SeGMA: Semi-Supervised Gaussian Mixture Auto-Encoder

Marek Śmieja, Maciej Wołczyk, Jacek Tabor, and Bernhard C. Geiger, Senior Member, IEEE

Abstract—We propose a semi-supervised generative model, SeGMA, which learns a joint probability distribution of data and their classes and which is implemented in a typical Wasserstein auto-encoder framework. We choose a mixture of Gaussians as a target distribution in latent space, which provides a natural splitting of data into clusters. To connect Gaussian components with correct classes, we use a small amount of labeled data and a Gaussian classifier induced by the target distribution. SeGMA is optimized efficiently due to the use of Cramer-Wold distance as a maximum mean discrepancy penalty, which yields a closed-form expression for a mixture of spherical Gaussian components and thus obviates the need of sampling. While SeGMA preserves all properties of its semi-supervised predecessors and achieves at least as good generative performance on standard benchmark data sets, it presents additional features: (a) interpolation between any pair of points in the latent space produces realistically-looking samples; (b) combining the interpolation property with disentangled class and style variables, SeGMA is able to perform a continuous style transfer from one class to another; (c) it is possible to change the intensity of class characteristics in a data point by moving the latent representation of the data point away from specific Gaussian components.

Index Terms—deep generative model, semi-supervised learning, Wasserstein Auto-Encoder, Gaussian mixture model.

I. INTRODUCTION

Deep generative models, such as the variational auto-encoder (VAE, [1]), Wasserstein auto-encoder (WAE, [2]) or generative adversarial network (GAN, [3]) play an important role in deep learning. They are capable of learning a probability distribution of complex high-dimensional data, which can be used to generate new examples. Their applications include image inpainting [4], 3D object reconstruction [5], sentence paraphrasing [6], and many more [7]–[9].

In more specialized applications where data is composed of classes, we may want to construct a separate generative model for every class rather than a single model for the entire data. Since, in practice, the access to labeled data is limited, it is often not possible to train these separate models using classical techniques. A step towards solving this problem was the introduction of semi-supervised versions of VAE models [10], [11]. These models extend their unsupervised predecessor by introducing an additional latent variable for encoding class labels. Making use of a small number of labeled examples together with a large collection of unlabeled data, they train a classifier together with an individual generative model for each class. Samples are produced by transforming a categorical, i.e., discrete, variable describing the class together with a latent code generated from a continuous target distribution using a decoder network.

In this paper, we present an alternative approach for constructing a collection of generative models for individual classes. Instead of introducing a classification network with an additional discrete latent variable representing the class, we use a classical mixture of Gaussians to provide a natural splitting of data in the single latent space of the auto-encoder. Using a small labeled data set, classes are assigned to components of this mixture of Gaussians by minimizing the cross-entropy loss induced by the class posterior distribution of a simple Gaussian classifier. The resulting mixture describes the distribution of the whole data, and representatives of individual classes are generated by sampling from its components, see Fig. 1 for illustration.

Our model, which we will call semi-supervised Gaussian mixture auto-encoder (SeGMA), is an adaptation of the Cramer-Wold auto-encoder [12], which is an instance of WAE models with maximum mean discrepancy (MMD) penalty [2]. The use of CWAE yields a closed-form expression for the MMD penalty for spherical Gaussians, which eliminates the need of sampling and propagating gradients through discrete variables which is not possible in a straightforward manner [13], Sec. 1.1]. Experimental results on MNIST, SVHN, and CelebA data sets show that SeGMA obtains comparable or even better generative performance than corresponding VAE models. Moreover, it has several advantages, which cannot be
obtained using these models:

- Due to the use of a single continuous latent space in which the class variable is encoded implicitly, we can interpolate between any two data points as in classical unsupervised generative models. In consequence, we are able to generate intermediate examples which mix properties of several classes. This property is difficult to obtain for semi-supervised VAE models, because they are trained directly on discrete class variables for which intermediate states are not necessarily meaningful.

- Despite lacking an architectural separation between the discrete class label and the continuous latent code, we demonstrate that SeGMA is able to disentangle the class of a data point from its style. In contrast to semi-supervised VAE models, in which this disentanglement is explicit, SeGMA allows to perform continuous style transfer. In other words, we can change the class variable smoothly, while preserving the style of examples. This is a consequence of interpolation property, see Fig. 2. While continuous style transfer is performed by moving a latent representation from the original Gaussian component towards the component of the target class, the intensity of the style w.r.t. certain class-discriminating characteristics can be increased by moving the latent representation away from specific Gaussian components.

- SeGMA is easy to implement in an existing WAE-MMD framework and is robust to the choice of hyperparameters (we use the same hyperparameters across all data sets). We obtain better generative performance than related VAE approaches despite using simpler neural networks and significantly lower-dimensional latent space – e.g., we use a classical encoder-decoder network with a 20-dimensional latent space for SVHN, while the method proposed by [11] consists of six networks with 300 dimensions for encoding latent codes. SeGMA is trained faster and in a more stable way due to the use of Cramer-Wold distance which eliminates the need of sampling. Finally, since we use a classical auto-encoder architecture, it is easier to apply convolutional networks than in semi-supervised VAE models, where continuous and discrete inputs have to be gathered together.

The remainder of this work is organized as follows: We discuss the similarities between our approach and the related works in semi-supervised and unsupervised generative models in Section II. We complete the theoretical framework of SeGMA in Section IV, where we include a regularization term based on a small labeled data set. For the specific choice of a mixture of Gaussians as a target distribution in latent space, we instantiate our theory in Section V and briefly discuss optimization issues. We conclude by showing experimental results and comparisons with state-of-the-art semi-supervised VAE models in Section VI.

II. RELATED WORK

There are a few works on unsupervised deep clustering, which use a mixture of Gaussians as a target distribution in latent space. The authors of [14] propose a generative model based on the VAE in which both the encoder and decoder are stochastic. They train their model by maximizing the evidence lower bound (ELBO) over the parameters of the Gaussian mixture model and the parameters of the encoder and decoder. Their variational posterior is a mean-field approximation, and they assume that the conditional distribution of the class label given the input features is equal to the conditional distribution of the class label given the latent code, cf. [14] eq. (16)]. A very similar model was recently introduced in [15], with the main difference that the decoder is deterministic and that, instead of maximizing the ELBO, a variational bound on the information bottleneck functional is optimized; the paper thus generalizes [16] in the sense that the latter proposed a spherical Gaussian as a target distribution in latent space. The authors further show that their cost function degenerates to the ELBO proposed in [14] for a specific choice of the information bottleneck trade-off parameter. In both [14] and [15], the discrete class variable is explicit only during generation; during inference, it is inferred by applying a simple Gaussian classifier in latent space, which makes the cost function independent of this class variable.

Despite being unsupervised, both [14] and [15] report that the obtained clusters agree very well with the class labels. That this need not be the case in an unsupervised setting is illustrated in [17], which proposed a slightly more complicated Gaussian mixture model in which the means and variances are learned by training the parameters of an additional neural network with a standard Gaussian distribution at its input. The authors show that, for MNIST, the clusters coincide with the individual classes and that the generative model allows separating style from class (cf. [17, Fig. 5]). In contrast, for harder datasets, such as SVHN, the clusters do not correspond to the classes in the data set, but to groups of images that are visually similar, cf. [17, Fig. 6]. The other works [14–16, 18] did not verify their generative performance on any datasets except MNIST.

Another approach for training deep generative models relies on using WAE [2]. The authors of [19] show that in some cases the optimization of a classical shallow Gaussian mixture model using sliced p-Wasserstein distance [20] leads to better parameters than those resulted from EM algorithm. Instead of a joint optimization of Wasserstein distance with neural network weights, they fit a Gaussian mixture model on a fixed embedding of data. The paper [18] explains the difficulties in training VAE models with discrete latent variables [21–23]. As a remedy they propose a WAE-MMD model with a mixture of Gaussians as a target distribution. This fully unsupervised model uses two latent variables (discrete and continuous) and is optimized by sampling from a target distribution.
The semi-supervised deep generative models proposed in the literature differ substantially from the unsupervised generative models discussed so far. The most important difference is that they have two explicit latent variables, a discrete one accounting for the class and a continuous one, commonly attributed to represent the style of the data point. Thus, these methods explicitly consider the discrete variable also during inference, e.g., by training a classifier network on the latent space in addition to an encoder network. For example, [10] proposed a generative model parameterized by a stochastic neural network taking the latent class and style variables as inputs. Similarly, encoder and classifier – computing the style and class variables, respectively – are implemented as stochastic neural networks. All model parameters are optimized by maximizing the ELBO over the unlabeled and labeled parts of the data set; for the former, the class variable is supplied via posterior inference using the classifier network. The authors of [11] improved upon [10] by adding a continuous auxiliary latent variable, thereby increasing the capacity of the model and improving the variational bound. By using neural networks for class inference, both [10] and [11] achieve good classification and generative performance with only a small labeled data set. The paper [24] follows a different approach and modifies the VAE model so that one of the continuous latent variables represents a clustering structure of the data. The authors of [25] build their semi-supervised model on GANs, but they focus directly on a classification task. They show that good semi-supervised learning requires a bad generator network; consequently, their generator does not produce realistic samples.

On the other hand, our setting is conceptually similar to generative deep clustering approaches which use mixtures of Gaussians as target distributions. Most of these works use a single continuous latent space (except the VAE-MMD approach [18], which uses two latent variables), but require sampling from some distribution during training. In contrast, the use of the Cramer-Wold distance in SeGMA allows fitting the encoded data to the target mixture using a closed-form expression. Furthermore, while the discussed works on clustering usually employ an auxiliary classifier to assign samples to clusters, we use a small labeled data set to align the Gaussian components of the target distribution with classes. This way, the class variable remains implicit for the unlabeled, but becomes explicit only for the labeled part of the data set. Finally, our focus is on the generative properties. In comparison, [14], [18] generated samples only for MNIST, [15] did not generate samples at all, and none of the mentioned works evaluate the quality of their samples using quantitative methods.

On the other hand, our work draws concepts from semi-supervised VAEs, which are comprised of (at least) two latent spaces, with one of them being discrete. The main difference to semi-supervised VAEs is that we propose using a single continuous latent space that allows us not only to transfer style to different classes, but also to interpolate between data points from different classes. Finally, our cost function is not based on variational principles, but is motivated by WAEs.

III. PRELIMINARIES: WASSERSTEIN AUTO-ENCODER AND CRAMER-WOLD DISTANCE

Our approach is based on the WAE with a MMD penalty [2]. As opposed to the VAE [1], WAE allows using deterministic, i.e., non-random, encoders mapping the input to a latent space via a function. To eliminate the need for sampling during training and to improve the model stability, we implement MMD using Cramer-Wold distance [12].

Let \( X = (x_i)_{i=1}^n \subset \mathbb{R}^N \) be a data set. A non-random auto-encoder consists of a deterministic encoder \( E: \mathbb{R}^N \rightarrow \mathbb{Z} \) and a deterministic decoder \( D: \mathbb{Z} \rightarrow \mathbb{R}^N \), where \( \mathbb{Z} = \mathbb{R}^D \) is a latent space (usually \( D < N \)). The encoder thus provides a lower-dimensional representation of \( X \) that the decoder shall be able to reconstruct with as small an error as possible. This goal is achieved by minimizing the mean squared error between input and output of the auto-encoder:

\[
\text{MSE}(X,E,D) = \frac{1}{n} \sum_{i=1}^{n} \| x_i - D(E(x_i)) \|^2, \tag{1}
\]

where \( \| \cdot \| \) denotes the Euclidean norm.

To make the auto-encoder generative, the reconstruction error is complemented by a regularization term that encourages the distribution of the low-dimensional representation \( E(X) \) to be similar to a target distribution \( P_Z \). Specifically, for a WAE with MMD penalty, the regularization term is chosen as the norm in some reproducing kernel Hilbert space \( \mathcal{H}_k \), i.e.,

\[
d_{\text{MMD}}(E(X), P_Z) = \| \int_{Z} k(z, \cdot) dP_Z\phi(z) - \int_{Z} k(z, \cdot) dP_Z(z) \|_{\mathcal{H}_k}, \tag{2}
\]

where \( P_Z\phi \) is the distribution of \( E(X) \) and where \( k: \mathbb{Z} \times \mathbb{Z} \rightarrow \mathbb{R} \) is a positive definite reproducing kernel. If the distribution of \( E(X) \) is similar to \( P_Z \) and if \( E \) and \( D \) are such that \( \text{MSE}(X; E, D) \) is small, then samples from \( X \) can be generated by sampling from \( P_Z \) and passing these samples to the decoder \( D \) [12] Remark 4.1.

During the training process, the comparison of the latent data representations \( E(X) \) with a target distribution \( P_Z \) is performed by sampling from \( P_Z \) and approximating [2] by averaging the kernel \( k \) evaluated at all pairs of samples [2, Algorithm 2]. Such a procedure is necessary even for a simple target distribution such as the standard Gaussian \( N(0, I) \). To eliminate the need for sampling, MMD can be implemented using the Cramer-Wold distance, which has a closed-form expression for spherical Gaussian distributions. In consequence, Cramer-Wold distance allows to compare latent data representations with a target distribution given by \( N(0, I) \) without sampling. This approach results in Cramer-Wold auto-encoder (CWAE) [12], which is an instance of WAE-MMD with inverse multiquadratics kernel [2, page 9].

The formula of Cramer-Wold distance \( d^2_{\gamma} \), where \( \gamma > 0 \) is a regularization parameter, is induced by a corresponding
scalar product $\langle \cdot , \cdot \rangle_\gamma$, which for two spherical, $D$-dimensional Gaussians $N(a, \alpha I), N(b, \beta I)$ is given by:

$$
\langle N(a, \alpha I), N(b, \beta I) \rangle_\gamma = \frac{1}{\sqrt{2\pi(\alpha + \beta + 2\gamma)}} \phi_D \left( \frac{||a - b||^2}{2(\alpha + \beta + 2\gamma)} \right),
$$

(3)

where $\phi_D(s) \approx (1 + \frac{4s}{2D-3})^{-\frac{1}{2}}$, for $D \geq 10$.

To evaluate (3) for a sample $Z = (z_i)_{i=1}^m$, we represent it as the uniform mixture of Gaussians with zero covariance, i.e. $Z = \frac{1}{m} \sum_{i=1}^m N(z_i, 0)$. If we put $P_Z = N(0, I)$, then the Cramer-Wold distance between this target distribution and the sample $Z$ equals:

$$
d_2^Z(Z, P_Z) = \langle Z - P_Z, Z - P_Z \rangle_\gamma = \langle Z, Z \rangle_\gamma - 2 \langle Z, P_Z \rangle_\gamma + \langle P_Z, P_Z \rangle_\gamma
$$
$$
= \frac{1}{m^2} \sum_{i=1}^m \sum_{j=1}^m \langle N(z_i, 0), N(z_j, 0) \rangle_\gamma
$$
$$
- \frac{2}{m} \sum_{i=1}^m \langle N(z_i, 0), N(0, I) \rangle_\gamma + \langle N(0, I), N(0, I) \rangle_\gamma
$$

(4)

where $\langle \cdot , \cdot \rangle_\gamma$ is given by (3). The parameter $\gamma$ can be seen as a kernel bandwidth and is commonly selected using Silverman’s rule of thumb for Gaussian densities.

### IV. Theoretical Model: Semi-Supervised Learning for Improved Class Representation

Classical WAE models allow us to describe the distribution of the data and to generate samples from it. In practice, data can come from several distinct classes. In such a case, we want to model a distribution of the whole data as well as to be able to generate samples from a given class.

To this end, we introduce a joint distribution $P_{Z,Y}$, which additionally encodes the latent class variable $Y$. On the one hand, marginalization over the class variable $Y$ yields the target distribution $P_Z$ to which the WAE fits the latent representation. On the other hand, to generate samples from a given class $y$, we fix this class in the distribution $P_{Z,Y}$, sample from the resulting conditional distribution $P_{Z|Y=y}$, and pass the obtained latent codes through the decoder $D$. Thus, $P_{Z,Y}$ should be parametrized such that both:

- samples from its marginal $P_Z$ have high quality,
- samples from $P_{Z|Y=y}$ are representatives of class $y$.

In practical cases, $P_Z$ could be a multi-modal distribution, with each mode corresponding to one class.

To parametrize $P_{Z,Y}$ (e.g., to assign the modes of the distribution $P_Z$ to individual classes), we follow a typical semi-supervised learning scenario and use a small number of labeled examples [26]. It is assumed that we have access to a labeled data set $(X_L,Y_L) = (x_i, y_i)_{i=n+1}^m$, where $X_L \subset \mathbb{R}^N$ and where $y_i \in \{1, \ldots, K\}$ denotes the class label. To incorporate knowledge coming from labeled examples in building our generative model, we use a classifier. More precisely, let $P_{Y|Z}$ be the class posterior probability. We complement the WAE objective with the cross-entropy between the true class label and the class label inferred from $P_{Y|Z}$:

$$
\mathcal{L}(\hat{P}_{Y|X_L} \| P_{Y|Z}) = \frac{1}{m-n} \sum_{i=n+1}^m - \log P_{Y|Z}(y_i|\mathcal{E}(x_i))
$$
$$
= \frac{1}{m-n} \sum_{i=n+1}^m - \log \frac{P_Y(y_i)P_{Z|Y=y_i}(\mathcal{E}(x_i))}{P_Z(\mathcal{E}(x_i))}
$$

(5)

This suggests that a good generative model in the proposed semi-supervised setting consists of an encoder $\mathcal{E}$ and a decoder $D$ such that

$$
\text{MSE}(\hat{X}, \mathcal{E}, D) + \alpha d_{\text{MMD}}(\mathcal{E}X, P_Z) + \beta \mathcal{L}(\hat{P}_{Y|X_L} \| P_{Y|Z})
$$

(6)

is minimized, where $\hat{X} = X \cup X_L$ and $\alpha, \beta$ are trade-off parameters.

### V. Practical Implementation

In this section, we present our choice for the distribution $P_{Z,Y}$, instantiate the cost function (6) for this choice and discuss its optimization.

In order to preserve the simplicity of target distribution as well as to include the information of classes, we choose $P_{Z,Y}$ to be a Gaussian mixture model. In this case, $P_Y$ is a categorical distribution from $K$ categories with prior probabilities $p_1, \ldots, p_K$, while $P_{Z|Y=k}$ is a multivariate Gaussian $N(\mu_k, \Sigma_k)$, which describes the distribution of class $k$ in latent space. The marginalization of $P_{Z,Y}$ over classes $Y$ gives a target distribution $P_Z$ which is a mixture of Gaussians with density $P_Z = \sum_{k=1}^K p_k N(\mu_k, \Sigma_k)$.

On the one hand, choosing $P_{Z,Y}$ to be a Gaussian mixture model makes it easy to generate latent codes for a given class $k$ by sampling from the conditional density $P_{Z|Y=k} = N(\mu_k, \Sigma_k)$. At the same time, the posterior probability used in semi-supervised setting simplifies to:

$$
P_{Y|Z}(k|z) = \frac{p_k N(\mu_k, \Sigma_k)(z)}{\sum_{l=1}^K p_l N(\mu_l, \Sigma_l)(z)}.
$$

(7)

Using such a simple Gaussian classifier in the feature space directly may fail; we show in our experiments that its embedding in the latent space yields satisfactory performance.

On the other hand, there appears the question how to compute $d_{\text{MMD}}(\mathcal{E}X, P_Z)$ for the mixture of Gaussians and how to train a network minimizing the WAE objective in this case. The simplest approach relies on sampling from the mixture density $P_Z$ and next computing the MMD distance between these samples and encoded data. The implementation of this step requires the reparameterization trick to backpropagation of gradients. However, since we have $K$ Gaussians, the number of samples should probably be $K$ times larger than for a single Gaussian to approximate this distribution well enough, which might negatively influence the training time.

Our choice to implement the MMD penalty with the Cramer-Wold distance [12] resolves this issue since, as we have outlined in Section III, it obviates the need for sampling.
As an added benefit, this significantly decreases training time and improves model stability. Following along the lines of \(^4\) and making use of \(^3\), the Cramer-Wold distance between a sample \(Z = (z_i)_{i=1}^m\) and a mixture of spherical Gaussians \(P = \sum_{k=1}^K p_k N(\mu_k, \sigma_k^2 I)\) can be computed in closed form:

\[
d^2(Z, P) = \frac{1}{m^2 2\pi(2\gamma)} \sum_{i=1}^m \sum_{j=1}^m \phi_D \left( \frac{||z_i - z_j||^2}{4\gamma} \right) - \frac{m}{2} \sum_{i=1}^m \sum_{k=1}^K 2p_k \frac{1}{m^2 2\pi(\sigma_k^2 + 2\gamma)} \phi_D \left( \frac{||z_i - \mu_k||^2}{2(\sigma_k^2 + 2\gamma)} \right) + \frac{1}{K} \sum_{k=1}^K \sum_{i=1}^m \frac{p_k}{m^2 2\pi(\sigma_k^2 + \sigma_i^2 + 2\gamma)} \phi_D \left( \frac{||\mu_k - \mu_i||^2}{2(\sigma_k^2 + \sigma_i^2 + 2\gamma)} \right).
\]

To use the CWAE with the target distribution \(P_Z\) being a mixture of Gaussians, it is sufficient to replace \(^2\) by \(^\dagger\) (in fact we take the logarithm of the squared Cramer-Wold distance to improve the balance between this term and the MSE, \(^\dagger\) Footnote 2). Taking all this together, we define the SeGMA objective function.

\textbf{Definition 1.} Let \(P_Z = \sum_{k=1}^K p_k N(\mu_k, I)\) be a target distribution and let \(X = X \cup X_L\) be composed of unlabeled and labeled data, where \(Y_L\) denotes labels of \(X_L\). The aim of SeGMA is to find minimizers of the following optimization problem:

\[
\min_{\mathcal{E}, \mathcal{D}, \{\mu_k\}, \{p_k\}} \text{MSE}(\hat{X}, \mathcal{E}, \mathcal{D}) + \alpha \log d^2(\mathcal{E}, \hat{X}, P_Z; \gamma) + \beta \mathcal{L}(\hat{P}_{Y|X_L}, P_Y|Z), \tag{9}
\]

where \(\alpha, \beta\) are trade-off parameters and where \(P_Y|Z\) and \(d^2\) are given in \((7)\) and \((8)\), respectively.

As it can be seen in this definition, we choose spherical Gaussian components with identity covariance matrices. One may argue that this choice is very restrictive, limiting the expressiveness of our model. In practice, however, encoder and decoder are implemented by deep neural networks; ensuring that these networks have sufficient capacity guarantees that the restriction to spherical Gaussians is unproblematic (which we show to be the case in our experiments). At the same time, the capacity of the encoder and decoder needs to be restricted to ensure that data points from the same class are mapped to the same component in latent space.

SeGMA is trained in an analagous way to CWAE with a slight modification caused by the use of labeled data. More precisely, we take a batch, which is composed of labeled and unlabeled data, and process it by the encoder and the decoder. It is a common practice that half of data in a batch is labeled \(^\dagger\). If we have additional knowledge about class proportions, we use these proportions for selecting labeled examples in each batch. The cross entropy \(\mathcal{L}\) is computed only for labeled examples, while MSE and \(d^2\) are evaluated for all data. During back-propagation, we update both weights of the encoder and decoder, as well as the means \(\mu_k\) of Gaussians. Class priors \(p_k\) are set to reflect the proportions of classes in the set of the known labels \(Y_k\). Updating the means of Gaussians allows us to better organize the class structure in the latent space. Namely, our model can place similar classes closer together, while significantly distinct ones can be put far apart. This property can be useful in analyzing the similarity between classes after successful training, which would not be possible using a separate discrete class variable.

### VI. Experiments

In this section, we present the results of our experiments. Our goal is to compare with similar methods on standard benchmark tasks as well as to present interesting properties of SeGMA, which are difficult to obtain using existing approaches.

#### A. Experimental setting

For the evaluation, we chose three datasets of varying complexity, namely MNIST \(^27\), SVHN \(^28\) and CelebA \(^29\), which are commonly used for comparing generative models \(^2\), \(^11\). For these datasets we randomly chose, respectively, 100, 1000 and 1000 labeled samples, while the rest of the total 60000, 604388 and 182637 samples remained unlabeled. Since CelebA labels consist of multiple tags (i.e. sex, presence of eyeglasses, presence of facial hair, etc.), we left only the two most balanced tags (‘smiling’ and ‘male’) and created four exhaustive and mutually exclusive classes: ‘not male, not smiling’, ‘not male, smiling’, ‘male, not smiling’ and ‘male, smiling’.

We compare SeGMA to previous semi-supervised generative models, M1+M2 \(^10\) and ADGM \(^11\). We reimplemented these methods based on an open repository\(^5\) and the description of these models in the papers\(^7\). We excluded methods, which do not focus on generative properties (although they are based on generative models), such as GANs \(^25\). According to the best of the authors’ knowledge these are the only deep models, which introduce partial supervision to learn probability distributions of specific classes (not only the whole data density).

Contrary to the pipelines presented in \(^10\), \(^11\), we used no preprocessing on any of the datasets except for CelebA, where we followed \(^2\) and cropped and then resized images to a resolution of 140×140 and 64×64, respectively. To show that SeGMA does not need much fine-tuning on the validation set (which is often impractical in semi-supervised settings with a small number of available labels), we used the same values of hyperparameters \((\alpha = 5, \beta = 10, \gamma = (4 N_c^{-2})^2\)\), where \(N_c\) is the number of samples per class in a single batch, learning

\(^1\)In principle, a sufficiently wide and shallow neural network can implement any function. Indeed, a powerful encoder network may be such that an unlabeled data point is mapped to a different component than a labeled data point regardless of their similarity. Restricting the capacity of the encoder ensures a “continuity” or “bounded variation” in the implemented function, guaranteeing that data points that are similar in feature space get mapped to points close in latent space.

\(^2\)https://github.com/wolhert/semi-supervised-pytorch

\(^3\)https://github.com/dpkingma/npips14-ssl for M1+M2 and https://github.com/larsmaaloe/auxiliary-deep-generative-models for ADGM.

\(^5\)We we unable to use original authors codes directly, because they are based on a version of Theano, which is no longer supported.
rate $= 3 \cdot 10^{-4}$) for all experiments and adapted only the network architecture to each data set. Specifically, for MNIST and SVHN we used fully connected networks with ReLU activation functions and layer sizes $1024 - 1024 - 10 - 1024 - 1024 - 784$ and $786 - 786 - 786 - 786 - 20 - 786 - 786 - 786 - 786 - 786 - 786 - 3072$, respectively (i.e., the latent space has dimension $D = 10$ and $D = 20$ for MNIST and SVHN). For M1+M2 and ADGM operating on MNIST and SVHN we stuck to the architectures proposed in [10] and [11], respectively. For CelebA, the architectural details can be found in the appendix. We do not use any regularizers (weight decay, dropout, batch normalization), since we want to show that our model works in the simplest possible setting. Additional regularization might further improve its performance.

B. Generative performance

First, we examine the quality of generated samples. Moreover, we verify whether the models are capable of generating representative examples of a given class. For this purpose, we generate samples from each Gaussian component and pass these points through the decoder.

Randomly selected samples are presented in Figures 3, 4 and 5 for subsequent datasets – each row in the images corresponds to samples related to a separate Gaussian component for SeGMA, and to samples determined by a separate discrete class variable in M1+M2 and ADGM, respectively. It is evident that SeGMA generates realistically-looking samples. The produced examples are diverse and as sharp as samples returned by the corresponding CWAE model, see [12, Figure 2]. While ADGM generates samples of comparable quality for MNIST, the images produced for SVHN are less colorful. For CelebA, it returns grainy images, which contain many anomalies. It may be caused by an encoder network, which has to combine convolutional layers applied to an image with dense layers applied to one-hot vector representing the class [3]. M1+M2 gives reasonable results only for MNIST while for other data sets, the images are blurry and there is not enough variance between different images which might follow from the mode collapse. We wish to mention that the results reported in [10] displayed better quality for SVHN. We believe that this is due to specific preprocessing and careful hyperparameter selection, which is difficult to accomplish in a typical semi-supervised setting where the number of labeled data available for a validation stage is limited.

To provide an additional quantitative assessment of sample quality, we calculate the Fréchet Inception Distance (FID) [30], which is a standard score for generative models. To calculate FIDs, we used 10000 images sampled from the target distribution in the latent space.

| Variant     | Model  | MNIST | SVHN | CelebA |
|-------------|--------|-------|------|--------|
| unsupervised| CWAE   | 20.76 | 49.30| 51.94  |
|             | SeGMA  | 17.79 | 61.11| 51.13  |
| semi-supervised| M1+M2 | 40.50 | 142.11| 70.96 |
|             | ADGM   | 14.50 | 55.54| 51.96  |
|             | SeGMA  | 12.51 | 63.80| 50.54  |

The authors of ADGM did not examine their method in the case of convolutional neural networks.
Fig. 6: Class interpolations trained on various datasets. The first and the last columns are the real samples.

TABLE II: Test errors on various datasets (lower is better).

| Model  | MNIST | SVHN | CelebA |
|--------|-------|------|--------|
| M1+M2  | 17.0% | 65.7%| 44.5%  |
| ADGM   | 4.1%  | 41.2%| 41.7%  |
| SeGMA  | 12.7% | 32.8%| 24.6%  |

TABLE III: FIDs of interpolations.

| Model  | MNIST | SVHN | CelebA |
|--------|-------|------|--------|
| M1+M2  | 56.38 | 176.89 | 88.24 |
| ADGM   | 21.75 | 76.66 | 63.60 |
| SeGMA  | 13.40 | 63.47 | 48.14 |

connection between the generativity, semi-supervision, and a mixture of Gaussians as a target distribution, we also show FIDs for an unsupervised variant of SeGMA (i.e. for $\beta = 0$) and for a CWAЕ with a single spherical Gaussian as a target distribution (i.e. for $\beta = 0$ and $K = 1$). It is evident from Table I that the FIDs of SeGMA and ADGM are comparable across datasets, which is slightly surprising when one looks at the samples generated by these models. It is interesting that the FID of CWAЕ is better than both versions of SeGMA on SVHN. It suggests that deep generative models can be trained more easily on unimodal target distributions than using more complex mixture of Gaussians. In this case, we need to pay an additional cost (i.e., slightly lower quality of samples) for building a generative model for each class. Nevertheless, this observation does not hold for CelebA and MNIST, where the information of class labels allows to build better generative models for the entire data.

Visual inspection of the results suggests that the components in each model correspond to the correct classes (examples in each row of the figures have the same class). There are only few errors (e.g., the digits "2" and "3" in the second and sixth row of Figure 3c or the digit "5" in the ninth row of Figure 4c). Notably, similar errors occur also in M1+M2 (e.g., digit "6" in the first row of Figure 4a) and ADGM (e.g., digit "8" in the last row of Figure 4b) despite the fact that these methods require explicit discrete latent variables. To get a further insight into this aspect, we measured the classification accuracy on test sets. More precisely, we encoded each test image using an encoder network and classify it using (7) in the latent space. It is clear from Table III that SeGMA gives better results than competitive methods on harder datasets such as SVHN and CelebA. It is consistent with previous observation that SeGMA obtained higher quality of samples on these sets.

C. Interpolation

ADGM and M1+M2 use the same Gaussian as a target distribution for all classes. To distinguish between different classes, this distribution is additionally parametrized by a one-hot vector representing $Y$. Training is performed by sampling from the categorical probability distribution $P_Y$, and, in consequence, these models are unable to use non-discrete class labels. As a result, they produce realistically-looking interpolations between samples in the same class, but have problems with smooth interpolation between samples in different classes. In contrast, SeGMA uses a single continuous latent space in which the discrete class label is implicit in the identity of the mode of a potentially multimodal target distribution (e.g., Gaussian component in the case of a mixture of Gaussians). In other words, the samples from all classes are placed in the same continuous space and thus we may be able to interpolate between them freely.

To confirm this claim experimentally, we randomly pick a pair of images and map them to the latent space. Next, we generate linear interpolations between these encoded points and decode these interpolations using a decoder network. To obtain analogical effect for ADGM, we interpolate both the latent codes and the one-hot representations of classes.
The results of ADGM and SeGMA are presented in the Figure 6 (we omit M1+M2 interpolations because of their poor quality). It can be seen that interpolations produced by SeGMA have better quality than the ones obtained using ADGM. It is evident that many interpolations generated by ADGM are outside of the true data density (e.g. images in the sixth column of the first, second, fourth and fifth rows in the case of MNIST). For SVHN and CelebA, interpolations are often blurry or unrealistic (second row of CelebA and fifth row for SVHN). Note that the interpolations produced by SeGMA can also pass through the regions of low density, which lie between Gaussian components (e.g. fourth row in the case of MNIST). This negative effect could be however partially fixed using more sophisticated interpolations than the linear one \[31\], \[32\], which is not fully justified for this type of distribution. Nevertheless, we can observe very interesting geometrical properties of the class structure obtained by SeGMA: The interpolation between "6" and "9" (first row) leads to generating a digit "4" (first row). This suggests that the class of digits "4" is localized between classes of digits "6" and "9". Similar effect can be observed for the second row, where the model passes through the class of digits "3".

The above results are confirmed by FID scores calculated for images generated from interpolations, see Table III. Specifically, we took two random images from the test data and encoded them into the latent space. Next, we randomly picked a point from the interpolation line and decoded it. We obtained 10000 samples this way, which were used for calculating FID against the real data. It is evident that FIDs calculated for SeGMA are significantly better than the ones obtained by competitive methods.

### D. Style Transfer and Class Intensity

Semi-supervised generative models based on the VAE generate images by decoding a data point sampled from the target distribution and a one-hot vector describing the class label. If we flip the class vector, but keep the latent code unchanged, then the model returns an image with similar style, but from a different class. In other words, these models disentangle the label feature in the latent space. In this experiment, we investigate whether a comparable style transfer can be achieved for our model.

In the case of SeGMA, we cannot simply change the class label, because we do not have an individual vector describing the class. However, we can move a latent code generated by one Gaussian component to the corresponding location w.r.t. the mode of another Gaussian component. In other words, we move a latent code \(\tilde{z}\) by a vector between the mean of target Gaussian \(N(\mu_t, I)\) and the mean of the initial Gaussian \(N(\mu_s, I)\) from which it was generated, i.e.:

\[
\tilde{z} = z + (\mu_t - \mu_s) \tag{10}
\]

In addition, we can perform the interpolation between \(z\) and \(\tilde{z}\) to change the class label gradually. Moving along this line in latent space is presumably more natural than moving along a corresponding line between two one-hot encoded class vectors, as it would be necessary for semi-supervised VAE models. In the continuous latent space, it is natural to assume that close points correspond to similar images; for one-hot encoded class vectors or a discrete latent space, the notion of closeness and similarity is inadequate in the first place.

We verify the above claims in the following experiment. We encode an image into the latent space and gradually change its class label in a direction to the randomly selected class according to (10). Sample results of this operation for SeGMA...
existing semi-supervised generative models. In particular, we points from different classes, which was not possible in space as the style variable, we can interpolate between data

Since a mixture of Gaussians as a target distribution. By connecting model, which combines a W AE-MMD framework with a

α to the picture. Examples of this operation are presented in the 'not male' class, we can add more masculine features face and then moving it away from the Gaussian representing far from Gaussian components connected with female images.

An interesting property of our model is that we can not only perform: 

\[ \hat{z} = z + \alpha (\mu_s - \mu_t) \] (11)

for some \( \alpha > 0 \). For example, by using an image of a male face and then moving it away from the Gaussian representing the 'not male' class, we can add more masculine features to the picture. Examples of this operation are presented in Fig. [8] for \( \alpha = 0.5 \). In the first three rows, the samples are moving away from the "not male/smiling" class, while in the fourth row, it is moving away from the "male/smiling" class. It can be observed that the man in the third row gains more masculine feature, while the woman in the fourth row gains more feminine features. This suggests that the presence of a beard is recognized as a typical male attribute and was encoded more feminine features. This suggests that the presence of a masculine feature, while the woman in the fourth row gains decreasing, e.g., female attributes resulted in growing a beard in male celebrities.

Due to the use of a simple auto-encoder architecture from a classical WAE model, SeGMA scales better with the complexity of the dataset than other semi-supervised generative approaches. In particular, SeGMA requires fewer dimensions in the latent space (20 dimensions for SVHN) than ADGM (300 dimensions for SVHN), which is composed on six neural networks. Making use of Cramer-Wold distance as MMD penalty, we do not need to sample while training the model, which speeds up the procedure and increases its stability. In contrast, the authors of ADGM recommend using multiple samples when estimating expectations in their model, which is costly both in time and computing resources. Our model is also more flexible when it comes to using different networks’ architectures, such as convolutional layers, than the previous semi-supervised models.

**APPENDIX**

For SeGMA, the encoder \( E \) consists of two convolutional layers with 32 filters, two convolutional layers with 64 filters, and two fully connected layers of size 786 – 786. The decoder \( D \) consists of three fully connected layers of size 786 – 786 – 1024, one transposed convolutional layer with 64 filters, two transposed convolutional layers with 32 filters, and a final transposed convolutional layer with 3 filters. The latent space has dimension \( D = 32 \).

For M1, the encoder \( E \) consists of two convolutional layers with 32 filters, two convolutional layers with 64 filters, and a fully connected layer of size 300. The decoder \( D \) consists of two fully connected layers of size 300 – 1024, one transposed convolutional layer with 64 filters, two transposed convolutional layers with 32 filters, and a final transposed convolutional layer with 3 filters. The latent space has dimension \( D = 32 \). For M2, encoder and decoder are fully connected with sizes 300 and 300 – 300, respectively. The latent space has dimension \( D = 50 \).

For ADGM, the encoder \( E \) consists of two convolutional layers with 32 filters and two convolutional layers with 64 filters. The result is a flattened vector. After that every edge in the probabilistic graph of this model is implemented by a neural network with two fully connected layers of size 500 – 500. Also the decoder \( D \) implements every edge in the probabilistic graph by a neural network with two fully connected layers of size 500 – 500. The resulting image is further processed by a transposed convolutional layer with 64 filters, two transposed convolutional layer with 32 filters, and a final transposed convolutional layer with 3 filters. The latent space has dimension \( D = 300 \).

All networks are implemented using ReLU activation functions and all filters are of size 4x4 and stride 2x2.

![Image](https://via.placeholder.com/150)

**Fig. 8:** Changing intensity of the label. The samples in the first row are moving from the anti-target classes, which is "not male/smiling" for the first three rows and "male/smiling" for the fourth row.

and analogous results for ADGM are presented in Figure 7. Although the style transfer leads to different images for SeGMA and for ADGM (see right-most images in Figure 7), it can be seen that the style is indeed maintained for SeGMA. In addition to that, the images obtained via interpolation are more natural for SeGMA. As mentioned, this is because ADGM encodes only discrete class labels while SeGMA treats it as continuous variable.

An interesting property of our model is that we can not only change the class of the presented data point, but also increase or decrease the intensity of certain stylistic aspects. We can achieve this property by moving the latent representation \( z \) of a data point away from a class which lacks the considered stylistic aspect. More precisely, let \( z \) be a latent code of an image, which belongs to the initial Gaussian \( N(\mu_s, I) \). We can move \( z \) away from an anti-target Gaussian \( N(\mu_t, I) \) by performing:

\[ \hat{z} = z + \alpha (\mu_s - \mu_t) \] (11)

VII. CONCLUSION

We constructed SeGMA, a semi-supervised generative model, which combines a WAE-MMD framework with a mixture of Gaussians as a target distribution. By connecting each component with a specific class, SeGMA is capable of generating class representatives of high quality. Since a discrete class label is implicitly encoded in the same latent space as the style variable, we can interpolate between data points from different classes, which was not possible in existing semi-supervised generative models. In particular, we can change the class labels gradually while preserving the style of a given data point. Moreover, SeGMA allows for increasing (decreasing) the influence of a given class by moving this example in a (opposite) direction of the corresponding Gaussian component. This property is illustrated in Fig. 8 where decreasing, e.g., female attributes resulted in growing a beard in male celebrities.

All networks are implemented using ReLU activation functions and all filters are of size 4x4 and stride 2x2.
REFERENCES

[1] D. P. Kingma and M. Welling, “Auto-encoding variational bayes,” arXiv preprint arXiv:1312.6114, 2013.
[2] I. Tolstikhin, O. Bousquet, S. Gelly, and B. Schoelkopf, “Wasserstein auto-encoders,” in Proc. International Conference on Learning Representations (ICLR), Vancouver, May 2018.
[3] I. Goodfellow, J. Pouget-Abadie, M. Mirza, B. Xu, D. Warde-Farley, S. Ozair, A. Courville, and Y. Bengio, “Generative adversarial nets,” in Proc. Advances in Neural Information Processing Systems (NIPS), 2014, pp. 2672–2680.
[4] R. A. Yeh, C. Chen, T. Yuan Lim, A. G. Schwing, M. Hasegawa-Johnson, and M. N. Do, “Semantic image inpainting with deep generative models,” in Proc. IEEE Conf. on Computer Vision and Pattern Recognition (CVPR), 2017, pp. 5485–5494.
[5] H. Fan, H. Su, and L. J. Guibas, “A point set generation network for 3d object reconstruction from a single image,” in Proc. IEEE Conf. on Computer Vision and Pattern Recognition (CVPR), 2017, pp. 605–613.
[6] K. Guu, T. B. Hashimoto, Y. Oren, and P. Liang, “Generating sentences by editing prototypes,” Transactions of the Association of Computational Linguistics, vol. 6, pp. 437–450, 2018.
[7] J.-Y. Zhu, P. Krähenbühl, E. Shechtman, and A. A. Efros, “Generative visual manipulation on the natural image manifold,” in Proc. European Conf. on Computer Vision. Springer, 2016, pp. 597–613.
[8] J.-Y. Zhu, T. Park, P. Isola, and A. A. Efros, “Unpaired image-to-image translation using cycle-consistent adversarial networks,” in Proc. IEEE Int. Conf. on Computer Vision (ICCV), 2017, pp. 2223–2232.
[9] A. Shrivastava, T. Pfister, O. Tuzel, J. Susskind, W. Wang, and R. Webb, “Learning from simulated and unsupervised images through adversarial training,” in Proc. IEEE Conf. on Computer Vision and Pattern Recognition (CVPR), 2017, pp. 2107–2116.
[10] D. P. Kingma, S. Mohamed, D. J. Rezende, and M. Welling, “Semi-supervised learning with deep generative models,” in Proc. Advances in Neural Information Processing Systems (NIPS), 2014, pp. 3581–3589.
[11] L. Maaløe, C. K. Sønderby, S. K. Sønderby, and O. Winther, “Auxiliary deep generative models,” in Int. Conf. on Machine Learning (ICML), 2016, pp. 1445–1453.
[12] J. Tabor, S. Knop, P. Spurek, I. Podolak, M. Mazur, and S. Jastrzębski, “Cramer-wold autoencoder,” arxiv preprint arXiv:1805.09235, 2018.
[13] J. T. Rolle, “Discrete variational autoencoders,” in Proc. International Conference on Learning Representations (ICLR), Toulon, Apr. 2017.
[14] Z. Jiang, Y. Zheng, H. Tan, B. Tang, and H. Zhou, “Variational deep embedding: An unsupervised and generative approach to clustering,” in Proc. of the Twenty-Sixth Int. Joint Conf. on Artificial Intelligence (IJCAI-17), 2017, pp. 1965–1972. [Online]. Available: https://doi.org/10.24963/ijcai.2017/273
[15] Y. Uğur, G. Arvanitakis, and A. Zaidi, “Variational information bottleneck for unsupervised clustering: Deep gaussian mixture embedding,” arxiv preprint arXiv:1905.11741, May 2019.
[16] A. A. Alemi, I. Fischer, J. V. Dillon, and K. Murphy, “Deep variational information bottleneck,” in Proc. International Conference on Learning Representations (ICLR), Toulon, Apr. 2017.
[17] N. Dilokthanakul, P. A. Mediano, M. Gamelo, M. C. Lee, H. Salimbeni, K. Arulkumaran, and M. Shanahan, “Deep unsupervised clustering with gaussian mixture variational autoencoders,” arxiv preprint arXiv:1911.02648, Nov. 2019.
[18] B. Gaujac, I. Feige, and D. Barber, “Gaussian mixture models with Wasserstein distance,” arxiv preprint arXiv:1806.04465, 2018.
[19] S. Kolouri, G. K. Rohde, and H. Hoffmann, “Sliced wasserstein distance for learning gaussian mixture models,” in Proc. IEEE Conf. on Computer Vision and Pattern Recognition (CVPR), 2018, pp. 3427–3436.
[20] S. Kolouri, S. R. Park, M. Thorpe, D. Slepcev, and G. K. Rohde, “Optimal mass transport: Signal processing and machine-learning applications,” IEEE signal processing magazine, vol. 34, no. 4, pp. 43–59, 2017.
[21] D. Lawson, C.-C. Chiu, G. Tucker, C. Raffel, K. Swersky, and N. Jaitly, “Learning hard alignments with variational inference,” in 2018 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP). IEEE, 2018, pp. 5799–5803.
[22] E. Jang, S. Gu, and B. Poole, “Categorical reparameterization with gumbel-softmax,” arXiv preprint arXiv:1611.01144, 2016.
[23] C. J. Maddison, A. Mnih, and Y. W. Teh, “The concrete distribution: A continuous relaxation of discrete random variables,” arxiv preprint arXiv:1611.00712, 2016.
[24] L. Maaløe, M. Fraccaro, and O. Winther, “Cagem: A cluster aware deep generative model,” in Workshop on Advances in Approximate Bayesian Inferences at Advances in Neural Information Processing Systems (NIPS), 2017.
[25] Z. Dai, Z. Yang, F. Yang, W. W. Cohen, and R. R. Salakhutdinov, “Good semi-supervised learning that requires a bad gan,” in Proc. Advances in Neural Information Processing Systems (NIPS), 2017, pp. 6510–6520.
[26] Y. Wang and S. Chen, “Safety-aware semi-supervised classification,” IEEE transactions on neural networks and learning systems, vol. 24, no. 11, pp. 1763–1772, 2013.
[27] Y. LeCun and C. Cortes, “MNIST handwritten digit database.” [Online]. Available: http://yann.lecun.com/exdb/mnist/
[28] Y. Netzer, T. Wang, A. Coates, A. Bissacco, B. Wu, and A. Y. Ng, “Reading digits in natural images with unsupervised feature learning,” in Workshop on Deep Learning and Unsupervised Feature Learning at Advances in Neural Information Processing Systems (NIPS), 2011. [Online]. Available: http://ufldl.stanford.edu/housenumbers/nips2011 housenumbers.pdf
[29] Z. Liu, P. Luo, X. Wang, and X. Tang, “Deep learning face attributes in the wild,” in Proc. Int. Conf. on Computer Vision (ICCV), Dec. 2015.
[30] M. Heusel, H. Ramsauer, T. Unterthiner, B. Nessler, and S. Hochreiter, “Gans trained by a two time-scale update rule converge to a local nash equilibrium,” in Proc. Advances in Neural Information Processing Systems (NIPS), 2017, pp. 6626–6637.
[31] D. Leinik, I. Sieradzki, and I. Podolak, “Distribution-interpolation trade off in generative models,” in Proc. Int. Conf. on Learning Representation (ICLR), 2019.
[32] L. Struski, J. Tabor, I. Podolak, and A. Nowak, “Interpolation in generative models,” arxiv preprint arXiv:1904.03445, 2019.