)

$$y_r \sim \text{Bernoulli}(\text{sigmoid}(\text{logit}_r)), \qquad r = 1, \dots, N_R.$$
 (D.28)

Here, α_s is the ability of student s, β_q is the easiness of question q, and $\exp(\log \gamma_q)$ is its discrimination. Latent variables: $z = (\{\alpha_s\}_{s=1}^{N_S}, \mu_\beta, \log \sigma_\beta, \log \sigma_\gamma, \{\beta_q\}_{q=1}^{N_Q}, \{\log \gamma_q\}_{q=1}^{N_Q}).$

Seeds The Seeds model [13] is a random effects logistic regression for analyzing seed germination data. It models the number of germinated seeds r_i out of N_i seeds in G = 21 experimental groups, using group-specific predictors $x_{1,i}$ and $x_{2,i}$.

$$\tau \sim \text{Gamma}(0.01, 0.01) \tag{D.29}$$

$$a_0, a_1, a_2, a_{12} \sim \mathcal{N}(0, 10)$$
 (D.30)

$$b_i \sim \mathcal{N}\left(0, 1/\sqrt{\tau}\right), \qquad i = 1, \dots, G$$
 (D.31)

$$\eta_i = a_0 + a_1 x_{1,i} + a_2 x_{2,i} + a_{12} x_{1,i} x_{2,i} + b_i, \qquad i = 1, \dots, G$$
(D.32)

$$r_i \sim \text{Binomial}(N_i, \text{sigmoid}(\eta_i)), \qquad i = 1, \dots, G.$$
 (D.33)

Here, $x_{1,i}$ and $x_{2,i}$ are indicator variables for experimental conditions (e.g., seed type and root extract). τ is the precision for the random effects b_i . Latent variables: $z=(\tau,a_0,a_1,a_2,a_{12},\{b_i\}_{i=1}^G)$.

Sonar The Sonar model [20] is a Bayesian logistic regression. It uses D = 61 features/coefficients \mathbf{x} to classify N = 208 sonar returns u_i into two categories $y_i \in \{0, 1\}$ (e.g., mines vs. rocks).

$$\mathbf{x} \sim \mathcal{N}\left(\mathbf{0}, \sigma_x^2 I_D\right) \tag{D.34}$$

$$y_i \sim \text{Bernoulli (sigmoid } (\mathbf{x}^\top u_i)), \quad i = 1, \dots, N.$$
 (D.35)

Here, $u_i \in \mathbb{R}^D$ is the feature vector for the *i*-th observation, I_D is the $D \times D$ identity matrix, and σ_x^2 is a predefined prior variance for the coefficients \mathbf{x} . The latent variables are $z = (\mathbf{x})$.

Ionosphere The Ionosphere model [40] is a Bayesian logistic regression. It uses D=35 features/coefficients \mathbf{x} to classify N=351 radar returns u_i from the ionosphere into two categories $y_i \in \{0,1\}$.

$$\mathbf{x} \sim \mathcal{N}\left(\mathbf{0}, \sigma_x^2 I_D\right) \tag{D.36}$$

$$y_i \sim \text{Bernoulli}\left(\text{sigmoid}\left(\mathbf{x}^{\top}u_i\right)\right), \quad i = 1, \dots, N.$$
 (D.37)

Here, $u_i \in \mathbb{R}^D$ is the feature vector for the *i*-th observation, I_D is the $D \times D$ identity matrix, and σ_x^2 is a predefined prior variance for the coefficients \mathbf{x} . The latent variables are $z = (\mathbf{x})$.

D.2 Implementation Details

The conditioning networks for the shift (m_i) , log-scale $(\log s_i)$, and translation (t_i) , for MIF and its variants) terms in both forward autoregressive flows (FAF) and inverse autoregressive flows (IAF) are constructed as follows, depending on the experimental context.

For **affine flows**, such as those used in the ablation studies in Section 5.3, each conditioning network (for m_i , $\log s_i$, or t_i) consists of a single linear layer. This layer directly maps the conditioning inputs to the required output parameters.

For flows requiring greater representational capacity, specifically in experiments evaluating network expressiveness (Figure 2) and for the comprehensive benchmarks (Table 3), the conditioning networks are implemented using a **two-component MLP-based architecture**. Each parameter $(m_i, \log s_i, \text{ or } t_i)$ is computed by summing the outputs of two parallel components, both of which operate on the same input conditioning variables:

- 1. A **linear component**: This is a direct linear transformation of the inputs, identical in architecture to the conditioners used in the affine flows.
- 2. An **MLP component**: This is a multi-layer perceptron (MLP) featuring a single hidden layer with ReLU activation functions, followed by a linear output layer. The size of the hidden layer (number of hidden units) is varied in experiments that assess the impact of network capacity (e.g., from 2⁰ to 2¹⁰ as illustrated in Figure 2).

The final value for m_i , $\log s_i$, or t_i is the sum of the outputs derived from these linear and MLP components.

For experiments involving baseline models from Blessing et al. [10], we utilized the implementations provided in their publicly available code repository to ensure consistency and fair comparison.

Table 6: Training time comparisons (seconds) between the default *Model-Informed Flow* (MIF) and a variant that conditions on the base noise ("MIF with ϵ ").

Model	D	Hidden Units	MIF (s)	MIF with ϵ (s)
		0	17.06	13.88
		64	28.40	23.22
Eight Schools	10	256	28.04	22.18
-		512	28.21	22.03
		1024	30.30	22.61
		0	18.23	14.70
		64	27.38	23.16
Funnel	10	256	27.04	22.42
		512	28.57	22.30
		1024	30.77	22.69
		0	63.81	16.06
		64	148.73	27.81
German Credit	125	256	208.44	54.92
		512	275.74	93.26
		1024	417.05	173.51
		0	84.25	15.78
		64	238.04	37.32
Radon	174	256	331.24	94.82
		512	453.70	168.28
		1024	699.73	338.63
		0	72.26	17.59
		64	196.64	33.15
IRT	143	256	253.17	67.95
		512	457.56	119.95
		1024	516.98	222.65
		0	458.28	28.97
		64	1981.14	384.45
MovieLens	882	256	4847.23	1387.64
		512	8634.91	3156.82
		1024	15873.45	6749.33

D.3 Training Time Comparisons

We report wall-clock training times (in seconds) across six benchmarks and varying hidden sizes. Table 6 compares our default Model-Informed Flow (MIF) against a variant that conditions on the base noise ("MIF with ϵ "), while Table 7 ablates the number of conditioning subnetworks: "3 networks" uses (m,s,t) and "2 networks (no t)" uses only (m,s). Overall, "MIF with ϵ " is consistently faster than the default MIF at comparable capacities, and removing the translation network (t) yields additional speedups with similar trends across datasets. We use D to denote latent dimensionality.

Table 7: Ablation on the number of conditioning subnetworks (seconds). "3 networks" uses shift, scale, and translation (m, s, t). "2 networks (no t)" removes the translation network and uses only (m, s) under the same training setup.

Model	D	Hidden Units	3 Networks (s)	2 Networks (no t) (s)
		0	17.06	16.98
		64	28.40	24.13
Eight Schools	10	256	28.04	24.81
		512	28.21	25.80
		1024	30.30	25.76
		0	18.23	18.63
		64	27.38	25.89
Funnel	10	256	27.04	25.85
		512	28.57	26.27
		1024	30.77	26.01
		0	63.81	52.68
		64	148.73	115.39
German Credit	125	256	208.44	139.90
		512	275.74	175.94
		1024	417.05	258.98
		0	84.25	77.52
		64	238.04	220.17
Radon	174	256	331.24	306.44
		512	453.70	419.42
		1024	699.73	647.75
		0	72.26	66.73
		64	196.64	181.92
IRT	143	256	253.17	234.43
		512	457.56	423.00
		1024	516.98	478.45
		0	458.28	423.65
MovieLens		64	1981.14	1832.85
	882	256	4847.23	4486.69
		512	8634.91	7992.34
		1024	15873.45	14687.99