Variational Inference with Locally Enhanced Bounds for Hierarchical Models

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Abstract
Hierarchical models represent a challenging setting for inference algorithms. MCMC methods struggle to scale to large models with many local variables and observations, and variational inference (VI) may fail to provide accurate approximations due to the use of simple variational families. Some variational methods (e.g. importance weighted VI) integrate Monte Carlo methods to give better accuracy, but these tend to be unsuitable for hierarchical models, as they do not allow for subsampling and their performance tends to degrade for high dimensional models. We propose a new family of variational bounds for hierarchical models, based on the application of tightening methods (e.g. importance weighting) separately for each group of local random variables. We show that our approach naturally allows the use of subsampling to get unbiased gradients, and that it fully leverages the power of methods that build tighter lower bounds by applying them independently in lower dimensional spaces, leading to better results and more accurate posterior approximations than relevant baselines.

1. Introduction
Hierarchical models (Kreft & De Leeuw, 1998; Gelman, 2006; Snijders & Bosker, 2011) represent a general class of probabilistic models which are used in a wide range of scenarios. They have been successfully applied in psychology (Vallerand, 1997), ecology (Royle & Dorazio, 2008; Cressie et al., 2009), political science (Lax & Phillips, 2012), collaborative filtering (Lim & Teh, 2007), and topic modeling (Blei et al., 2003), among others. While these models may take a wide range of forms, a widely used one consists on a tree structure, where a set of global variables $\theta$ controls the distribution over local variables $z_i$ in multiple independent groups (see Figure 1 (left)). Then, after observing some data $y_i$ from each group, the inference problem consists on accurately approximating the posterior distribution over the global and local variables.

Inference is often difficult in hierarchical models. MCMC methods, on the one hand, struggle to scale to big models and datasets due to their incapacity to handle subsampling (Betancourt, 2015; Bardenet et al., 2017). Variational inference (VI) methods, on the other hand, are naturally compatible with subsampling, and thus represent a more scalable alternative (Hoffman et al., 2013; Titsias & Lázaro-Gredilla, 2014; Agrawal & Domke, 2021). Their accuracy, however, is sometimes limited by the use of simple variational families, such as factorized Gaussians.

Recently, many methods have been proposed to integrate Monte Carlo methods into variational inference to give tighter bounds and better posterior approximations (henceforth tightening methods). These include importance weighting (Burda et al., 2016) and many others (Salimans et al., 2015; Wolf et al., 2016; Maddison et al., 2017; Domke & Sheldon, 2019; Thin et al., 2021; Zhang et al., 2021; Geffner & Domke, 2021b). While these methods have shown good performance in practice, we observe that a direct application of them may be unsuitable with hierarchical models. There are two reasons for this. First, the posterior distributions for hierarchical models are often high dimensional—the dimensionality typically grows linearly with the number of local variables. This is problematic as the performance of tightening methods tends to degrade in higher dimensions. Second, current tightening methods are incompatible with subsampling, leading to slow inference.

Practitioners are thus faced with a choice: They can use powerful but inefficient methods (variational inference with tightening methods), or faster methods with lower accuracy (plain variational inference).

We propose locally-enhanced bounds, a new family of variational objectives for hierarchical models that enjoys much of the best of both worlds. The main idea involves applying tightening methods at a local level, separately for each set of local variables $z_i$, while using a regular variational approximation (e.g. Gaussian, normalizing flow) to model the posterior distribution over the global variables. This is naturally compatible with subsampling, making inference more efficient. Additionally, it maintains much of the bene-
2. Preliminaries

2.1. Hierarchical Models

While hierarchical models may take a wide range of forms (Gelman & Hill, 2006), in this work we focus on a two-level formulation, using $\theta$ to denote the global variables, and $z_i$ and $y_i$ to denote the local variables and observations of group $i$. By letting $z = (z_1, \ldots, z_M)$ and $y = (y_1, \ldots, y_M)$, the corresponding probabilistic model is given by

$$p(\theta, z, y) = p(\theta) \prod_{i=1}^{M} p(z_i, y_i|\theta)$$

(1)

where the exact form of $p(z_i, y_i|\theta)$ depends on the application. Often, $y_i$ is conditionally independent of $\theta$ given $z_i$, and so $p(z_i, y_i|\theta) = p(y_i|z_i)p(z_i|\theta)$. In addition, $y_i$ often consists on $N_i$ observations $y_{i1}, \ldots, y_{iN_i}$ that are conditionally independent given $z_i$, and so $p(y_i|z_i) = \prod_{j=1}^{N_i} p(y_{ij}|z_i)$. However neither of these simplifications is required.

2.2. Variational Inference

Variational Inference is a popular method used to approximate posterior distributions. Given some model $p(z, y)$, where $y$ is observed data and $z$ latent variables, the goal of variational inference is to find a simpler distribution $q(z)$ to approximate the target $p(z|y)$ (Jordan et al., 1999; Wainwright et al., 2008; Blei et al., 2017). VI does this by finding the parameters of $q(z)$ that maximize the evidence lower bound (ELBO), a lower bound on the log-marginal likelihood $\log p(y)$, given by

$$\mathcal{L}_{\text{VI}}(q(z)||p(z, y)) = \mathbb{E}_{q(z)} \log \frac{p(z, y)}{q(z)}.$$  

(2)

It can be shown that this is equivalent to minimizing the KL-divergence from $q(z)$ to the true posterior $p(z|y)$.

2.3. Tighter Bounds for Variational Inference

While VI has been successfully applied in a wide range of tasks (Blei et al., 2017; Zhang et al., 2017), its performance is sometimes limited by the use of simple approximating families for $q(z)$, such as Gaussians. A popular approach to address this drawback involves using tighter lower bounds on the log-marginal likelihood (Burda et al., 2016; Zhang et al., 2021), which lead to better posterior approximations (Domke & Sheldon, 2018; 2019).
Locally Enhanced Bounds for Hierarchical Models

Importance Weighting (IW) (Burda et al., 2016; Cremer et al., 2017) uses $K$ samples $z^k \sim q(z^k)$ to build a lower bound on the log-marginal likelihood $\log p(y)$ as

$$
\mathcal{L}_{\text{IW}}^K(q(z)||p(z,y)) = \mathbb{E}_{\prod_k q(z^k)} \log \frac{1}{M} \sum_{k=1}^K \frac{p(z^k,y)}{q(z^k)},
$$

which is provably tighter than the variational inference bound from Equation (2) for any $K \geq 1$.

Annealed Importance Sampling (AIS) (Neal, 2001) is another method that can be used to build tighter bounds. It defines a sequence of $K-1$ (unnormalized) densities $\pi^1(z), \ldots, \pi^{K-1}(z)$ that gradually bridge from $q(z)$ to $p(z,y)$. Then, it augments $q(z)$ using MCMC transitions $T^k(z^{k+1}|z^k)$ that hold the corresponding bridging density $\pi^k$ invariant, and builds a lower bound on $\log p(y)$ as

$$
\mathcal{L}_{\text{AIS}}^K(q(z)||p(z,y)) = \mathbb{E}_{q(z^1)} \log \frac{p(z^K,y)}{q(z^1)} \frac{1}{M} \sum_{k=1}^{K-1} \frac{\pi^k(z^k)}{\pi^{k+1}(z^{k+1})},
$$

where $z^k$ represents the $k$-th variable generated by the MCMC-augmented sampling process. It has been observed that AIS with Hamiltonian Monte Carlo kernels (Neal et al., 2011; Betancourt, 2017) often yields tight lower bounds in practice (Sohl-Dickstein & Culpepper, 2012; Grosse et al., 2015; Wu et al., 2017). However, since the HMC transitions include a correction step, the resulting bound is not differentiable. Thus, low variance reparameterization gradients cannot be used to tune the method’s many parameters.

Uncorrected Hamiltonian Annealing (UHA) (Geffner & Domke, 2021b; Zhang et al., 2021) is a method that addresses the non-differentiability drawback suffered by Hamiltonian AIS. It does so by mimicking the construction used by Hamiltonian AIS, but using uncorrected HMC kernels for the transitions. Then, UHA builds a differentiable lower bound on the log-marginal likelihood $\log p(y)$ as

$$
\mathcal{L}_{\text{UHA}}^K(q(z)||p(z,y)) = \mathbb{E}_{q(z^1,K,\rho^1,K)} \log \frac{p(z^K,y)}{q(z^1)} \prod_{k=1}^{K-1} \frac{r(\rho^{k+1})}{r(\hat{\rho}^k)},
$$

where $\rho^k$ and $\hat{\rho}^k$ are the momentum variables generated by HMC at each step $k$, and $z^1$ and $z^K$ are the first and last samples from the chain, respectively. We give full details on AIS and UHA in Appendix B.

All these methods have been observed to provide lower bounds that are significantly tighter than the original one used by variational inference, resulting in better posterior approximations (Domke & Sheldon, 2019).

3. Locally Enhanced Bounds for Hierarchical Models

This section introduces our method. We begin with a brief description on the use of variational inference and tightening methods for hierarchical models and their limitations. We then introduce our new family of variational bounds, locally-enhanced bounds, which addresses these limitations.

3.1. Variational Inference for Hierarchical Models

Given a hierarchical model $p(\theta, z, y)$ and some observations for $y$, we can approximate the posterior distribution $p(\theta, z|y)$ using VI with a variational distribution $q(\theta, z)$. There are many potential choices for the approximating distribution. One could use, for instance, a Gaussian with a diagonal or dense covariance (Challis & Barber, 2013). However, best results have been observed using a distribution that follows the true posterior’s factorization (Hoffman & Blei, 2015; Agrawal & Domke, 2021)

$$
q(\theta, z) = q(\theta) \prod_{i=1}^M q(z_i|\theta),
$$

which explicitly avoids modeling dependencies not present in the target posterior. Then, the parameters of $q(\theta, z)$ are trained by maximizing the objective

$$
\mathcal{L}_{\text{VI}}(q(\theta, z)||p(\theta, z, y)) = \mathbb{E}_{q(\theta,z)} \left[ \log \frac{p(\theta)}{q(\theta)} + \sum_{i=1}^M \log \frac{p(z_i,y_i|\theta)}{q(z_i|\theta)} \right].
$$

While computing this objective’s exact gradient is typically intractable, an unbiased estimate can be efficiently obtained by applying the reparameterization trick (Kingma & Welling, 2013; Rezende et al., 2014; Titsias & Lázaro-Gredilla, 2014) and subsampling $M' < M$ local terms. The fact that VI allows for subsampling makes the method a particularly attractive choice for cases where the number of groups $M$ is large.

3.2. Unsuitability of Tightening Methods for Hierarchical Models

One can directly apply tightening methods to variational inference for hierarchical models. However, this may work poorly when the number of groups $M$ is large. This is because these methods provide less tightening in high dimensions (particularly importance weighting (Bengtsson et al., 2021)).

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1For simplicity, the notation for the transitions and bridging densities ignores their dependency on $y$, which is fixed.

2The reparameterization trick is applicable for distributions $q(\theta, z)$ parameterized by $w$ for which the sampling process can be divided in two steps: Sampling a $w$-independent noise variable $\epsilon \sim q_0(\epsilon)$, and then obtaining the sample $(\theta, z)$ as a $w$-dependent differentiable transformation $(\theta, z) = T_\omega(\epsilon)$.  

This section introduces our method. Our goal is to apply importance weighting objective for hierarchical models

\[
\mathcal{L}^K_{IW}(q(\theta, z) \parallel p(\theta, z, y)) = 
\mathbb{E}_{q(z^y)} \left[ \log \frac{1}{K} \sum_{k=1}^{K} \frac{p(\theta^k)}{q(\theta^k)} \prod_{i=1}^{M} \frac{p(z^k_i, y_i | \theta^k)}{q(z^k_i | \theta^k)} \right].
\] (7)

There does not appear to be any way to estimate the objective above subsampling \(M' < M\) groups without introducing bias. This is problematic for stochastic optimization, as using no subsampling leads to expensive gradient evaluations and a slow overall optimization process, but the use of biased gradients may lead to suboptimal parameters (Naesseth et al., 2020; Geffner & Domke, 2021a) or may cause the optimization process to diverge (Ajalleian & Stich, 2020).

Importance weighting is not unique in this regard. Other methods, such as annealed importance sampling or uncorrected Hamiltonian annealing, also lead to objectives that do not allow unbiased subsampling either (Zhang et al., 2021).

### 3.3. Variational Inference with Locally Enhanced Bounds

This section introduces our method. Our goal is to apply tightening methods to boost variational inference’s performance on hierarchical models while avoiding the aforementioned issues. We propose to achieve this by applying tightening methods only for the local variables, separately for each group \(i = 1, \ldots, M\). This leads to a new family of variational objectives, which we call locally-enhanced bounds. Our construction of this new family of bounds is based on the concept of a bounding operator.

**Definition 3.1 (Bounding operator).** An operator \(\mathcal{L}(\cdot; | \cdot)\) is a bounding operator if, for any distributions \(q(z)\) and \(p(z, y)\), it satisfies \(\mathcal{L}(q(z) || p(z, y)) \leq \log p(y)\).

Example bounding operators we have seen so far include plain VI (Equation (2)), importance weighted VI (Equation (3)), and uncorrected Hamiltonian annealing (Equation (4)).

Building locally-enhanced bounds is simple. We begin by observing that the typical objective used by VI with hierarchical models, shown in Equation (6), can be re-written as

\[
\mathcal{L}_{VI}(q(\theta, z) \parallel p(\theta, z, y)) = \mathbb{E}_{q(z^y)} \left[ \log \frac{p(\theta)}{q(\theta)} + \sum_{i=1}^{M} \frac{\log p(z_i | y_i)}{\log q(z_i | \theta)} \right]
\]

\[= \mathbb{E}_{q(\theta)} \left[ \log \frac{p(\theta)}{q(\theta)} + \sum_{i=1}^{M} \mathcal{L}_{VI}(q(z_i | \theta) || p(z_i, y_i | \theta)) \right].
\] (8)

Then, a locally-enhanced bound is obtained by replacing \(\mathcal{L}_{VI}\) in the last line of Equation (8) by any other bounding operator. One could use any of the tightening techniques described in Section 2.3, such as importance weighting or uncorrected Hamiltonian annealing. (One could also use AIS, though this yields a non-differentiable objective.) The following theorem shows that bounds constructed this way always yield valid variational objectives.

**Theorem 3.2.** Let \(p(\theta, z, y) = p(\theta) \prod_{i=1}^{M} p(z_i, y_i | \theta)\) and \(q(\theta, z) = q(\theta) \prod_{i=1}^{M} q(z_i | \theta)\) be any distributions, and let \(\mathcal{L}(\cdot; | \cdot)\) be a bounding operator. Then,

\[
\mathbb{E}_{q(\theta)} \left[ \log \frac{p(\theta)}{q(\theta)} + \sum_{i=1}^{M} \mathcal{L}(q(z_i | \theta) || p(z_i, y_i | \theta)) \right] \leq \log p(y).
\] (9)

In particular, the gap in the above inequality is

\[
\mathbb{E}_{q(\theta)} \left[ \log \frac{p(\theta)}{q(\theta)} \right] + \sum_{i=1}^{M} \mathbb{E}_{q(z_i | \theta)} \left[ \log \frac{p(z_i, y_i | \theta)}{q(z_i | \theta)} \right].
\] (10)

We include a proof in Appendix A. Theorem 3.2 states that we can build a valid locally-enhanced variational bound by using Equation (9) with any valid bounding operator \(\mathcal{L}(\cdot; | \cdot)\). Some examples include, for instance, \(\mathcal{L}_{IW}^K\) or \(\mathcal{L}_{UHA}^K\), corresponding to importance weighting and uncorrected Hamiltonian annealing, introduced in Section 2.3. Equivalently, this construction can be seen as applying the corresponding tightening method at a local level, separately for each group, as shown in Figure 1.

For concreteness, consider importance weighting and its corresponding bounding operator \(\mathcal{L}_{IW}^K\). Following the construction described above, we get a locally-enhanced bound of

\[
\mathbb{E}_{q(\theta)} \left[ \log \frac{p(\theta)}{q(\theta)} + \sum_{i=1}^{M} \mathbb{E}_{q(z_i | \theta)} \left[ \log \frac{1}{K} \sum_{k=1}^{K} \frac{p(z^k_i, y_i | \theta)}{q(z^k_i | \theta)} \right] \right].
\] (11)

**Benefits of locally-enhanced bounds** The benefits of using locally-enhanced bounds are twofold. First, they naturally allow the use of subsampling. This can be seen by noting that the generic locally-enhanced bound from Equation (9) can be estimated without bias using a subset of local variables \(I \subset \{1, \ldots, M\}\) as

\[
\mathbb{E}_{q(\theta)} \left[ \log \frac{p(\theta)}{q(\theta)} + \frac{M}{|I|} \sum_{i \in I} \mathcal{L}(q(z_i | \theta) || p(z_i, y_i | \theta)) \right],
\] (12)

where \(|I|\) denotes the size of the set \(I\). This is in contrast to direct applications of tightening methods, which are incompatible with subsampling.
Second, they fully leverage the power of tightening methods by applying them separately for each set of local variables, which are often low-dimensional. In fact, for hierarchical models with \( M \) groups, the local variables’ dimensionality is, on average, \( M \) times smaller than that of the full model. Then, one may expect tightening methods to perform well when applied this way. We verify this empirically in Section 5, where we observe that locally-enhanced bounds obtained with importance weighting tend to be considerably better than those obtained by applying the same method directly for the full model all at once.

**Tightness of locally-enhanced bounds** Equation (9) shows that better tightening methods lead to tighter locally-enhanced bounds. However, Equation (10) states that, even in the ideal case where the perfect bounding operator is available,\(^3\) locally-enhanced bounds are only able to fully close the variational gap if the variational approximation over global variables \( q(\theta) \) is a perfect approximation of the true posterior \( p(\theta|y) \). If this is not the case, the application of a perfect tightening method yields a variational gap of \( \text{KL}(q(\theta)||p(\theta|y)) \).

Often, this does not represent a significant drawback. In practice, for moderately large datasets, the true posterior over global variables \( p(\theta|y) \) is informed by a large number of observations, and thus we might expect it to concentrate and roughly follow a Gaussian distribution. In such cases, accurate approximations can be obtained using a Gaussian variational family. Moreover, even in cases where the true global posterior is non-Gaussian (e.g. small dataset), one could use a more flexible family for \( q(\theta) \), such as normalizing flows (Tabak & Turner, 2013; Rezende & Mohamed, 2015). This can be done efficiently, as the dimensionality of \( \theta \) is often moderately low and, more importantly, does not depend on the number of groups \( M \) nor number of observations.

### 4. Related Work

There is a lot of work on related topics, such as the development of more flexible variational approximations (Tabak & Turner, 2013; Rezende & Mohamed, 2015), better tightening methods (Salimans et al., 2015; Domke & Sheldon, 2019), and more efficient variational methods for hierarchical models (Agrawal & Domke, 2021). Most of these represent contributions orthogonal to ours, and can be used jointly with our locally-enhanced bounds.

Normalizing flows (Tabak & Turner, 2013; Rezende & Mohamed, 2015; Kingma et al., 2016; Tomczak & Welling, 2016), for instance, are a powerful method to build flexible variational approximations using invertible parametric transformations. Since they typically require a large number of parameters, they are sometimes impractical for very high dimensional problems, such as those that arise when working with hierarchical models with many latent variables. Despite this, they can be used jointly with our method. One could use flows for each local approximation \( q(z_i|\theta) \) and/or for the global approximation \( q(\theta) \), and then optimize their parameters by maximizing a locally-enhanced bound.

Additionally, many powerful tightening methods have been developed (Agakov & Barber, 2004; Burda et al., 2016; Salimans et al., 2015; Domke & Sheldon, 2019; Geffner & Domke, 2021b; Zhang et al., 2021). All these methods can be easily used to build locally-enhanced bounds following our construction from Section 3.3.

Specifically for hierarchical models, Hoffman & Blei (2015) introduced a flexible framework for fast stochastic variational inference. Their approach, however, requires conjugacy, limiting its applicability. To overcome this limitation, Agrawal & Domke (2021) proposed a parameter efficient algorithm that uses a single amortization network (Kingma & Welling, 2013) to parameterize all local approximations \( q(z_i|\theta) \). This approach is compatible with our method, as this amortized variational distribution can be used with locally-enhanced bounds.

Finally, concurrently with this work, Jankowiak & Phan (2021) proposed several promising extensions for uncorrected Hamiltonian Annealing (Geffner & Domke, 2021b; Zhang et al., 2021). One of them involves its use for hierarchical models, applying it independently for each set of local variables. This is equivalent to a locally-enhanced bound built using uncorrected Hamiltonian Annealing. Although this is a minor focus of their work, it can be seen as an instance of our general framework.

### 5. Experiments

This section presents an empirical evaluation of our new bounding technique. We perform variational inference using locally-enhanced bounds on multiple hierarchical models with real and synthetic datasets. We use a variational distribution \( q(\theta, z) = q(\theta) \prod_{i=1}^{M} q(z_i) \), where the approximation for the global variables \( q(\theta) \) is set to be a factorized Gaussian, and the local approximations \( q(z_i) \) are taken to be independent of \( \theta \) and also set to factorized Gaussians.\(^4\)

We test locally-enhanced bounds obtained using importance weighting and uncorrected Hamiltonian annealing for \( K \in \{5, 10, 15\} \). We compare against plain VI, which trains the parameters of \( q(\theta, z) \) by maximizing the \( \mathcal{L}_{\text{VI}} \) objective from Equation (6) (this corresponds to the “branch” approach from Agrawal & Domke (2021)), and against a direct/global application of importance weighting.

\(^3\)That is \( \mathcal{L}(q(z_i)||p(z_i, y_i)) = \log p(y_i) \).

\(^4\)We parameterize Gaussians using their mean and log-scale.
which uses the objective from Equation (7).

We optimize using Adam (Kingma & Ba, 2014) with a step-size $\eta = 0.001$. For the plain VI baseline and the locally-enhanced bounds, we use subsampling with $M^S = 10$ to estimate gradients at each step using the reparameterization trick (Kingma & Welling, 2013; Titsias & Lázaro-Gredilla, 2014; Rezende et al., 2014). We do not use subsampling with the global application of importance weighting, as the method does not support it. We initialize all methods to maximizers of the ELBO, and train for 50k steps. All results are reported together with their standard deviation, obtained by using five different random seeds.

We clarify that the global importance weighting baseline is also trained for 50k steps, using a full-batch approach to compute gradients at each iteration. This results in an optimization process that is significantly more expensive than that of other methods (locally-enhanced bounds and plain VI) which support subsampling.

5.1. Synthetic data

Model We consider the hierarchical model given by

$$p(\mu_z, \psi_z, \psi_y, z, y) = \mathcal{N}(\mu_z|0, 1)\mathcal{N}(\psi_z|0, 1)$$

$$\mathcal{N}(\psi_y|0, 1) \prod_{i=1}^{M}\mathcal{N}(z_i|\mu_z, e^{\psi_y}) \prod_{j=1}^{N_i}\mathcal{N}(y_{ij}|z_i x_{ij}, e^{\psi_y}),$$

(13)

where $x_{ij}$ is external information available for all observations $y_{ij}$. In this case, $\theta = (\mu_z, \psi_z, \psi_y)$ and $z$ represent the global and local variables respectively. While the above model defines the local variables $z_i$ to be one dimensional, they can also be defined to have an arbitrary dimension $d_z > 1$, by setting $\mathcal{N}(z_i|1_{d_z}, \mu_z, I_{d_z}, e^{\psi_y})$ and $\mathcal{N}(y_{ij}|z_i^T x_{ij}, e^{\psi_y})$.

Datasets We generated several datasets by sampling from the hierarchical model above. We consider different number of groups $M \in \{10, 50, 100\}$, and observations per group $N \in \{10, 30\}$. In all cases, we sample components of $x_{ij} \in \mathbb{R}^{d_z}$ independently from a standard Gaussian.

Results Results for all the generated datasets are shown in Figure 2. It can be observed that the use of locally-enhanced bounds yields significant improvements over plain VI, with the performance gap increasing for the larger values of $K$. It can also be observed that the use of locally-enhanced bounds leads to better results than the ones obtained using the global importance weighting baseline. While this baseline is somewhat competitive for the smaller models (left plots in Figure 2), it is severely outperformed by the use of locally-enhanced bounds in the larger models (right plots in Figure 2). This is despite the fact that the baseline is significantly more expensive to run, as it does not allow subsampling.

All results in Figure 2 were obtained for datasets which have

![Figure 2. Locally-enhanced bounds yield much tighter lower bounds than the baselines. The figure shows inference results using locally-enhanced bounds on synthetic datasets of different sizes. The plots show the final lower bound achieved by different methods after training for 50k steps. Both locally-enhanced methods and global IW converge to plain VI for $K = 1$. The dimensionality of the local variables $z_i$ is taken to be $d_z = 5$ for the datasets with $N = 10$ observations per group, and $d_z = 20$ for the datasets with $N = 30$ observations.](image-url)
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Figure 3. Locally-enhanced bounds yield much tighter lower bounds than Plain VI. The figure shows inference results using locally-enhanced bounds on MovieLens datasets of different sizes. The plots show the final lower bound achieved by different methods after training for 50k steps. Both locally-enhanced methods and global IW converge to plain VI for $K = 1$.

Figure 4. Locally-enhanced bounds yield much tighter lower bounds than the baselines. The figure shows inference results using locally-enhanced bounds on a synthetic dataset generated with $M = 100$ groups and a different number of observations per group (see main text). The plot shows the final lower bound achieved by different methods after training for 50k steps. Both locally-enhanced methods and global IW converge to the baseline plain VI for $K = 1$.

the same number of observations for all local groups. To verify the effect that changing this may have, we ran additionally simulations using a dataset which contained different number of observations for different groups. Specifically, we considered a dataset composed of $M = 100$ groups, out of which 50 have only 2 observations, 30 have 5 observations, and 20 have 30 observations. Results are shown in Figure 4. The same conclusion holds, with locally-enhanced bounds significantly outperforming the baselines.

5.2. Real data: Movie Lens

We now show results obtained using data from MovieLens100K (Harper & Konstan, 2015). This database contains 100k ratings from several users on 1700 movies, where each movie comes with a feature vector $x \in \{0,1\}^{18}$ containing information about its genre. While the original ratings consist on discrete values between 1 and 5, we binarize them, assigning 0 as “dislike” to ratings (1, 2, 3), and 1 as “like” to ratings (4, 5).

Model We consider the hierarchical model given by

$$p(\mu_z, \psi_z, z, y) = \mathcal{N}(\mu_z|0, I)\mathcal{N}(\psi_z|0, I)$$

$$\prod_{i=1}^M \mathcal{N}(z_i|\mu_z, \psi_z) \prod_{j=1}^N \mathcal{B}(y_{ij}|z_i^T x_{ij}),$$

where $x_{ij} \in \{0,1\}^{18}$ represents the feature vector for the $j$-th movie ranked by the $i$-th user, $\mu_z \in \mathbb{R}^{18}$ and $\psi_z \in \mathbb{R}^{18}$ represent the global variables $\theta$, and $z_i \in \mathbb{R}^{18}$ represents the local variables for group $i$, in this case the $i$-th user.

Datasets We used data from MovieLens100K to generate several datasets with a varying number of users and ratings per user. Specifically, we consider three different number of users $M \in \{10, 50, 100\}$ and two different number of ratings per user $N \in \{30, 200\}$.

Results Results are shown in Figure 3. Similarly to the results observed for the synthetic dataset, it can be observed
that the use of locally-enhanced bounds leads to significant improvements over the baselines, with the performance gap increasing for the larger values of $K$ and for the bigger models.

6. Discussion and Future Work

We introduced locally-enhanced bounds, a new type of variational objective obtained by applying tightening methods at a local level for hierarchical models following Equation (1). The approach combines the efficiency of plain variational inference and the power of tightening methods while avoiding their drawbacks.

We identify two interesting directions for future work. First, identifying what divergence is being minimized. Tightening methods can often be mapped to the minimization of some divergence in an augmented space (Domke & Sheldon, 2018; 2019). We think that understanding exactly what divergence is being minimized by each of the proposed locally-enhanced bounds would be quite useful in order to fully understand their potential. We believe this could be done using ideas from (Domke & Sheldon, 2019).

And second, how can we develop more general locally-enhanced bounds for hierarchical models that do not follow a two level tree structure? Developing methods able to automatically exploit conditional independences in arbitrary hierarchical models to build locally-enhanced bounds would be extremely useful in practice.

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A. Proof of Theorem 3.2

Proof. We have

\[
\log p(y) = \mathbb{E}_{q(\theta)} \log \left( \frac{p(\theta)}{q(\theta)} \frac{p(y|\theta) q(\theta)}{p(\theta|y)} \right) \\
= \mathbb{E}_{q(\theta)} \left[ \log \frac{p(\theta)}{q(\theta)} + \log p(y|\theta) + \log \frac{q(\theta)}{p(\theta|y)} \right] \\
= \mathbb{E}_{q(\theta)} \left[ \log \frac{p(\theta)}{q(\theta)} + \sum_{i=1}^{M} \log p(y_i|\theta) \right] + \text{KL}(q(\theta)\|p(\theta|y)) \\
= \mathbb{E}_{q(\theta)} \left[ \log \frac{p(\theta)}{q(\theta)} + \sum_{i=1}^{M} \mathcal{L}(q(z_i|\theta)\|p(z_i, y_i|\theta)) \right] \\
+ \sum_{i=1}^{M} \mathbb{E}_{q(\theta)} \left[ \log p(y_i|\theta) - \mathcal{L}(q(z_i|\theta)\|p(z_i, y_i|\theta)) \right] + \text{KL}(q(\theta)\|p(\theta|y)).
\]

In the final equality, note that all terms on the second line are non-negative: the KL-divergence by definition and \( \log p(y_i|\theta) - \mathcal{L}(q(z_i|\theta)\|p(z_i, y_i|\theta)) \) by assumption. \( \square \)

B. Details for AIS and UHA

This section introduces the details for AIS and UHA. We begin with a detailed description AIS, explain how it can be used with HMC transition kernels, and finally move on to UHA, which is built on those ideas.

Annealed Importance Sampling (AIS) AIS can be seen as an instance of the auxiliary VI framework (Agakov & Barber, 2004). Given an initial approximation \( q(z) \) and an unnormalized target distribution \( p(z) \), AIS proceeds in four steps.

1. It builds a sequence of unnormalized densities \( \pi^1(z), \ldots, \pi^{K-1}(z) \) that gradually bridge from \( q(z) \) to the target \( p(z) \).

2. It defines the forward transitions \( T^k(z^{k+1}|z^k) \) as an MCMC kernel that leaves the bridging density \( \pi^k \) invariant, and the backward transitions \( U^k(z^k|z^{k+1}) \) as the reversal of \( T^k \) with respect to \( \pi^k \).

3. It uses the transition \( T^k \) and \( U^k \) to augment the variational and target density. This yields the augmented distributions

\[
q(z^{1:K}) = q(z^1) \prod_{k=1}^{K-1} T^k(z^{k+1}|z^k) \\
p(z^{1:K}) = p(z^K) \prod_{k=1}^{K-1} U^k(z^k|z^{k+1}).
\]

4. It uses the augmented distributions to build the augmented ELBO, a lower bound on the log-normalizing constant of \( p(z) \) as

\[
\mathbb{E}_{q(z^{1:K})} \log \frac{p(z^K)}{q(z^1)} \prod_{k=1}^{K-1} \frac{T^k(z^k|z^{k+1})}{U^k(z^k|z^{k+1})}.
\]

Then, using that \( T^k(z^{k+1}|z^k)\pi^k(z^k) = U^k(z^k|z^{k+1})\pi^k(z^{k+1}) \), the ratio from Equation (17) simplifies to

\[
\mathbb{E}_{q(z^{1:K})} \log \frac{p(z^K)}{q(z^1)} \prod_{k=1}^{K-1} \frac{\pi^k(z^k)}{\pi^{k+1}(z^{k+1})}.
\]

This is the AIS lower bound. Its tightness depends on the specific Markov kernels used, with more powerful kernels leading to tighter bounds.
While closely related to Hamiltonian AIS, the use of uncorrected transition means that \( U \), which can be easily estimated using samples from the augmented proposal \( q(z) \), where \( \bar{\pi} = \pi \), and the bridging densities \( \pi^k(z) \) with a momentum variable \( \rho \sim r(\rho) \). Then, the transitions \( T^k(z^{k+1}, \rho^{k+1}|z^k, \rho^k) \) and \( U^k(z^k, \rho^k|z^{k+1}, \rho^{k+1}) \) as an HMC kernel and its reversal, respectively.

It has been observed that Hamiltonian AIS may yield tight lower bounds on the log marginal likelihood (Sohl-Dickstein & Culpepper, 2012; Grosse et al., 2015; Wu et al., 2017). Its main drawback, however, is that, due the use of a correction step in contrast to Hamiltonian AIS, it yields differentiable lower bounds that admit reparameterization gradients. This simplifies tuning all of the method’s parameters, which has been observed to yield large gains in practice (Geffner & Domke, 2021; Zhang et al., 2021).

Uncorrected Hamiltonian Annealing (UHA) UHA can be seen as a differentiable alternative to Hamiltonian AIS. It closely follows its derivation. It extends the variational distribution and target with the momentum variables \( \rho \), sets \( T^k(z^{k+1}, \rho^{k+1}|z^k, \rho^k) \) and \( U^k(z^k, \rho^k|z^{k+1}, \rho^{k+1}) \), and builds the ELBO using these augmented distributions as

\[
\mathbb{E}_{q(z^{1:K}, \rho^{1:K})} \log \frac{p(z^K) r(\rho^K)}{q(z^1) r(\rho^1)} \prod_{k=1}^{K-1} \frac{U^k(z^k, \rho^k|z^{k+1}, \rho^{k+1})}{T^k(z^{k+1}, \rho^{k+1}|z^k, \rho^k)}. \tag{19}
\]

The main difference with Hamiltonian AIS comes in the choice for the transition. UHA sets \( T^k \) to be an uncorrected HMC kernel targeting the bridging density \( \pi^k(z, \rho) \). This transition consists on two steps, (partially) re-sampling the momentum from a distribution \( s(\cdot|\rho^k) \) that leaves \( r(\rho) \) invariant, followed by the simulation of Hamiltonian dynamics without a correction step. Formally, this can be expressed as

\[
\begin{align*}
T^k(z^{k+1}, \rho^{k+1}|z^k, \rho^k) : \\
1. \quad & \tilde{\rho}^k \sim s(\cdot|\rho^k) \\
2. \quad (z^{k+1}, \rho^{k+1}) = \text{Dynamics}(z^k, \tilde{\rho}^k).
\end{align*} \tag{20}
\]

Similarly, UHA defines the backward transition \( U^k \) as the uncorrected reversal of an HMC kernel that leaves \( \pi^k(z, \rho) \) invariant (see Geffner & Domke (2021b) for details).

While closely related to Hamiltonian AIS, the use of uncorrected transition means that \( U^k \) is no longer the reversal of \( T^k \). Therefore, the simplification for the ratio \( U^k / T^k \) used by AIS to go from Equation (17) to Equation (18) cannot be used. However, Geffner & Domke (2021b) and Zhang et al. (2021) showed that the ratio between these uncorrected transitions yields a simple expression,

\[
\frac{U^k(z^k, \rho^k|z^{k+1}, \rho^{k+1})}{T^k(z^{k+1}, \rho^{k+1}|z^k, \rho^k)} = \frac{r(\rho^k)}{r(\tilde{\rho}^k)}, \tag{21}
\]

where \( \tilde{\rho}^k \) is defined in Equation (20). Then, the bound from Equation (19) can be expressed as (Geffner & Domke, 2021b; Zhang et al., 2021)

\[
\mathbb{E}_{q(z^{1:K}, \rho^{1:K})} \log \frac{p(z^K)}{q(z^1)} \prod_{k=1}^{K-1} \frac{r(\rho^{k+1})}{r(\tilde{\rho}^k)}, \tag{22}
\]

which can be easily estimated using samples from the augmented proposal \( q(z^{1:K}, \rho^{1:K}) \). UHA’s main benefit is that, in contrast to Hamiltonian AIS, it yields differentiable lower bounds that admit reparameterization gradients. This simplifies tuning all of the method’s parameters, which has been observed to yield large gains in practice (Geffner & Domke, 2021b; Zhang et al., 2021).