Variational Inference for Monte Carlo Objectives

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Introduction

- Variational training of directed generative models has been widely adopted.
  - Results depend heavily on the choice of the variational posterior.
  - A variational posterior that is too simple can prevent the model from using much of its capacity.
  - Making it more expressive is one way to avoid this (see e.g. DRAW, normalizing flows).
- Simpler (orthogonal) alternative: optimize a tighter lower bound on the log-likelihood by throwing more computation at the problem.
  - Burda et al. (2016) used the reparameterization trick to implement this approach in variational autoencoders.
- We develop a more general version than can also handle the harder case of models with discrete latent variables.
  - We use the availability of multiple samples to implement highly effective variance reduction at virtually no additional cost.

Motivation

- Continuous latent variables are not always appropriate.
  - Some properties of the world, such as absence/presence, number of objects, are fundamentally discrete.
  - Dependencies between between discrete latent variables can be easier to capture (e.g. DARN).
- Inference-based learning provides a principled way of training deep models without backpropagation.
  - Inferring the latent variable values effectively makes them observed, breaking the flow of gradients through them.
  - An inference network propagates the information contained in the target/output, which is captured by the backpropagated gradient in differentiable/reparameterized models.

Multi-sample objective for variational inference

- The standard variational lower bound on $\log P_\theta(x)$ with a variational posterior $Q(h|x)$:

$$\mathcal{L}(x) = E_{Q(h|x)}\left[\log \frac{P(x,h)}{Q(h|x)}\right] = \log P(x) + E_{Q(h|x)}\left[\log \frac{P(h|x)}{Q(h|x)}\right].$$

  - There is a big penalty for having regions with $Q(h|x) \gg P(h|x)$.
  - As a result, the learned $Q(h|x)$ provides very incomplete coverage of $P(h|x)$.

- A tighter lower bound on $\log P_\theta(x)$ (IWAE, Burda et al., 2016):

$$\mathcal{L}^K(x) = E_{Q(h^{1:K}|x)}\left[\log \frac{1}{K}\sum_{k=1}^{K} \frac{P(x,h^k)}{Q(h^k|x)}\right]$$

  - Now we have K shots at hitting a high-probability region of $P(h|x)$.
  - The learned $Q(h|x)$ is now less conservative.

Monte-Carlo objectives

- Generalization: Objectives of the form

$$\mathcal{L}^K(x) = E_{Q(h^{1:K}|x)}\left[\log \frac{1}{K}\sum_{k=1}^{K} f(x, h^k)\right],$$

  where $h^1, ..., h^K$ are independent samples from some distribution $Q(h|x)$.
- Special case: If $f(x, h)$ is an unbiased Monte Carlo estimator of $P(x)$, then so is $\hat{I}(h^{1:K}) = \frac{1}{K}\sum_{k=1}^{K} f(x, h^k)$.
  - $E_{Q(h^{1:K}|x)}\left[\log \hat{I}(h^{1:K})\right]$ is a lower bound on $\log P(x)$.
  - Can think of $\log \hat{I}(h^{1:K})$ as a *stochastic* lower bound on $\log P(x)$.
  - The bound becomes tighter as K increases, converging to $\log P(x)$ in the limit.
- $Q(h|x)$ can be thought of as a proposal distribution as opposed to a variational posterior.

Examples of Monte Carlo objectives

- The simplest case involves Monte Carlo sampling from the prior:

$$\mathcal{L}^K(x) = E_P\left[\log \frac{1}{K}\sum\nolimits_{k=1}^{K} P(x|h^k)\right] \text{ with } h^k \sim P(h).$$

- Importance sampling with a learned proposal is usually much more efficient:

$$\mathcal{L}^K(x) = E_{Q(h^{1:K}|x)}\left[\log \frac{1}{K}\sum\nolimits_{k=1}^{K} \frac{P(x, h^k)}{Q(h^k|x)}\right].$$

- Many other possibilities:
    - Can incorporate variance reduction techniques from IS such as control variates.
    - Can use α-divergence based objectives.

Gradients of the lower bound

- We would like to maximize the objective

$$\mathcal{L}^K(x) = E_{Q(h^{1:K}|x)}\left[\log \frac{1}{K}\sum_{k=1}^{K} f(x, h^k)\right] = E_{Q(h^{1:K}|x)}\left[\log \hat{I}(h^{1:K})\right].$$

- Its gradient can be expressed as

$$\frac{\partial}{\partial\theta}\mathcal{L}^K(x) = E_{Q(h^{1:K}|x)}\left[\sum_j \log \hat{I}(h^{1:K})\frac{\partial}{\partial\theta}\log Q(h^j|x)\right] + E_{Q(h^{1:K}|x)}\left[\sum_j \tilde{w}^j \frac{\partial}{\partial\theta}\log f(x, h^j)\right]$$

where $\tilde{w}^j \equiv \frac{f(x,h^j)}{\sum_{k=1}^{K} f(x,h^k)}$.

  - The second term is easy to estimate.
  - The first term is much harder.

Estimating the gradients (NVIL-style)

- Can use the Neural Variational Inference and Learning (NVIL) estimator developed for the single-sample variational objective.
- Applying it to the multi-sample objective gives:

$$\frac{\partial}{\partial\theta}\mathcal{L}^K(x) \simeq \sum_j (\log \hat{I}(h^{1:K}) - b(x)) \tfrac{\partial}{\partial\theta} \log Q(h^j|x)$$
$$+ \sum_j \tilde{w}^j \tfrac{\partial}{\partial\theta} \log f(x, h^j),$$

  with $h^k \sim Q(h|x)$
  - $b(x)$ is a predictor/baseline trained to predict $\log \hat{I}(h^{1:K})$.
- Drawback: uses the same learning signal for all h^k, even though some samples will be much better than others.
  - There is no credit assignment within a set of K samples.

Disentangling the learning signals

- Would like to have a different learning signal for each sample.
- Key observation: since the K samples are independent, when considering the learning signal for one of the samples, can treat all other samples as constant.
  - Can "subtract-out" the effect of the other samples to isolate the effect of the sample of interest.
- What to subtract from $\log \hat{I}(h^{1:K})$?
  - Something very close to it that does not depend on the sample of interest.
- One idea: train a baseline-like predictor for $f(x, h^j)$.
  - This introduces additional complexity.
  - Can we avoid learning an extra mapping?

VIMCO: simple local learning signals

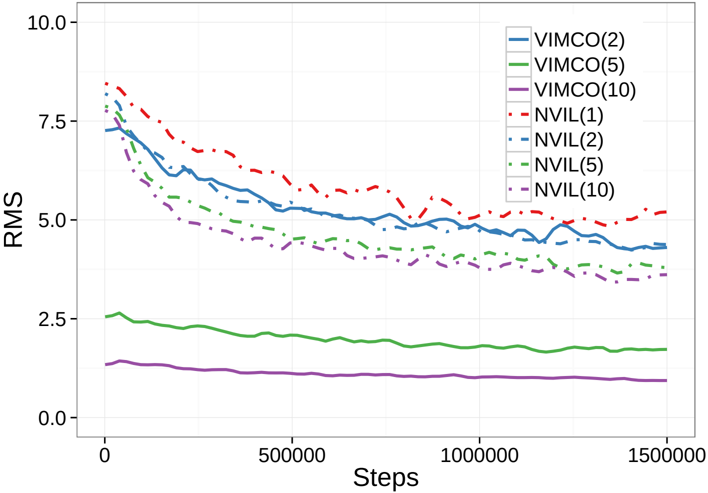
- Better idea: estimate $f(x, h^j)$ from the other $K - 1$ $f(x, h^k)$.
- Two natural choices for estimating $f(x, h^j)$ are:
  - the arithmetic mean: $\hat{f}(x, h^{-j}) = \frac{1}{K-1} \sum_{k \neq j} f(x, h^k)$
  - the geometric mean: $\hat{f}(x, h^{-j}) = \exp\left(\frac{1}{K-1} \sum_{k \neq j} \log f(x, h^k)\right)$
- This gives the following local learning signals:

$$\hat{L}(h^j | h^{-j}) = \log \frac{1}{K} \sum_{k=1}^{K} f(x, h^k) - \log \frac{1}{K} \left(\sum_{k \neq j} f(x, h^k) + \hat{f}(x, h^{-j}) \right).$$

- The second term can be seen as a hand-crafted sample-dependent baseline *with no free parameters*.
- VIMCO local learning signals work well without any additional variance reduction.

Variance reduction: VIMCO vs. NVIL

The magnitude (root mean square) of the learning signal for VIMCO and NVIL as a function of the number of samples used in the objective and the number of parameter updates.

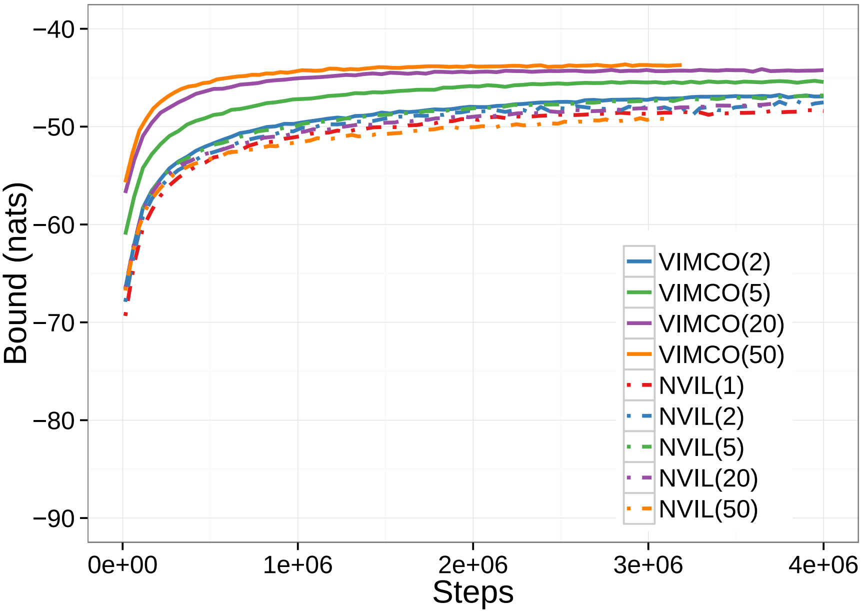


Generative modelling: 200-200-200 SBN on MNIST

Estimates of the negative log-likelihood (in nats) for generative modelling on MNIST. The model is an SBN with three latent layers of 200 binary units.

Number of samples	Training alg. VIMCO	NVIL	RWS
1	—	95.2	—
2	93.5	93.6	94.6
5	92.8	93.7	93.4
10	92.6	93.4	93.0
50	91.9	96.2	92.5

Structured prediction with inference (MNIST)



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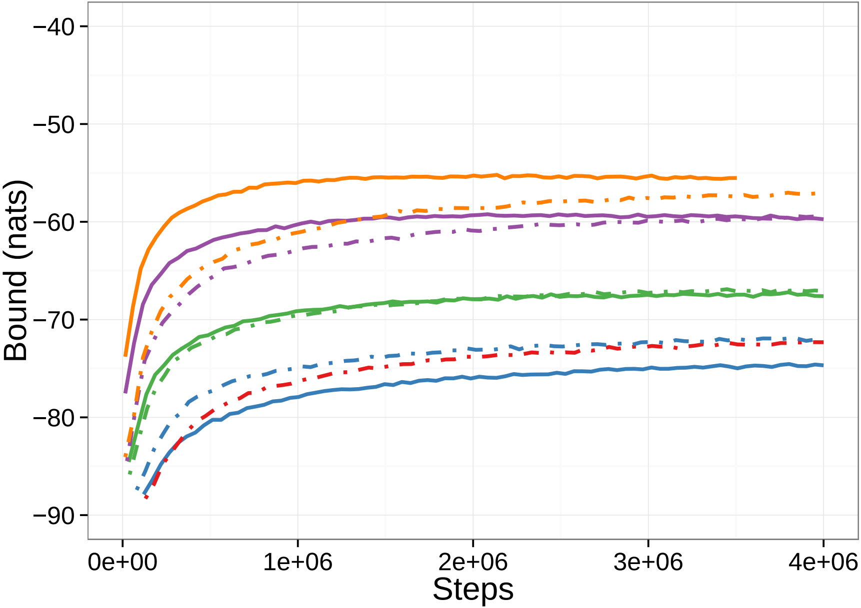
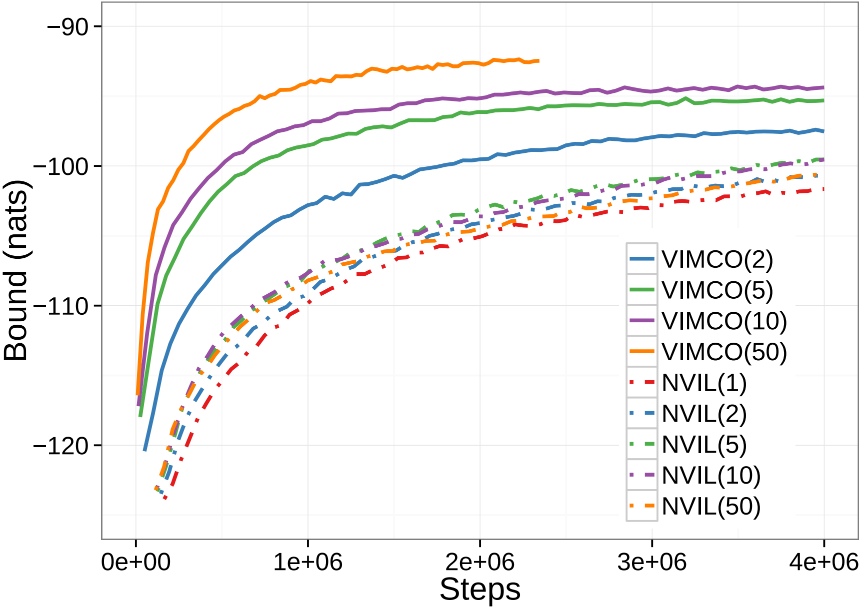


Conclusions

- A principled, unbiased approach to optimizing multi-sample variational objectives that just works.
  - Implements effective variance reduction essentially for free.
  - Does not need a learned baseline to work well.
- Performs better than NVIL and Reweighted Wake Sleep.
- Can handle both discrete and continuous latent variables and can be combined with the reparameterization trick.

Thank you!

Generative modelling: 200-200-200 SBN on MNIST



Structured prediction: completion examples