Filtering Variational Objectives

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Abstract

The evidence lower bound (ELBO) appears in many algorithms for maximum likelihood estimation (MLE) with latent variables because it is a sharp lower bound of the marginal log-likelihood. For neural latent variable models, optimizing the ELBO jointly in the variational posterior and model parameters produces state-of-the-art results. Inspired by the success of the ELBO as a surrogate MLE objective, we consider the extension of the ELBO to a family of lower bounds defined by a Monte Carlo estimator of the marginal likelihood. We show that the tightness of such bounds is asymptotically related to the variance of the underlying estimator. We introduce a special case, the *filtering variational objectives* (FIVOs), which takes the same arguments as the ELBO and passes them through a particle filter to form a tighter bound. FIVOs can be optimized tractably with stochastic gradients, and are particularly suited to MLE in sequential latent variable models. In standard sequential generative modeling tasks we present uniform improvements over models trained with ELBO, including some whole nat-per-timestep improvements.

1 Introduction

Statistical latent variable models relying on neural networks have become enormously popular in recent years. They have many millions of parameters and high computational requirements, though gradient descent learning in these models is straightforward when the objective function and its gradients are tractable. Thus, the development of new objectives for learning such models can have a large impact on practice. There are currently a few dominant approaches for training neural latent variable models: (1) optimizing a lower bound on the marginal log-likelihood [1, 2], (2) restricting the class of models to be invertible [3], or (3) using likelihood-free methods, such as density ratio estimation [4, 5, 6, 7]. While likelihood-free methods are popular and result in models that generate crisp samples, they do not compare as favourably in quantitative log-likelihood evaluations [8, 9]. In this work we focus on the first approach, and introduce *filtering variational objectives* (FIVOs), objectives for maximum likelihood estimation in latent variable models.

The EM algorithm is the classic algorithm of the first kind [10]. EM takes as arguments the model and a variational posterior and optimizes a lower bound (ELBO) on the marginal log-likelihood a.k.a. evidence. The ELBO is sharp, achieving equality when the variational posterior is the true posterior [11, 12]. Because EM requires an inference step, the most common approach for neural latent variable models is to directly optimize a Monte Carlo approximation of the ELBO jointly in all of the arguments [13, 1, 2, 14, 15]. Unfortunately, when the family of variational posteriors is restricted, learning in this way tends to force the model's posterior to satisfy the factorizing assumptions of the variational family. One strategy for addressing this is to decouple the tightness of the bound from quality of the variational posterior. For example, [16] observed that the typical variational ELBO is

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obtained as the log importance weight of a single sample from an importance sampler with proposal given by the variational posterior, and that using N samples from the same proposal produces a tighter bound, known as IWAE.

Indeed, it follows from Jensen's inequality that the log of *any* unbiased positive Monte Carlo estimator of the marginal likelihood will result in a bound that can be optimized for MLE. The contributions of this work are (a) a more considered study of this general case and (b) a special case defined by a particle filter. We call the general bounds Monte Carlo objectives (MCOs) [17], because they transform a Monte Carlo estimator into an objective for MLE. We provide basic results for MCOs, including that the tightness of an MCO is asymptotically related to the variance of the estimator from which it is constructed. As a special case, we introduce the filtering variational objectives (FIVOs), MCOs defined by a particle filter's estimator of the marginal likelihood [18, 19]. The essence of the filter's computation is simple: in the forward pass it propagates a set of latent variable trajectories using a combination of importance sampling and resampling steps. From this lattice of states, the objective is a log-sum-exp over the trajectories at each time step, then a sum over time. Thus, FIVOs are constructed from the same variational posterior as the ELBO, but tend to converge faster [20, 21] than the IWAE for models with sequential structure [22].

The paper is organized as follows. In Section 2 we review the ELBO and maximum likelihood estimation in latent variable models. In Section 3 we define Monte Carlo objectives and describe their basic properties. We define filtering variational objectives in Section 4, discuss details of their optimization, and present a sharpness result. In Section 5 we cover related work. In Section 6 we present experiments showing that training sequential generative models with FIVOs produce far better likelihood scores on held out data than when training with ELBO or IWAE.

2 Background

2.1 Latent Variable Models and Maximum Likelihood Estimation

Let x be an $\mathcal{X}$-valued random variable representing our observation. We assume that x was generated dependent on an unobserved $\mathcal{Z}$-value latent variable z. The goal of maximum likelihood estimation (MLE) is to recover the density $p \in \mathcal{P}$ that maximizes the marginal log-likelihood $\log p(x)$,

$$p^* = \underset{p \in \mathcal{P}}{\operatorname{argmax}} \log \left(\int p(x, z) \, dz \right) \tag{1}$$

In applications with neural networks, the densities $p \in \mathcal{P}$ are normally parameterized differentiably by parameters θ [23, 24, 25], and optimizing the likelihood via stochastic gradient ascent in θ suffices for state of the art results [26]. Instead, the central difficulty in carrying out this optimization is that the likelihood function is defined via an integration over the unobserved variables. Such integrals are usually intractable, if the variables are non-Gaussian or their relationship non-linear.

2.2 The Evidence Lower Bound (ELBO)

One strategy to circumvent the difficulty of marginalization is to optimize a lower bound (ELBO) on the marginal log-likelihood [27, 28, 29, 11, 12]. The ELBO is defined by a second distribution q, the variational posterior, which approximates the true posterior $p(z|x)$. The key feature of the ELBO is that it is a sharp lower bound, *i.e.,* equality holds when the variational posterior is identical to the true posterior. This allows us to relate improvements in the ELBO to improvements in the likelihood.

In detail, let $q(z|x)^1$ denote a conditional density on $\mathcal{Z}$ given x. The ELBO is defined as,

$$\mathcal{L}(x, p, q) = \underset{q(z|x)}{\mathbb{E}} \left[\log \frac{p(x, z)}{q(z|x)} \right] . \tag{2}$$

By Jensen's inequality (see Section 3) we see that $\mathcal{L}(x, p, q) \leq \log p(x)$. Crucially, for any fixed p, if the variational posterior q is taken from the family of all distributions, then the ELBO is tight at the true posterior [30, 31]: If $q^*(x, p) = \operatorname{argmax}_q \mathcal{L}(x, p, q)$, then $q^*(x, p)(z) = p(z|x)$ and

$$\mathcal{L}(x, p, q^*(x, p)) = \log p(x). \tag{3}$$

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[1] An underlying assumption here is that q puts mass on any event with positive mass under p.

Thus, the joint optimum of the ELBO in p and q is exactly the MLE. The observation that optimizing over q corresponds to inference leads to the EM algorithm, which interleaves inference and maximization [10, 32, 33]. EM rarely applies to neural models, because inference is intractable.

Instead, gradient ascent on a Monte Carlo estimator of the ELBO is common practice [13]. We assume that p and q are parameterized in a differentiable way by distinct parameters θ and ϕ, respectively. A naive gradient step would consist of sampling $z \sim q_\phi(z|x)$ and following $\nabla_{\theta,\phi}(\log p_\theta(x,z) - \log q_\phi(z|x))$ and $(\log p_\theta(x,z) - \log q_\phi(z|x))\nabla_\phi \log q_\phi(z|x)$. These gradients follow the ELBO's in expectation, but variance reduction techniques are usually necessary [14, 34, 17]. This can be improved if q_ϕ is a reparameterizable distribution [1, 2]. Reparameterizable distributions are those that can be simulated by sampling from some fixed distribution $\epsilon \sim d(\epsilon)$ and applying a deterministic transformation $z = f_\phi(x, \epsilon)$. With reparametrization, the ELBO becomes,

$$\mathcal{L}(x, p_\theta, q_\phi) = \mathbb{E}_d \left[\log \frac{p_\theta(x, f_\phi(x, \epsilon))}{q_\phi(f_\phi(x, \epsilon)|x)} \right] . \tag{4}$$

When p_θ, q_ϕ, and f_ϕ are differentiable, optimization proceeds by sampling ϵ, and taking a stochastic gradient step $\nabla_{\theta,\phi}(\log p_\theta(x, f_\phi(x, \epsilon)) - \log q_\phi(f_\phi(x, \epsilon)|x))$. Again reparameterized gradients follow the ELBO's in expectation, but they tend to have lower variance [35]. Optimizing the ELBO jointly in this way is justified, but in practice the ELBO places a harsh penalty on the mismatch between q_ϕ and the true posterior. This tends to reduce the capacity of the model p_θ to match the modelling assumptions of the variational posterior q_ϕ—justifying the consideration of tighter bounds.

3 Monte Carlo Objectives (MCOs)

In this section we study Monte Carlo objectives (MCOs) [17], a generalization of the ELBO constructed by taking the $\log$ of a positive unbiased estimator of the marginal likelihood. The key property of MCOs is that they approximate the marginal log-likelihood from below. There are many Monte Carlo estimators of marginal likelihoods [36, 37, 38, 39, 40], so we seek a tool for comparing the quality of their corresponding MCO. The measure of quality that we consider is the tightness of the MCO on the marginal log-likelihood, which we show is related to the variance of the estimator that defines it.

One can verify that the ELBO is a lower bound by using Jensen's inequality. Because log is concave,

$$\mathbb{E}_{q(z|x)} \left[\log \frac{p(x, z)}{q(z|x)} \right] \leq \log \int \frac{p(x, z)}{q(z|x)} q(z|x) \, dz = \log p(x). \tag{5}$$

In this argument, the property of $p(x, z)/q(z|x)$ used is that its expected value is $p(x)$ when $x \sim q(z|x)$. More generally, let $\hat{p}_N(x)$ denote an unbiased estimator of the marginal likelihood, $\mathbb{E}[\hat{p}_N(x)] = p(x)$. Here $N \in \mathbb{N}$ roughly represents the amount of computation, e.g., the number of samples needed to simulate $\hat{p}_N(x)$. The basic idea is that we will treat $\log \hat{p}_N(x)$ as an objective in and of itself, and it will stochastically lower bound $\log p(x)$.

Definition 1. Monte Carlo Objectives. Let $\hat{p}_N(x)$ be an unbiased positive estimator of $p(x)$, then

$$\mathcal{L}_N(x, p) = \mathbb{E}[\log \hat{p}_N(x)] \tag{6}$$

is a Monte Carlo objective over $p \in \mathcal{P}$.

The unbiased estimator underlying the ELBO is a single importance weight. The IWAE bound [16] corresponds to N averaged importance weights,

$$\mathcal{L}_N^{\text{IWAE}}(x, p, q) = \mathbb{E}_{q(z^i|x)} \left[\log \left(\frac{1}{N} \sum_{i=1}^N \frac{p(x, z^i)}{q(z^i|x)} \right) \right] \tag{7}$$

As long as the support of $q(z|x)$ includes the support of $p(z|x)$ then $\hat{p}_N(x)$ converges to $p(x)$ almost surely as $N \to \infty$ (known as strong consistency). The advantage of a consistent estimator is that its MCO can be driven towards $\log p(x)$ by increasing N. In some cases this convergence will be monotonic, [16]. Because this will not be be true in general, we show that the tightness of $\mathcal{L}_N(x, p)$ is asymptotically related to $\text{var}(\hat{p}_N(x))$, i.e., the variance of the underlying estimator. This is useful because it provides us with a tool to compare the rate of convergence for different MCOs. We summarize their key characteristics:

Proposition 1. Properties of Monte Carlo Objectives. *Let $\mathcal{L}_N(x, p)$ be a Monte Carlo objective defined by an unbiased positive estimator $\hat{p}_N(x)$ of $p(x)$. Then,*

(a) *(Bound)* $\mathcal{L}_N(x, p) \leq \log p(x)$.

(b) *(Consistency) If $\log \hat{p}_N(x)$ is uniformly integrable and $\hat{p}_N(x)$ is strongly consistent, then*
$$\mathcal{L}_N(x, p) \overset{N \to \infty}{\longrightarrow} \log p(x).$$

(c) *(Asymptotic Bias) Let $g(N) = \mathbb{E}[(\hat{p}_N(x) - p(x))^6]$ be the 6th central moment. If the 1st inverse moment $\limsup \mathbb{E}[\hat{p}_N(x)^{-1}] < \infty$ is bounded, then*
$$\log p(x) - \mathcal{L}_N(x, p) = \frac{1}{2} \operatorname{var}\left(\frac{\hat{p}_N(x)}{p(x)}\right) + \mathcal{O}(\sqrt{g(N)}). \tag{8}$$

Proof. See Appendix. □

Whether we can compute stochastic gradients of $\mathcal{L}_N(x, p)$ efficiently depends on the specific form of the estimator and the underlying random variables. Another consideration is the variance of its gradients. [16] showed that the mean absolute deviation of MCOs is bounded by the bias. For estimators satisfying a central limit theorem, we can expect their moments to be sub-Gaussian, and by properties (b) and (c), one can expect the signal to noise ratio of the learning signal to improve with N. These considerations motivate the MCO defined by a particle filter's estimator of the marginal likelihood: (a) for models with sequential structure the relative variance of these estimators scales favorable to importance sampling, (b) these estimators can mostly be reparameterized, and (c) many satisfy central limit theorems [41, 42].

4 Filtering Variational Objectives (FIVOs)

We introduce the filtering variational objectives (FIVOs) as a family of MCOs specialized to enable effective optimization of latent variable models with sequential structure. When the data generation process is inherently sequential *e.g.,* audio and text, the relative variance of an importance sampling estimator can scale exponentially in the number of steps whereas. Particle filters extend simple importance sampling, and provide estimators whose relative variance tends to scale more favourably with the number of steps—linearly in some cases. More generally, graphical models can be serialized to produce particle filter whose estimate of the marginal likelihood has lower variance [22].

We suppose our observations are sequences of n $\mathcal{X}$-valued random variables denoted $x_{1:n}$, where $x_{i:j} \equiv (x_i, \ldots, x_j)$ represents a sequence from x_i to x_j, inclusive. We also assume that the data generation process relies on a sequence of n unobserved $\mathcal{Z}$-valued latent variables denoted $z_{1:n}$. For the purpose of exposition, we focus on sequential latent variable models that factorize as a sequence of tractable conditionals, $p(x_{1:n}, z_{1:n}) = p_1(x_1, z_1) \prod_{k=2}^n p_k(x_k, z_k | x_{1:k-1}, z_{1:k-1})$. An example is the hidden Markov model (HMM), in which the density of the process factorizes as $p(x_{1:n}, z_{1:n}) = p_1(z_1) g(x_1 | z_1) \prod_{k=1}^n p_k(z_k | z_{k-1}) g(x_k | z_k)$ into a Markov model over the latent space $p_1(z_1) \prod_{k=1}^n p_k(z_k | z_{k-1})$ and conditional densities $g(x_k | z_k)$ over the observations.

A particle filter is a sequential Monte Carlo algorithm which propagates a population of N weighted particles steps 1 to n using a combination of importance sampling and resampling steps. More specifically, the particle filter takes as arguments an observation $x_{1:n}$, the number of particles N, the model distribution p, and a variational posterior $q(z_{1:n} | x_{1:n})$ factored over k,

$$q(z_{1:n} | x_{1:n}) = \prod_{k=1}^n q_k(z_k | x_{1:k}, z_{1:k-1}). \tag{9}$$

The particle filter maintains a population $\{w_{k-1}^i, z_{1:k-1}^i\}_{i=1}^N$ of particles $z_{1:k-1}^i$ with weights w_{k-1}^i. At step k, each particle proposes an extension with the proposal distribution $q_k(z_k^i | x_{1:k}, z_{1:k-1}^i)$. The weights are multiplied by the incremental importance weights,

$$\alpha_k(z_{1:k}^i) = \frac{p_k(x_k, z_k^i | x_{1:k-1}, z_{1:k-1})}{q_k(z_k^i | x_{1:k}, z_{1:k-1})}, \tag{10}$$

Algorithm 1 Simulating $\mathcal{L}_{\mathrm{N}}^{\mathrm{FIVO}}(x_{1:n}, p, q)$

1: **FIVO**$(x_{1:n}, p, q, N)$:
2: $\{w_0^i\}_{i=1}^N = \{1/N\}_{i=1}^N$
3: **for** $k \in \{1, \dots, n\}$ **do**
4:     **for** $i \in \{1, \dots, N\}$ **do**
5:        $z_k^i \sim q_k(z_k | x_{1:k}, z_{1:k-1}^i)$
6:        $z_{1:k}^i = \mathbf{CONCAT}(z_{1:k-1}^i, z_k^i)$
7:     $\hat{p}_k = \left(\sum_{i=1}^N w_{k-1}^i \alpha_k(z_{1:k}^i) \right)$
8:     $\hat{p}_N(x_{1:k}) = \hat{p}_N(x_{1:k-1})\hat{p}_k$
9:     $\{w_k^i\}_{i=1}^N = \{w_{k-1}^i \alpha_k(z_{1:k}^i)/\hat{p}_k\}_{i=1}^N$
10:     **if** resampling criteria satisfied by $\{w_k^i\}_{i=1}^N$ **then**
11:        $\{w_k^i, z_{1:k}^i\}_{i=1}^N = \mathbf{RSAMP}(\{w_k^i, z_{1:k}^i\}_{i=1}^N)$
12: **return** $\log \hat{p}_N(x_{1:n})$

13: **RSAMP**$(\{w^i, z^i\}_{i=1}^N)$:
14: **for** $i \in \{1, \dots, N\}$ **do**
15:     $a \sim \text{Categorical}(\{w^i\}_{i=1}^N)$
16:     $y^i = z^a$
17: **return** $\{\frac{1}{N}, y^i\}_{i=1}^N$

and renormalized. If the current weights satisfy a resampling criteria, then a resampling step is performed and N particles are sampled in proportion to their weights from the current population with replacement. After resampling the weights are reset to $1/N$. Otherwise, the population is copied to the next step along with the accumulated weights. See Algorithm 1 and Figure 1.

The quantity $\hat{p}_N(x_{1:n})$ computed by Algorithm 1 is an unbiased strongly consistent estimator of $p(x_{1:n})$ [41, 42, 43, 44]. Thus, it defines an MCO:

Definition 2. Filtering Variational Objectives. Let $\log \hat{p}_N(x_{1:n})$ be the output of Algorithm 1 with inputs $(x_{1:n}, p, q, N)$, then $\mathcal{L}_{\mathrm{N}}^{\mathrm{FIVO}}(x_{1:n}, p, q) = \mathbb{E}[\log \hat{p}_N(x_{1:n})]$ is a filtering variational objective.

As long as $\log \hat{p}_N(x_{1:n})$ is uniformly integrable, then $\mathcal{L}_{\mathrm{N}}^{\mathrm{FIVO}}(x_{1:n}, p, q)$ approaches $\log p(x_{1:n})$ almost sure. Crucially, the resampling step can dramatically decrease the relative variance of the estimator over simple importance sampling. In fact, $\mathcal{L}_{\mathrm{N}}^{\mathrm{FIVO}}(x_{1:n}, p, q)$ is only distinguished from $\mathcal{L}_{\mathrm{N}}^{\mathrm{IWAE}}(x_{1:n}, p, q)$ by the resampling step; if resampling is removed, the FIVO reduces to IWAE. In some scenarios, for example in an HMM, resampling reduces the scaling order of the relative variance from exponential in n to linear in n [20, 19]. Thus, we expect $\mathcal{L}_{\mathrm{N}}^{\mathrm{FIVO}}(x_{1:n}, p, q)$ to be a tighter bound than the $\mathcal{L}(x_{1:n}, p, q)$ or the $\mathcal{L}_{\mathrm{N}}^{\mathrm{IWAE}}(x_{1:n}, p, q)$. Intuitively resampling allows us to discard particles with low weight, and refocus the distribution of particles to regions of higher mass under the posterior. Of course, resampling is a greedy process, and it is possible that a particle discarded at step k, could have attained a high mass at step n. Thus, in practice, the best trade-off is to exploit adaptive resampling schemes, and in this work we make use of the standard ESS adaptive decision. We note that there is a large literature on the effect of resampling, alternative resampling schemes, and additional algorithmic advances on the standard particle filter framework presented here [19]. Note, there is an informative view of particle filters as simple importance sampling over an extended space [43]. In this extended space, the FIVO bound is just an ELBO from the particle filter distribution to a certain target process.

4.1 Optimization

FIVOs can be optimized with the same basic stochastic gradient ascent framework used for the ELBO. We assume that p and q are parameterized in a differentiable way by distinct θ and ϕ. A single gradient update comprises running Algorithm 1 forward, storing the states, and computing a gradient in a backward pass conditioned on the forward values. If we do not make assumptions on the sampling process, then the gradients through stochastic values are the score functions of each decision scaled by the future learning signal. We include this general gradient in the Appendix, but in practice it is preferable to reparameterize the sampling of q_k. When the values z_k^i are reparameterized, the gradient flows through the lattice of states z_k^i created in the forward process (see Figure 1). If 1_k indicates a resampling time, then the gradient simplifies to

$$\nabla_{\theta,\phi} \log \hat{p}_N(x_{1:n}) + \sum_{k=1}^n \sum_{i=1}^N 1_k (\log \hat{p}_N(x_{1:n}) - \log \hat{p}_N(x_{1:k})) \nabla_{\theta,\phi} \log w_k^i . \qquad (11)$$

In practice, the resampling gradients $\nabla_{\theta,\phi} \log w_k^i$ can add orders of magnitude to the variance of this estimator. We found the best results were achieved by omitting them and following the biased gradient $\nabla_{\theta,\phi} \log \hat{p}_N(x_{1:n})$.
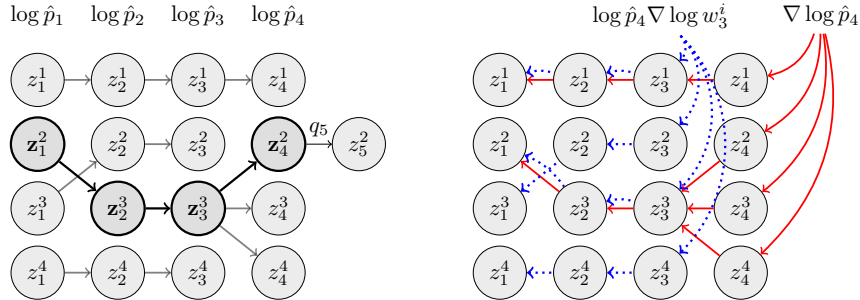
Figure 1: Visualization of the FIVO. (left) The forward computation produces a lattice of latent states. (right) The backward gradient (in the reparameterized case) flows through that lattice, gradients from the objective at time 4 shown in solid red and resampling gradients at time 3 shown in dotted blue.

4.2 Sharpness

As with the ELBO and IWAE, the FIVO is a variational objective taking as an argument the variational posterior q. One may wonder whether FIVO admits the true posterior as its optimum $q^*(x_{1:n}, p) = \mathrm{argmax}_q \mathcal{L}_N^{\mathrm{FIVO}}(x_{1:n}, p, q)$, and whether FIVO equals the marginal log-likelihood at q^*. Unfortunately, this is not necessarily the case for all classes of models p. However, the bound is sharp if we restrict the class of models to those such that given $x_{1:k-1}$, $z_{1:k-1}$ and x_k are independent.

Proposition 2. Sharpness of Filtering Variational Objectives. *Let* $\mathcal{L}_N^{\mathrm{FIVO}}(x_{1:n}, p, q)$ *be a FIVO, and* $q^*(x_{1:n}, p) = \mathrm{argmax}_q \mathcal{L}_N^{\mathrm{FIVO}}(x_{1:n}, p, q)$. *If* p *has independence structure such that* $p(z_{1:k-1}|x_{1:k}) = p(z_{1:k-1}|x_{1:k-1})$ *for* $k \in \{2, \dots, n\}$, *then*

$$q^*(x_{1:n}, p)(z_{1:n}) = p(z_{1:n}|x_{1:n}) \quad and \quad \mathcal{L}_N^{\mathrm{FIVO}}(x_{1:n}, p, q^*(x_{1:n}, p)) = \log p(x_{1:n}) .$$

Proof. See Appendix. □

Unfortunately many common models (like the HMM) are not in this class. The problem is that the resampling step responds to the conditional density of p at each step k as if it were the final step. This prevents the filter from matching posteriors that must account for future observations. Allowing q_k to condition on $x_{k+1:n}$ does not alleviate this problem. In a sense, this is the price we have to pay for greedily exploiting the sequential structure of p in a single forward pass. Yet, for the experiments we consider, any effects from this are minor compared to the advantage of optimizing a tighter bound.

5 Related Work

The marginal log-likelihood is a central quantity in statistics and probability, and there has long been an interest in bounding it [30]. The literature relating to the bounds we called Monte Carlo objectives has typically focused on the problem of estimating the marginal likelihood itself. [45, 46] use Jensen's inequality in a forward and reverse estimator to detect the failure of inference methods. IWAE [16] is a clear influence on this work, and the FIVO can be seen as an extension of this bound. The ELBO enjoys a long history [11] and there have been efforts to improve the ELBO itself. [47] generalize the ELBO by considering arbitrary operators of the model and variational posterior. More closely related to this work is a body of work improving the ELBO by increasing the expressiveness of the variational posterior. For example [48, 49] augment the variational posterior with deterministic transformations with fixed Jacobians, [50] extend the variational posterior to admit a Markov chain.

The specific problem of learning in neural models with latent variables is also well studied [51]. [52] learn a neural q posterior for the purpose of inference, but they optimize the reverse KL. [53] uses importance sampling to approximate gradients under the posterior. [54] introduce specific sequential Monte Carlo improvements of this method for sequential neural models. These are distinct from our contribution in the sense that inference for the sake of estimation is the ultimate goal. To our knowledge the idea of treating the output of inference as an objective in and of itself, while not completely novel, has not been fully appreciated in the literature. Although, this idea shares inspiration with methods that optimize the convergence of Markov chains [55].
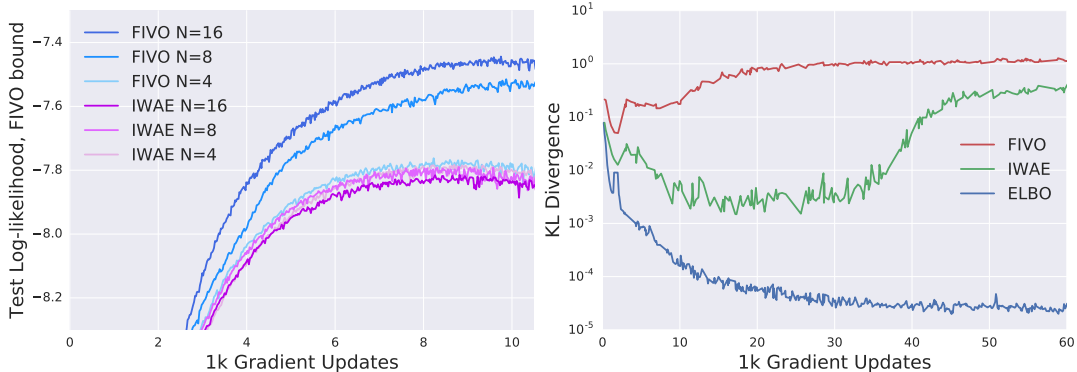
Figure 2: (Left) Learning curves comparing models trained with $\mathcal{L}_N^{\text{FIVO}}$ and $\mathcal{L}_N^{\text{IWAE}}$ for different N on the Piano-midi.de dataset. (Right) The KL divergence between $p(z_{1:n})$ and $q(z_{1:n}|x_{1:n})$ for models trained with ELBO, IWAE, and FIVO on the JSB chorales dataset with $N = 16$.

6 Experiments

We sought to understand: (a) how optimizing the ELBO, IWAE, and FIVO bounds compare in terms of final model log-likelihoods, (b) whether there are differences in how the trained models use the stochastic state, and (c) how IWAE and FIVO scale with the number of particles. To explore these questions, we trained variational recurrent neural networks (VRNN) [56] with the ELBO, IWAE, and FIVO bounds on two benchmark sequential modeling tasks: modeling natrual speech waveforms and modeling polyphonic music. These datasets are known to be difficult to model without stochastic latent states [57].

The VRNN is a sequential latent variable model that combines a deterministic recurrent neural network (RNN) with stochastic latent states z_k at each step. The observation distribution x_k is conditioned directly on z_k and indirectly on $z_{1:k-1}$ via the RNN's state $h_k(z_{k-1}, x_{k-1}, h_{k-1})$. For a length n sequence the model's posterior factorizes into the conditionals

$$p_1(z_1)q_1(x_1|z_1) \prod_{k=2}^{n} p_k(z_k|h_k(z_{k-1}, x_{k-1}, h_{k-1}))g_k(x_k|z_k, h_k(z_{k-1}, x_{k-1}, h_{k-1})). \quad (12)$$

Similarly the variational posterior factorizes as

$$q_1(z_1|x_1) \prod_{k=2}^{n} q_k(z_k|h_k(z_{k-1}, x_{k-1}, h_{k-1}), x_k). \quad (13)$$

All latent variables are factorized Gaussians, and the observation distributions depend on the dataset. The RNN is a single-layer LSTM and the conditionals are parameterized by fully connected neural networks with one hidden layer of the same size as the LSTM hidden layer. We used the residual parameterization [57] for the variational posterior.

When training with the ELBO, we used batch sizes of $4N$ to match the computational budget of IWAE and FIVO (neglecting the insignificant resampling computation). To evaluate each model p, we computed $\mathcal{L}(x_{1:n}, p, q), \mathcal{L}_{64}^{\text{IWAE}}(x_{1:n}, p, q), \mathcal{L}_{64}^{\text{FIVO}}(x_{1:n}, p, q)$, and report the maximum because all are stochastic lower bounds on the log likelihood. For training set performance see the Appendix.

To reduce the variance from the gradient terms arising from the resampling events, we used a linear baseline in the number of remaining timesteps. Still, we found that the unbiased FIVO gradients had high variance. This variance is almost entirely due to the gradients corresponding to resampling events, accounting for 6 orders of magnitude (Appendix Figure 3). Thus, we report results using only the first term of Eq. (11) to compute gradient estimates.

6.1 Polyphonic Music

We evaluated VRNNs trained with the ELBO, IWAE, and FIVO bounds on 4 polyphonic music datasets: the Nottingham folk tunes, the JSB chorales, the MuseData library of classical piano and orchestral music, and the piano-midi.de MIDI archive [58]. Each dataset is split into standard train,

N	Bound	Nottingham	JSB	MuseData	piano-midi
4	ELBO	-3.23	-8.61	-7.12	-7.79
	IWAE	-3.21	-8.59	-7.17	-7.81
	FIVO	**-2.86**	**-6.95**	**-6.55**	**-7.72**
8	ELBO	-3.60	-8.60	-7.11	-7.83
	IWAE	-3.30	-7.53	-7.10	-7.81
	FIVO	**-2.62**	**-6.69**	**-6.36**	**-7.49**
16	ELBO	-3.54	-8.60	-7.17	-7.83
	IWAE	-2.95	-7.55	-7.08	-7.81
	FIVO	**-2.58**	**-6.60**	**-6.09**	**-7.19**

		TIMIT	
N	Bound	64 units	512 units
4	ELBO	35,908	36,981
	IWAE	35,984	34,067
	FIVO	**40,211**	**41,834**
8	ELBO	35,612	37,902
	IWAE	36,835	38,074
	FIVO	**40,912**	**41,666**

Table 1: Test set performance of models trained with different bounds and numbers of particles on polyphonic music and TIMIT.

valid, and test sets and is represented as a sequence of 88-dimensional vectors denoting the notes active at the current timestep. We mean-centered the input data, and we modeled the output as a set of 88 factorized Bernoulli variables. We initialized the output biases of the VRNN to the training set statistics. For the results reported in Table 1, the Nottingham model used 64 units, the JSB Chorales model used 32 units, the MuseData model used 256 units, and the piano-midi.de model used 64 units. We report bounds on average log likelihood per timestep.

Models trained on the FIVO bound significantly outperformed models trained with either the ELBO or the IWAE bounds on all four datasets (Table 1). In some cases, the improvements exceeded 1.0 nat *per timestep*, and in all cases, optimizing FIVO with $N = 4$ outperformed optimizing either IWAE or ELBO for $N = \{4, 8, 16\}$. A known pathology when training stochastic latent state models with the ELBO bound is that the stochastic states are unused, and as a result, the inference network collapses to the model [59]. To investigate this, we plot the KL divergence from $q(z_{1:n}|x_{1:n})$ to $p(z_{1:n})$ averaged over the dataset (Figure 2). Indeed, the KL of models trained with ELBO collapsed during training, whereas the KL of models trained with FIVO remained high, even while achieving a higher log likelihood bound. In Figure 2, we also investigated how the log likelihood bound of models trained with IWAE and FIVO scaled with the number of particles, N. FIVO continued to benefit as N increased through $\{4, 8, 16\}$ while IWAE suffered diminishing returns.

6.2 Speech

The TIMIT dataset is a standard benchmark for sequential models that contains 6300 utterances with an average duration of 3.1 seconds spoken by 630 different speakers. The 6300 utterances are divided into a training set of size 4620 and a test set of size 1680. We further divide the training set into a validation set of size 231 and a training set of size 4389, with the splits exactly as in [57]. Each TIMIT utterance is represented as a sequence of real-valued amplitudes which we split into a sequence of 200-dimensional frames, as in [56], [57]. Data preprocessing was limited to mean centering and variance normalization as in [57]. For TIMIT, the output distribution was a factorized Gaussian, and we report the average log likelihood bound per sequence. Again, models optimized with the FIVO bound significantly outperformed models optimized with IWAE or ELBO, see Table 1.

7 Conclusions

We introduced the family of filtering variational objectives, a class of lower bounds on the log marginal likelihood that extend the evidence lower bound. FIVOs are suited for MLE in neural latent variable models. We trained models with the ELBO, IWAE, and FIVO bounds and found that the models trained with FIVO significantly outperformed other models across all four polyphonic music modeling tasks and a speech waveform modeling task. Although our experiments used data sequential in time, the FIVO is not restricted to time series. Future work will include exploring control variates for the resampling gradients, FIVOs defined by more sophisticated filtering algorithms, and new MCOs based on differentiable operators like leapfrog operators with deterministically annealed temperatures. In general, we hope that this paper inspires the machine learning community to take a fresh look at the literature of marginal likelihood estimators—seeing them as objectives instead of algorithms for inference.

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Appendix of Filtering Variational Objectives

Gradients of $\mathcal{L}_{\mathrm{N}}^{\mathrm{FIVO}}(x_{1:n}, p, q)$. We formulate an unbiased gradient of $\mathcal{L}_{\mathrm{N}}^{\mathrm{FIVO}}(x_{1:n}, p, q)$ under no assumptions about the forward sampling process. There are two types of stochastic values in Algorithm 1., the latent variables z_k^i and the resampling decisions, and we must take gradients with respect to each. Where 1_k is an indicator as to whether a resampling event has occurred at step k,

$$\nabla_{\theta,\phi} \log \hat{p}_N(x_{1:n}) \; + \; \sum_{k=1}^{n} \sum_{i=1}^{N} \left(\log \frac{\hat{p}_N(x_{1:n})}{\hat{p}_N(x_{1:k-1})} \nabla_\phi \log q_{k,\phi}(z_k^i | x_{1:k}, z_{1:k-1}^i) \right.$$
$$\left. + 1_k \log \frac{\hat{p}_N(x_{1:n})}{\hat{p}_N(x_{1:k})} \nabla_{\theta,\phi} \log w_k^i \right) \tag{14}$$

Proof of Proposition 1. Let $\hat{p}_N(x)$ be an unbiased positive estimator of $p(x)$. Let $\mathcal{L}_N(x, p) = \mathbb{E}[\log \hat{p}_N(x)]$ be the Monte Carlo objective defined by $\hat{p}_N(x)$.

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(a) By Jensen's inequality,

$$\mathcal{L}_N(x, p) = \mathbb{E}[\log \hat{p}_N(x)] \leq \log \mathbb{E}[\hat{p}_N(x)] = \log p(x)$$

(b) Let $\hat{p}_N(x)$ be strongly consistent and $\log \hat{p}_N(x)$ uniformly integrable. $\hat{p}_N(x)$ converges almost surely to $p(x)$, and by continuity of log we get that $\log \hat{p}_N(x)$ converges almost surely to $\log p(x)$. Because $\log \hat{p}_N(x)$ is uniformly integrable, we get $\mathcal{L}_N(x, p) \to \log p(x)$.

(c) Let $g(N) = \mathbb{E}[(\hat{p}_N(x) - p(x))^6]$, and assume $\limsup \mathbb{E}[(\hat{p}_N(x))^{-1}] < \infty$. Define the relative error

$$\Delta = \frac{\hat{p}_N(x) - p(x)}{p(x)} \tag{15}$$

Then the bias $\log p(x) - \mathcal{L}_N(x, p) = -\mathbb{E}[\log(1 + \Delta)]$. Now, Taylor expand $\log(1 + \Delta)$ about 0,

$$\log(1 + \Delta) = \Delta - \frac{1}{2}\Delta^2 + \int_0^\Delta \left(\frac{1}{1+x} - 1 + x\right) dx \tag{16}$$

$$= \Delta - \frac{1}{2}\Delta^2 + \int_0^\Delta \left(\frac{x^2}{1+x}\right) dx \tag{17}$$

and in expectation

$$-\mathbb{E}[\log(1 + \Delta)] = \frac{1}{2}\Delta^2 - \mathbb{E}\left[\int_0^\Delta \left(\frac{x^2}{1+x}\right) dx\right] \tag{18}$$

Our aim is to show

$$\left|\mathbb{E}\left[\int_0^\Delta \frac{x^2}{1+x} dx\right]\right| \in \mathcal{O}(g(N)^{1/2}) \tag{19}$$

In particular, by Cauchy-Schwarz

$$\left|\mathbb{E}\left[\int_0^\Delta \left(\frac{x^2}{1+x}\right) dx\right]\right| \leq \mathbb{E}\left[\left|\int_0^\Delta \frac{1}{(1+x)^2} dx\right|^{1/2} \left|\int_0^\Delta x^4 dx\right|^{1/2}\right] \tag{20}$$

$$= \mathbb{E}\left[\left|\frac{\Delta}{1+\Delta}\right|^{1/2} \left|\frac{\Delta^5}{5}\right|^{1/2}\right] \tag{21}$$

$$= \mathbb{E}\left[\left|\frac{1}{1+\Delta}\right|^{1/2} \left|\frac{\Delta^6}{5}\right|^{1/2}\right] \tag{22}$$

and again by Cauchy-Schwarz

$$\leq \left(\mathbb{E}\left[\left|\frac{1}{1+\Delta}\right|\right]\right)^{1/2} \left(\mathbb{E}\left[\frac{\Delta^6}{5}\right]\right)^{1/2} \tag{23}$$

and we're done.

Proof of Proposition 2. Assume $p(z_{1:k-1}|x_{1:k}) = p(z_{1:k-1}|x_{1:k-1})$ for all $k \in \{2, \ldots, n\}$. We will show $\mathcal{L}_N^{\text{FIVO}}(x_{1:n}, p, q) = \log p(x_{1:n})$ at $q(z_k|z_{1:k-1}, x_{1:k}) = p(z_k|z_{1:k-1}, x_{1:k})$. We will do this by induction, showing that every particle has a constant weight and that $\hat{p}_N(x_{1:n}) = p(x_{1:n})$ is a constant. For $k = 1$ we have

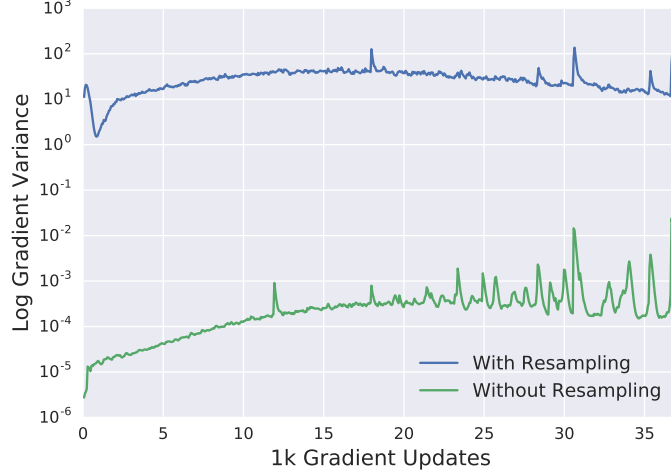$$\alpha_1^i(z_1) = \frac{p_1(x_1, z_1)}{p(z_1|x_1)} = p_1(x_1) \tag{24}$$

Figure 3: Variance of FIVO gradients with and without resampling terms along the trajectory generated by a training run trained without resampling terms. The variance of the gradients with resampling terms is several orders of magnitude larger than the gradients without resampling terms, making it difficult to train with the resampling terms. These curves are generated from training on the JSB chorales.

Thus, all particles have the same weight and $\hat{p}_1 = p_1(x_1)$. Now for any k we have that the weights must be $1/N$ since the particles all have the same weight and

$$\alpha_k^i(z_{1:k}) = \frac{p_k(x_k, z_k | z_{1:k-1}, x_{1:k-1})}{p(z_k | z_{1:k-1}, x_{1:k})} \tag{25}$$

$$= \frac{p(z_{1:k}, x_{1:k})}{p(z_{1:k-1}, x_{1:k-1}) p(z_k | z_{1:k-1}, x_{1:k})} \tag{26}$$

$$= \frac{p(x_{1:k})}{p(x_{1:k-1})} \frac{p(z_{1:k} | x_{1:k})}{p(z_{1:k-1} | x_{1:k-1}) p(z_k | z_{1:k-1}, x_{1:k})} \tag{27}$$

$$= \frac{p(x_{1:k})}{p(x_{1:k-1})} \frac{p(z_{1:k} | x_{1:k})}{p(z_{1:k-1} | x_{1:k}) p(z_k | z_{1:k-1}, x_{1:k})} \tag{28}$$

$$= \frac{p(x_{1:k})}{p(x_{1:k-1})} \tag{29}$$

and thus,

$$\hat{p}_N(x_{1:n}) = p_1(x_1) \prod_{k=2}^{n} \frac{p(x_{1:k})}{p(x_{1:k-1})} = p(x_{1:n}) \tag{30}$$

Implementation details We initialized weights using the Xavier initialization [60] and used the Adam optimizer [61] with a batch size of 4. We performed a grid search over learning rates $\{3 \times 10^{-4}, 1 \times 10^{-4}, 3 \times 10^{-5}, 1 \times 10^{-5}\}$ and picked the run and early stopping step by the validation performance. During training, we did not truncate sequences and performed full backpropagation through time.

N	Bound	Nottingham		JSB Chorales		MuseData		Piano-MIDI.de	
		Train	Test	Train	Test	Train	Test	Train	Test
	ELBO	-3.03	-3.23	-5.38	-8.61	-5.42	-7.12	-7.06	-7.79
4	IWAE	-3.02	-3.21	-5.23	-8.59	-5.22	-7.17	-7.18	-7.81
	FIVO	**-2.25**	**-2.86**	**-4.22**	**-6.95**	**-5.16**	**-6.55**	**-6.32**	**-7.72**
	ELBO	-3.04	-3.60	-6.10	-8.60	-5.93	-7.11	-7.33	-7.83
8	IWAE	-3.15	-3.30	-6.18	-7.53	-5.71	-7.10	-6.71	-7.81
	FIVO	**-1.98**	**-2.62**	**-5.10**	**-6.69**	**-5.47**	**-6.36**	**-6.22**	**-7.49**
	ELBO	-3.39	-3.54	-6.10	-8.60	-6.18	-7.17	-7.23	-7.83
16	IWAE	-2.18	-2.95	-4.60	-7.55	-5.74	-7.08	-7.04	-7.81
	FIVO	**-2.12**	**-2.58**	**-4.42**	**-6.60**	**-5.58**	**-6.09**	**-6.44**	**-7.19**

Table 2: Performance of the VRNN on the polyphonic music datasets trained with different bounds and numbers of particles.

N	Bound	TIMIT			
		64 units		512 units	
		Train	Test	Train	Test
	ELBO	36,095	35,908	35,765	36,981
4	IWAE	35,519	35,984	36,833	34,067
	FIVO	**39,636**	**40,211**	**40,940**	**41,834**
	ELBO	35,617	35,612	38,467	37,902
8	IWAE	35,822	36,835	37,161	38,074
	FIVO	**40,019**	**40,912**	**40,963**	**41,666**

Table 3: Performance of the VRNN on the TIMIT dataset trained with different bounds and numbers of particles.