Abstract

Even though Variational Autoencoders (VAEs) are widely used for semi-supervised learning, the reason why they work remains unclear. In fact, the addition of the unsupervised objective is most often vaguely described as a regularization. The strength of this regularization is controlled by down-weighting the objective on the unlabeled part of the training set. Through an analysis of the objective of semi-supervised VAEs, we observe that they use the posterior of the learned generative model to guide the inference model in learning the partially observed latent variable. We show that given this observation, it is possible to gain finer control on the effect of the unsupervised objective on the training procedure. Using importance weighting, we derive two novel objectives that prioritize either one of the partially observed latent variable, or the unobserved latent variable. Experiments on the IMDB English sentiment analysis dataset and on the AG News topic classification dataset show the improvements brought by our prioritization mechanism and exhibit a behavior that is inline with our description of the inner working of Semi-Supervised VAEs.

1 Introduction

Variational Autoencoders (VAEs) are a class of deep learning models that combine the efficiency of Amortized Variational Inference with the representational power of deep learning (Zhang et al., 2019). They have been successfully applied to a range of Natural Language Processing (NLP) tasks such as text generation (Bowman et al., 2016; Fang et al., 2019), multimodal generative modeling (Shi et al., 2019), disentangled representation learning (John et al., 2019; Chen et al., 2019), and linguistically informed representation learning (Wolf-Sonkin et al., 2018; Zhang et al., 2020), inter alia. Their successes can be attributed to their efficient learning process, their two-way mapping ability, and other properties such as the disentanglement they induce (Rolinek et al., 2019; Li et al., 2020; Higgins et al., 2019) and the resulting smoothness in their latent space (Bowman et al., 2016).

VAEs are also prevalently used for semi-supervised learning, as described in the pioneer work of Kingma et al. (2014). For that matter, the VAE’s successes have been established through numerous works (e.g. Tomczak and Welling, 2018; Chen et al., 2018; Corro and Titov, 2019), but to the best of our knowledge, their successes or failures are most often attributed to a regularization (or over-regularization) on the latent representations (Chen et al., 2018; Wolf-Sonkin et al., 2018; Yacoby et al., 2020)

In this work, we aim to deepen our understanding of the interaction between the generative model and the classification model in Semi-supervised VAEs. Our contributions can be summed up as follows:

1. After laying out the technical background (section 3), we clarify analytically that the improvements yielded by SSVAEs over sheer supervision comes from the generative model guiding the inference model with its posterior on the distribution of the partially observed latent variable (section 4)

2. We design a technique for focusing the learning process on either of the unobserved or the partially-observed latent variable to improve the learning performance while still lower-bounding the log-likelihood (section 5)

3. We offer experimental evidence that aligns with the our conception of the inner workings of SSVAEs, and that encourages the use of our prioritization mechanism in semi-supervised learning (section 6).
2 Related Works

Semi-supervision with VAEs has received a lot of attention in the recent years. After the pioneer work of Kingma et al. (2014) on image classification, the method was extended to more tasks such as morphological inflections (Wolf-Sonkin et al., 2018), controllable speech synthesis (Habib et al., 2019), Parsing (Corro and Titov, 2019), Sequential Labeling (Chen et al., 2018) and many more. Systems have also been tweaked in various manners to improve the learning performance. Tomczak and Welling (2018) uses a mixture of variational posteriors with pseudo inputs to prevent the unsupervised loss from causing over-regularization. As latent variables are stochastic, Zhang et al. (2019) proposes using a deterministic ancestor of a single latent variable in a VAE to perform classification, and constrain this deterministic ancestor with an adversarial term to have it abide by the values of the random latent variable. Gururangan et al. (2020) introduces a low resource pretraining scheme using VAEs to transfer representational capabilities from in-domain unlabeled data, to downstream tasks using minimum computational power. In a broad sens, the current state of the art on the tasks we used for this study in semi-supervised learning Chen et al. (2020) relies on a carefully crafted training scheme of representation mixing between labeled and unlabeled samples, and on contextual pretrained embeddings from (Devlin et al., 2019).

Our work is also in line with literature taking interest in building deep graphical models that relate observations to latent variables with known meanings. As such, Siddharth et al. (2017) builds a general framework for training deep graphical models using VAEs, and provides techniques (also using importance weighting) to estimate the ELBo no matter the dependency structure of the graphical model.

3 Background

In the following, we will denote our observable data by $x$, our unknown latent variables by $z$, and the partially observed latent variable that we want to predict by $y$.

3.1 Semi-Supervised Learning with VAEs

We will take interest in the widely used form of SSVAEs, namely what is referred to as the M2 model from the work of Kingma et al. (2014). In the most general case\footnote{Contrary to the work of Kingma et al. (2014), we will not assume independence between $z$ and $y$ in our derivations}, our generative model is $p_\theta(x) = \int p_\theta(x|z) p_\theta(y,z)dydz$. The loss function $J^\alpha$ from this model is constructed as the summation between 3 losses\footnote{The original formulation mixed sums and expectations. We only use expectations here for uniformity, and because the 3 quantities are calculated as averages over batches in the implementation for them to be equally scaled.}:

$$J^\alpha = \mathbb{E}_{(x,y)\sim p^*(x,y)}[\mathcal{L}(x,y)] + \mathbb{E}_{x\sim\hat{p}(x)}[\mathcal{U}(x)] + \alpha \mathbb{E}_{(x,y)\sim p^*(x,y)}[-\log q_\phi(y|x)] \tag{1}$$

Where $p^*$ is the distribution of our true data, $q_\phi$ is the approximate posterior (encoder) on $y$ and $z$, and $p_\theta$ is our generative model (decoder) with $p_\theta(z,y)$ being the prior on $z$ and $y$. $\mathcal{L}$ and $\mathcal{U}$ are explicit as follows:

$$\log p_\theta(x,y) \geq \mathbb{E}_{z\sim q_\phi(z|x,y)} \left[ \log p_\theta(x|y,z) + \log p_\theta(y,z) - \log q_\phi(z|x,y) \right] = -\mathcal{L}(x,y) = \text{ELBo}(x,y) \tag{2}$$

$$\log p_\theta(x) \geq \mathbb{E}_{(y,z)\sim q_\phi(y,z|x)} \left[ \log p_\theta(x|y,z) + \log p_\theta(y,z) - \log q_\phi(y,z|x) \right] = -\mathcal{U}(x) = \text{ELBo}(x) \tag{3}$$

The ELBo (Evidence Lower Bound) is a lower bound on the true log-likelihood (Kingma and Welling, 2019). In equation 1, the addition of the last term (weighted by $\alpha$) may seem to be driven by the need for a classification loss, but it can actually be derived as part of the lower bound for $\log p_\theta(x,y)$ (together with $-\mathcal{U}$) if we consider a symmetric Dirichlet prior for the categorical distribution on $y$ with parameter $\alpha$ (Kingma et al., 2014). $-J^\alpha$ is therefore a sound lower bound for $\log p_\theta(x) + \log p_\theta(x,y)$.

Notice here that $\mathcal{L}$ and $\mathcal{U}$ respect the following equalities (c.f. Appendix A):

$$\mathcal{L}(x,y) = \log p_\theta(x,y) - \text{KL}[q_\phi(z|x,y)||p_\theta(z|x,y)] \tag{4}$$
Although VAEs are an ubiquitous generative modeling choice, they only lower bound the true marginal log-likelihood. In that sense, various subsequent works have brought tighter lower bounds to the true log-likelihood such as (Masrani et al., 2019), (Ding and Freedman, 2019), and (Burda et al., 2016). For this study, we chose to make use of IWAEs (Burda et al., 2016) as it is a mature technique that found its way into more applicative works such as that of Shi et al. (2019). For a use case involving two latent variables (y and z), the IWAE lower bound can be written as follows:

\[
\log p_\theta(x) \geq \mathcal{L}_k(x) = \\
\mathbb{E}_{(y_1,z_1),..., (y_k,z_k) \sim q_\phi(y,z|x)} \left[ \log \frac{1}{k} \sum_{i=1}^{k} p_\theta(y_i,z_i|x) \right] \\
\left[ \log \frac{1}{k} \sum_{i=1}^{k} q_\phi(y_i,z_i|x) \right]
\]

The particularity of this lower bound (when contrasted to that of a VAE), is that it is equal to ELBo when \( k = 1 \), and reaches the exact log-likelihood as \( k \) goes to infinity. In other words, it departs from equation 4 at \( k = 1 \), and anneals the Kullback-Leibler divergence in it as \( k \) goes to infinity. We will make use of the Semi-Supervised IWAE (SSIWAE) objective in the experimental section, which is simply obtained by replacing the ELBo in equations 2 and 3 by a tighter importance weighted lower bound. Implications will be discussed in section 5.

### 4 How Do Semi-Supervised VAEs Improve Upon Supervised Learning?

For semi-supervision, \( z \) is often assumed to be independent from \( y \) (Corro and Titov, 2019), but some works do build hierarchical inference processes between \( y \) and \( z \) (Chen et al., 2018). To keep our work valid for both cases, we won’t assume independence between \( z \) and \( y \) for this section.

In the process of jointly learning generation and supervised inference, we will first think about how the former can help the latter. Generation can be learned given only the samples \( x \), while supervised inference needs both \( x \) and \( y \). It is useful here not to think about semi-supervision as two separate learning processes, but rather as a process where the supervised signal is composed of a classical sample-wise learning signal, as well as an overall coherence statistic that is being validated with regard to the generative model. We could give rise to such statistics validation without biasing the classical supervised maximum likelihood learning objective in the following manner:

\[
\phi = \arg \max_\phi \mathcal{L}(y|x; \phi) \\
= \arg \max_\phi \mathbb{E}_{x,y \sim p^*(x,y)} \left[ \log q_\phi(y|x) \right] \\
= \arg \max_\phi \mathbb{E}_{x,y \sim p^*(x,y)} \left[ \alpha \log q_\phi(y|x) \\
- \text{KL}[q_\phi(y|x)||p^*(y|x)] \right]
\]
Where $\alpha$ is a positive weight. These equalities stand because they are equalities between the $\arg\max$ of each quantity, and not the quantities themselves. In fact, for an expressive enough approximation family $q_{\phi}$, our approximation is maximized at $q_{\phi} = p^*$ nullifying the KL-divergence. As a result, for an expressive enough $q_{\phi}$ this addition will not bias our learning objective. Since the KL term samples $y$ from $q_{\phi}$ and not $p^*$, it can indeed be calculated as a statistic over only the samples of $x$ (an expectation over only $x$) as is required for the unsupervised part of semi-supervised learning objectives. Equation 10 can therefore be written as follows:

$$\arg\max_{\phi} E_{x,y \sim p^*(x,y)} \left[ \log q_{\phi}(y|x) \right] - E_{x \sim p^*(x)} \left[ \text{KL}[q_{\phi}(y|x)||p^*(y|x)] \right] \quad (11)$$

Additionally, if the family of approximations $p_{\theta}$ also contains $p^*$, we can write equation 11 as follows:

$$\arg\max_{\phi} \arg\max_{\theta} E_{x,y \sim p^*(x,y)} \left[ \alpha \log q_{\phi}(y|x) + \log p_{\theta}(x,y) \right] - E_{x \sim p^*(x)} \left[ \text{KL}[q_{\phi}(y|x)||p_{\theta}(y|x)] \right] \quad (12)$$

Consequently, given that we would like to learn a generative model to guide our supervised model, a joint estimator that takes the following form could be used:

$$\arg\max_{\phi} \arg\max_{\theta} E_{x,y \sim p^*(x,y)} \left[ \alpha \log q_{\phi}(y|x) + \log p_{\theta}(x,y) \right] + E_{x \sim p^*(x)} \left[ \log p_{\theta}(x) - \text{KL}[q_{\phi}(y|x)||p_{\theta}(y|x)] \right] \quad (13)$$

Noticeably, this formalism closely resembles that of $-J^\alpha$ in equation 6. The difference is in the Kullback-Leibler terms. While the objective in equation 13 only minimizes Kullback-Leibler divergence between $q_{\phi}(y|x)$ and $p_{\theta}(y|x)$, equation 6 includes a Kullback-Leibler between $q_{\phi}(y, z|x)$ and $p_{\theta}(y, z|x)$ and another between $q_{\phi}(z|x, y)$ and $p_{\theta}(z|x, y)$. As stated before, the form that $J^\alpha$ takes in equation 6 is interesting in that it isolates the effect on the encoder in its Kullback-Leibler terms. Accordingly, the effect of semi-supervision with VAEs on a supervised learning process stems from these terms. The Kullback-Leibler terms, in both the objective we constructed in equation 13 and $J^\alpha$ in equation 6, work towards bringing the $y$ we sample from the approximate posterior closer to that of the true posterior, which is the guidance provided by the generative model. It is this guidance that we deem responsible for the improvement brought by semi-supervision over sheer supervision. However, the terms that influence the inference network in equation 6, when optimized, also bring together the $z$ samples from the approximate posterior and those from the true posterior. We find it important to study the difference between the effect of the objective from equation 13, and that of $-J^\alpha$. In that sense, we will present a tractable estimator for the objective in equation 13.

5 Rebuilding semi-supervised VAEs with importance weighting

The problematic terms in equation 13 are $\log p_{\theta}(x, y)$ and the second expectation, $\log p_{\theta}(x, y)$ can be lower-bounded by the IWAE objective when considering $(x, y)$ an observation and $z$ a latent variable:

$$\log p_{\theta}(x, y) \geq E_{z_1, \ldots, z_k \sim q_{\phi}(z|x, y)} \left[ \log \frac{1}{k} \sum_{i=1}^{k} \frac{p_{\theta}(x, y, z_i)}{q_{\phi}(z_i|x, y)} \right]$$

$$= \text{IWAE}(x, y, k) \quad (14)$$

The content of the second expectation in equation 13 can be lower-bounded by the following estimator that partially uses the IWAE formalism, making it the Partially Importance Weighted Objective (PIWO):

$$\log p_{\theta}(x) - \text{KL}[q_{\phi}(y|x)||p_{\theta}(y|x)] \geq E_{y \sim q_{\phi}(y|x)} \left[ \frac{1}{k} \sum_{i=1}^{k} \frac{p_{\theta}(x, y, z_i)}{q_{\phi}(y, z_i|x)} \right]$$

$$= \text{PIWO}(x, k) \quad (15)$$

Its derivation is explicited in Appendix B. Therefore, This estimator lower-bounds the
AppendixC): A question naturally arises bound when $k-J$ to $z$ sense, and using the analogue process, we derive a case $y$ the learning effort on $i$) process being dominated by the generation part. The supervised data has far lower data complexity than $z$ effort on $model is learned by concentrating the learning needs to be delayed until after a good generative

ii) guidance from the generative model overfits the few examples at hand and needs scarce, multiple scenarios are likely: $y$ could be tempted to concentrate the learning effort on $\alpha$ when $k=1$ and reaches the objective in equation 13 asymptotically when $k$ goes to infinity. We will refer to the lower bound in equation 16 as the Semi-Supervised PIWO (SSPIWO). The above formalism prioritizes having $y$ abide by the true posterior over having both $y$ and $z$ abide by it like in Semi-supervised VAEs (equation 6). A question naturally arises here: Is it always better to prioritize guiding $y$ with the true posterior?

In a setup where annotated data is abundant, one could be tempted to concentrate the learning effort on $y$. However, in a setup where labels are scarce, multiple scenarios are likely: i) $y$ overfits the few examples at hand and needs guidance from the generative model ii) Learning $y$ needs to be delayed until after a good generative model is learned by concentrating the learning effort on $z$ iii) Due to the difference in size, the supervised data has far lower data complexity than the unsupervised data, which leads to the learning process being dominated by the generation part. Case i) needs an objective that can concentrate the learning effort on $y$ like SSPIWO. However, case ii) needs to concentrate learning on $z$. In that sense, and using the analogue process, we derive a $z$ centered learning objective that is similarly equal to $-\mathcal{J}^\alpha$ at $k=1$ and reaches the following lower bound when $k$ goes to infinity (full derivation in AppendixC):

$$
\log p_\theta(x) + \log p_\theta(x, y) \geq \\
\mathbb{E}_{(x,y) \sim p^\star(x,y)} \left[ \alpha \log q_\phi(y|x) + \right. \\
\log p_\theta(x, y) - \text{KL}[q_\phi(z|x, y) \| p_\phi(z|x, y)] \\
+ \mathbb{E}_{x \sim p^\star(x)} \left[ \log p_\theta(x) - \text{KL}[q_\phi(z|x) \| p_\phi(z|x)] \\
\geq \text{SSPIWO}(x, y, k) \right. \tag{17}
$$

We dub this objective the Semi-Supervised inverse Partially Importance Weighted Objective (SSPIWO).

Finally, case iii) requires down-weighting the generative objective as a whole from the inference network’s learning objective. Given that weighting down the whole generative objective (or raising $\alpha$) has proven to be an effective strategy in semi-supervision with VAEs, the importance weighting used in SSIAE should also induce an improvement over vanilla SSVAEs. In fact, the SSIAE objective, as stated in 3.2, asymptotically anneals the Kullback-Leibler divergence between posterior approximations and the true posteriors, which we deem responsible for the generative modelling’s influence on the supervised learning process.

We synthesize the claims we aim to study in the following hypotheses: $H1$ : "SSPIWO improves upon SSVAE and SSPIWO in labeled data abundant regimes", $H2$ : "The effect of complete importance weighting (SSIAE) is similar to that of down-weighting the generative objective’s influence on the classifier using a higher $\alpha$", and $H3$ : "The prioritization importance weighting objectives SSPIWO brings a lever for improvement that is different than that of down-weighting the generative objective".

6 Experiments

6.1 Experimental Setup

Datasets Sequence classification tasks are a classical testbed for semi-supervised learning. Therefore, we use the following datasets:

- The binary sentiment analysis dataset IMDB. This dataset consists in 25K supervised examples and 50K unsupervised examples. The task here is to try to classify the sentiment expressed in movie reviews into negative, or positive sentiments. (Maas et al., 2011)
- the text classification dataset AG News (Zhang et al., 2015). This task is 4-way topic classification task. We use 32K labeled examples as was done in (Xu et al., 2017) and 64K unlabeled examples to obtain similar proportions to IMDB.

The supervised examples are divided into 5 splits. For all experiments, we report the average accuracy over 5 runs, swapping each time the split we use for validation (early stopping, and $\alpha$ selection). The
unlabeled training set is always fixed.

![Graphical Models](image)

Figure 1: Generative (left) and inference (right) Graphical Models

**Graphical Model** The graphical inference and generative models are depicted in figure 1. The white latent variables are Gaussian latent variables, while the grayed out ones are categorical. For the inference network, we model $y$ and $z$ as two conditionally independent latent variables (refer to Appendix D for a brief discussion of our objectives in the structured posterior case). In the generative model, we set the prior on $z$ to be a standard Gaussian, while $y$ is generated from a Categorical whose parameters are conditioned on $z$ through a learnable module. This design choice stems from the fact that we want the supervised $y$ in the inference model to be regularized by a distribution that depends on the example at hand. In fact, using independent priors would lead to regularizing $y$ with the marginal distribution of $y$ in the training set, while our modeling choice will provide $y$ with guidance that is specific to the current sample.

Finally, $x$ is generated auto-regressively using $y, z$, and its value at the previous time-step (the previous word).

**Architectural choices and hyper-parameters**

In the inference (encoding) step, the Gaussian latent variables $z$ and $y$ are given by $q(x, y|x) = q(y|x)q(z|x)$. They are both obtained by passing $x$ through the same pretrained 300-dimensional fastText (Bojanowski et al., 2016) embedding layer, then taking the last state from a common 2-layered BiLSTM with 200 hidden states. Their parameters are then obtained by passing this last state through 3 separate linear layers (1 for $\mu_z$, 1 for $\sigma_z$, and 1 for $\text{logits}_y$). $\sigma_z$ is obtained using an additional softplus activation gate. $z$ has size 100 and the embeddings for $y$ have size 50.

As for the decoding step, we model a structured prior $p(z, y) = p_\theta(y|z)p(z)$ where $p$ is a standard Gaussian and $p_\theta$ a linear layer yielding $\text{logits}_y$. The sampled $z$ and $y$ are then concatenated with the previous word at each generation step to obtain the next word using a 1-layered LSTM with size 200.

The experiments are conducted for the Semi-Supervised (SS) objectives "None" (pure supervision), "VAE", "PIWO", "iPIWO", and "IWAE". We try different supervision rates (percentages of supervised data with regard to total labeled training examples) ranging from 0.1% to 100%.

All experiments use a batch size of 32, a 0.5 dropout rate, and 4e-3 learning rate with the Adam optimizer (Kingma and Ba, 2015). For better efficiency, we reduce the vocabulary of the datasets to the 10000 most frequent words and we set the maximum sentence length to 256 tokens for IMDB and to 64 for AG News. No notable performance decay has been observed with these restrictions.

The stochasticity of the training procedure (random batches, latent variable samples, etc) brings variability in our experiments through phenomena that are out of the scope of this study. Nonetheless, we expect our hypotheses to be validated by the overall behavior of our results. The code for our experiments is publicly available.

**Training Procedure** To prevent posterior collapse, the kullback-leibler divergence is linearly annealed over the 3000 following steps as was done by Bowman et al. (2016). For the multisample models (SSIWAE, SSPIWO, and SSiPIWO) we use 5 importance samples. We use the STL objective (Roeder et al., 2017) for ELBo, and the DReG objective (Tucker et al., 2019) for importance weighted objectives, as these have been shown to lessen gradient variance without biasing the training procedure.

If the accuracy doesn’t improve for 4 epochs, the training is halted and the accuracy of the best epoch is reported.

**6.2 Results**

We compare the different objectives we are interested in, using different proportions of the labeled datasets. We picked the value for $\alpha$ that performed the best on the development set for each

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1[https://github.com/ghazi-f/SSPIWO]
Table 1: Accuracies on IMDB and AGNEWS on their respective test sets. The best semi-supervised accuracy for each part of the table, and each supervision proportion is given in bold. The standard deviation for the 5 runs is between parentheses.

| dataset | SS | 0.1%  | 0.3%  | 1%    | 3%    | 10%   | 30%   | 100%  |
|---------|----|-------|-------|-------|-------|-------|-------|-------|
| IMDB    | None | 52.86(1.73) | 51.73(1.71) | 54.69(3.00) | 56.19(4.14) | 73.10(1.91) | 82.48(0.55) | 86.65(0.44) |
|         | VAE  | 53.13(1.87) | 53.99(2.11) | 57.58(1.37) | 61.47(1.38) | 72.45(1.18) | 82.44(0.85) | 86.43(0.64) |
|         | PIWO | 53.33(1.21) | 53.91(2.57) | 56.32(1.33) | 60.81(1.79) | 74.52(1.30) | 82.99(0.54) | 87.05(0.50) |
|         | iPIWO| 53.17(1.87) | 52.70(1.69) | 55.97(1.92) | 59.71(2.84) | 74.51(0.76) | 82.56(1.11) | 86.61(0.91) |
|         | iVAE | 53.74(1.54) | 53.33(2.07) | 56.28(2.42) | 61.73(1.36) | 74.11(1.86) | 82.32(0.74) | 86.50(0.20) |
| AGNEWS  | None | 56.63(4.22) | 68.49(5.69) | 78.68(1.47) | 82.82(2.24) | 85.91(0.29) | 88.38(0.48) | 90.24(0.32) |
|         | VAE  | 60.23(2.54) | 71.21(1.50) | 78.73(0.86) | 82.14(0.96) | 85.81(0.78) | 88.26(0.25) | 90.13(0.29) |
|         | PIWO | 61.83(4.41) | 71.18(2.74) | 78.55(1.12) | 82.38(0.73) | 86.10(0.42) | 88.26(0.31) | 90.24(0.20) |
|         | iPIWO| 63.01(2.20) | 72.21(1.43) | 77.24(1.68) | 82.56(0.98) | 85.79(0.69) | 88.06(0.10) | 90.03(0.35) |
|         | iVAE | 62.40(3.22) | 70.75(4.42) | 77.82(2.17) | 82.61(0.93) | 85.28(1.04) | 87.99(0.44) | 90.12(0.20) |

Table 2: Average $\log_{10}(\alpha)$ values across experiments

| dataset | SSVAE | SSIWO | SSPIWO | SSIWAE |
|---------|-------|-------|--------|--------|
| IMDB    | 1.86  | 1.14  | 1.86   | 1.29   |
| AG News | 1.57  | 1.43  | 2.0    | 0.86   |

HSR regime In the HSR regime, despite high variances, it can be seen that the the highest score is consistently obtained with SSIW. SSPIWO outperforming SSVAE and SSPIWO constitutes evidence confirming hypothesis $H1$. Additionally, SSPIWO improving upon SSVAE and SSIW in an experiment where we searched for $\alpha$ establishes that the benefit of its prioritization is complimentary to the benefit of varying $\alpha$ and thus distinct (as stated by hypothesis $H3$).

LR regime As discussed in section 5, there are different factors at play in the low supervision regime making it difficult for one objective to always outperform the others. This undermines the fact that even though SSPIWO is able to bring improvement, avoiding overfitting through careful architectural choices is still of great importance.

Studying the values of $\alpha$ A last observation we made in our experiments is reported in table 2, when inspecting the values of $\alpha$ that yielded the best performance for each objective. We can see that SSVAE selected values of $\alpha$ that were, in average, higher than those selected by SSIW by a large margin. This suggests that SSIW already down-weights the influence of the unsupervised objective to a certain extent, which is in line with Hypothesis $H2$. Now looking at the prioritization objectives, we can also see in both experiments that SSPIWO has higher or equal $\alpha$ values than SSVAE, and that SSPIWO selects $\alpha$ values that are lower than those of SSVAE. Focusing on the partially observed latent variable rather than the unsupervised latent variable seems to allow for more learning signal from the unsupervised objective. This evidence further supports our claim about the core of the improvement brought by Semi-Supervised VAEs over purely supervised learning (section 4).

Relationship to multitask learning We consider it most interesting to remember that semi-supervision with generative models is a special case of multi-task learning where the performance on a main task is improved by jointly training for a proxy unsupervised task. Compatibility between multiple tasks in multi-task learning has been studied in numerous works. In the special case of NLP, the work of Binge and Sogaard (2017) has shown that a major explanatory factor for the compatibility between main tasks and auxiliary tasks was whether gradients rose at similar moments during single task training. Results from our work show that it is possible to
alter the influence of the unsupervised proxy task in a sound manner so that a task that hindered learning the main task (c.f. VAE vs None in table 1 for 10% to 100% of IMDB) becomes beneficial for it (c.f. PIWO vs None results in the same setup). Therefore, importance weighting is a promising avenue of research to find training schemes for multivariate VAE based graphical models that improve compatibility between main tasks and auxiliary tasks.

7 Discussion & Conclusion

Our work enabled better control on the learning process of semi-supervision with deep generative models. We conducted an analysis on the objective used in these models, which led to an alternative objective that could improve upon the vanilla SSVAE objective while still lower-bounding the true joint likelihood. The improvements brought by SSPIWO proved to be distinct from that of the weighting mechanism classically used in SSVAEs. We stated 3 Hypotheses in the theoretical section, which were in line with the results provided by our experimental section. We now know that SSVAEs guide a partially observed variable by having it abide by their true posterior. We also know of a way to prioritize this guidance over learning other variability factors for the generative model, or conversely, how to prioritize factorizing the generative model into unknown factors while putting a minimum effort into aligning these factors with information from supervised variables. SSPIWO enables better injection of information about a known variability factor into a latent variable in regimes where labeled data is highly available. VAEs possessing a latent variable with a specific meaning are useful for semi-supervision, but also yield a model where the inference network can better explain the observations, and where the generative model can perform generation conditioned on specific values of the known factor. For suitably sized networks, SSPIWO could therefore improve such systems.

Although our study has brought to light new information about SSVAEs, it is limited with regard to two aspects. The first is that our new objectives use importance weighting, which linearly increases the memory cost of training. This disables the use of higher batch sizes for hardware with limited memory, or requires resorting to techniques such as gradient accumulation to lighten the memory constraints at the cost of a longer run time. The second limit is that this study focuses only on improving the classification score, while disregarding the generation score. We find it important for the whole joint likelihood lower-bounded by our objectives to be well estimated, leading to a model that can properly estimate labels from observation and conditionally generate observations on given labels. As such, we strongly advocate for the investigation of partially importance weighted objectives for conditional generation in future works.

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A Derivations for equations 5 and 4

The following equality is known to be valid for an ELBo featuring $x$ as an observation and $z$ as a latent variable (Kim et al., 2019):

$$
E_{z \sim q_\phi(z|x)} \left[ \log p_\theta(x|z) \right]
+ \log p_\theta(z) - \log q_\phi(z|x)
= \log p_\theta(x) - KL[q_\phi(z|x)||p_\theta(z|x)]
$$

Equation 5 (resp. equation 4) is a direct application for this equality in a case where the observation is $x$ (resp. $(x, y)$) and the latent variable is $(y, z)$ (resp. $z$).

B Partially Importance Weighted Objective Derivation

We depart from the ELBo expressed considering only $y$ as a latent variable. The property exhibited by ELBo in equation 18 becomes as follows:

$$
\log p_\theta(x) - KL[q_\phi(y|x)||p_\theta(y|x)]
= E_{y \sim q_\phi(y|x)} \left[ \log p_\theta(x|y) \right] - KL[q_\phi(y|x)||p_\theta(y)]
$$

The left hand side is the content of the second expectation in equation 13 that we would like to estimate. The second term of the right hand size is tractable, but the first term is intractable. In fact, it would require marginalizing $p_\theta(x|y, z)p(z)$ over all possible values of $z$, and sampling from $p(z)$ is too inefficient for this to be done. Here we simply used the IWAE objective to lower-bound the first term (log-likelihood of $x$ conditioned on $y$):

$$
E_{y \sim q_\phi(y|x)} \left[ \log p_\theta(x|y) \right] \geq \sum_{k=1}^{K} \frac{1}{K} \left[ \log \frac{1}{K} \sum_{i=1}^{K} p_{x, z_i}(x, z_i|y) \right]
$$

Inequality 20 turns to an equality when $k$ goes to infinity. Replacing the first term in the right hand side of equation 19 with its lower bound from equation 20 leads to the PIWO lower bound:

$$
\log p_\theta(x) - KL[q_\phi(y|x)||p_\theta(y|x)]
\geq \sum_{k=1}^{K} \frac{1}{K} \left[ \log \frac{1}{K} \sum_{i=1}^{K} p_{x, z_i}(x, z_i|y) \right] - KL[q_\phi(y|x)||p_\theta(y)]
$$

The last equality just integrates the decomposed Kullback-Leibler term into the expectation to make it more compact.
The quantity we aim to estimate is the following:

$$\text{SSiPIWO}(x, y, k) \leq \mathbb{E}_{(x,y) \sim p^*(x,y)} \left[ \alpha \log q_\phi(y|x) + \log p_\theta(x, y) - \text{KL}[q_\phi(z|x, y)||p_\theta(z|x, y)] \right]$$

$$+ \mathbb{E}_{x \sim p^*(x)} \left[ \log p_\theta(x) - \text{KL}[q_\phi(z|x)||p_\theta(z|x)] \right]$$

(22)

The first expectation is clearly the same as in $J^\alpha$ and will be trivially estimated using $\mathcal{L}(x, y)$ and $q_\phi(y|x)$.

For the term in the second expectation, we can use the exact derivation we used for PIWO while swapping the role of $y$ and $z$. In fact, this quantity is subject to the equality:

$$\log p_\theta(x) - \text{KL}[q_\phi(z|x)||p_\theta(z|x)] = \mathbb{E}_{z \sim q_\phi(z|x)} [\log p_\theta(x)] - \text{KL}[q_\phi(z|x)||p_\theta(z)]$$

(23)

It can thus be analogously lower-bounded by:

$$\log p_\theta(x) - \text{KL}[q_\phi(z|x)||p_\theta(z|x)] \geq \mathbb{E}_{z \sim q_\phi(z|x)} \left[ \sum_{i=1}^{k} \frac{1}{k} \log p_\theta(x, y_i, z) \right]$$

$$= \text{iPIWO}(x, k)$$

(24)

The full estimator for SSiPIWO is therefore

$$\text{SSiPIWO}(x, y, k) = \mathbb{E}_{(x,y) \sim p^*(x,y)} \left[ \alpha \log q_\phi(y|x) - \mathcal{L}(x, y) \right]$$

$$+ \mathbb{E}_{x \sim p^*(x)} \left[ \text{iPIWO}(x, k) \right]$$

(25)

D About Structured Approximate Posteriors

Modeling latent variables in the approximate posterior as independent latent variables is a choice that is most often sufficient. This ensues from the fact that, in most cases, observations are completely informative on the latent variables. Nevertheless, PIWO as can be seen in equation 21 requires sampling from $q_\phi(z|x, y)$ and, as a consequence, can only be computed exactly in cases where our variational posterior factors as $q_\phi(y, z|x) = q_\phi(z|x, y)q_\phi(y|x)$ (which includes the independence case). Otherwise, a lower bound to PIWO may be derived using a procedure similar to that used in (Siddharth et al., 2017) in section 2.1.

Of course, the analogous argument stands for iPIWO when swapping $z$ and $y$. .