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, 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. 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 \[20, 21\]
that 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 \( \log p(x) \),

\[
    p^* = \underset{p \in \mathcal{P}}{\text{argmax}} \log \left( \int p(x, z) \, dz \right) \quad (1)
\]

In applications with neural networks, the densities \( p \in \mathcal{P} \) are normally parameterized differentiably
by parameters \( \theta \) \[23, 24, 25\], and optimizing the likelihood via stochastic gradient ascent in \( \theta \) 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 \( q(z|x) \) denote a conditional density on \( \mathcal{Z} \) given \( x \). The ELBO is defined as,

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

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 \( q^*(x, p) = \text{argmax}_q \mathcal{L}(x, p, q) \), then \( q^*(x, p)(z) = p(z|x) \) and

\[
    \mathcal{L}(x, p, q^*(x, p)) = \log p(x). \quad (3)
\]

\footnote{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 $\theta$ and $\phi$, 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 $q_\phi$ is a reparameterizable distribution [1, 2]. Reparameterizable distributions are those constructed by taking the average importance weights, and of itself, and it will stochastically lower bound $\log f_\phi(x, \epsilon)$. With reparameterization, the ELBO becomes,

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

When $p_\theta, q_\phi$, and $f_\phi$ are differentiable, optimization proceeds by sampling $\epsilon$, 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 $q_\phi$ and the true posterior. This tends to reduce the capacity of the model $p_\theta$ to match the modelling assumptions of the variational posterior $q_\phi$ — 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,

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

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

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

(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

$$\log p(x) - \mathcal{L}_N(x, p) = \frac{1}{2} \text{var} \left( \frac{\hat{p}_N(x)}{p(x)} \right) + O(\sqrt{g(N)}).$$

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. [10] 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 favorably 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 $n$ $X$-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 $Z$-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, $p(x_{1:n}, z_{1:n}) = p_1(x_1, z_1) \prod_{k=2}^{n} p_k(x_k | x_{1:k-1}, z_{1:k-1})$. An example is the hidden Markov model (HMM), in which the density of the process factorizes as $p(x_{1:n}, z_{1:n}) = p_1(z_1) g(x_1 | z_1) \prod_{k=2}^{n} p_k(z_k | z_{k-1}) g(x_k | z_k)$ 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 $k$,

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

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,

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

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

1: $\text{FIVO}(x_{1:n}, p, q, N);$
2: $\{w^{i}_{k}\}_{i=1}^{N} = \{1/N\}_{i=1}^{N};$
3: for $k \in \{1, \ldots, n\}$ do
4:   for $i \in \{1, \ldots, N\}$ do
5:     $z^{i}_{k} \sim q_{k}(z^{i}_{k}|x_{1:k-1});$
6:     $z^{1:i}_{k} = \text{CONCAT}(z^{1:i-1}_{k}, z^{i}_{k});$
7:     $\hat{p}_{k} = \sum_{i=1}^{N} w^{i}_{k-1} \alpha_{k}(z^{1:i}_{k});$
8:     $\hat{p}_{N}(x, y) = \hat{p}_{N}(x_{1:n}|\tau_{k}) / \hat{p}_{k};$
9:     $\{w^{i}_{k}\}_{i=1}^{N} = (w^{i}_{k-1} \alpha_{k}(z^{i}_{k}) / \hat{p}_{k})_{i=1}^{N};$
10: if resampling criteria satisfied by $\{w^{i}_{k}\}_{i=1}^{N}$ then
11:     $\{w^{i}_{k}, z^{i}_{k}\}_{i=1}^{N} = \text{RSAMP}(\{w^{i}_{k}, z^{i}_{k}\}_{i=1}^{N});$
12: return $\log \hat{p}_{N}(x_{1:n});$
13: $\text{RSAMP}(\{w^{i}_{k}, z^{i}_{k}\}_{i=1}^{N});$
14: for $i \in \{1, \ldots, N\}$ do
15:     $a \sim \text{Categorical}(\{w^{i}_{k}\}_{i=1}^{N});$
16:     $y^{i} = z^{a};$
17: return $\left(\frac{1}{N}, y^{i}\right)_{i=1}^{N};$

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 $\mathcal{L}^{\text{FIVO}}_{N}(x_{1:n}, p, q)$ is a filtering variational objective.

As long as $\log \hat{p}_{N}(x_{1:n})$ is uniformly integrable, then $\mathcal{L}^{\text{FIVO}}_{N}(x_{1:n}, p, q)$ 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, $\mathcal{L}^{\text{FIVO}}_{N}(x_{1:n}, p, q)$ is only distinguished from $\mathcal{L}^{\text{IWAE}}_{N}(x_{1:n}, p, q)$ 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 $\mathcal{L}^{\text{FIVO}}_{N}(x_{1:n}, p, q)$ to be a tighter bound than the $\mathcal{L}(x_{1:n}, p, q)$ or the $\mathcal{L}^{\text{IWAE}}_{N}(x_{1:n}, p, q)$. 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

FIVO 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 $\theta$ and $\phi$. 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 $z^{i}_{k}$ are reparameterized, the gradient flows through the lattice of states $z^{i}_{k}$ created in the forward process (see Figure 1). If $1_{k}$ indicates a resampling time, then the gradient simplifies to

$$\nabla_{\theta, \phi} \log \hat{p}_{N}(x_{1:n}) + \sum_{k=1}^{n} \sum_{i=1}^{N} 1_{k} (\log \hat{p}_{N}(x_{1:n}) - \log \hat{p}_{N}(x_{1:k})) \nabla_{\theta, \phi} \log w^{i}_{k}. \quad (11)$$

In practice, the resampling gradients $\nabla_{\theta, \phi} \log w^{i}_{k}$ 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 $\nabla_{\theta, \phi} \log \hat{p}_{N}(x_{1:n})$.
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 \( q^*(x_{1:n}, p) = \text{argmax}_q \mathcal{L}^{\text{FIVO}}_N(x_{1:n}, p, q) \), 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 \( \mathcal{L}^{\text{FIVO}}_N(x_{1:n}, p, q) \) be a FIVO, and \( q^*(x_{1:n}, p) = \text{argmax}_q \mathcal{L}^{\text{FIVO}}_N(x_{1:n}, p, q) \). 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 \( k \in \{2, \ldots, n\} \), then

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

**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. 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 \([55]\).
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 natural 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 \(x_n\) 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

\[
p_k(z_k | x_{1:k}) = \prod_{k=2}^{n} p_k(z_k | h_k(z_{k-1}, x_{k-1}, h_{k-1})) g_k(x_k | z_k, h_k(z_{k-1}, x_{k-1}, h_{k-1})).
\] (12)

Similarly the variational posterior factorizes as

\[
q_k(z_k | x_{1:k}) = \prod_{k=2}^{n} q_k(z_k | h_k(z_{k-1}, x_{k-1}, h_{k-1}), x_k).
\] (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 \(L(x_{1:n}, p, q), L_{64}^{\text{IWAE}}(x_{1:n}, p, q), L_{64}^{\text{FIVO}}(x_{1:n}, p, q)\), 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,
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.
References

[1] Diederik P Kingma and Max Welling. Auto-encoding variational Bayes. *arXiv preprint arXiv:1312.6114*, 2013.

[2] Danilo Jimenez Rezende, Shakir Mohamed, and Daan Wierstra. Stochastic backpropagation and approximate inference in deep generative models. *arXiv preprint arXiv:1401.4082*, 2014.

[3] Laurent Dinh, Jascha Sohl-Dickstein, and Samy Bengio. Density estimation using real nvp. *arXiv preprint arXiv:1605.08803*, 2016.

[4] Ian Goodfellow, Jean Pouget-Abadie, Mehdi Mirza, Bing Xu, David Warde-Farley, Sherjil Ozair, Aaron Courville, and Yoshua Bengio. Generative adversarial nets. In *Advances in neural information processing systems*, pages 2672–2680, 2014.

[5] Sebastian Nowozin, Botond Cseke, and Ryota Tomioka. f-gan: Training generative neural samplers using variational divergence minimization. *arXiv preprint arXiv:1606.00709*, 2016.

[6] Dustin Tran, Rajesh Ranganath, and David M Blei. Deep and hierarchical implicit models. *arXiv preprint arXiv:1702.08896*, 2017.

[7] Shakir Mohamed and Balaji Lakshminarayanan. Learning in implicit generative models. *arXiv preprint arXiv:1610.03483*, 2016.

[8] Yuhuai Wu, Yuri Burda, Ruslan Salakhutdinov, and Roger Grosse. On the quantitative analysis of decoder-based generative models. *arXiv preprint arXiv:1611.04273*, 2016.

[9] I. Danihelka, B. Lakshminarayanan, B. Uria, D. Wierstra, and P. Dayan. Comparison of Maximum Likelihood and GAN-based training of Real NVPs. *arXiv preprint arXiv:1705.05263*, 2017.

[10] Arthur P Dempster, Nan M Laird, and Donald B Rubin. Maximum likelihood from incomplete data via the EM algorithm. *J. R. Stat. Soc. Ser. B Stat. Methodol.*, pages 1–38, 1977.

[11] Michael J Jordan, Zoubin Ghahramani, Tommi S Jaakkola, and Lawrence K Saul. An introduction to variational methods for graphical models. *Machine learning*, 37(2):183–233, 1999.

[12] Matthew J. Beal. *Variational algorithms for approximate Bayesian inference*. 2003.

[13] Matthew D Hoffman, David M Blei, Chong Wang, and John William Paisley. Stochastic variational inference. *Journal of Machine Learning Research*, 14(1):1303–1347, 2013.

[14] Rajesh Ranganath, Sean Gerrish, and David Blei. Black box variational inference. In *Artificial Intelligence and Statistics*, pages 814–822, 2014.

[15] Alp Kucukelbir, Dustin Tran, Rajesh Ranganath, Andrew Gelman, and David M Blei. Automatic differentiation variational inference. *arXiv preprint arXiv:1603.00788*, 2016.

[16] Yuri Burda, Roger Grosse, and Ruslan Salakhutdinov. Importance weighted autoencoders. *arXiv preprint arXiv:1509.00519*, 2015.

[17] Andriy Mnih and Danilo J Rezende. Variational inference for Monte Carlo objectives. *arXiv preprint arXiv:1602.06725*, 2016.

[18] Neil J Gordon, David J Salmond, and Adrian FM Smith. Novel approach to nonlinear/non-gaussian bayesian state estimation. In *IEE Proceedings F (Radar and Signal Processing)*, volume 140, pages 107–113. IET, 1993.

[19] Arnaud Doucet and Adam M. Johansen. A tutorial on particle filtering and smoothing: Fifteen years later. In D. Crisan and B. Rozovsky, editors, *The Oxford Handbook of Nonlinear Filtering*, pages 656–704. Oxford University Press, 2011.

[20] Frédéric Cérou, Pierre Del Moral, and Arnaud Guyader. A nonasymptotic theorem for unnormalized Feynman–Kac particle models. *Ann. Inst. H. Poincaré B*, 47(3):629–649, 2011.

[21] Jean Bérard, Pierre Del Moral, and Arnaud Doucet. A lognormal central limit theorem for particle approximations of normalizing constants. *Electron. J. Probab.*, 19(94):1–28, 2014.

[22] Christian Andersson Naesseth, Fredrik Lindsten, and Thomas B Schön. Sequential monte carlo for graphical models. In *Advances in Neural Information Processing Systems*, pages 1862–1870, 2014.
[23] Hugo Larochelle and Iain Murray. The neural autoregressive distribution estimator. In *AISTATS*, 2011.

[24] Benigno Uria, Iain Murray, and Hugo Larochelle. A deep and tractable density estimator. In *ICML*, pages 467–475, 2014.

[25] Aaron van den Oord, Nal Kalchbrenner, and Koray Kavukcuoglu. Pixel recurrent neural networks. *arXiv preprint arXiv:1601.06759*, 2016.

[26] Aaron van den Oord, Sander Dieleman, Heiga Zen, Karen Simonyan, Oriol Vinyals, Alex Graves, Nal Kalchbrenner, Andrew Senior, and Koray Kavukcuoglu. Wavenet: A generative model for raw audio. *arXiv preprint arXiv:1609.03499*, 2016.

[27] Lawrence K Saul, Tommi Jaakkola, and Michael I Jordan. Mean field theory for sigmoid belief networks. *Journal of Artificial Intelligence Research*, 4(1):61–76, 1996.

[28] Tommi S Jaakkola and Michael I Jordan. Computing upper and lower bounds on likelihoods in intractable networks. In *Proceedings of the twelfth international conference on Uncertainty in Artificial Intelligence*, pages 340–348. Morgan Kaufmann Publishers Inc., 1996.

[29] Zoubin Ghahramani and Michael I Jordan. Factorial hidden Markov models. In *Advances in Neural Information Processing Systems*, pages 472–478, 1996.

[30] R. M Neal and Geoffrey E Hinton. A view of the EM algorithm that justifies incremental, sparse, and other variants. In *Learning in graphical models*, pages 355–368. Springer, 1998.

[31] Andriy Mnih and Karol Gregor. Neural variational inference and learning in belief networks. *arXiv preprint arXiv:1402.0030*, 2014.

[32] Yarin Gal. *Uncertainty in Deep Learning*. PhD thesis, University of Cambridge, 2016.

[33] Siddhartha Chib. Marginal likelihood from the Gibbs output. *Journal of the American Statistical Association*, 80(394):1133–1141, 1995.

[34] Xiao-Li Meng and Wing Hung Wong. Simulating ratios of normalizing constants via a simple identity: a theoretical exploration. *Statistica Sinica*, pages 831–860, 1996.

[35] Andrew Gelman and Xiao-Li Meng. Simulating normalizing constants: From importance sampling to bridge sampling to path sampling. *Statistical science*, pages 163–185, 1998.

[36] Roger B Grosse, Zoubin Ghahramani, and Ryan P Adams. Sandwiching the marginal likelihood using bidirectional Monte Carlo. *arXiv preprint arXiv:1511.02543*, 2015.

[37] Yuri Burda, Roger Grosse, and Ruslan Salakhutdinov. Accurate and conservative estimates of MRF log-likelihood using reverse annealing. In *Artificial Intelligence and Statistics*, pages 102–110, 2015.
Appendix of Filtering Variational Objectives

Gradients of $\mathcal{L}^{FIVO}_{N}(x_{1:n}, p, q)$. We formulate an unbiased gradient of $\mathcal{L}^{FIVO}_{N}(x_{1:n}, p, q)$ under no assumptions about the forward sampling process. There are two types of stochastic values in Algorithm 1, the latent variables $z_i^k$ 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 $k$,

$$
\nabla_{\theta, \phi} \log \hat{p}_N(x_{1:n}) + \sum_{k=1}^{n} \sum_{i=1}^{N} \left( \log \frac{\hat{p}_N(x_{1:n})}{\hat{p}_N(x_{1:k-1})} \nabla_{\phi} \log q_{k, \phi}(z_i^k | x_{1:k}, z_i^{1:k-1}) + 1_k \log \frac{\hat{p}_N(x_{1:n})}{\hat{p}_N(x_{1:k})} \nabla_{\theta, \phi} \log w_i^k \right)
$$

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 $\hat{p}_N(x)$. 


(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 \( \lim \sup \mathbb{E}[(\hat{p}_N(x))^{-1}] < \infty \). Define the relative error

\[ \Delta = \frac{\hat{p}_N(x) - p(x)}{p(x)} \]

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

\[ \log(1 + \Delta) = \Delta - \frac{1}{2} \Delta^2 + \int_0^\Delta \left( \frac{1}{1 + x} - 1 + x \right) \, dx \]

and in expectation

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

Our aim is to show

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

In particular, by Cauchy-Schwarz

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

\[ = \mathbb{E} \left[ \frac{\Delta}{1 + \Delta} \right]^{1/2} \left( \frac{\Delta^5}{5} \right)^{1/2} \]

\[ = \mathbb{E} \left[ \frac{1}{1 + \Delta} \right]^{1/2} \left( \frac{\Delta^6}{5} \right)^{1/2} \]

and again by Cauchy-Schwarz

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

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 \( \mathcal{L}^{\text{VBO}}_N(x_{1:n}, p, q) = \log p(x_{1:n}) \) 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

\[ \alpha_1^*(z_1) = \frac{p_1(x_1, z_1)}{p(z_1 | x_1)} = p_1(x_1) \]
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

\[
\alpha_k(z_{1:k}) = \frac{p_k(x_k, z_k | z_{1:k-1}, x_{1:k-1})}{p(z_k | z_{1:k-1}, x_{1:k})}
\]

and thus,

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

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

| N  | Bound | Nottingham | JSB Chorales | MuseData | Piano-MIDI.de |
|----|-------|------------|--------------|----------|---------------|
|    |       | Train      | Test         | Train    | Test          | Train | Test |
| 4  | ELBO  | -3.03      | -3.23        | -5.38    | -8.61         | -5.42 | -7.12 | -7.06 | -7.79 |
|    | 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 |
| 8  | ELBO  | -3.04      | -3.60        | -6.10    | -8.60         | -5.93 | -7.11 | -7.33 | -7.83 |
|    | 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 |
| 16 | ELBO  | -3.39      | -3.54        | -6.10    | -8.60         | -6.18 | -7.17 | -7.23 | -7.83 |
|    | 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 3: Performance of the VRNN on the TIMIT dataset trained with different bounds and numbers of particles.

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

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

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