Learning Selection Bias and Group Importance: Differentiable Reparameterization for the Hypergeometric Distribution

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Abstract

Partitioning a set of elements into a given number of groups of a priori unknown sizes is a critical task in many applications. It can be characterized by a hypergeometric distribution, which describes biased sampling without replacement based on the relative importance between classes of samples. Due to hard constraints, this discrete distribution is not differentiable in its standard formulation, prohibiting its use in modern machine learning frameworks. Hence, previous works mostly fall back on suboptimal heuristics or simplified assumptions. In this work, we propose a differentiable reparameterization trick for the multivariate noncentral hypergeometric distribution. We introduce reparameterizable gradients to enable learning of the importance or the selection bias between groups. We highlight the applicability and usability of the proposed formulation in two different experiments: weakly-supervised learning and clustering.

1 Introduction

Many machine learning approaches, such as deep generative models, rely on differentiable sampling procedures. Most notably, the reparameterization trick for Gaussian distributions [24, 44]. Another example is the categorical distribution, used in either generative models with latent categorical variables [25] or attention mechanisms [52]. The concrete distribution [37] or Gumbel-Softmax trick [21] has recently boosted its usage in stochastic networks. Unlike the high-variance gradients of score-based methods such as REINFORCE [50], these works enable reparameterized and low-variance gradients with respect to the categorical weights. Based on the Gumbel-Softmax trick, reparameterization procedures in combination with continuous relaxations for discrete distributions and other previously non-differentiable algorithms gained attraction in machine learning research [17, 43, 51]. Despite enormous progress in recent years, the extension to more complex probability distributions is still missing or comes with a trade-off regarding differentiability or computational speed [20].

In this work, we propose a differentiable reparameterization for the hypergeometric distribution. This discrete probability distribution describes the probability of $x$ successes out of $n$ trials from a total population of size $N$ with $m$ members belonging to the success class [46]. The classical application is sampling without replacement, for which an urn model is the standard example. In the univariate case, the urn consists of marbles in two different colors, whereas in the multivariate case, there are marbles in $c$ different colors. The hypergeometric distribution plays an important role in various areas of science, such as biology, social and computer science. Applications go from modeling gene mutations and recommender systems to analyzing social networks [3, 7, 35]. It is essential wherever the choice of a single element influences the distribution over classes of the remaining components.
Previous work mainly uses the hypergeometric distribution implicitly to model assumptions or as a tool to prove theorems. However, to the best of our knowledge, it is not yet integrated into the learning processes themselves.

Our differentiable reparameterization integrates the hypergeometric distribution into stochastic networks and modern learning frameworks. By combining a sequence of categorical distributions, we enable reparameterizing a more complex but well-defined distribution. Additionally, the hypergeometric distribution allows us to introduce dependencies between elements or samples in cases where previous work had to assume independence.

We highlight the advantages of our new formulation in two different experiments. Our first experiment demonstrates the potential of the hypergeometric distribution for a weakly-supervised learning task where we assign latent dimensions to groups of unknown size. Our second experiment integrates the hypergeometric distribution into a variational clustering algorithm. We model the number of samples per cluster using an adaptive hypergeometric distribution prior. By doing so, we overcome the simplified i.i.d. assumption and establish a dependency structure between dataset samples.

Our contributions are the following:

1. We introduce a differentiable reparameterization for the hypergeometric distribution, which uses the Gumbel-Softmax trick in combination with sequential sampling.
2. The proposed formulation enables learning selection bias and group importance from data.
3. We highlight the versatility of the proposed method in two different experiments.

2 Related Work

In recent years, finding continuous relaxations for discrete distributions and non-differentiable algorithms to integrate them into differentiable pipelines gained popularity. Jang et al. [21] and Maddison et al. [37] concurrently proposed the Gumbel-Softmax gradient estimator. It enabled reparameterized gradients with respect to parameters of the categorical distribution and their use in differentiable models. Methods to select \( k \) elements - instead of only one - were subsequently introduced. Kool et al. [27, 28] implement sequential sampling without replacement using a stochastic beam search. Kool et al. [29] extend the sequential sampling procedure to a reparameterizable estimator using REINFORCE. Grover et al. [17] proposed a relaxed version of a sorting procedure that simultaneously serves as a differentiable and reparameterizable top-\( k \) elements selection procedure. Xie and Ermon [51] proposed a relaxed subset selection algorithm to select a given number \( k \) out of \( n \) elements. Paulus et al. [43] generalized stochastic softmax tricks to combinatorial spaces. Unlike Kool et al. [29], who also use a sequence of categorical distributions, the proposed method describes a differentiable reparameterization for the more complex but well-defined hypergeometric distribution. Differentiable reparameterizations of complex distributions with learnable parameters enable new applications, as shown in Section 5.

The classical use case for the hypergeometric probability distribution is sampling without replacement, for which urn models serve as the standard example. The hypergeometric distribution is used as modeling distribution in simulations of social evolution [30, 40, 41], tracking of human neurons and gene mutations [35, 36], network analysis [7], and recommender systems [3]. Additionally, it is used as modeling assumption in submodular maximization [11, 18], \( k \)-means clustering variants [9], or random permutation graphs [5]. Despite not being differentiable, current sampling schemes for the multivariate hypergeometric distribution are a trade-off between numerical stability and computational efficiency [13, 14, 32].

3 Preliminaries

Urn models are typical examples of the hypergeometric probability distribution. Suppose we think of an urn with marbles in different colors. Then, \( c \in \mathbb{N}_+ \) is the number of different classes (e.g. marble colors in the urn), \( \mathbf{m} = [m_1, \ldots, m_c] \in \mathbb{N}_+^c \) describes the number of elements per class (e.g. marbles per color), \( N = \sum_{i=1}^{c} m_i \) is the total number of elements (e.g. all marbles in the urn) and...

\[ \text{Huijben et al. [20] provide a great review article of the Gumbel-Max trick and its extensions describing recent algorithmic developments and applications.} \]
Let \( n \in \{0, \ldots, N\} \) be the number of elements (e.g., marbles) to draw. The multivariate hypergeometric distribution describes the probability of drawing \( \mathbf{x} = [x_1, \ldots, x_c] \in \mathbb{N}_+^c \) marbles by sampling without replacement such that \( \sum_{i=1}^c x_i = n \).

So far, every marble in the urn is picked equally likely, and there is no selection bias. The number of selected class samples is proportional to the ratio between class elements and the total number of elements in the urn. Often this assumption is too restrictive, and selection bias is a desired model property. Biased generalizations, which make certain colors more likely to be picked, exist for the univariate case. We focus on the multivariate distribution as the univariate distribution is only a special case.

An additional variable \( \omega_i \in \mathbb{R}_{0+} \) for every class \( i \) introduces selection bias between classes. In the literature, two different versions of the noncentral hypergeometric distribution exist, Fisher’s [12] and Wallenius’ [8, 48] distribution. Due to limitations of the latter [13], we will refer to Fisher’s version of the noncentral hypergeometric distribution in the remaining part of this work.

**Definition 3.1 (Multivariate Fisher’s Noncentral Hypergeometric Distribution).** A random vector \( \mathbf{X} \) follows Fisher’s noncentral multivariate distribution, if its joint probability mass function is given by [12]

\[
P(\mathbf{X} = \mathbf{x}; \omega) = p_{\mathbf{X}}(\mathbf{x}; \omega) = \frac{1}{P_0} \prod_{i=1}^c \binom{m_i}{x_i} \omega_i^{x_i}, \quad \text{where} \quad P_0 = \sum_{(y_1, \ldots, y_c) \in S} \prod_{i=1}^c \binom{m_i}{y_i} \omega_i^{y_i} \tag{1}
\]

and \( \binom{n}{k} = \frac{n!}{k!(n-k)!} \). The support \( S \) of the PMF is given by

\[
S = \left\{ \mathbf{x} \in \mathbb{Z}_{0+}^c : \forall i \quad x_i \leq m_i, \sum_{i=1}^c x_i = n \right\} \tag{2}
\]

The multivariate distribution is parameterized by the total number of samples per class \( m_i \), the number of samples to draw \( n \) and the group importances \( \omega \). In this work, we assume \( m_i \) and \( n \) fixed per experiment. Therefore, and to reduce clutter, we only use \( \omega \) as distribution parameter in Equation (1) and the remaining part in this work.

The class importance \( \omega \) is a crucial modeling parameter in applying the noncentral hypergeometric distribution (see [8]). It resembles latent factors like importance, fitness, or adaptation capabilities of a class of elements, which are often more challenging to measure in field experiments than the sizes of different populations. Introducing a differentiable and reparameterizable formulation enables the learning of selection bias and group importance from data. We highlight this in Section 5. We provide a more detailed introduction to the hypergeometric distribution in Appendix A.

### 4 Method

Multiple sampling procedures exist for the noncentral hypergeometric distribution [14]. We choose the conditional sampling algorithm because it scales linearly with the number of classes and not with the number of states as in previous works [32]. This procedure uses the conditional probability equation given by

\[
p_{\mathbf{X}}(\mathbf{x}; \omega) = p_{X_1}(x_1; \omega) \prod_{i=2}^c p_{X_i}(x_i|\{\bigcup_{j<i} x_j\}; \omega) \tag{3}
\]

The first class \( X_1 \) is sampled from the marginal distribution \( p_{X_1}(x_1; \omega) \), then the following classes \( X_i, i > 1 \) are sampled from the conditional distribution given all previously sampled classes \( p_{X_i}(x_i|\{x_1, \ldots, x_{i-1}\}; \omega) \) [23]. Broadly speaking, the sampling algorithm consists of 3 parts:

1. Reformulate the multivariate distribution as a sequence of interdependent and conditional univariate distributions.
2. Calculate the PMF of the respective univariate distributions.
3. Sample from this conditional distribution utilizing the Gumbel-Softmax trick.

The sampling algorithm is described in Algorithm 1 using pseudo-code. We explain and discuss all steps in the following sections of this paper.
we derive the calculation of the PMF for the univariate distribution only. For the multivariate
As described in the introduction to Section 4, we use a conditional sampling scheme. We sample
Algorithm 1
Sampling From Multivariate Noncentral Hypergeometric Distribution. The different
blocks are explained in more detail in Sections 4.1 to 4.3
Input: \( m \in \mathbb{Z}_{0+}^c, \omega \in \mathbb{R}_{0+}^c, n \in \mathbb{N}, \tau \in \mathbb{R}_+ \)
Output: \( x \in \mathbb{Z}_{0+}^c, \{ \alpha_i \in \mathbb{R}^{m_i} \}_{i=1}^c, \{ \tilde{r}_i \in \mathbb{R}^{m_i} \}_{i=1}^c \)
for \( i \in \{ 1, \ldots, c \} \) do
\[
L \leftarrow i, R \leftarrow \bigcup_{j=i+1}^c j \quad \text{# Formulate the multivariate as a univariate}
\]
\[
m \rightarrow m_L, m_R \in \mathbb{Z}_{0+}, \omega \rightarrow \omega_L, \omega_R \in \mathbb{R}_{0+} \quad \text{# distribution (Section 4.1)}
\]
x_L, \alpha_L, \tilde{r}_L \leftarrow \text{sampleUNCHG}(m_L, m_R, \omega_L, \omega_R, n, \tau) \quad \text{# Sample from univariate distribution}
\]
n \leftarrow n - x_L \quad \text{# Re-assign classes for next step}
\]
x_i \leftarrow x_L, \alpha_i \leftarrow \alpha_L, \tilde{r}_i \leftarrow \tilde{r}_L \quad \text{# Assign values for next class}
\]
end for
return \( x, \{ \alpha_i \}_{i=1}^c, \{ \tilde{r}_i \}_{i=1}^c \)

function \text{SAMPLEUNCHG}(m_i, m_j, \omega_i, \omega_j, n, \tau)
\]
\[
\alpha_i \leftarrow \text{calcLogPMF}(m_i, \omega_i, n) \quad \text{# Section 4.2}
\]
x_i, \tilde{r}_i \leftarrow \text{contRelaxSample}(\alpha_i, \tau) \quad \text{# Section 4.3}
\]
return \( x_i, \alpha_i, \tilde{r}_i \)
end function

4.1 Sequential Sampling Using Conditional Distributions
As described in the introduction to Section 4, we use a conditional sampling scheme. We sample from a sequence of conditional univariate distributions instead of a single multivariate one. In the first step, we define class \( i = 1 \) as the success class and merge the remaining classes \( i > 1 \) into a single, negative class. We then sample \( x_1 \) elements from class \( i = 1 \) out of \( n \) elements we sample in total. In the second step, we define class \( i = 2 \) as success class and, again, merge the remaining classes \( i > 2 \) into a single, negative class. We then sample \( x_2 \) elements from class \( i = 2 \). Because we already sampled \( x_1 \) elements in the first step, the number of elements to sample is \( n - x_1 \) elements at this stage. From step 1 to step 2, the number of elements to sample from (e.g. the total number of marbles in the urn) changes from \( N_1 = \sum_{i=1}^n m_i \) to \( N_2 = N_1 - m_1 \). We continue with this procedure until no class is left to be sampled from, i.e. \( i = c \) [14].

There are, of course, various algorithms for creating univariate distributions out of subsets of classes. Independent of the algorithm, we define the two new classes as \( L \) and \( R \), and the respective parameters are given by [14]

\[
m_L = \sum_{i \in L} m_i, \quad m_R = \sum_{r \in R} m_r, \quad \omega_L = \sum_{i \in L} \omega_i \cdot m_i, \quad \omega_R = \sum_{r \in R} \omega_r \cdot m_r
\]

In this work, we follow a straightforward approach. As described above, we select a single class \( i \) as set \( L \) and the remaining classes as set \( R \). Afterwards, we choose a single class \( j \) from set \( R \) as our new set \( L \). We leave the exploration of different and more sophisticated subset selection strategies for future work.

This method produces biased samples for noncentral distributions as merging multiple classes into one is only approximately equal to the univariate noncentral distribution. The choice of classes to merge might influence the quality of the approximation [14]. Note that the proposed method introduces bias compared to a non-differentiable reference distribution with the same \( \omega \) (see Section 5.1) and not the underlying and desired true selection bias. We can still recover the true selection bias because a different \( \omega \) can overcome the bias introduced by the conditional sampling and merging procedure.

4.2 Calculate Probability Mass Function
In Section 4.1, we derive a sequential sampling procedure for the hypergeometric distribution. In this sequential procedure we repeatedly simulate a univariate distribution to simplify sampling. Therefore, we derive the calculation of the PMF for the univariate distribution only. For the multivariate extension, see Appendix B.1.
The PMF $p_{X_L}(x_L; \omega)$ for the hypergeometric distribution of two classes $L$ and $R$ defined by $m_L, m_R, \omega_L, \omega_R$ and $n$ is given as

$$p_{X_L}(x_L; \omega) = \frac{1}{P_0} \binom{m_L}{x_L} \omega_L^{x_L} \binom{m_R}{n-x_L} \omega_R^{n-x_L} \tag{5}$$

$P_0$ is defined as in Equation (1), $\omega_L, \omega_R$ and their derivation from $\omega$, and $m_L, m_R, n$ as in Equation (4). The large exponent of $\omega$ and the combinatorial terms can lead to numerical instabilities making the direct calculation of the PMF in Equation (5) infeasible. Calculations in log-domain increase numerical stability for such large domains, while keeping the relative ordering.

**Lemma 4.1.** The unnormalized log-probabilities

$$\log p_{X_L}(x_L; \omega) = x_L \cdot \log \omega_L + (n - x_L) \log \omega_R + \psi_F(x_L) + C \tag{6}$$

define the unnormalized weights of a categorical distribution that follows Fisher’s noncentral hypergeometric distribution. $C$ is a constant and $\psi_F(x_L)$ is defined as follows

$$\psi_F(x_L) = -\log (\Gamma(x_L + 1) \Gamma(n - x_L + 1)) - \log (\Gamma(m_L - x_L + 1) \Gamma(m_R - n + x_L + 1)) \tag{7}$$

We provide the proof to Lemma 4.1 in Appendix B.2. This subsection relates to the calculation of the PMF function in Algorithm 1. Common automatic differentiation frameworks\(^2\) have numerically stable implementations of $\log \Gamma(x)$. Therefore, Equation (7) and more importantly Equation (6) can be calculated efficiently and reliably.

Using the multivariate form of Lemma 4.1 (see Appendix B.1), it is possible to directly calculate the categorical weights for the multivariate states. A multivariate state is defined as valid combination of $X = x$. It would result in a significant speed-up for large number of classes $c$ compared to the conditional sampling procedure. However, the number of multivariate states is $\prod_{i=1}^{c} m_i$, which quickly results in unfeasible memory requirements. Therefore, we would be restricted to settings with no practical relevance.

### 4.3 Continuous Relaxation

Continuous relaxations describe procedures to make discrete distributions differentiable with respect to their parameters [20]. We make use of the Gumbel-Softmax trick to reparameterize the conditional distributions. The Gumbel-Softmax trick enables a reparameterization of categorical distributions that allows the computation of gradients with respect to the distributions parameters. We state Lemma 4.2, and provide a proof in Appendix B.3.

**Lemma 4.2.** The Gumbel-Softmax trick can be applied to the conditional distribution $p_{X_i}(x_i|x_{-i})$ of class $i$ given the already sampled classes $k < i$.

Lemma 4.2 connects the Gumbel-Softmax trick to the hypergeometric distribution. Hence, reparameterizing enables gradients with respect to the parameter $\omega$ of the hypergeometric distribution:

$$u \sim U(0,1), \quad g_i = -\log(-\log(u)), \quad \tilde{r}_i = \alpha_i(\omega) + g_i \tag{8}$$

where $u \in [0, 1]^{m_i+1}$ is a random sample from an i.i.d. uniform distribution $U$, $g_i$ is therefore i.i.d. gumbel noise. $\tilde{r}_i$ are the perturbed conditional probabilities for class $i$ given the class conditional unnormalized log-weights $\alpha_i(\omega)$. Note the difference between the categorical and the hypergeometric distribution concerning the Gumbel-Softmax trick. Whereas the (unnormalized) category weights are also the distribution parameters for the former, the log-weights $\alpha_i$ for class $i$ are a function of the class importance $\omega$ and the pre-defined $x_i = [0, \ldots, m_i]$ for the latter.

$$\alpha_i(\omega) = \log p_{X_i}(x_i; \omega) = [\log p_{X_i}(0; \omega), \ldots, \log p_{X_i}(m_i; \omega)] \tag{9}$$

We use the softmax function to generate $(m_i + 1)$-dimensional sample vectors from the perturbed unnormalized weights $\tilde{r}_i/\tau$, where $\tau$ is the temperature parameter. Softmax is the continuous and differentiable approximation to the argmax function. Due to Lemma 4.2 and the translation-invariance of the arg max-function, the softmax function is invariant to constant shifts and we do not need to calculate the constant $C$ in Equation (6). We refer the reader to Jang et al. [21] or Maddison

\(^2\)E.g. Tensorflow [1] or PyTorch [42]
Figure 1: Comparing random variables from the proposed distribution to a reference distribution. We draw samples from a multivariate noncentral hypergeometric distribution consisting of 3 classes. \( m_i = 200 \) \( \forall \ i \) and \( n = 180 \). The class weights \( \omega_1 \) and \( \omega_3 \) for classes 1 and 3 are set to 1.0, \( \omega_2 \) is increased from 1.0 to 10.0 with a step size of 1.0 (defined as \( w_2 \) in the figure legend). Figure 1a shows histograms of the number of elements for class 2. We see that the behaviour across different class weights \( \omega_2 \) is very similar between the proposed and the reference implementation. This behaviour is also reflected in values of the KS test and their respective \( p \)-values in Figure 1b.

et al. [37] for more details on the Gumbel-Softmax trick itself. This procedure corresponds to the `reSample` function in Algorithm 1.

Sampling without replacement and the hard constraint \( \sum_i x_i = n \) make the sequential sampling from predefined categorical distributions impossible without dynamically changing category weights. Hence, assigning distribution parameters would not be independent anymore from sampling. For the hypergeometric distribution, instead, we introduce a sampling scheme that adapts the categorical weights based on the parameter \( \omega \) by taking advantage of Lemma 4.1 and Equation (9). This is crucial and enables taking gradients with respect to the distribution parameters \( \omega \), equal to reparameterization tricks of other distributions.

5 Experiments

We perform three experiments that demonstrate the accuracy of the proposed method and highlight the versatility and applicability of the multivariate hypergeometric distribution to different important areas of machine learning. We first test the proposed formulation of the hypergeometric sampling procedure against a reference implementation. Second, we show how the hypergeometric distribution finds groups of shared generative factors in the weakly-supervised setting. Our third experiment demonstrates that variational clustering algorithms benefit from the hypergeometric distribution prior.

5.1 Kolmogorov-Smirnov Test

To assess the accuracy of the proposed method, we evaluate it against a reference distribution using the Kolmogorov-Smirnov test [26, 45, KS]. It is a nonparametric test to estimate the equality of two distributions for continuous and discrete probability distributions. We compare the class conditional hypergeometric distributions against a reference distribution from SciPy [47]. As described in Section 4 class conditional distributions are used to sample from the multivariate distribution. For this experiment, we use a multivariate hypergeometric distribution of three classes. We perform a sensitivity analysis with respect to the class weights \( \omega \). We keep \( \omega_1 \) and \( \omega_3 \) fixed at 1.0, and \( \omega_2 \) is increased from 1.0 to 10.0 in steps of 1.0. For every value of \( \omega_2 \), we sample 50000 i.i.d. random vectors. The KS test quantifies a distance between the empirical distributions of two groups of samples. Hence, a small test value implies that the underlying distributions are similar. The null distribution of this test is calculated under the null hypothesis that the two groups of samples are drawn from the same distribution. We would like the test to fail to reject the null hypothesis in our setting. In this case, the same distribution generated the two groups of samples, i.e. the two underlying distributions are equal. We can only reject the null hypothesis if the \( p \)-value is below the significance threshold \( t = 0.05 \). Vice versa, \( p > 0.05 \) implies that we cannot reject the null hypothesis, which is desirable for our application.
Estimation of shared factors

learned representation

Figure 2: Evaluation of three different methods on the weakly-supervised learning experiment with respect to two different tasks. We compare our HypergeometricVAE against two previous methods, LabelVAE and AdaptiveVAE. First (Figure 2a), we evaluate the models’ ability to estimate the number of shared generative factors between a pair of images. The performance is reported using mean squared error (MSE) between the true and the estimated number of shared factors (lower is better). Second (Figure 2b), we assess the quality of the learned latent representation. The performance is reported using classification accuracy with respect to the generative factors. We report the mean accuracy over all generative factors (higher is better). The proposed model (Hypergeometric) outperforms existing models (Label, Adaptive) by a margin in estimating the number of shared factors while reaching almost the same performance in the quality of latent representations.

Figure 1 shows the histogram of class 2 for all values of \( \omega_2 \) (Figure 1a) and the results of the KS test for all classes (Figure 1b). The histograms for classes 1 and 3 are in the Appendix (Figure 3). We see that the proposed and the reference distribution histograms are visually similar. Additionally, the calculated distances of the KS-test are small, and the corrected \( p > 0.05 \). We correct the \( p \)-values for false discovery rate of multiple comparisons as we are performing \( c = 3 \) tests per joint distribution. We use the Benjamini-Hochberg correction [4]. In Figure 1b, we see that the test clearly fails to reject the null hypothesis in 30 out of 30 cases. For all tests, \( p \)-values are well above the threshold, and many are close to 1.0. The results of the KS test strongly imply that the proposed continuous relaxation and sampling procedure follow a noncentral hypergeometric distribution.

5.2 Weakly-Supervised Learning

In this experiment, we induce weak-supervision through pairs of images that may share part of their generating factors. We do not know the actual number of generative factors nor the number of shared latent factors. We use the setting and code from Locatello et al. [34] and compare the models on the mpi3d toy dataset [15]. We train all models as variational autoencoders [24, VAE] to maximize an evidence lower bound (ELBO) on the marginal log-likelihood of images. We perform the same experiment for multiple dataset versions with different numbers of independent generative factors \( k \). By independent, we mean generative factors that do not encode the same information for a pair of images.

We compare three methods, which all try to infer shared and independent latent factors. All methods individually encode both images to some latent representation, aggregate them to get a shared latent representation, and then identify the independent dimensions that should be replaced with the shared ones. The difference among methods is only in the selection process of shared factors. The first one assumes that the number of independent factors is known [6, 19, LabelVAE]. Like in Locatello et al. [34], we assume this to be 1 for all experiments. The second method relies on an adaptive heuristic to infer the number of shared latent factors [34, AdaptiveVAE]. First, they calculate the Kullback-Leibler (KL) divergence between pairs (across images) of latent factors. Then, their heuristic defines a threshold to determine whether a pair of factors encodes the same information, i.e., is shared, or not.

In our approach (HypergeometricVAE), we model the number of shared and independent latent factors of a pair of images as a multivariate hypergeometric distribution with unknown \( \omega \in \mathbb{R}_{d+}^2 \). For \( d \) being the number of latent factors, we have \( m_i = d \) where \( i \in \{1, 2\} \) and the number of elements to draw \( n = d \). Given class weights \( \omega \), we are able to sample estimates for the \( k \) independent and \( d - k \) shared factors. The proposed formulation allows to infer such \( \omega \) and simultaneously learn...
We investigate the use of the multivariate noncentral hypergeometric distribution in a deep clustering task. Several techniques have been proposed in the literature to combine long-established clustering algorithms, such as K-means or Gaussian Mixture Models, with the flexibility of deep neural networks to learn better representations of high-dimensional data [39]. Among those, Jiang et al. [22], Dilokthanakul et al. [10], and Manduchi et al. [38] include a trainable Gaussian Mixture prior distribution in the latent space of a VAE. A Gaussian Mixture model permits a probabilistic approach to clustering where an explicit generative assumption of the data is defined. All methods are optimized using stochastic gradient variational Bayes [24, 44]. A major drawback of the above models is that the samples are either assumed to be i.i.d. or they require pairwise side information, which limits their applicability in real-world scenarios.

5.3 Deep Variational Clustering

We see that our model reaches comparable performance to the baseline methods. Given the general works, it is not explicitly designed for weakly-supervised learning but achieves results more than comparable to field-specific models. Additionally, the proposed method gives accurate estimates of the nature of the method, the positive results of the proposed method are surprising. Unlike previous works, it is not explicitly designed for weakly-supervised learning but achieves results more than comparable to field-specific models.

Table 1: Evaluation of the clustering experiment on the MNIST datasets. We compare the methods on 3 different dataset versions, namely i) uniform class distribution ii) subsampling with 80% of samples and iii) subsampling with only 60% of samples. We subsample half of the classes. Accuracy (Acc), normalized mutual information (NMI), and adjusted rand index (ARI) are used as evaluation metrics. Higher is better for all metrics. Mean and standard deviations are computed across 5 runs.

| Dataset Version | Uniform | Categorical | Hypergeometric |
|-----------------|---------|-------------|----------------|
| **Uniform**     | Acc (%) | 92.0 ± 3.0  | 87.2 ± 5.0     | 93.8 ± 2.0    |
|                 | NMI (%) | 84.8 ± 2.2  | 81.8 ± 1.9     | 86.3 ± 3.0    |
|                 | ARI (%) | 84.2 ± 4.3  | 78.3 ± 4.6     | 86.9 ± 4.0    |
| **Subsampling 80%** | Acc (%) | 90.8 ± 4.0  | 87.4 ± 4.7     | 92.5 ± 0.5    |
|                 | NMI (%) | 84.1 ± 2.2  | 81.8 ± 2.3     | 84.6 ± 0.8    |
|                 | ARI (%) | 83.2 ± 3.6  | 78.2 ± 5.0     | 84.4 ± 1.0    |
| **Subsampling 60%** | Acc (%) | 83.5 ± 3.9  | 86.5 ± 4.9     | 89.7 ± 4.3    |
|                 | NMI (%) | 80.7 ± 1.4  | 81.3 ± 2.9     | 82.9 ± 2.2    |
|                 | ARI (%) | 77.6 ± 2.6  | 77.7 ± 6.3     | 81.5 ± 3.9    |
The multivariate noncentral hypergeometric distribution can be easily integrated in VAE-based clustering algorithms to overcome limitations of current approaches. Given a dataset $X = \{x_i\}_{i=1}^N$ that we wish to cluster into $K$ groups, we consider the following generative assumptions:

$$c \sim p(c; \pi), \quad z_i \sim p(z_i | c_i) = \mathcal{N}(z_i | \mu_{c_i}, \sigma_{c_i}^2), \quad x_i \sim p_0(x_i | z_i) = \text{Ber} (\mu_{x_i}) \quad (10)$$

where $c = \{c_i\}_{i=1}^N$ are the cluster assignments, $z_i \in \mathbb{R}^D$ are the latent embeddings of a VAE and $x_i$ is assumed to be binary for simplicity. In other words, we assume the data is generated from a random process where the cluster assignments are first drawn from a prior probability $p(c; \pi)$, then each latent embedding $z_i$ is sampled from a Gaussian distribution, whose mean and variance depend on the selected cluster $c_i$. Finally, the sample $x_i$ is generated from a Bernoulli distribution whose parameter $\mu_{x_i}$ is the output of a neural network parameterized by $\theta$, as in the classical VAE. With these assumptions, the latent embeddings $z_i$ follow a mixture of Gaussian distributions, whose means and variances, $\{\mu_{c_i}, \sigma_{c_i}^2\}_{i=1}^K$, are tunable parameters.

Previous work [22] modeled the prior distribution as $p(c; \pi) = \prod_i p(c_i) = \prod_i \text{Cat}(c_i | \pi)$ with either tunable or fixed parameters $\pi$. In this task, we instead replace this prior with the multivariate noncentral hypergeometric distribution with weights $\pi$ and $K$ classes where every class relates to a cluster. Hence, we sample the number of samples per cluster (or cluster size) following Definition 3.1. The hypergeometric distribution permits to create a dependence between samples. The prior probability of a sample to be assigned to a given cluster is not independent of the remaining samples anymore, allowing us to loosen the over-restrictive i.i.d. assumption.

We explore the effect of three different prior probabilities in Equation (10), namely (i) the categorical distribution, by setting $p(c; \pi) = \prod_i \text{Cat}(c_i | \pi)$; (ii) the uniform distribution, by fixing $\pi_i = 1/K$ for $i = 1 \ldots K$; and (iii) the multivariate noncentral hypergeometric distribution. We compare them on three different MNIST versions [31]. The first version is the standard dataset which has a balanced class distribution. For the second and third dataset version we explore different ratios of subsampling for half of the classes. The subsampling rates are 80% in the moderate and 60% in the severe case. In Table 1 we evaluate the methods with respect to their clustering accuracy (Acc), normalized mutual information (NMI) and adjusted rand index (ARI).

As can be seen, the hypergeometric prior distribution shows fairly good clustering performance in all datasets. Although the uniform distribution performs reasonably well, it assumes the clusters have equal importance. Hence it might fail in more complex scenarios. On the other hand, the categorical distribution has subpar performance compared to the uniform distribution, even in the moderate subsampling setting. This might be due to the additional complexity given by the learnable cluster weights, which results in unstable results. On the contrary, the additional complexity does not seem to affect the performance of the proposed hypergeometric prior but instead boosts its clustering performance, especially in the imbalanced dataset. In an additional study in Appendix C.3.3, we are able to show that the model is able to learn the weights, $\pi$, which reflect the subsampling rates of each cluster (see Figure 6).

6 Conclusion

We propose a reparameterization trick for the multivariate noncentral hypergeometric distribution in this work. In combination with the Gumbel-Softmax trick, this new formulation enables reparameterized gradients with respect to the class weights $\omega$ of the hypergeometric distribution. We show the various possibilities of the hypergeometric distribution in machine learning by applying it to two common areas, clustering, and weakly-supervised learning. In both applications, methods using the hypergeometric distribution reach state-of-the-art performance. We believe this work is an essential step toward integrating the hypergeometric distribution into more machine learning algorithms. Applications in biology and social sciences represent potential directions for future work.

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**Checklist**

1. For all authors...
   
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper’s contributions and scope? *[Yes]* See Sections 4 and 5

   (b) Did you describe the limitations of your work? *[Yes]* See Section 4 and more specifically Sections 4.1 and 4.2

   (c) Did you discuss any potential negative societal impacts of your work? *[N/A]* We do not see direct negative societal impact of our research.
(d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]

2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes] See Sections 3 and 4 and Appendices A and B
   (b) Did you include complete proofs of all theoretical results? [Yes] See Appendices B.2 and B.3

3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] See Appendix C and supplementary material
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] See Appendix C
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] See Figures 2 and 5, Table 1, and Appendix C.1
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] See Appendix C

4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes]
   (b) Did you mention the license of the assets? [Yes] All tools used are open-source and cited accordingly
   (c) Did you include any new assets either in the supplemental material or as a URL? [Yes] Code is attached as supplementary material
   (d) Did you discuss whether and how consent was obtained from people whose data you’re using/curating? [N/A]
   (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A]

5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]
A Preliminaries

The hypergeometric distribution is a discrete probability distribution that describes the probability of \( x \) successes in \( n \) draws without replacement from a finite population of size \( N \) with \( m \) elements that are part of the success class. Unlike the binomial distribution, which describes the probability distribution of \( x \) successes in \( n \) draws with replacement.

**Definition A.1 (Hypergeometric Distribution [16])**. A random variable \( X \) follows the hypergeometric distribution, if its probability mass function (PMF) is given by

\[
P(X = x) = p_X(x) = \frac{\binom{m}{x} \binom{N-m}{n-x}}{\binom{N}{n}}
\]  

Urn models are typical examples of the hypergeometric probability distribution. Suppose we think of an urn with marbles in two different colors, e.g. green and purple, we can label as success the drawing of a green marble. Then \( N \) defines the total number of marbles and \( m \) the number of green marbles in the urn. \( x \) is the number of green marbles, and \( n - x \) is the number of drawn purple marbles.

The multivariate hypergeometric distribution describes an urn with more than two colors, e.g. green, purple, and yellow in the simplest case with three colors. As described in Johnson [23], the definition is given by:

**Definition A.2 (Multivariate Hypergeometric Distribution)**. A random vector \( X \) follows the multivariate hypergeometric distribution, if its joint probability mass function is given by

\[
P(X = x) = p_X(x) = \frac{\prod_{i=1}^{c} \binom{m_i}{x_i}}{\binom{N}{n}}
\]  

where \( c \in \mathbb{N}_+ \) is the number of different classes (e.g. marble colors in the urn), \( m = [m_1, \ldots, m_c] \in \mathbb{N}_+^c \) describes the number of elements per class (e.g. marbles per color), \( N = \sum_{i=1}^{c} m_i \) is the total number of elements (e.g. all marbles in the urn) and \( n \in \{0, \ldots, N\} \) is the number of elements (e.g. marbles) to draw. The support \( S \) of the PMF is given by

\[
S = \left\{ x \in \mathbb{Z}_{0+}^c : \forall i \quad x_i \leq m_i, \quad \sum_{i=1}^{c} x_i = n \right\}
\]

B Methods

B.1 PMF for the multivariate Fisher’s noncentral distribution

In this section, we give a detailed derivation for the calculation of the log-probabilities of the multivariate Fisher’s noncentral hypergeometric distribution. We end up with a formulation that is proportional to the actual log-probabilities. Because the ordering of categories is not influenced by scaling with a constant factor (addition/subtraction in log domain), these are unnormalized log-probabilities of the multivariate Fisher’s noncentral hypergeometric distribution.

\[
p_X(x; \omega) = \frac{1}{P_0} \prod_{i=1}^{c} \binom{m_i}{x_i} \omega_i^{x_i}
\]

---

3Although the distribution itself is older, Gonin [16] were the first to name it hypergeometric distribution.
where $P_0$ is defined as in Equation (1). From there it follows

$$
\log p_X(x; \omega) = \log \left( \frac{1}{P_0} \prod_{i=1}^{c} \left( \frac{m_i}{x_i} \right)^{\omega_i^{x_i}} \right)
$$

(15)

$$
= \log \left( \frac{1}{P_0} \right) + \log \left( \prod_{i=1}^{c} \left( \frac{m_i}{x_i} \right)^{\omega_i^{x_i}} \right)
$$

(16)

$$
= \log \left( \frac{1}{P_0} \right) + \sum_{i=1}^{c} \log \left( \left( \frac{m_i}{x_i} \right)^{\omega_i^{x_i}} \right)
$$

(17)

$$
= \log \left( \frac{1}{P_0} \right) + \sum_{i=1}^{c} \left( \log \left( \frac{m_i}{x_i} \right) + \log (\omega_i^{x_i}) \right)
$$

(18)

$$
= \log \left( \frac{1}{P_0} \right) + \sum_{i=1}^{c} \left( \log \left( \frac{m_i}{x_i} \right) + x_i \log (\omega_i) \right)
$$

(19)

Constant factor can be removed as the argmax is invariant to scaling with a constant factor which equals addition or subtraction in log-space. It follows

$$
\log p_X(x; \omega) = \sum_{i=1}^{c} \left( \log \left( \frac{m_i}{x_i} \right) + x_i \log (\omega_i) \right) + C
$$

(20)

$$
= \sum_{i=1}^{c} \left( \log \frac{1}{x_i! (m_i - x_i)!} + x_i \log (\omega_i) \right) + \tilde{C}
$$

(21)

$$
= \sum_{i=1}^{c} \left( - \log (\Gamma(x_i + 1) \Gamma(m_i - x_i + 1)) + x_i \log (\omega_i) \right) + \tilde{C}
$$

(22)

In the last line we used the relation $\Gamma(k + 1) = k!$. After setting $C = \tilde{C}$, it directly follows

$$
\log p_X(x; \omega) = \sum_{i=1}^{c} x_i \log \omega_i + \psi_F(x) + C
$$

(24)

where $\psi_F(x) = - \sum_{i=1}^{c} \log (\Gamma(x_i + 1) \Gamma(m_i - x_i + 1))$.

The Gamma function is defined in Whittaker and Watson [49] as

$$
\Gamma(z) = \int_{0}^{\infty} x^{z-1} e^{-x} dx
$$

(25)

### B.2 Proof for Lemma 4.1

**Proof.** Factors that are constant for all $x$ do not change the relative ordering between different values of $x$. Hence, removing them preserves the ordering of values $x$ [2].

$$
\log p_{X_L}(x_L; \omega) = \log \left( \frac{1}{P_0} \left( \frac{m_L}{x_L} \right)^{\omega_L^{x_L}} \left( \frac{m_R}{n - x_L} \right)^{\omega_R^{n - x_L}} \right)
$$

(26)

$$
= \log \left( \frac{m_L}{x_L} \right) + \log \left( \frac{m_R}{n - x_L} \right) + \log (\omega_L^{x_L}) + \log (\omega_R^{n - x_L}) + C
$$

(27)

Using the definition of the binomial coefficient (see Section 3) and its relation to the Gamma function\(^4\) $\Gamma(k + 1) = k!$, it follows

$$
\log p_{X_L}(x_L; \omega) = x_L \cdot \log \omega_L + (n - x_L) \cdot \log \omega_R - \log (\Gamma(x_L + 1) \Gamma(n - x_L + 1)) - \log (\Gamma(m_L - x_L + 1) \Gamma(m_R - n + x_L + 1)) + C
$$

(28)

With $\psi_F(x)$ as defined in Equation (7), Equation (6) follows directly.

---

\(^4\)see Appendix B.1 for the definition on the Gamma function
Figure 3: Comparing random variables drawn from the proposed distribution to a reference distribution.
Figure 4: As an additional evaluation, we perform analysis on how disentangled the latent representations are. And related to that, we assess the quality of the learned latent representation using a linear classifier. We see that the dynamics over different $k$ seems to be related for the disentanglement and downstream performance of the learned latent representations.

B.3 Proof for Lemma 4.2

Proof. When sampling class $i$, we draw $x_i$ samples from class $i$ where $x_i \leq m_i$. The conditional distribution $p_{X_i}(x_i|\{x_k\}_{k=1}^{i-1}; \omega)$ for class $i$ given the already sampled classes $k < i$ simultaneously defines the weights of a categorical distribution. Sampling $x_i$ elements from class $i$ can be seen as selecting the $x_i$th category from the distribution defined by the weights $p_{X_i}(x_i|\{x_k\}_{k=1}^{i-1}; \omega)$. Therefore,

$$\sum_{0 \leq x_i \leq m_i} p_{X_i}(x_i|\{x_k\}_{k=1}^{i-1}; \omega) = 1,$$

which allows us to apply the Gumbel-Max trick and, respectively, the Gumbel-Softmax trick.

C Experiments

All our experiments were performed on our internal compute cluster, equipped with NVIDIA RTX 2080. Every training and test run used only a single NVIDIA RTX 2080. The weakly-supervised runs took approximately 3-4 hours each, where the clustering runs only took about 3 hours each.

C.1 Kolmogorov-Smirnov Test

As described in Section 5.1 in the main text, we report the histograms of all classes next to each other here in Figure 3. We can see that class 1 and class 3 have (at least visually) the same distribution over histograms for different values of $\omega_2$. And they also match their respective reference histograms.

C.2 Weakly-Supervised Learning

C.2.1 Method, Implementation and Hyperparameters

In this section we give more details on the used methods. We make use of the disentanglement_lib [33] which is also used in the original paper we compare to [34]. The baseline algorithms [6, 19] are already implemented in disentanglement_lib. For details on the implementation of models, we refer to the original paper. We did not change any hyperparameters or network settings. All experiments were performed using $\beta = 1.0$ as this is the best performing $\beta$ according to Locatello et al. [34]. For all experiments we train 5 models with different random seeds.

All experiments are performed using GroupVAE [19]. Using GroupVAE, shared latent factors are aggregated using an arithmetic mean. Bouchacourt et al. [6] assume also knowledge about shared and independent latent factors. Different to GroupVAE, their ML-VAE aggregates shared latent factors by using the Product of Experts (i.e. geometric mean).
C.2.2 HypergeometricVAE (in more detail)

In our approach (HypergeometricVAE), we model the number of shared and independent latent factors of a pair of images as a hypergeometric distribution with unknown $\omega$. In reference to the urn model, shared and independent factors each correspond to one color and the urn contains $d$ marbles of each color, where $d$ is the dimensionality of the latent space. Given the correct weights $\omega$ and when drawing from the urn $d$ times, the number of each respective color corresponds, in expectation, to the correct number of independent/shared factors. The proposed formulation allows to simultaneously infer such $\omega$ and learn the latent representation in a fully differentiable setting within the weakly-supervised pipeline by Locatello et al. [33].

To integrate the procedure described above in this framework, we need two additional building blocks. First, we introduce a function that returns $\omega$. To achieve this, we use a single dense layer followed by a tangens hyperbolicus activation function which returns logits $\tilde{\omega}$. The input to this layer is a vector $\gamma$ containing the symmetric version of the KL divergences between pairs of latent distributions, i.e. for latent $P$ and $Q$, the vector contains $\frac{1}{2}(KL(P||Q) + KL(Q||P))$. An estimation $\hat{\omega}$ is than given by $\exp(\tilde{\omega})$. Second, sampling from the hypergeometric distribution with these weights leads to an estimate $\hat{k}$. Consequently, we need a method to select $\hat{k}$ factors out of the $d$ that are given. Similar to the original paper, we select the factors achieving the highest symmetric KL-divergence. In order to do this, we sort $\gamma$ in descending order using the stochastic sorting procedure $\text{neuralsort}$ [17]. This enables us to select the top $\hat{k}$ independent as well as the bottom $d - \hat{k}$ shared latent factors. Like AdaptiveVAE, we substitute the shared factors by the mean value of the original latent code before continuing the VAE forward pass in the usual fashion.

C.2.3 Data

The mpi3d dataset [15] consists of frames displaying a robot arm and is based on 7 generative factors.

- object color
- object shape
- object size
- camera height
- background color
- horizontal axis
- vertical axis

For more details on the dataset and in general, we refer to https://github.com/rr-learning/disentanglement_dataset.

C.2.4 Downstream task on the learned latent representations

For the downstream task we sample randomly 10000 samples from the training set and 5000 samples from the test set. For every generative factor of the dataset, an individual classifier is trained on the 10000 training samples. Afterwards, every classifier evaluates the latent representations of the 5000 test samples. The classification accuracies of the individual classifiers is averaged into a single average accuracy. The average accuracy is the one reported.

C.2.5 Additional Results

Disentanglement Originally, Locatello et al. [34] proposed their method in the context of learning disentangled representation in a weakly-supervised setting. Figure 4a shows the result of the comparison. We see that the proposed does not quite reach the disentanglement performance of the other two methods. The DCI score evaluates the disentanglement of the single frame representations which is not based on pairs of information. For future work, it would be more interesting to us to investigate the disentanglement between shared and independent latent factors.

Hypergeometric Prior In the presented results we learned good estimations for $\omega$ without imposing any constraints. In addition, we wanted to see if we were able to learn better representations when
imposing a hypergeometric prior that would enable us to inject knowledge about the dataset. In our case, we knew that at least one factor was independent for any two samples. This can be modeled by a hypergeometric prior with $\omega_1 = 1$ and $\omega_2 = d$, i.e. by giving $d$ times more weight to shared factors than independent ones. The results using an additional hypergeometric prior over three different seeds on the disentanglement, shared factor estimation and classification task can be seen in Figure 5. There seems to be some kind of trade-off between accurately estimating the number of shared factors and achieving good performance on disentanglement/downstream classification. We suspect that further hyperparameter fitting and more sensible prior models could lead to better results over all three tasks. Further exploration of hypergeometric priors as well as finding alternative approaches to infer $\omega$ parameters is left for future work.

C.3 Clustering

In this section, we provide the interested reader with more details on the clustering experiments. In the following we describe the models, the optimisation procedure and the implementation details used in the clustering task.
We follow a deep variational clustering approach as described by Jiang et al. [22]. In particular, assuming the generative process described in Equation (10), we can write the joint probability of the data, also known as the likelihood function, as

\[
p(X) = \sum_c \int \int p(X, Z, c) = \sum_c \int \int p(c; \pi)p(X|Z)p(Z|c) = \sum_c p(c; \pi) \prod_i \int p(x_i|z_i)p(z_i|c_i)
\]  

(30)

Different from Jiang et al. [22], the prior probability \( p(c; \pi) \) cannot be factorized as \( p(c_i; \pi) \) for \( i = 1, \ldots, K \) are not independent. By using a variational distribution \( q_\phi(Z, c|X) \), we have the following evidence lower bound

\[
\log p(X) \geq E_{q_\phi(Z, c|X)} \left[ \log \left( \frac{p(c; \pi)p(X|Z)p(Z|c)}{q_\phi(Z, c|X)} \right) \right] = \mathcal{L}_{ELBO}.
\]  

(31)

For sake of simplicity, we assume the following amortized mean-field variational distribution, as in previous work [10, 22]:

\[
q_\phi(Z, c|X) = q_\phi(Z|X)q_\phi(c|X) = \prod_i q_\phi(z_i|x_i)q_\phi(c_i|x_i).
\]  

(32)

From where it follows

\[
\mathcal{L}_{ELBO} = E_{q_\phi(Z|X)q_\phi(c|X)} [\log p(c|\pi) + \log p(X|Z) + \log p(Z|c) - \log q_\phi(Z, c|X)]
\]  

(33)

\[
\begin{aligned}
&- E_{q_\phi(Z|X)} [\log q_\phi(Z|X)] - E_{q_\phi(Z|X)q_\phi(c|X)} [\log q_\phi(c|X)].
\end{aligned}
\]  

(34)

In the ELBO formulation all terms, except the first one, can be efficiently calculated as in previous work [22]. For the remaining term, we rely on the following sampling scheme

\[
E_{q_\phi(Z|X)q_\phi(c|X)} [\log p(c|\pi)] = \sum_c \int Z q_\phi(Z|X)q_\phi(c|X) \log p(c|\pi))
\]  

(35)

\[
= \sum_c \prod_i \int_{z_i} q_\phi(z_i|x_i)q_\phi(c_i|x_i) \log p(c|\pi)
\]  

(36)

\[
= \sum_{i=1}^L \log p(c^l|\pi),
\]  

(37)

where we use the SGVB estimator and the Gumbel-Softmax trick [21] to sample from the variational distributions \( q_\phi(z_i|x_i) \) and \( q_\phi(c_i|x_i) \) respectively. The latter is set to a categorical distributions with weights given by:

\[
p(c_i|z_i; \pi) = \frac{\mathcal{N}(z_i|\mu_{c_i}, \sigma_{c_i}^2)\pi_{c_i}}{\sum_k \mathcal{N}(z_i|\mu_k, \sigma_k^2)\pi_k},
\]  

(38)

where \( L \) is the number of Monte Carlo samples and it is set to 1 in all experiments.

### C.3.2 Implementation Details

To implement our model we adopted a feed-forward architecture for both the encoder and decoder of the VAE with four layers of 500, 500, 2000, 500 units respectively, where \( D = 10 \). The VAE is pretrained using the same layer-wise pretraining procedure used by Jang et al. [21]. Each data set is divided into training and test sets, and all the reported results are computed on the latter. We employed the same hyper-parameters for all experiments. In particular, the learning rate is set to 0.001, the batch size is set to 128 and the models are trained for 1000 epochs. Additionally, we used an annealing schedule for the temperature of the Gumbel-Softmax trick.

### C.3.3 Additional Results

In Figure 6, we are able to show that the learned class weights \( \omega \) match the true subsampling rates used in the experiments. This means that the learned selection bias corresponds to the true bias in the dataset.