REINTERPRETING IMPORTANCE-WEIGHTED AUTOENCODERS

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ABSTRACT

The standard interpretation of importance-weighted autoencoders is that they maximize a tighter lower bound on the marginal likelihood than the standard evidence lower bound. We give an alternate interpretation of this procedure: that it optimizes the standard variational lower bound, but using a more complex distribution. We formally derive this result, present a tighter lower bound, and visualize the implicit importance-weighted distribution.

1 BACKGROUND

The importance-weighted autoencoder (IWAE; Burda et al. (2016)) is a variational inference strategy capable of producing arbitrarily tight evidence lower bounds. IWAE maximizes the following multi-sample evidence lower bound (ELBO):

\[ \log p(x) \geq \mathbb{E}_{z_1 \ldots z_k \sim q(z|x)} \left[ \log \left( \frac{1}{k} \sum_{i=1}^{k} p(x, z_i) q(z_i|x) \right) \right] = L_{IWAE}[q] \] (IWAE ELBO)

which is a tighter lower bound than the ELBO maximized by the variational autoencoder (VAE; Kingma & Welling (2014)):

\[ \log p(x) \geq \mathbb{E}_{z \sim q(z|x)} \left[ \log \left( \frac{p(x, z)}{q(z|x)} \right) \right] = L_{VAE}[q]. \] (VAE ELBO)

2 DEFINING THE IMPLICIT DISTRIBUTION \( \tilde{q}_{IW} \)

In this section, we derive the implicit distribution that arises from importance sampling from a distribution \( p \) using \( q \) as a proposal distribution. Given a batch of samples \( z_2 \ldots z_k \) from \( q(z|x) \), the following is the unnormalized importance-weighted distribution:

\[ \tilde{q}_{IW}(z|x, z_2:k) = \frac{1}{k} \sum_{j=1}^{k} \frac{p(x, z_j)}{q(z_j|x)} q(z|x) = \frac{1}{k} \left( \frac{p(x, z_j)}{q(z_j|x)} + \sum_{j=2}^{k} \frac{p(x, z_j)}{q(z_j|x)} \right) \]

(1)

True posterior

|   | \( k = 1 \) | \( k = 10 \) | \( k = 100 \) |
|---|---|---|---|

Figure 1: Approximations to a complex true distribution, defined via \( q_{EW} \). As \( k \) grows, this approximation approaches the true distribution.
Here are some properties of the approximate IWAE posterior:

- When $k = 1$, $\tilde{q}_{IW}(z|x, z_{2:k})$ equals $q(z|x)$.
- When $k > 1$, the form of $\tilde{q}_{IW}(z|x, z_{2:k})$ depends on the true posterior $p(z|x)$.
- As $k \to \infty$, $E_{z_{2:k} \sim \tilde{q}_{IW}(z|x, z_{2:k})}$ approaches the true posterior $p(z|x)$ pointwise.

See the appendix for details. Importantly, $\tilde{q}_{IW}(z|x, z_{2:k})$ is dependent on the batch of samples $z_{2} \ldots z_{k}$. See Fig. 3 in the appendix for a visualization of $\tilde{q}_{IW}$ with different batches of $z_{2} \ldots z_{k}$.

2.1 Recovering the IWAE Bound from the VAE Bound

Here we show that the IWAE ELBO is equivalent to the VAE ELBO in expectation, but with a more flexible, unnormalized $\tilde{q}_{IW}$ distribution, implicitly defined by importance reweighting. If we replace $q(z|x)$ with $\tilde{q}_{IW}(z|x, z_{2:k})$ and take an expectation over $z_{2} \ldots z_{k}$, then we recover the IWAE ELBO:

$$
E_{z_{2:k} \sim q(z|x)}[\mathcal{L}_{VAE}[\tilde{q}_{IW}(z|z_{2:k})]] = E_{z_{2:k} \sim q(z|x)} \left[ \int \tilde{q}_{IW}(z|z_{2:k}) \log \left( \frac{p(x,z)}{\tilde{q}_{IW}(z|x, z_{2:k})} \right) dz \right]
$$

$$
= E_{z_{2:k} \sim q(z|x)} \left[ \int \tilde{q}_{IW}(z|z_{2:k}) \log \left( \frac{1}{k} \sum_{i=1}^{k} \frac{p(x,z_{i})}{q(z_{i}|x)} \right) dz \right]
$$

$$
= E_{z_{1:k} \sim q(z|x)} \left[ \log \left( \frac{1}{k} \sum_{i=1}^{k} \frac{p(x,z_{i})}{q(z_{i}|x)} \right) \right] = \mathcal{L}_{IWAE}[q]
$$

For a more detailed derivation, see the appendix. Note that we are abusing the VAE lower bound notation because this implies an expectation over an unnormalized distribution. Consequently, we replace the expectation with an equivalent integral.

2.2 Expected Importance Weighted Distribution $q_{EW}$

We can achieve a tighter lower bound than $\mathcal{L}_{IWAE}[q]$ by taking the expectation over $z_{2} \ldots z_{k}$ of $\tilde{q}_{IW}$. The expected importance-weighted distribution $q_{EW}(z|x)$ is a distribution given by:

$$
q_{EW}(z|x) = E_{z_{2:k} \sim q(z|x)}[\tilde{q}_{IW}(z|x, z_{2:k})] = E_{z_{2:k} \sim q(z|x)} \left[ \frac{p(x,z)}{\frac{1}{k} \sum_{i=1}^{k} \frac{p(x,z_{i})}{q(z_{i}|x)} + \sum_{j=2}^{k} \frac{p(x,z_{j})}{q(z_{j}|x)}} \right]
$$

(2)

See section 5.2 for a proof that $q_{EW}$ is a normalized distribution. Using $q_{EW}$ in the VAE ELBO, $\mathcal{L}_{VAE}[q_{EW}]$, results in an upper bound of $\mathcal{L}_{IWAE}[q]$. See section 5.3 for the proof, which is a special case of the proof in Naesseth et al. (2017). The procedure to sample from $q_{EW}(z|x)$ is shown in Algorithm 1. It is equivalent to sampling-importance-resampling (SIR).

2.3 Visualizing the Nonparametric Approximate Posterior

The IWAE approximating distribution is nonparametric in the sense that, as the true posterior grows more complex, so does the shape of $\tilde{q}_{IW}$ and $q_{EW}$. This makes plotting these distributions challenging. A kernel-density-estimation approach could be used, but requires many samples. Thankfully, equations (1) and (2) give us a simple and fast way to approximately plot $\tilde{q}_{IW}$ and $q_{EW}$ without introducing artifacts due to kernel density smoothing.

Figure 1 visualizes $q_{EW}$ on a 2D distribution approximation problem using Algorithm 2. The base distribution $q$ is a Gaussian. As we increase the number of samples $k$ and keep the base distribution fixed, we see that the approximation approaches the true distribution. See section 5.6 for 1D visualizations of $\tilde{q}_{IW}$ and $q_{EW}$ with $k = 2$.

3 Resampling for Prediction

During training, we sample the $q$ distribution and implicitly weight them with the IWAE ELBO. After training, we need to explicitly reweight samples from $q$. 
Algorithm 1 Sampling $q_{EW}(z|x)$

1: $k \leftarrow$ number of importance samples  
2: for $i$ in 1..$k$ do  
3: $z_i \sim q(z|x)$  
4: $w_i = \frac{p(x,z_i)}{q(z_i|x)}$  
5: Each $\tilde{w}_i = \frac{w_i}{\sum_{i=2}^k w_i}$  
6: $j \sim \text{Categorical}(\tilde{w})$  
7: Return $z_j$

Algorithm 2 Plotting $q_{EW}(z|x)$

1: $k \leftarrow$ number of importance samples  
2: $S \leftarrow$ number of function samples  
3: $L \leftarrow$ locations to plot  
4: $\hat{f} = \text{zeros}(|L|)$  
5: for $s$ in 1..$S$ do  
6: $z_2 \ldots z_k \sim q(z|x)$  
7: $\hat{p}(x) = \sum_{i=2}^k \frac{p(x,z_i)}{q(z_i|x)}$  
8: for $z$ in $L$ do  
9: $\hat{f}[z] += \frac{p(x,z)}{\hat{p}(x) + \hat{p}(x)}$  
10: Return $\hat{f}/S$

Figure 2: Reconstructions of MNIST samples from $q(z|x)$ and $q_{EW}$. The model was trained by maximizing the IWAE ELBO with $K=50$ and 2 latent dimensions. The reconstructions from $q(z|x)$ are greatly improved with the sampling-resampling step of $q_{EW}$.

In figure 2, we demonstrate the need to sample from $q_{EW}$ rather than $q(z|x)$ for reconstructing MNIST digits. We trained the model to maximize the IWAE ELBO with $K=50$ and 2 latent dimensions, similar to Appendix C in Burda et al. (2016). When we sample from $q(z|x)$ and reconstruct the samples, we see a number of anomalies. However, if we perform the sampling-resampling step (Alg. 1), then the reconstructions are much more accurate. The intuition here is that we trained the model with $q_{EW}$ with $K = 50$ then sampled from $q(z|x)$ ($q_{EW}$ with $K = 1$), which are very different distributions, as seen in Fig. 1.

4 Discussion

Bachman & Precup (2015) also showed that the IWAE objective is equivalent to stochastic variational inference with a proposal distribution corrected towards the true posterior via normalized importance sampling. We build on this idea by further examining $\tilde{q}_{IW}$ and by providing visualizations to help better grasp the interpretation. To summarize our observations, the following is the ordering of lower bounds given specific proposal distributions,

$$\log p(x) \geq L_{VAE}[q_{EW}] \geq \mathbb{E}_{z_2 \ldots z_k \sim q(z|x)} [L_{VAE}[\tilde{q}_{IW}(z|z_2:k)]] = L_{IWAE}[q] \geq L_{VAE}[q]$$

In light of this, IWAE can be seen as increasing the complexity of the approximate distribution $q$, similar to other methods that increase the complexity of $q$, such as Normalizing Flows (Jimenez Rezende & Mohamed, 2015), Variational Boosting (Miller et al., 2016) or Hamiltonian variational inference (Salimans et al., 2015). With this interpretation in mind, we can possibly generalize $\tilde{q}_{IW}$ to be applicable to other divergence measures. An interesting avenue of future work is the comparison of IW-based variational families with alpha-divergences or operator variational objectives.
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5 APPENDIX

5.1 DETAILED DERIVATION OF THE EQUIVALENCE OF VAE AND IWAE BOUND

Here we show that the expectation over $z_2...z_k$ of the VAE lower bound with the unnomalized importance-weighted distribution $\tilde{q}_{W, L_{VAE}[\tilde{q}_W(z|z_{2:k})]}$, is equivalent to the IWAE bound with the original $q$ distribution, $L_{\text{IWAE}}[q]$.

$$
\mathbb{E}_{z_2...z_k \sim q(z|x)}[L_{\text{VAE}}[\tilde{q}_W(z|z_{2:k})]] = \mathbb{E}_{z_2...z_k \sim q(z|x)} \left[ \int_z \tilde{q}_W(z|x, z_{2:k}) \log \left( \frac{p(x, z)}{\tilde{q}_W(z|x, z_{2:k})} \right) dz \right] 
$$

(3)

$$
= \mathbb{E}_{z_2...z_k \sim q(z|x)} \left[ \int_z \tilde{q}_W(z|x, z_{2:k}) \log \left( \frac{p(x, z)}{\frac{1}{k} \sum_{i=1}^{k} p(x, z_i)} \right) dz \right] 
$$

(4)

$$
= \mathbb{E}_{z_2...z_k \sim q(z|x)} \left[ \int_z \tilde{q}_W(z|x, z_{2:k}) \log \left( \frac{1}{k} \sum_{i=1}^{k} \frac{p(x, z_i)}{q(z_i|x)} \right) dz \right] 
$$

(5)

$$
= \mathbb{E}_{z_2...z_k \sim q(z|x)} \left[ \int_z k \sum_{i=1}^{k} \frac{p(x, z_i)}{q(z_i|x)} \log \left( \frac{1}{k} \sum_{i=1}^{k} \frac{p(x, z_i)}{q(z_i|x)} \right) dz \right] 
$$

(6)

$$
= \mathbb{E}_{z_2...z_k \sim q(z|x)} \left[ \int_z k \sum_{i=1}^{k} \frac{p(x, z_i)}{q(z_i|x)} \log \left( \frac{1}{k} \sum_{i=1}^{k} \frac{p(x, z_i)}{q(z_i|x)} \right) dz \right] 
$$

(7)

$$
= \mathbb{E}_{z_2...z_k \sim q(z|x)} \left[ \int_z k \sum_{i=1}^{k} \frac{p(x, z_i)}{q(z_i|x)} \log \left( \frac{1}{k} \sum_{i=1}^{k} \frac{p(x, z_i)}{q(z_i|x)} \right) dz \right] 
$$

(8)

$$
= \mathbb{E}_{z_2...z_k \sim q(z|x)} \left[ \frac{k}{\sum_{j=1}^{k} \frac{p(x, z_j)}{q(z_j|x)}} \log \left( \frac{1}{k} \sum_{i=1}^{k} \frac{p(x, z_i)}{q(z_i|x)} \right) \right] 
$$

(9)

$$
= \mathbb{E}_{z_2...z_k \sim q(z|x)} \left[ \frac{\sum_{i=1}^{k} \frac{p(x, z_i)}{q(z_i|x)}}{\sum_{j=1}^{k} \frac{p(x, z_j)}{q(z_j|x)}} \log \left( \frac{1}{k} \sum_{i=1}^{k} \frac{p(x, z_i)}{q(z_i|x)} \right) \right] 
$$

(10)

$$
= \mathbb{E}_{z_2...z_k \sim q(z|x)} \left[ \log \left( \frac{1}{k} \sum_{i=1}^{k} \frac{p(x, z_i)}{q(z_i|x)} \right) \right] 
$$

(11)

$$
= L_{\text{IWAE}}[q] 
$$

(12)

(8): Change of notation $z = z_1$.

(10): $z_i$ has the same expectation as $z_1$ so we can replace $k$ with the sum of $k$ terms.
5.2 Proof that \(q_{EW}\) is a normalized distribution

\[
\int_z q_{EW}(z|x)dz = \int_z E_{z_2...z_k \sim q(z|x)} [q_{IW}(z|x,z_{2:k})]dz
\]

(13)

\[
= \int_z E_{z_2...z_k \sim q(z|x)} \left[ \frac{p(x,z)}{\frac{1}{k} \left( \frac{p(x,z)}{q(z|x)} + \sum_{j=2}^{k} \frac{p(x,z_j)}{q(z_j|x)} \right)} \right]dz
\]

(14)

\[
= \int_z \frac{q(z|x)}{q(z|x)} E_{z_2...z_k \sim q(z|x)} \left[ \frac{p(x,z)}{\frac{1}{k} \left( \frac{p(x,z)}{q(z|x)} + \sum_{j=2}^{k} \frac{p(x,z_j)}{q(z_j|x)} \right)} \right]dz
\]

(15)

\[
= E_{z \sim q(z|x)} E_{z_2...z_k \sim q(z|x)} \left[ \frac{p(x,z)}{\frac{1}{k} \left( \frac{p(x,z)}{q(z|x)} + \sum_{j=2}^{k} \frac{p(x,z_j)}{q(z_j|x)} \right)} \right]
\]

(16)

\[
= E_{z_1...z_k \sim q(z|x)} \left[ \frac{p(x,z_1)}{\frac{1}{k} \left( \sum_{j=1}^{k} \frac{p(x,z_j)}{q(z_j|x)} \right)} \right]
\]

(17)

\[
= k \cdot E_{z_1...z_k \sim q(z|x)} \left[ \frac{p(x,z_1)}{\frac{1}{k} \left( \sum_{j=1}^{k} \frac{p(x,z_j)}{q(z_j|x)} \right)} \right]
\]

(18)

\[
= \sum_{i=1}^{k} E_{z_1...z_{i-1}z_{i+1}...z_k \sim q(z|x)} \left[ \frac{p(x,z_i)}{\frac{1}{k} \left( \sum_{j=1}^{k} \frac{p(x,z_j)}{q(z_j|x)} \right)} \right]
\]

(19)

\[
= E_{z_1...z_k \sim q(z|x)} \left[ \frac{1}{\frac{1}{k} \left( \sum_{j=1}^{k} \frac{p(x,z_j)}{q(z_j|x)} \right)} \right]
\]

(20)

\[
= E_{z_1...z_k \sim q(z|x)} \left[ \frac{1}{\frac{1}{k} \left( \sum_{j=1}^{k} \frac{p(x,z_j)}{q(z_j|x)} \right)} \right]
\]

(21)

\[
E_{z_1...z_k \sim q(z|x)} [1] = 1
\]

(22)

(17): Change of notation \(z = z_1\).
(19): \(z_i\) has the same expectation as \(z_1\) so we can replace \(k\) with the sum of \(k\) terms.
(20): Linearity of expectation.
5.3 Proof that $\mathcal{L}_{VAE}[q_{EW}]$ is an upper bound of $\mathcal{L}_{IWAE}[q]$

Proof provided by Christian Naesseth.

Let $\tilde{p}(x|z_{1:k}) = \frac{1}{k} \left( \frac{p(x, z_1)}{q(z_1|x)} + \sum_{j=2}^{k} \frac{p(x, z_j)}{q(z_j|x)} \right)$

$$\mathcal{L}_{VAE}[q_{EW}] = E_{z \sim q_{EW}} \left[ \log \left( \frac{p(x, z)}{q_{EW}(z|x)} \right) \right]$$

$$= E_{z \sim q_{EW}} \left[ \log \left( \frac{p(x, z)}{\mathcal{E}_{q(z_{2:k}|x)} \left[ \frac{p(x, z)}{p(x|z_{1:k})} \right] } \right) \right]$$

$$= E_{z \sim q_{EW}} \left[ \log \left( \frac{1}{\mathcal{E}_{q(z_{2:k}|x)} \left[ \frac{1}{p(x|z_{1:k})} \right] } \right) \right]$$

$$= E_{z \sim q_{EW}} \left[ -\log \left( \mathcal{E}_{q(z_{2:k}|x)} \left[ \frac{p(x|z_{1:k})}{\tilde{p}(x|z_{1:k})} \right] \right) \right]$$

$$= -\int_z p(x, z) \mathcal{E}_{q(z_{2:k}|x)} \left[ \frac{\tilde{p}(x|z_{1:k})}{p(x|z_{1:k})} \right] \log \left( \mathcal{E}_{q(z_{2:k}|x)} \left[ \frac{p(x|z_{1:k})}{\tilde{p}(x|z_{1:k})} \right] \right) dz$$

$$\geq -\int_z p(x, z) \mathcal{E}_{q(z_{2:k}|x)} \left[ \frac{\tilde{p}(x|z_{1:k})}{p(x|z_{1:k})} \right] \log \left( \frac{p(x|z_{1:k})}{\tilde{p}(x|z_{1:k})} \right) dz$$

$$= \int_z p(x, z) \int_{z_{2:k}} q(z_{2:k}|x) \frac{\tilde{p}(x|z_{1:k})}{p(x|z_{1:k})} \log \left( \frac{p(x|z_{1:k})}{\tilde{p}(x|z_{1:k})} \right) dz$$

$$= \int_{z_{1:k}} q(z_{1:k}|x) \log \left( \frac{p(x, z_1)}{q(z_1|x)} \right) \log \left( \frac{1}{k} \sum_{j=1}^{k} \frac{p(x, z_j)}{q(z_j|x)} \right) dz$$

$$= \sum_{i=1}^{k} \int_{z_{1:k}} q(z_{1:k}|x) \log \left( \frac{1}{k} \sum_{j=1}^{k} \frac{p(x, z_j)}{q(z_j|x)} \right) dz$$

$$= \int_{z_{1:k}} q(z_{1:k}|x) \log \left( \frac{1}{k} \sum_{j=1}^{k} \frac{p(x, z_j)}{q(z_j|x)} \right) dz$$

For (28): Given that $f(A) = -\text{AlogA}$ is concave for $A > 0$, and $f(E[x]) \geq E[f(x)]$, then $f(E[x]) = -E[x]\log E[x] \geq E[-x\log x]$.

(30): Change of notation $z = z_1$.

(34): $z_1$ has the same expectation as $z_1$ so we can replace $k$ with the sum of $k$ terms.
5.4 Proof that $q_{EW}$ is closer to the true posterior than $q$

The previous section showed that $\mathcal{L}_{IWAE}(q) \leq \mathcal{L}_{VAE}(q_{EW})$. That is, the IWAE ELBO with the base $q$ is a lower bound to the VAE ELBO with the importance weighted $q_{EW}$. Due to Jensen’s inequality and as shown in Burda et al. (2016), we know that the IWAE ELBO is an upper bound of the VAE ELBO: $L_{IWAE}(q) \geq L_{VAE}(q_{EW})$. Furthermore, the log marginal likelihood can be factorized into: $\log(p(x)) = L_{VAE}(q_{EW}) + KL(q\|p)$, and rearranged to: $KL(q\|p) = \log(p(x)) - L_{V AE}(q_{EW})$.

Following the observations above and substituting $q_{EW}$ for $q$:

$$KL(q_{EW}\|p) = \log(p(x)) - L_{V AE}(q_{EW})$$ (39)

$$\leq \log(p(x)) - L_{IWAE}(q)$$ (40)

$$\leq \log(p(x)) - L_{VAE}(q) = KL(q\|p)$$ (41)

Thus, $KL(q_{EW}\|p) \leq KL(q\|p)$, meaning $q_{EW}$ is closer to the true posterior than $q$ in terms of KL divergence.

5.5 In the limit of the number of samples

Another perspective is in the limit of $k = \infty$. Recall that the marginal likelihood can be approximated by importance sampling:

$$p(x) = E_{q(z|x)} \left[ \frac{p(x, z)}{q(z|x)} \right] \approx \frac{1}{k} \sum_{i} p(x, z_i) q(z_i|x)$$ (42)

where $z_i$ is sampled from $q(z|x)$. We see that the denominator of $\tilde{q}_{IW}$ is approximating $p(x)$. If $p(x,z)$ is bounded, then it follows from the strong law of large numbers that, as $k$ approaches infinity, $\tilde{q}_{IW}$ converges to the true posterior $p(z|x)$ almost surely. This interpretation becomes clearer when we factor out the true posterior from $\tilde{q}_{IW}$:

$$\tilde{q}_{IW}(z|x, z_{2:k}) = \frac{p(x)}{\frac{1}{k} \sum_{j=2}^{k} \frac{p(x, z_j)}{q(z_j|x)}} p(z|x)$$ (43)

We see that the closer the denominator becomes to $p(x)$, the closer $\tilde{q}_{IW}$ is to the true posterior.

5.6 Visualizing $\tilde{q}_{IW}$ and $q_{EW}$ in 1D

Figure 3: Visualization of 1D $\tilde{q}_{IW}$ and $q_{EW}$ distributions. The blue $p(z)$ distribution and the green $q(z)$ distribution are both normalized. The three instances of $\tilde{q}_{IW}(z|z_2)$ ($k = 2$) have different $z_2$ samples from $q(z)$ and we can see that they are unnormalized. $q_{EW}(z)$ is normalized and is the expectation over 30 $\tilde{q}_{IW}(z|z_2)$ distributions. The $\tilde{q}_{IW}$ distributions were plotted using Algorithm 2 with $S = 1$. 