Amortized Variational Inference: When and Why?

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Abstract

Amortized variational inference (A-VI) is a method for approximating the intractable posterior distributions that arise in probabilistic models. The defining feature of A-VI is that it learns a global inference function that maps each observation to its local latent variable's approximate posterior. This stands in contrast to the more classical factorized (or mean-field) variational inference (F-VI), which directly learns the parameters of the approximating distribution for each latent variable. In deep generative models, A-VI is used as a computational trick to speed up inference for local latent variables. In this paper, we study A-VI as a general alternative to F-VI for approximate posterior inference. A-VI cannot produce an approximation with a lower Kullback-Leibler divergence than F-VI's optimal solution, because the amortized family is a subset of the factorized family. Thus a central theoretical problem is to characterize when A-VI still attains F-VI's optimal solution. We derive conditions on both the model and the inference function under which A-VI can theoretically achieve F-VI's optimum. We show that for a broad class of hierarchical models, including deep generative models, it is possible to close the gap between A-VI and F-VI. Further, for an even broader class of models, we establish when and how to expand the domain of the inference function to make amortization a feasible strategy. Finally, we prove that for certain models—including hidden Markov models and Gaussian processes—A-VI cannot match F-VI's solution, no matter how expressive the inference function is. We also study A-VI empirically. On several examples, we corroborate our theoretical results and investigate the performance of A-VI when varying the complexity of the inference function. When the gap between A-VI and F-VI can be closed, we find that the required complexity of the function need not scale with the number of observations, and that A-VI often converges faster than F-VI.

1 Introduction

A latent variable model is a probabilistic model of observations $\mathbf{x} = x_{1:N}$ with local latent variables $\mathbf{z} = z_{1:N}$ and global latent parameters θ . Consider the model where the joint distribution factorizes as

$$p(\theta, \mathbf{z}, \mathbf{x}) = p(\theta) \prod_{n=1}^{N} p(z_n) p(x_n \mid z_n, \theta),$$
 (1)

and where $p(z_n)$ and $p(x_n \mid z_n, \theta)$ have the same distributional forms for all n. This factorization underlies many probabilistic models, including probabilistic principal component analysis [5, 21, 28] and deep generative models [17, 24, 29]. More generally Eq. 1 characterizes a *simple hierarchical model* [1], a subclass of Bayesian hierarchical models [8, 22] with a factorized prior on z.

With a model in Eq. 1 and an observed dataset \mathbf{x} , the central computational problem is to approximate the posterior distribution of the latent variables $p(\theta, \mathbf{z} \mid \mathbf{x})$. For most models of interest, however, the posterior is intractable to compute exactly. While there are many approaches to tackle this problem, this paper focuses on *variational inference* (VI) [4, 7, 13, 31].

Preprint. Under review.

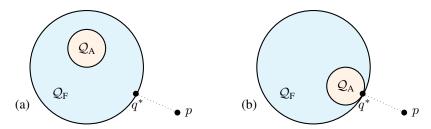


Figure 1: Ordering of the variational families. The variational family Q_A for A-VI is a subset of the variational family Q_F for F-VI. (a) In general, F-VI can achieve a lower KL-divergence than A-VI. (b) Under certain conditions, however, A-VI may still achieve the same optimal solution q^* as F-VI.

The modus operandi of VI is to set a parameterized family of approximate distributions Q and find the member of the family that minimizes the Kullback-Leibler (KL) divergence between the approximation and the posterior,

$$q^* = \arg\min_{q \in \mathcal{Q}} \mathrm{KL}\left(q(\theta, \mathbf{z}) \mid\mid p(\theta, \mathbf{z} \mid \mathbf{x})\right). \tag{2}$$

The solution to this optimization is then used as a proxy for the exact posterior. (In practice, VI finds a local optimum of this objective.)

To fully specify the VI objective of Eq. 2, we must decide on the variational family Q over which to optimize. Many applications of VI use the *fully factorized family*, also known as the *mean-field family*. It is the set of distributions where each variable is independent,

$$Q_{\mathrm{F}} = \left\{ q : q(\theta, \mathbf{z}) = q_0(\theta) \prod_{n=1}^{N} q_n(z_n) \right\}, \tag{3}$$

where the notation q_n clarifies that there is a separate factor for each latent variable. An algorithm that optimizes Eq. 2 over Q_F is a *factorized variational inference* (F-VI) algorithm.

While the factorized family involves a separate variational factor $q_n(z_n)$ for each latent variable, recent applications of VI have explored the *amortized variational family* [e.g 1, 17, 29]. As for the factorized family, the latent variables are independent. But in the amortized family the variational distribution of the local variable z_n is governed by an *inference function* $f_{\phi}(x_n)$,

$$Q_{\mathcal{A}}(\mathcal{F}) = \left\{ q : q(\theta, \mathbf{z}) = q_0(\theta) \prod_{n=1}^{N} q(z_n; f_{\phi}(x_n)); f_{\phi} \in \mathcal{F} \right\}, \tag{4}$$

where \mathcal{F} denotes a class of inference functions over which we optimize. With this family, optimizing Eq. 2 amounts to fitting $q_0(\theta)$ and the function f_{ϕ} by learning the parameters ϕ . Such an algorithm is called *amortized variational inference* (A-VI).

The canonical application of A-VI is in the *variational autoencoder* (VAE) [17, 29]. A VAE fits a variational posterior to a deep generative model. The model is defined with a low-dimensional latent variable $z_n \in \mathbb{R}^d$ and high-dimensional observations $x_n \in \mathbb{R}^p$. Its joint distribution factorizes as in Eq. 1, where the conditional likelihood $p(x_n \mid z_n, \theta)$ is formed by feeding z_n into a neural network with parameters θ (the "decoder"). To approximate the posterior, a VAE uses A-VI. Its inference function $f_{\phi}(x)$ is also a neural network (the "encoder"), which takes in a data point x_n and returns the parameters to an approximate posterior of its local latent variable $q(z_n; f_{\phi}(x_n))$.

Why use A-VI? In the context of VAEs, the motivation for A-VI is scale [17]. While F-VI requires fitting a separate variational factor q_n for each of the N datapoints, A-VI may be more efficient since what we learn about ϕ is *amortized* across data points. Further, AVI can speed up calculations of held-out likelihoods, since it does not need to refit the local variational factors of the new data. (That said, in this paper we focus on using AVI for posterior inference, rather than for posterior predictive distributions.) There has also been interest in extending A-VI beyond VAEs [9], for example for latent Dirichlet allocation models [27] and other classes of hierarchical models [2]. Here, our goal is to formally study the role of A-VI as a general purpose alternative to F-VI.

Contributions. We first provide an elementary proof that the "amortization gap" is always positive, meaning that the optimal result of F-VI is either as close or closer to the posterior as the optimal result of A-VI. This follows from the fundamental ordering $Q_A(\mathcal{F}) \subseteq Q_F$ for any \mathcal{F} . We then ask:

Under what conditions can A-VI still achieve the same optimal approximation as F-VI? This question amounts to distinguishing two scenarios illustrated in Figure 1. In the first case, $\mathcal{Q}_A(\mathcal{F})$ is a subset of $\mathcal{Q}_A(\mathcal{F})$ and does <u>not</u> contain F-VI's optimal solution; in the second case, $\mathcal{Q}_A(\mathcal{F})$ is still a subset of $\mathcal{Q}_A(\mathcal{F})$, but this time it contains the optimal solution.

We show that the potential for A-VI to achieve F-VI's solution amounts to solving an *amortization* interpolation problem between x_n and the optimal variational factors of F-VI. For a solution to exist, two conditions must be met: (i) the interpolation problem must be well-posed, which is a condition on the model $p(\theta, \mathbf{z}, \mathbf{x})$; and (ii) the class of inference functions \mathcal{F} must be sufficiently expressive, which is a condition on the inference algorithm.

A well-posed interpolation problem requires the existence of a *learnable inference function*, a property which does not hold for all latent variable models. We show that it does hold for simple hierarchical models (Eq. 1), and we discuss how the existence of a learnable function can be understood as a manifestation of partial pooling in hierarchical models [8]. For other models, we show that a learnable inference function exists only if we extend the input of the inference function beyond x_n , thus generalizing our usual notion of amortization. Finally we provide important examples, such as the hidden Markov model and Gaussian process, where a learnable inference function does not exist and so where accurate A-VI is not available.

We then empirically study different classes of inference functions \mathcal{F} , and how their expressivity relates to the performance of A-VI. We find that the number of parameters of the inference function does not need to scale with N for A-VI to achieve F-VI's solution. In contrast, the number of parameters for F-VI scales with N. We demonstrate this phenomenon on an anlyatical example and across several numerical experiments. Furthermore we find that when \mathcal{F} is sufficiently expressive, A-VI often converges faster than F-VI to the optimal solution. Last we examine an example where a learnable inference function exists only if we increase the inference function's domain; accordingly, extending the input of the learning inference function improves the performance of A-VI.

Related work. In the context of VAEs, Cremer et al. [6] studied the difference in the optimal KL-divergence achieved by A-VI and F-VI. Several strategies have been proposed to reduce the so-called amortization gap [10, 14, 15, 18]. The bulk of our analysis consists in understanding when might the gap be null for VAEs and more generally for latent variable models. In cases where the gap cannot be closed, our results provide justification for a more general use of methods such as semi-amortized VI [14, 15].

Much of our work concerns the special case of hierarchical models, which has been extensively studied in the context of VI [1, 3, 11, 12, 25]. Most relevant to our work, Agrawal and Domke [1] studied amortization when using a "branch" approximation, $q(\theta, \mathbf{z}) = q(\theta) \prod_n q_n(z_n \mid \theta)$ [3, 11, 25], and constructed a map $f_{\phi}(\theta, x_n)$ to $q_n(z_n \mid \theta) \approx p(z_n \mid \mathbf{x}, \theta) = p(z_n \mid x_n, \theta)$. In their approach, the inference function takes both θ and x_n as its input. Our work considers the marginal factor $q_n(z_n) \approx p(z_n \mid \mathbf{x}) \neq p(z_n \mid x_n)$, which is obtained after marginalizing out θ and arises when using a fully factorized approximation (Eq. 3). That said, our theoretical analysis allows for the domain of the inference function to be extended and can be applied to the branch approximation.

2 Ordering of the variational families

We first set up some theoretical facts about A-VI and F-VI, and articulate the conditions under which the A-VI solution is as accurate as the F-VI solution. We make no assumptions in this section about the model $p(\theta, \mathbf{z}, \mathbf{x})$, which in general is not a simple hierarchical model (Eq. 1)—for example, the prior on \mathbf{z} may not factorize.

We assume that both families (Eqs. 3 and 4) use the same type of distribution for $q_0(\theta)$ and so we focus on the variational distributions of z_n . For each local latent variable z_n , F-VI assigns a marginal distribution $q_n(z_n\,;\,\nu_n)$ from a parametric family \mathcal{Q}_ℓ with parameter $\nu_n\in\mathcal{N}$. The joint family \mathcal{Q}_F is then defined as the product of marginals $q_0(\theta\,;\,\nu_0)\prod_{n=1}^N q_n(z_n\,;\,\nu_n)$. Minimizing the KL-divergence of Eq. 2 yields the optimal variational parameters $\nu^*=(\nu_0^*,\nu_1^*,\cdots,\nu_N^*)$.

Let \mathcal{X} be the space of x_n . A-VI fits a function $f_{\phi}: \mathcal{X} \to \mathcal{N}$ over a family of inference functions \mathcal{F} parameterized by ϕ . For example, suppose \mathcal{Q}_{ℓ} is a univariate Gaussian. Then we can use a neural network as our inference function which takes in x_n and returns the mean and variance of the approximating Gaussian for z_n . The KL-divergence of Eq. 2 is minimized with respect to the

network's weights. More generally, Q_{ℓ} may be any parametric distribution and the inference function may also be a polynomial, an expansion of basis functions, and more.

The first proposition states that the optimal variational distribution found by A-VI can be no better than the optimal variational distribution found by F-VI, i.e. the amortization gap is always positive.

Proposition 2.1. For any class of inference functions \mathcal{F} , $\mathcal{Q}_A(\mathcal{F})$ is a subset of \mathcal{Q}_F . Hence A-VI cannot achieve a lower KL-divergence than the optimal solution for F-VI, that is

$$\min_{q \in \mathcal{Q}_{A}(\mathcal{F})} KL\left(q(\theta, \mathbf{z}) \mid\mid p(\theta, \mathbf{z} \mid \mathbf{x})\right) \ge \min_{q \in \mathcal{Q}_{F}} KL\left(q(\theta, \mathbf{z}) \mid\mid p(\theta, \mathbf{z} \mid \mathbf{x})\right). \tag{5}$$

Proof. Any distribution in $\mathcal{Q}_A(\mathcal{F})$ can be found in \mathcal{Q}_F by (i) matching $q_0(\theta)$, and (ii) matching the variational parameters ν_n to $f_{\phi}(x_n)$. Thus $\mathcal{Q}_A(\mathcal{F}) \subseteq \mathcal{Q}_F$, and Eq. 5 follows.

We now ask: under what conditions can A-VI achieve the same minimum KL-divergence as F-VI? To do so, A-VI must construct a function from x_n to F-VI's optimal variational factors. This defines the amortization interpolation problem.

Proposition 2.2. Consider a model $p(\theta, \mathbf{z}, \mathbf{x})$ over N observations and latent variables. Suppose that for any $\mathbf{x} = x_{1:N}$ there exists $f_{\phi} \in \mathcal{F}$ which solves the amortization interpolation problem, that is

$$f_{\phi}(x_n) = \nu_n^*, \ \forall n. \tag{6}$$

Then

$$\min_{q \in \mathcal{Q}_{A}(\mathcal{F})} KL\left(q(\theta, \mathbf{z}) \mid\mid p(\theta, \mathbf{z} \mid \mathbf{x})\right) = \min_{q \in \mathcal{Q}_{F}} KL\left(q(\theta, \mathbf{z}) \mid\mid p(\theta, \mathbf{z} \mid \mathbf{x})\right). \tag{7}$$

With this proposition in place, we investigate the following questions:

- 1. Is there a class of inference functions \mathcal{F} that solves the amortization interpolation problem?
- 2. If so, how expressive does \mathcal{F} need to be to contain a solution?

Existing literature, notably on VAEs, has primarily focused on the second question [e.g 6, 15]. However when considering latent variable models more generally, we first need to carefully check that the interpolation problem is well-posed. Indeed if $x_n = x_m$ but $q(z_n; \nu_n^*) \neq q(z_m; \nu_m^*)$, then the interpolation problem does <u>not</u> admit a solution no matter how expressive $\mathcal F$ is. This immediately suggests a condition under which the interpolation problem is solvable.

Proposition 2.3. For a model $p(\theta, \mathbf{z}, \mathbf{x})$, the amortization interpolation problem can be solved if and only if for any $\mathbf{x} = x_{1:N}$ there exists a (dataset-dependent) function $f_{\mathbf{x}} : \mathcal{X} \to N$ such that

$$f_{\mathbf{x}}(x_n) = \nu_n^*, \ \forall n. \tag{8}$$

Proof. Suppose $f_{\mathbf{x}}$ exists. Then $x_n = x_m$ implies $q(z_n; \nu_n^*) = q(z_m; \nu_m^*)$ and the interpolation problem can be solved, for example with a polynomial of degree $\mathcal{O}(N)$. Conversely, suppose the interpolation problem is solvable. Then it must be the case that $x_n = x_m$ implies $q(z_n; \nu_n^*) = q(z_m; \nu_m^*)$ and the function $f_{\mathbf{x}}$ exists.

We call $f_{\mathbf{x}}$ a *learnable inference function* and emphasize that its existence is a property of the model $p(\theta, \mathbf{z}, \mathbf{x})$. In the next section, we will see that the existence of $f_{\mathbf{x}}$ is a verifiable property.

If a learnable inference function exists, we can ask how expressive does \mathcal{F} need to be to solve the amortization interpolation problem. The expressiveness of \mathcal{F} may be measured for example by the degree of the learning polynomials or the width of the learning neural networks. The existence of f_x guarantees that a brute-force approach works, e.g. with polynomials of degree $\mathcal{O}(N)$. But this may be overkill: a less expressive class of inference functions may still solve the interpolation problem. Then A-VI can achieve F-VI's solution even when $\mathcal{Q}_A(\mathcal{F})$ is a much smaller space than \mathcal{Q}_F ; see Figure 1b.

3 When does a learnable inference function exist?

A first step in understanding whether A-VI should be applied to a model is to establish the existence of a learnable inference function. That is we need to check that $x_n = x_m$ implies $\nu_n^* = \nu_m^*$ and moreover that x_n provides all the information we need to distinguish the different factors of $q(z_n; \nu_n^*)$. In this section, we show this for the simple hierarchical model of Eq. 1.

We first present a lemma that characterizes the optimal variational parameters of F-VI for any model. **Lemma 3.1.** (CAVI rule) Consider a probabilistic model $p(\theta, \mathbf{z}, \mathbf{x})$. The optimal solution for F-VI verifies,

$$q(z_n; \nu_n^*) \propto \exp\left\{\mathbb{E}_{q(\theta; \nu_0^*)}\left[\mathbb{E}_{q(\mathbf{z}_{-n}; \nu^*)}\left[\log p(\theta, \mathbf{z}, \mathbf{x})\right]\right]\right\},\tag{9}$$

where $\mathbb{E}_{q(\mathbf{z}_{-n}; \nu^*)}$ is the expectation with respect to all z_j 's except z_n .

Lemma 3.1 comes from the coordinate-ascent VI update rule for F-VI [4, equation 17], which tells us how to choose $q(z_n; \nu_n)$ to minimize the KL-divergence, while maintaining the other factors in the approximating distribution fixed. Applying this rule at the optimal solution gives Lemma 3.1.

The CAVI rule uses the factorization of q but makes no assumption about the model. Applying this rule to the simple hierarchical model, we obtain the following result (details in the Appendix).

Theorem 3.2. Consider the simple hierarchical model $p(\theta, \mathbf{z}, \mathbf{x})$ in Eq. 1. The optimal solution for *F-VI* can be written as a learnable inference function,

$$q(z_n; \nu_n^*) = k_{\mathbf{x}}(x_n) \ p(z_n) \ \exp\left\{ \mathbb{E}_{q(\theta; \nu_0^*)} \left[\log p(x_n \, | \, z_n, \theta) \right] \right\}$$
 (10)

where $k_{\mathbf{x}}(x_n) = \left[\int_{\mathcal{Z}} p(z) \exp\{\mathbb{E}_{q(\theta; \nu_0^*)}[\log p(x_n \mid z, \theta)]\right]^{-1}$ is a normalizing constant.

We emphasize that $q(z_n\,;\,\nu_n^*)$ depends on every element of ${\bf x}$ through the integral with respect to $q(\theta\,;\,\nu_0^*)$. But the right side of Eq. 10 constitutes a learnable dataset-dependent function from x_n to the optimal variational distribution $q(z_n\,;\,\nu_n^*)$. Since a parametric distribution is uniquely defined by its parameter, we also have a map between x_n and ν_n^* . Thus the amortization interpolation problem admits a solution, which can be solved for an expressive enough class of inference functions.

3.1 An illustrative example: linear probabilistic model

So far our discussion has been general but fairly abstract. We now provide a concrete example where the learnable inference function $f_{\mathbf{x}}$ can be written in closed form. Furthermore we find that in this example the inference function f_{ϕ} can solve the amortization interpolation problem by learning $f_{\mathbf{x}}$ with a constant number of variational parameters, no matter how large N is.

Consider the following simple hierarchical model,

$$p(\theta) \propto 1; \ p(z_n) = \text{normal}(0, 1); \ p(x_n \mid z_n, \theta) = \text{normal}(\theta + \tau z, \sigma),$$
 (11)

where $\theta \in \mathbb{R}$, and $\tau \in \mathbb{R}$ and $\sigma \in \mathbb{R}$ are fixed. In our notation, the second argument of normal() is the standard deviation. For this example, FVI's optimal solution can be worked out analytically.

Theorem 3.3. Let $q(z_n; \nu^*)$ be the optimal solution returned by F-VI, when optimizing over the family of Gaussians with a diagonal covariance matrix. Then

$$\mathbb{E}_{q(z_n;\nu_n^*)}(z_n) = \frac{\tau}{\sigma^2 + \tau^2}(x_n - \bar{x}); \ \operatorname{Var}_{q(z_n;\nu^*)}(z_n) = \xi^2, \tag{12}$$

where ξ is a constant with respect to \mathbf{x} .

The proof is in the Appendix. The bulk of the proof is to work out the posterior distribution analytically and show that

$$p(z_n \mid \mathbf{x}) = \text{normal}\left(\frac{\tau}{\sigma^2 + \tau^2}(x_n - \bar{x}), s\right),$$
 (13)

for some constant s. Showing this requires careful manipulations of Gaussian integrals, as well as some linear algebra. Since the posterior is normal, we can then calculate exactly F-VI's optimum [20, 30]. Now the optimal mean is a linear function,

$$\mathbb{E}_{q(z_n; \nu_n^*)}(z_n) = \alpha_0(\mathbf{x}) + \alpha x_n; \ \alpha_0(\mathbf{x}) = -\frac{\tau \bar{x}}{\sigma^2 + \tau^2}; \ \alpha = \frac{\tau}{\sigma^2 + \tau^2}.$$
 (14)

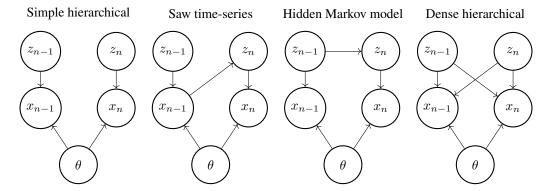


Figure 2: For the simple hierarchical model (Eq. 1), a learnable inference function $f_{\mathbf{x}}: \mathcal{X} \to \mathcal{Q}_{\ell}$ such that $f_{\mathbf{x}}(x_n) = q(z_n; \nu_n^*)$ exists. The saw time-series requires learning a map with two inputs (x_{n-1}, x_n) . For the Hidden Markov and dense hierarchical models, there may not be a learnable inference function. In the dense hierarchical model, there is an edge between every element of \mathbf{z} and every element of \mathbf{x} .

The standard-deviation is simply a constant. For A-VI to match the optimal solution returned by F-VI, we therefore need to learn a linear function for the mean and a constant standard deviation ξ . Hence regardless of the number of observations N, we can achieve F-VI's optimal solution by learning 3 variational parameters.

This example provides intuition behind Theorem 3.2, which connects A-VI to classical ideas in hierarchical Bayesian modeling. In the considered example, the posterior (Eq. 13) demonstrates a key property of hierarchical models, termed *partial pooling* [8]: the posterior mean of z_n depends on both the local observation x_n and, to a lesser degree, on the non-local observations through \bar{x} . Even though $p(z_n \mid \mathbf{x}) \neq p(z_n \mid x_n)$, the posterior density of each latent variable is distinguished by the local influence of x_n , while the global influence of \bar{x} is the same for all latent variables. As a result

$$x_n = x_m \implies p(z_n \mid \mathbf{x}) = p(z_m \mid \mathbf{x}),$$
 (15)

and a learnable inference function exists. More generally the above implication holds for simple hierarchical models (Eq. 1).

3.2 Extension of the analysis to other models

We now examine other models (Figure 2) to highlight that a learnable inference function, $f_x: \mathcal{X} \to N$ may not exist. In one example, we demonstrate that A-VI can attain F-VI's optimal solution if we expand the domain of the inference functions. In another example, we establish that such a strategy is not feasible.

Saw time series. In the "saw" time series, each latent variable z_n depends on the realization of the previous latent variable x_{n-1} . This may be seen as a time series with missing data. The joint is

$$p(\theta, \mathbf{z}, \mathbf{x}) = p(\theta) \prod_{n=1}^{N} p(z_n \mid x_{n-1}) p(x_n \mid z_n, \theta).$$
 (16)

Applying the CAVI rule to this distribution, we get the following result.

Theorem 3.4. For the saw time series model given by Eq. 16, the optimal solution for F-VI is

$$q(z_n; \nu_n^*) = k_{\mathbf{x}}(x_{n-1}, x_n) \ p(z_n \mid x_{n-1}) \exp\left\{ \mathbb{E}_{q(\theta; \nu_0^*)}[\log p(x_n \mid z_n, \theta)] \right\}, \tag{17}$$

where, overloading the notation, k_x is the normalizing constant.

Eq. 17 defines a data-set dependent function from x_{n-1} and x_n to the optimal variational factor. There is no learnable inference function, $f_{\mathbf{x}}: \mathcal{X} \to \mathcal{N}$, however, there exists a learnable function

 $f_{\mathbf{x}}: \mathcal{X} \times \mathcal{X} \to \mathcal{N}$, such that $f_{\mathbf{x}}(x_{n-1}, x_n) = \nu_n^*$ for all n. In this case extending the domain of the inference function ensures the existence of a solution to the amortization interpolation problem.

Hidden Markov model (HMM). We now consider another time series. The joint of the HMM is

$$p(\theta, \mathbf{z}, \mathbf{x}) = p(\theta) \prod_{n=1}^{N} p(z_n \mid z_{n-1}) p(x_n \mid z_n, \theta).$$
(18)

Our next theorem states that there is in general no learnable inference function $f: \mathcal{X} \to \mathcal{Q}_{\ell}$ and furthermore expanding the domain of the inference functions still yields no learnable function.

Theorem 3.5. Consider the HMM of Eq. 18. Let \mathbf{w}_n be a subset of \mathbf{x} . There exist hidden Markov models with no learnable function $f_{\mathbf{x}}: \mathcal{W} \to N$ such that $f_{\mathbf{x}}(\mathbf{w}_n) = \nu_n^*$ for all n.

The proof is obtained by constructing an example, and showing explicitly that even when all the elements of x are equal, the variational parameters take different different values. The details are in the Appendix. Here we provide a conceptual explanation for this result.

In the simple hierarchical and in the saw time series models the existence of a learnable inference function (respectively over \mathcal{X} and $\mathcal{X} \times \mathcal{X}$) is due to the fact that each data point either has a local or a global influence on $q(z_n; \nu_n^*)$. In the case of an HMM, there is no common global influence: any observation x_m will have a different influence on the variational factor for each latent variable z_n . Moreover, each observation is, to a varying degree, local to any latent variable. A similar reasoning can be applied to the dense hierarchical model (Figure 2), an example of which is a Gaussian process model.

We end this section by considering the case where for a particular realization of the data, the elements of $\mathbf x$ are all distinct. We can expect this for continuous data or high-dimensional discrete data (e.g. images). Then, no matter which model $p(\theta, \mathbf z, \mathbf x)$ we use, we can always use brute-force interpolation to obtain $f_{\phi}(x_n) = \nu_n^*$ for instance with a high degree polynomial or a neural network that memorizes a set of input/output pairs. In fact brute-force is likely our only option. Unfortunately such an approach requires using a class of inference functions $\mathcal F$ whose size scales with N, which is computationally expensive and does not align with current practices of A-VI.

4 Numerical experiments

We corroborate our theoretical results on several examples and explore the trade-off between the complexity of the inference function, the quality of the approximation, and the convergence time of the optimization. The code to reproduce the experiments can be found at https://github.com/charlesm93/amortized_vi.

Experimental setup. We cannot compute the KL-divergence and instead maximize the evidence lower-bound (ELBO),

$$\mathbb{E}_{q(\mathbf{z},\theta;\,\nu)}\left[\log p(\theta,\mathbf{z},\mathbf{x}) - \log q(\theta,\mathbf{z})\right]. \tag{19}$$

While this objective function cannot be computed exactly, we estimate it with 100 draws from the current approximation $q(\mathbf{z}, \theta; \nu)$.

We employ the Adam optimizer [16] in PyTorch [23] and use the reparameterization trick to evaluate the gradients. For most examples we use a learning rate of 1e-3. For the VAE examples, we start the learning rate at 1e-4 and progressively reduce the rate. To account for the stochastic nature of the algorithm, we repeat each experiment 10 times. In all experiments, we run a *constant factor algorithm*, which assigns the same factor \bar{q} to each latent variable z_n . The constant factor and F-VI may be seen respectively as the poorest and richest variational families.

Linear probabilistic model. We begin with the analytical example from Section 3.1. We draw θ and z_n from standard normals, and simulate N=10,000 observations. A-VI's inference function is a polynomial of degree d. We require a polynomial of degree d=1 to learn the optimal variational mean, which is a linear function of x_n (Theorem 3.3). Figure 3 shows the optimization paths over 5,000 steps for a single seed and Table 1 summarizes the results over 10 seeds. The final EBLO for each algorithm is estimated by averaging the last 500 ELBO estimations. As expected, A-VI attains the same outcome as F-VI for $d \ge 1$. We also find that A-VI is nearly an order of magnitude faster than F-VI with the best result achieved with d=1.

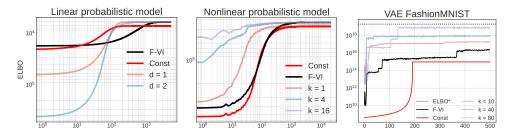


Figure 3: Examples of optimization paths. As benchmarks, we use F-VI and a constant factor algorithm which assigns the same distribution to all $q(z_n)$. A-VI is then run using different classes of inference functions: (left) varying the degree d of a learning polynomial; (middle, right) varying the width k of an inference neural network.

			Conv, $\epsilon = 0.1$	Conv, $\epsilon = 0.01$
Model	Method	Max ELBO	Median (Min, Max)	Median (Min, Max)
Linear	F-VI	-6088	1200 (1110, 2950)	2135 (1960, 4160)
	Const.	-7232	Х	Х
	d = 1	-6088	180 (70, 340)	365 (200, 580)
	d = 2	-6088	395 (100, 620)	700 (190, 900)
Nonlinear	F-VI	-3.240e+4	440 (410, 480)	1280 (1200, 2680)
	k = 1	-3.564e+4	X (540, X)	Х
	k = 2	-3.259e+4	540 (50, X)	X
	k = 4	-3.239e+4	160 (20, X)	1045 (230, X)
	k = 16	-3.240e+4	60 (40, X)	555 (170, X)

Table 1: Experimental results for linear and nonlinear probabilistic models. The results are computed across 10 seeds. The two right most columns give the number of iterations required to achieve convergence to the optimal ELBO (per F-VI's benchmark) within 10% ($\epsilon = 0.1$) or 1% ($\epsilon = 0.01$). An " χ " indicates the algorithm does not attain the optimal ELBO.

Nonlinear probabilistic model. This example is a variation on the previous model, with a nonlinear likelihood,

$$p(x_n \mid z_n, \theta) = \operatorname{normal}(\theta + z_n(1 + \sin(z_n)), \cos(z_n)). \tag{20}$$

The inference function is a neural network with two hidden layers of width k and ReLu activation. A-VI matches F-VI's solution for $k \geq 4$. This time, an overparameterized neural network, e.g. k = 16, yields faster convergence (Table 1). While A-VI typically converges faster than F-VI, we also find instances where A-VI fails to converge after 20,000 iterations even when using an expressive class of inference functions \mathcal{F} . F-VI behaves in a more stable manner.

Deep generative model. Next we consider a VAE on which we perform full Bayesian inference: that is we jointly estimate the posterior distribution for the latent variables \mathbf{z} and for the weights of the decoder θ . The likelihood is a Gaussian with fixed variance and the mean is given by a two-layer neural network of width 40 with a leaky ReLU activation function. We consider two data sets: MNIST [19] and FashionMNIST [32]. To alleviate the computational burden, we use a subset of 10,000 images and run the optimization for 500 steps, with each step using the full data.

We do not believe that Adam maximizes the ELBO in 500 iterations, especially given the non-convex loss functions at hand (Figure 3). This points at a limitation of our theoretical analysis, which focused on the optimal KL-divergence. For many problems, the relevant question is not how far *can* the optimizer go, rather how far does it actually go. As a "silver" benchmark, we run F-VI for another 500 iterations, initialized at the best output obtained with A-VI, which is a semi-amortized approach [15]. We then report the highest achieved ELBO over 10 seeds as ELBO*. We estimate the achieved ELBO by averaging the final 20 steps and report our results in Figure 4. For MNIST, A-VI returns results

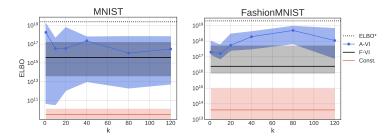


Figure 4: Achieved ELBO after 500 steps for varying widths k of the inference network. The solid line is the median ELBO and the shaded region extends between the minimum and maximum ELBO. (left) For MNIST, a narrow neural network performs as well as F-VI. (right) For FashionMNIST, A-VI consistently outperforms F-VI, with a wider inference network yielding better results.

comparable to F-VI even when using a narrow neural network. In FashionMNIST, A-VI consistently outperforms F-VI with a wider network yielding better results.

Saw time series. In this final example, we explore the benefits of extending the domain of the inference function. We simulate N = 1,000 observations from a saw time series (eq. 16),

$$x_0 = 0$$
; $p(z_n \mid x_{n-1}) = \text{normal}(x_{n-1}, 1)$; $p(x_n \mid z_n) = \text{normal}(\alpha(\theta + z_n), 1)$, (21)

which generates a Markov chain with missing values. Once again, we fit a neural network with two hidden layers of width k. Additionally, we allow the network to either take in x_n or (x_{n-1},x_n) when mapping to $q_n(z_n)$. Only with the expanded output does A-VI attain F-VI's optimum for $k \geq 4$. Using only x_n produces a suboptimal approximation even when using a comparatively wide inference network (e.g. k=20). Figure 5 demonstrates this behavior for one optimization path. Additional experimental results can be found in Appendix.

5 Discussion

In this paper, we derive conditions under which A-VI may achieve the same optimal solution as F-VI. Closing the gap between the two algorithms

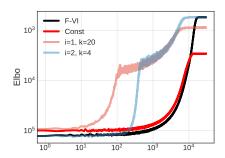


Figure 5: Optimization path for saw time series. When using a single input (i = 1 case), A-VI cannot achieve F-VI's solution even with a relatively broad inference network. The problem is solved by extending the input (i = 2 case).

amounts to solving an amortized interpolation problem (Proposition 2.2). For the interpolation problem to be solvable, the model $p(\theta, \mathbf{z}, \mathbf{x})$ must admit a learnable inference function (Proposition 2.3). We show how to check this condition on several models, notably by using the CAVI rule (Lemma 3.1). We demonstrate the existence of a learnable inference function for simple hierarchical models, which encompasses many canonical models in Machine Learning (Theorem 3.2). When a learnable inference function exists, we empirically find that the number of variational parameters for A-VI does not need to scale with N unlike for F-VI.

A direction for future work is to extend our theoretical analysis to other VI algorithms. An example we already alluded to is the branch factorization [1, 3, 11, 25]. Another interesting case would be to amortize a Gaussian approximation with a dense covariance matrix.

We would also like to better understand the optimization paths induced by different choices of inference functions. When does a more expressive inference class burden the optimization, as seen for the linear probabilistic model, and when does overparameterization lead to more efficient optimization, as in the case of the nonlinear probabilistic model? A more in-depth analysis could help us understand how to choose the class of inference functions, which remains an outstanding tuning parameter for A-VI.

A final direction to pursue is to study how accurate A-VI is when applied to held-out data. We believe the *generalization gap* [7, 26] can also be analyzed by setting up an implicit interpolation problem, this time with constraints to not overfit. More generally understanding the role of A-VI for online learning, i.e. how well can $f_{\phi}(x_{N+1})$ approximate $p(z_n \mid \mathbf{x}, x_{N+1})$, constitutes an interesting research venue.

6 Acknowledgment

We thank Lawrence Saul, Robert Gower, and Justin Domke for helpful discussions, and Achille Nazaret for feedback on this manuscript.

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Appendix

- A Missing proofs for Section 3: "Mapping local variables to the optimal solution of F-VI"
- A.1 Proof of Theorem 3.2: learnable inference function for the simple hierarchical model

Applying the CAVI rule (Lemma 3.1) to Eq. 1,

$$q(z_n; \nu^*) \propto \exp \left\{ \mathbb{E}_{q(\theta; \nu_0^*)} \left[\mathbb{E}_{q(\mathbf{z}_{-n}; \nu^*)} \left[\log p(\theta) + \sum_{j=1}^n \log p(z_j) + \log p(x_j \mid z_j, \theta) \right] \right] \right\}$$

$$\propto \exp \left\{ \mathbb{E}_{q(\theta; \nu_0^*)} \left[\mathbb{E}_{q(\mathbf{z}_{-n}; \nu^*)} \left[\log p(z_n) + \log p(x_n \mid z_n, \theta) \right] \right] \right\}.$$

To obtain the result, note none of the terms inside the expectation depend on \mathbf{z}_{-n} and that we can pull out $\log p(z_n)$ from the expectation with respect to θ .

A.2 Analytical results for the illustrative example

We prove Theorem 3.3, which provides an exact expression for the mean and variance of $q(z_n; \nu^*)$, the optimal solution returned by F-VI when applied to the linear generative model. Recall that in the model of interest, $\theta \in \mathbb{R}$, and we introduce the fixed standard deviations, $\tau \in \mathbb{R}$ and $\sigma \in \mathbb{R}$. Next

$$p(\theta) \propto 1; \ p(z_n) = \text{normal}(0, 1); \ p(x_n) = \text{normal}(\theta + \tau z_n, \sigma).$$
 (22)

Since the posterior distribution, $p(\theta, \mathbf{z} \mid \mathbf{x})$ is normal, $q(z_n; \nu^*)$ can be worked out analytically using the results by [e.g 20, 30]. Specifically,

$$q(z_n; \nu_n^*) = \operatorname{normal}\left(\mu_n, \frac{1}{\left[\Sigma^{-1}\right]_{nn}}\right),\tag{23}$$

where μ_n is the posterior mean for z_n and Σ is the posterior covariance matrix. It remains to find an analytical expression for the posterior distribution.

Lemma A.1. The marginal posterior distribution is given by

$$p(z_n \mid \mathbf{x}) = \text{normal}\left(\frac{\tau}{\sigma^2 + \tau^2}(x_n - \bar{x}), s\right),$$
 (24)

for some s, constant with respect to x.

Proof. From Bayes' rule

$$\log p(\mathbf{z}, \theta \mid \mathbf{x}) = k - \frac{1}{2} \sum_{n=1}^{N} z_n^2 - \frac{1}{2\sigma^2} \sum_{n=1}^{N} (x_n - \theta - \tau z_n)^2$$

$$= k - \frac{1}{2} \sum_{n=1}^{N} z_n^2 - \frac{1}{2\sigma^2} \sum_{n=1}^{N} \theta^2 + (x - \tau z_n)^2 - 2\theta(x_n - \tau z_n)$$

$$= k - \frac{1}{2} \sum_{n=1}^{N} z_n^2 - \frac{1}{2\sigma^2} \left(n\theta^2 + \sum_{n=1}^{N} (x_n - \tau z_n)^2 - 2\theta \sum_{n=1}^{N} (x_n - \tau z_n) \right) (25)$$

where k is a constant with respect to \mathbf{z} and θ . Moving forward, we overload the notation for k to designate any such constant. As expected, Eq. 25 is quadratic in θ and \mathbf{z} .

Remark A.2. At this point, the proof may take two directions: in one, we work out the precision matrix, Φ (i.e. the inverse covariance matrix) for $p(\mathbf{z}, \theta \mid \mathbf{x})$ and invert it to obtain the posterior mean for each z_n . Constructing Φ is straightforward and necessary to show the covariance of $q(z_n; \nu_n^*)$ is constant with respect to \mathbf{x} . However, inverting Φ requires recursively applying the Sherman-Morrison formula three times, which is algebraically tedious. The other direction is to marginalize out θ . We can then construct the precision matrix, Ψ , for $p(\mathbf{z} \mid \mathbf{x})$, which only requires a single application of the Sherman-Morrison formula to invert. We opt for the second direction, noting both options are rather involved.

To marginalize out θ , we complete the square and perform a Gaussian integral,

$$\log p(\mathbf{z}, \theta \mid \mathbf{x}) = k - \frac{1}{2} \sum_{n=1}^{N} z_n^2 - \frac{n}{2\sigma^2} \left[\theta^2 + \frac{1}{n} \sum_{n=1}^{N} (x_n - \tau z_n)^2 - 2\theta \sum_{n=1}^{N} (x_n - \tau z_n) + \left(\frac{1}{n} \sum_{n=1}^{N} (x_n - \tau z_n) \right)^2 - \left(\frac{1}{n} \sum_{n=1}^{N} (x_n - \tau z_n) \right)^2 \right]$$

$$= k - \frac{1}{2} \sum_{n=1}^{N} z_n^2 - \frac{n}{2\sigma^2} \left[\left(\theta - \frac{1}{n} \sum_{n=1}^{N} (x_n - \tau z_n) \right)^2 + \frac{1}{n} \sum_{n=1}^{N} (x_n - \tau z_n)^2 - \left(\frac{1}{n} \sum_{n=1}^{N} (x_n - \tau z_n) \right)^2 \right]$$

$$(26)$$

Then

$$\log p(\mathbf{z} \mid \mathbf{x}) = k - \frac{1}{2} \sum_{n=1}^{N} z_n^2 - \frac{1}{2\sigma^2} \left[\sum_{n=1}^{N} (x_n - \tau z_n)^2 - \frac{1}{n} \left(\sum_{n=1}^{N} (x_n - \tau z_n) \right)^2 \right].$$
 (27)

Expanding the square,

$$\left(\sum_{n=1}^{N} (x_n - \tau z_n)\right)^2 = \sum_{n=1}^{N} (x_n - \tau z_n)^2 + 2\sum_{j \le n} (x_n - \tau z_n)(x_j - \tau z_j). \tag{28}$$

Plugging this in and factoring out τ , we get

$$\log p(\mathbf{z} \mid \mathbf{x}) = k - \frac{1}{2} \sum_{n=1}^{N} z_n^2 - \frac{\tau^2}{2\sigma^2} \left[\sum_{n=1}^{N} \left(1 - \frac{1}{n} \right) \left(\frac{x_n}{\tau} - z_n \right)^2 - \frac{2}{n} \sum_{j < n} \left(\frac{x_n}{\tau} - z_n \right) \left(\frac{x_j}{\tau} - z_j \right) \right]. \tag{29}$$

Now the standard expression for a multivariate Gaussian is

$$\log p(\mathbf{z} \mid \mathbf{x}) = k - \frac{1}{2} (\mathbf{z} - \boldsymbol{\mu})^T \Psi(\mathbf{z} - \boldsymbol{\mu}) = k - \frac{1}{2} \left(\sum_{n=1}^N \Psi_{nn} (z_n - \mu_n)^2 + 2 \sum_{j < n} \Psi_{jn} (z_n - \mu_n) (z_j - \mu_j) \right),$$
(30)

where μ is the mean and Ψ the precision matrix. We solve for the mean and precision matrix by matching the coefficients in the above two expressions for z_n , $z_n z_j$, and z_n^2 , which respectively produce the following equations:

$$\sum_{j=1}^{N} \Psi_{nj} \mu_{j} = \frac{\tau}{\sigma^{2}} (x_{n} - \bar{x})$$
(31)

$$\Psi_{nj} = -\frac{\tau^2}{n\sigma^2}, \ \forall n \neq j$$
 (32)

$$\Psi_{nn} = 1 + \frac{\tau^2}{\sigma^2} \left(1 - \frac{1}{N} \right). \tag{33}$$

This immediately gives us the precision matrix. Eq. 31 may be rewritten in matrix form as

$$\boldsymbol{\mu} = \frac{\tau}{\sigma^2} \Psi^{-1} [\mathbf{x} - \bar{x} \mathbf{1}], \tag{34}$$

where 1 is the N-vector of 1's. Let $\alpha = \Psi_{nj}$, for any $n \neq j$, and $\beta = \Psi_{nn} - \alpha$. Then

$$\Psi = \beta I + \alpha \mathbf{1} \mathbf{1}^T, \tag{35}$$

Applying the Sherman-Morrison formula, we obtain the covariance matrix,

$$\Psi^{-1} = (\beta I + \alpha \mathbf{1} \mathbf{1}^{T})^{-1}$$

$$= \beta^{-1} I - \frac{\beta^{-1} I \alpha \mathbf{1} \mathbf{1}^{T} \beta^{-1} I}{1 + \alpha \mathbf{1}^{T} \beta^{-1} I \mathbf{1}}$$

$$= \beta^{-1} I - \frac{\alpha \beta^{-1}}{\beta + N \alpha} \mathbf{1} \mathbf{1}^{T}.$$
(36)

Notice that Ψ^{-1} does not depend on x and that it's diagonal elements are all equal. Moreover $(\Psi^{-1})_{nn}$ gives us the constant, s. Next let

$$a = \beta^{-1} \frac{\tau}{\sigma^2}; \quad b = -\frac{\alpha \beta^{-1}}{\beta + N\alpha} \frac{\tau}{\sigma^2}.$$
 (37)

Then $\mu = (aI + b\mathbf{1}\mathbf{1}^T)[\mathbf{x} - \bar{x}\mathbf{1}\mathbf{1}^T]$ and moreover

$$\mu_n = a(x_n - \bar{x}) + b \sum_{j=1}^N x_j - \bar{x}$$

$$= a(x_n - \bar{x})$$

$$= \frac{\tau}{\sigma^2} \left(\frac{\tau^2 + \sigma^2}{\sigma^2}\right)^{-1} (x_n - \bar{x})$$

$$= \frac{\tau}{\sigma^2 + \tau^2} (x_n - \bar{x}),$$

as desired.

To complete the proof of Theorem 3.4, we need to show that the variances of $q(z_n; \nu^*)$ is constant with respect to \mathbf{x} ; that they are equal for each z_n follows from the symmetry of the problem. We already constructed the precision matrix, Ψ , for $p(\mathbf{z} \mid \mathbf{x})$, but we actually need to study the full precision matrix, Φ , of $p(\theta, \mathbf{z} \mid \mathbf{x})$. We use the index 0 to denote the columns (or rows) corresponding to θ .

Lemma A.3. The posterior precision matrix, Φ , of $p(\theta, \mathbf{z} \mid \mathbf{x})$ verties

$$\Phi_{00} = \frac{N}{\sigma^2}; \quad \Phi_{0j} = \frac{\tau}{2\sigma^2} \text{ if } j > 0; \quad \Phi_{nn} = 1 + \frac{\tau^2}{\sigma^2} \text{ if } i > 0; \quad \Phi_{nj} = 0, \text{ if } n \neq j.$$
(38)

Crucially, Φ is constant with respect to \mathbf{x} .

Proof. Consider Eq. 25, rewritten here for convenience,

$$\log p(\mathbf{z}, \theta \mid \mathbf{x}) = k - \frac{1}{2} \sum_{n=1}^{N} z_n^2 - \frac{1}{2\sigma^2} \left(N\theta^2 + \sum_{n=1}^{N} (x_n - \tau z_n)^2 - 2\theta \sum_{n=1}^{N} (x_n - \tau z_n) \right).$$

The standard Gaussian form is

$$\log p(\mathbf{z}, \theta \mid \mathbf{x}) = k - \frac{1}{2} \left[\Phi_{00}(\theta - \nu)^2 + \sum_{n=1}^{N} \Phi_{nn}(z_n - \mu_n)^2 + 2 \left(\sum_{j=1}^{N} \Phi_{0j}(\theta - \nu)(z_j - \mu_j) + \sum_{j < n} \Phi_{nj}(z_n - \mu_n)(z_j - \mu_j) \right) \right]. (39)$$

Matching coefficients for θ^2 , θz_j , $z_n z_j$ and z_n^2 , we obtain respectively

$$\Phi_{00} = \frac{N}{\sigma^2}; \ \Phi_{0j} = \frac{\tau}{2\sigma^2} \text{ if } j > 0; \ \Phi_{nn} = 1 + \frac{\tau^2}{\sigma^2} \text{ if } n > 0; \ \Phi_{nj} = 0, \text{ if } n \neq j.$$

The variance of $q(z_n; \nu^*)$ is obtained by inverting the diagonal elements of Φ . By symmetry, $\operatorname{Var}_{q^*}(z_n) = \xi \ \forall n$, where ξ is a constant which does not depend on \mathbf{x} . This completes the proof of Theorem 3.4.

A.3 Proof of Theorem 3.5: non-existence of a learnable inference function for hidden Markov models

Before stating the proof, let us quickly examine why the proof used for the simple hierarchical model does not work here. This time when applying the CAVI rule (Lemma 3.1) to the hidden Markov model, we get

$$q(z_n; \nu_n^*) \propto \exp\left\{\mathbb{E}_{q(\theta; \nu_0^*)} \log p(x_n \mid z_n, \theta) + \mathbb{E}_{q(z_{n-1}; \nu^*)} \log p(z_n \mid z_{n-1}) + \mathbb{E}_{q(z_{n+1}; \nu^*)} \log p(z_{n+1} \mid z_n)\right\}.$$

Because the prior on \mathbf{z} does not factorize, we pick up two additional terms through $p(z_n \mid z_{n-1})$ and $p(z_{n+1} \mid z_n)$, which prevents us from finishing the proof as we did in Section A.1. Nonetheless we should be mindful that the above does not immediately give us counter-example in which a learnable inference function does not exist.

Now to the proof. Our strategy is to construct an example for which the optimal F-VI solution (using a factorized Gaussian approximation) can be written in a (nearly) closed form, and show that the optimal variational factors ν_n^* take different values even when all the values of \mathbf{x} are equal. Then for any subset $\mathbf{w}_n \in \mathbf{x}$, we have $\mathbf{w}_n = \mathbf{w}_m$ but $\nu_n^* \neq \nu_m^*$. This provides our counter-example.

Consider the model

$$p(z_0) \propto 1$$
; $p(z_n \mid z_{n-1}) = \text{normal}(z_{n-1}, 1)$; $p(x_n \mid z_n) = \text{normal}(z_n, 1)$, (41)

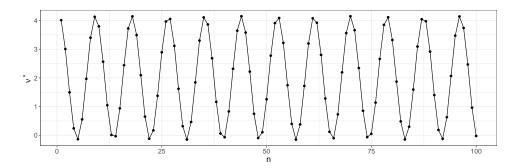


Figure 6: Optimal variational means when using a Gaussian F-VI on a hidden Markov model (Eq. 41). Even though the elements of x are all equal, the optimal variational means take on different values.

where θ is held fixed (and ignored for the rest of this analysis). Applying Bayes' rule and expanding

$$\log p(\mathbf{z} \mid \mathbf{x}) = k - \frac{1}{2} \sum_{n=1}^{N} (z_n - z_{n-1})^2 + (x_n - z_n)^2$$
$$= -\frac{1}{2} \sum_{n=1}^{N} 2z_n^2 + z_{n-1}^2 - 2x_n z_n - 2z_n z_{n-1},$$

which is a quadratic form in z and hence a Gaussian. Matching the coefficients for z_n , $z_n z_i$ and z_n^2 to the standard expression for a multivariate Gaussian (Eq. 39), we get

$$\sum_{j=1}^{N} \Psi_{nj} \mu_{j} = -2x_{n}$$

$$\Psi_{nj} = -2 \quad \text{if } j = n - 1 \text{ or } j = n + 1$$

$$\Psi_{nn} = 3 \quad \text{if } n \ge 1$$

$$\Psi_{00} = 1.$$
(42)
$$(43)$$

$$(44)$$

$$(45)$$

$$\Psi_{nj} = -2 \quad \text{if } j = n - 1 \text{ or } j = n + 1$$
 (43)

$$\Psi_{nn} = 3 \quad \text{if } n \ge 1 \tag{44}$$

$$\Psi_{00} = 1.$$
 (45)

All non-specified elements of Ψ go to 0. Moreover the precision matrix Ψ is tri-diagonal. The posterior mean solves the linear problem,

$$\mu = -2\Psi^{-1}\mathbf{x}.\tag{46}$$

Since the variational family and the target are both Gaussian, the optimal variational mean is simply the posterior mean [20, 30] and $\nu^* = \mu$. Even though the elements of x are all equal, it is in general not the case that the elements of ν^* are constant.

To see this explicitly, we take N=100 and $x_1=x_2=\cdots=x_N=1$, and find that the elements of ν^* are indeed distinct (Figure 6). This shows that there exists a hidden Markov model and a realization of the data x such that no learnable inference function exists.

B Additional experimental results

All experiments are conducted in Python 3.9.15 with PyTorch 1.13.1 and CUDA 12.0 using an NVIDIA RTX A6000 GPU.

For all models, we use a factorized Gaussian approximation and learn the variational mean and variational variance (directly in the case of F-VI or through an inference function when running A-VI).

Nonlinear probabilistic model. Table 2 provides the complete results for the nonlinear probabilistic experiment. This includes the performance of the constant factor algorithm and a more extensive number of neural network widths for A-VI. When using a large width, i.e. k = 24 and k = 32, we found on several runs that the Adam optimizer was unstable, with the evaluated loss becoming NaN. We report such cases as failures to converge.

			Conv, $\epsilon = 0.1$	Conv, $\epsilon = 0.01$
Model	Method	Max ELBO	Median (Min, Max)	Median (Min, Max)
Nonlinear	F-VI	-3.240e+4	440 (410, 480)	1280 (1200, 2680)
	Const.	-3.670e+4	Х	Х
	k = 1	-3.564e+4	X (540, X)	Х
	k = 2	-3.259e+4	540 (50, X)	Х
	k = 4	-3.239e+4	160 (20, X)	1045 (230, X)
	k = 8	-3.239e+4	65 (20, 9080)	1060 (110, X)
	k = 16	-3.239e+4	60 (40, X)	555 (170, X)
	k = 24	-3.239e+4	65 (30, 17930)	520 (160, 17930)
	k = 32	-3.239e+4	45 (20, X)	250 (20, X)

Table 2: Experimental results for the nonlinear probabilistic model. The results are computed across 10 seeds. The two right most columns give the number of iterations required to achieve convergence to the optimal ELBO (per F-VI's benchmark) within 10% ($\epsilon=0.1$) or 1% ($\epsilon=0.01$). An "X" indicates the algorithm does not attain the optimal ELBO.

			Conv, $\epsilon=0.1$	Conv, $\epsilon=0.01$
Model	Method	Max ELBO	Median (Min, Max)	Median (Min, Max)
Saw time series	F-VI	-553.10	15925 (15750, 16060)	17595 (17330, 17800)
	Const.	-2933.14	Х	Х
	i = 1, k = 4	-891.83	Х	Х
	i = 1, k = 6	-891.88	Х	Х
	i = 1, k = 10	-885.98	Х	Х
	i = 1, k = 20	-885.39	Х	Х
	i = 2, k = 2	-553.05	6870 (5070, X)	9085 (7500, X)
	i=2, k=4	-553.05	6305 (2220, 17490)	7780 (3620, X)
	i = 2, k = 6	-553.07	5025 (3240, 8050)	7235 (5460, 9200)
	i = 2, k = 10	-553.07	4650 (3240, 8050)	7145 (3470, 9510)

Table 3: Experimental results for the saw time series model. i indicates the number of input for the neural network: if i = 1, the network takes in x_n and if i = 2, it takes in (x_{n-1}, x_n) .

Deep generative models. We provide additional details on the models. For both the MNIST and FashionMNIST data sets, we use a likelihood neural network with two hidden layers and leaky ReLU activation function (with coefficient 0.2).

For MNIST, we apply a sigmoid transformation to the output of the likelihood network. This gives us the parameter of a Bernoulli likelihood with which we model the binary outcome: "0" if the pixel is white, "1" if it is black. For numerical stability, we perturb p_{ij} with a jitter term $\varepsilon=$ 1e-10 to prevent the log likelihood from going to infinity when $p_{nj}=0$ or $p_{nj}=1$. This is important during the early stages of the optimization.

For FashionMNIST, we use a Gaussian likelihood with a fixed standard deviation. The log density then corresponds to the mean squared error with respect to the likelihood mean. The mean is outputed by the likelihood neural network.

To improve the stability of the Adam optimizer, we gradually reduce the learning rate. The optimization is divided into three phases of equal length. During the first phase, the learning rate is 1e-4, and it is reduced by a factor of 10 at the beginning of each new phase.

Saw time-series. Table 3 summarises the results for the saw time series experiment. For the neural network with two inputs, increasing the width of the neural network does not improve the final ELBO but it improves the convergence rate.