MaskAAE: Latent space optimization for Adversarial Auto-Encoders

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Abstract

The field of neural generative models is dominated by the highly successful Generative Adversarial Networks (GANs) despite their challenges, such as training instability and mode collapse. Auto-Encoders (AE) with regularized latent space provide an alternative framework for generative models, albeit their performance levels have not reached that of GANs. In this work, we hypothesise that the dimensionality of the AE model's latent space has a critical effect on the quality of generated data. Under the assumption that nature generates data by sampling from a "true" generative latent space followed by a deterministic function, we show that the optimal performance is obtained when the dimensionality of the latent space of the AE-model matches with that of the "true" generative latent space. Further, we propose an algorithm called the Mask Adversarial Auto-Encoder (MaskAAE), in which the dimensionality of the latent space of an adversarial auto encoder is brought closer to that of the "true" generative latent space, via a procedure to mask the spurious latent dimensions. We demonstrate through experiments on synthetic and several real-world datasets that the proposed formulation yields betterment in the generation quality.

1 INTRODUCTION

The objective of a probabilistic generative model is to learn to sample new points from a distribution given a finite set of data points drawn from it. Deep generative models, especially the Generative Adversarial Networks (GANs) (Goodfellow et al. (2014)) have shown remarkable success in this task by generating high quality data (Brock et al. (2019)). GANs implicitly learn to sample from the data distribution by transforming a sample from a simplistic distribution (such as Gaussian) to the sample from the data distribution by optimising a min-max objective through an adversarial game between a pair of function approximators called the generator and the discriminator. Although GANs generate high-quality data, they are known to suffer from problems like instability of training (Arora et al. (2017); Salimans et al. (2016)), degenerative supports for the generated data (mode collapse) (Arjovsky and Bottou (2017); Srivastava et al. (2017)) and sensitivity to hyper-parameters (Brock et al. (2019)).

Auto-Encoder (AE) based generative models (Zhao et al. (2017); Kingma and Welling (2013); Makhzani et al. (2016); Tolstikhin et al. (2018)) provide an alternative to GAN based models. The fundamental idea is to learn a lower dimensional latent representation of data through a deterministic or stochastic encoder and learn to generate (decode) the data through a decoder. Typically, both the encoder and decoder are realised through learnable family of function approximators or deep neural networks. To facilitate the generation process, the distribution over the latent space is forced to follow a known distribution so that sampling from it is feasible. Despite resulting in higher data-likelihood and stable training, the quality of generated data of the AE-based models is known to be far away from state-of-the-art GAN models (Dai and Wipf (2019); Grover et al. (2018); Theis et al. (2015)).

While there have been several angles of looking at the shortcomings of the AE-based models (Dai and Wipf (2019); Hoshen et al. (2019); Kingma et al. (2016); Tomczak and Welling (2017); Klushyn et al. (2019); Bauer and Mnih (2019); van den Oord et al. (2017)), an important question seems to have remained unaddressed: How does the dimensionality of the latent space (bottle-neck

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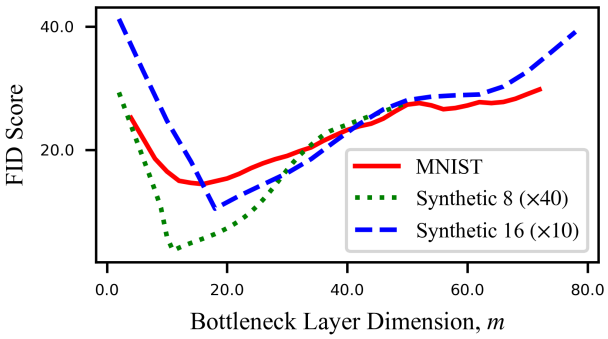


Figure 1: FID score for a Wasserstein Auto-Encoder with varying latent dimensionality m for 2 synthetic datasets of 'true' latent dimensions, $n = 8$ and $n = 16$ and MNIST. It is seen that the generation quality gets worse on both the sides of a certain latent dimensionality. FID scores have been scaled appropriately to bring them in the same range

layer) affect the generation quality in AE-based models?

It is a well-known fact that most of the naturally occurring data effectively lies in a manifold with dimension much lesser than its original dimensionality (Cayton (2005); Law and Jain (2006); Narayanan and Mitter (2010)). Intuitively, this suggests that with functions that Deep Neural Networks learn, there exists an optimal number of latent dimensions, since "lesser" or "extra" number of latent dimensions may result in loss of information and noisy generation, respectively. This observation is also corroborated by empirical evidence provided in Fig. 1 where a state-of-the-art AE-based generative model (Wasserstein Auto-Encoder Tolstikhin et al. (2018)) is constructed on two synthetic (detailed in Section 5) and MNIST datasets, with varying latent dimensionality (everything else kept the same). It is seen that the generation quality metric (FID) follows a U-shaped curve. Thus, to obtain optimal generation quality, a brute-force search over a large range of values of latent dimensionality may be required, which is practically infeasible. Motivated by the aforementioned observations, in this work, we explore the role of latent dimensionality in AE-based generative models, with the following contributions:

1. We model the data generation as a two-stage process comprising of sampling from a "true" latent space followed by a deterministic function.

2. We provide theoretical understanding on the role of the latent space dimensionality on the generation quality, by formalizing the requirements for a faithful generation in of AE-based generative models with deterministic encoder and decoder networks.

3. Owing to the obliviousness of the dimensionality of the "true" latent space in real-life data, we propose a method to algorithmically "mask" the spurious dimensions in AE-based models (and thus call our model the MaskAAE).

4. We demonstrate the efficacy of the proposed model on synthetic as well as large-scale image datasets by achieving better generation quality metrics compared to the state-of-the-art AE-based models.

2 RELATED WORK

Let $\boldsymbol{x}$ denote data points lying in the space $\mathcal{X}$ conforming to an underlying distribution $\Upsilon(\boldsymbol{x})$, from which a generative model desires to sample. An Auto-Encoder based model constructs a lower-dimensional latent space $\mathcal{Z}$ to which the data is projected through an (probabilistic or deterministic) Encoder function, E_κ. An inverse projection map is learned from $\mathcal{Z}$ to $\mathcal{X}$ through a Decoder function D_ψ, which can be subsequently used as a sampler for $\Upsilon(\boldsymbol{x})$. For this to happen, it is necessary that the distribution of points over the latent space $\mathcal{Z}$ is regularized (to some known distribution $\Pi(\boldsymbol{z})$) to facilitate explicit sampling from $\Pi(\boldsymbol{z})$, so that decoder can generate data taking samples from $\Pi(\boldsymbol{z})$ as input. Most of the AE-based models maximize the data likelihood (or a lower bound on it), which is shown (Kingma and Welling (2013); Hoffman and Johnson (2016)) to consist of the sum of two critical terms - (i) the likelihood of the Decoder generated data and, (ii) a divergence measure between the assumed latent distribution, $\Pi(\boldsymbol{z})$, and the distribution imposed on the latent space by the Encoder, $\Psi(\boldsymbol{z}) = \int \Psi(\boldsymbol{z}|\boldsymbol{x})\Upsilon(\boldsymbol{x})d\boldsymbol{x}$, (Hoffman and Johnson (2016); Makhzani et al. (2016)). This underlying commonality, suggests that the success of an AE-based generative model depends upon simultaneously optimising the aforementioned terms. The first criterion is fairly easily ensured in all AE models by minimizing a surrogate function such as the reconstruction error between the samples of the true data and output of the decoder, which can be made arbitrarily small (Burgess et al. (2017); Dai and Wipf (2019); Alain and Bengio (2014)) by increasing the network capacity. It is well recognized that the quality of the generated data relies heavily on achieving the second criteria of bringing the Encoder imposed latent distribution $\Psi(\boldsymbol{z})$ close to the assumed latent prior distribution $\Pi(\boldsymbol{z})$ (Dai and Wipf (2019); Hoffman and Johnson (2016); Burgess et al. (2017)). This can be achieved either by (i) assuming a pre-defined primitive distribution for $\Pi(\boldsymbol{z})$ and modifying the Encoder such that $\Psi(\boldsymbol{z})$ follows assumed $\Pi(\boldsymbol{z})$ (Kingma and Welling (2013); Makhzani et al. (2016); Tolstikhin et al. (2018); Chen et al. (2018); Higgins et al. (2017);

Kim and Mnih (2018); Kingma et al. (2016)) or by (ii) modifying the latent prior $\Pi(\boldsymbol{z})$ to follow whatever distribution $\big(\Psi(\boldsymbol{z})\big)$ Encoder imposes on the latent space (Tomczak and Welling (2017); Bauer and Mnih (2019); Klushyn et al. (2019); Hoshen et al. (2019); van den Oord et al. (2017)).

The seminal paper on VAE (Kingma and Welling (2013)) proposes a probabilistic Encoder which is tuned to output the parameters of the conditional posterior $\Psi(\boldsymbol{z}|\boldsymbol{x})$ which is forced to follow the Normal distribution prior assumed on $\Pi(\boldsymbol{z})$. However, the minimization of the divergence between the conditional latent distribution and the prior in the VAE leads to trade-off between the reconstruction quality and the latent matching, as this procedure also leads to the minimization of the mutual information between $\mathcal{X}$ and $\mathcal{Z}$, which in turn reduces Decoder's ability to render good reconstructions (Kim and Mnih (2018)). This issue is partially mitigated by altering the weights on the two terms of the ELBO during optimization (Higgins et al. (2017); Burgess et al. (2017)), or through introducing explicit penalty terms in the ELBO to strongly penalize the deviation of $\Psi(\boldsymbol{z})$ from assumed prior $\Pi(\boldsymbol{z})$ (Chen et al. (2018); Kim and Mnih (2018)). Adversarial Auto-Encoders (AAE) (Makhzani et al. (2016)) and Wasserstein Auto-Encoders (WAE) (Tolstikhin et al. (2018)) address this issue, by taking advantage of adversarial training to minimize the divergence between $\Psi(\boldsymbol{z})$ and $\Pi(\boldsymbol{z})$, via deterministic Encoder and Decoder networks. There also have been attempts in employing the idea of normalizing flow for distributional estimation for making $\Psi(\boldsymbol{z})$ close to $\Pi(\boldsymbol{z})$ (Kingma et al. (2016); Rezende and Mohamed (2015)). These methods, although improve the generation quality over vanilla VAE while providing additional properties such as disentanglement in the learned space, fail to match the generation quality of GAN and its variants.

In another class of methods, the latent prior $\Pi(\boldsymbol{z})$ is made learnable instead of being fixed to a primitive distribution so that it matches with Encoder imposed $\Psi(\boldsymbol{z})$. In VamPrior (Tomczak and Welling (2017)), the prior is taken as a mixture density whose components are learned using pseudo-inputs to the Encoder. Klushyn et al. (2019) introduces a graph-based interpolation method to learn the prior in a hierarchical way. In van den Oord et al. (2017); Kyatham et al. (2019), discrete latent space is employed, using vector quantization schemes where the prior is learned using a discrete auto-regressive model. While these prior matching methods provide various advantages, there is no mechanism to ward-off the 'spurious' latent dimensions that are known to degrade the generation quality. While there exists a possibility that the Decoder learns to ignore those spurious dimensions by making the corresponding weights zero there is no guarantee or empirical evidence of neglecting those dimensions. Another indirect approach to handle this issue is to add noise to the input data and prevent variance collapse in the latent space through explicit regularization (Rubenstein et al. (2018)). However, this approach avoids the problem instead of solving it. The closest work to ours is 2-stage VAE (Dai and Wipf (2019)), in which the authors show that VAEs struggle to match the latent distribution to an isotropic standard Gaussian when there is a mismatch between the original data manifold dimension and the latent space capacity. To resolve this, they propose two VAEs, where the first one maps the data to a latent code having the same dimension as the latent space capacity, and the second stage then maps the latent spaced mapped in the first stage to an isotropic Gaussian (see supplementary for a detailed discussion).

To summarize, it is observed that without additional modifications, in vanilla AE-based models, the existence of superfluous latent dimensions degrades the generation quality. We formally address this problem, presenting a novel theoretical analysis of the issues involved, and also provide a method to ameliorate this problem by explicitly masking the spurious dimensions in the latent space of AE based models.

3 EFFECT OF LATENT DIMENSIONALITY

3.1 PRELIMINARIES

In this section, we theoretically examine the effect of latent dimensionality on the quality of generated data in AE based generative models. We show that if dimensionality of the latent space $\mathcal{Z}$ is more than the *optimal* dimensionality (to be defined), $\Pi(\boldsymbol{z})$ and $\Psi(\boldsymbol{z})$ diverge too much whereas it being less leads to information loss.

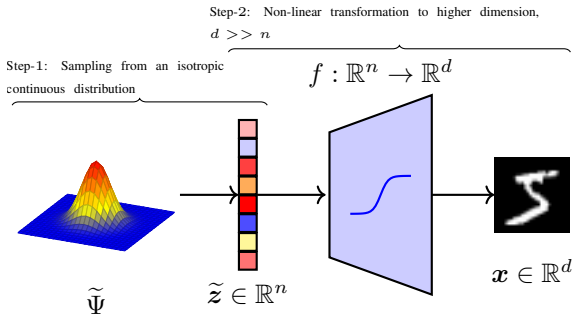


Figure 2: Depiction of the assumed data generation process. Samples drawn from a 'true' latent distribution $\widetilde{\Psi}(\widetilde{\mathbf{z}})$ are passed through a function f to obtain $\boldsymbol{x}$.

To begin with, we allow a certain inductive bias in assuming that nature generates data as described in Figure 2 using the following two-step process: First sam-

ple from some isotropic continuous latent distribution in n-dimensions (call this $\widetilde{\Psi}$ over $\widetilde{\mathcal{Z}}$), and then pass this through a function $f : \mathbb{R}^n \rightarrow \mathbb{R}^d$, where d is the dataset dimensionality. Typically $d >> n$, thereby making data to lie on a low-dimensional manifold in R^d. Since $\widetilde{\mathcal{Z}}$ can intuitively be viewed as the latent space from which the nature is generating the data, we call n the *true latent dimension* and function f, as the *data-generating function*. Note that within this ambit, $\widetilde{\mathcal{Z}}$ forms the domain of f and it is unique only up to its range with following properties:

A1 f is *L-lipschitz*: $\exists$ some finite $L \in \mathbb{R}^+$ satisfying $||f(\widetilde{\boldsymbol{z}}_1) - f(\widetilde{\boldsymbol{z}}_2)|| \leq L||\widetilde{\boldsymbol{z}}_1 - \widetilde{\boldsymbol{z}}_2||,\ \forall \widetilde{\boldsymbol{z}}_1, \widetilde{\boldsymbol{z}}_2 \in \widetilde{\mathcal{Z}}$.

A2 There does not exist $f^* : \mathbb{R}^{n'} \rightarrow \mathbb{R}^d, n' < n$ satisfying A1 such that the range of f is a subset of the range of f^*.

The first property is satisfied by a large class of functions, including neural networks and the second simply states that n, the dimension of the domain (generative latent space) of f is minimal[1]. Hence, it is reasonable to impose these restrictions on data-generating functions. (An illustrative example for A2 is provided in the supp.)

3.2 CONDITIONS FOR GOOD GENERATION

In this section, we formulate the conditions required for faithful generation in latent variable generative models. Let $\Gamma(\boldsymbol{x}, \boldsymbol{z})$ and $\Gamma'(\boldsymbol{x}, \boldsymbol{z})$ denote the true and the (implicitly) inferred joint distribution of the observed and latent variables. The goal of the latent variable generative models is to minimize the negative log-likelihood of $\Gamma'(\boldsymbol{x}, \boldsymbol{z})$ under $\Gamma(\boldsymbol{x}, \boldsymbol{z})$:

$$\mathcal{L}(\Gamma, \Gamma') = - \mathop{\mathbb{E}}_{\boldsymbol{x}, \boldsymbol{z} \sim \Gamma} \big[\log(\Gamma'(\boldsymbol{x}, \boldsymbol{z})) \big] \tag{1}$$

An AE-based generative model would attempt to minimize Eq. 1 by learning two parametric functions, $E_\kappa \triangleq g : \mathbb{R}^d \rightarrow \mathbb{R}^m$ (m is hereafter referred to as *assumed latent dimension / model capacity*) and $D_\psi \triangleq g' : \mathbb{R}^m \rightarrow \mathbb{R}^d$, to approximate the distributions $\Psi(\boldsymbol{z}|\boldsymbol{x})$ and $\Gamma(\boldsymbol{x}|\boldsymbol{z})$, respectively. Further, Eq. 1 can be split into two terms, and the objective of any AE-model can be restated as:

$$\min \Bigg(\underbrace{\mathop{\mathbb{E}}_{\Gamma}[-\log(\Gamma'(\boldsymbol{x}|\boldsymbol{z}))]}_{\text{R1}} + \underbrace{\mathop{\mathbb{E}}_{\Gamma}[\log \frac{1}{\Gamma'(\boldsymbol{z})}]}_{\text{R2}} \Bigg) \tag{2}$$

If E_κ and D_ψ are deterministic (as in the case of AAE (Makhzani et al. (2016)) [2], WAE (Tolstikhin et al. (2018)) etc.), then the two terms in Eq. 2 can be cast as the following two requirements (see the supp. for the proof):

R1 $f(\widetilde{\boldsymbol{z}}) = g'(g(f(\widetilde{\boldsymbol{z}})))\ \forall\ \widetilde{\boldsymbol{z}}\ \in \mathbb{R}^n$. This condition states that the reconstruction error between the real and generated data should be minimal.

R2 The Cross Entropy $\mathcal{H}(\Psi, \Pi)$ between the chosen prior Ψ, and Π on $\mathcal{Z}$ is minimal.

With this, we state and prove the conditions required to ensure R1 and R2 are met with assumed data generation process.

Theorem 1. *With the assumption of data generating process mentioned in Sec.3.1, requirements R1 and R2 (Sec.3.2), can be satisfied iff assumed latent dimension m is equal to true latent dimension n.*

Proof: We prove by contradicting either R1 or R2, in assuming both the cases of $m < n$ or $m > n$.

Case A ($m < n$)*:* For R1 to hold, the range of f must be a subset of the range of g'. Further, since g' is a Neural Network, it satisfies A1. But, by A2, such a function cannot exist if $m < n$.

Case B ($m > n$): For the sake of simplicity, let us assume that $\widetilde{\mathcal{Z}}$ is a unit cube[3] in $\mathbb{R}^n$. We show in Lemma 1 and 2 that in this case, R2 will be contradicted if $m > n$. The idea is to first show that the range of $g \circ f$ will have Lebesgue measure 0 (Lemma 1) and this leads to arbitrarily large $\mathcal{H}$ (Lemma 2).

Lemma 1: Let $\Omega : [0, 1]^\alpha \rightarrow \mathbb{R}^\beta$ be an $L - lipschitz$ function. Then its range $R \in \mathbb{R}^\beta$ has Lebesgue measure 0 in $\mathbb{R}^\beta$ dimensions if $\beta > \alpha$.

Proof: For some $\epsilon \in \mathbb{N}$, consider the set of points:

$$\text{S}=\Big\{ \big(\tfrac{a_0 + 0.5}{\epsilon}, \ldots, \tfrac{a_{\alpha-1} + 0.5}{\epsilon} \big) \Big| a_i \in \{0, \ldots, \epsilon - 1\} \Big\}.$$

Construct closed balls around them having radius $\frac{\sqrt{\alpha}}{2\epsilon}$. It is easy to see that every point in the domain of Ω is contained in at least one of these balls. This is because,

[1] If there exists such an f^*, then that would become the generating function with n' being minimal.

[2] Makhzani et al. (2016), in their work, have observed that the performance of stochastic and deterministic networks are comparable. Thus, We consider only deterministic networks for theoretical analysis and experimentation in our work.

[3] One can easily obtain another function $\nu : [0, 1]^n \rightarrow \widetilde{\mathcal{Z}}$ that scales and translates the unit cube appropriately. Note that for such a ν to exist, we need $\widetilde{\mathcal{Z}}$ to be bounded, which may not be the case for certain distributions like the Gaussian distributions. Such distributions, however, can be approximated successively in the limiting sense by truncating at some large value Rudin et al. (1964)

for any given point, the nearest point in S can be at-most $\frac{1}{2\epsilon}$ units away along each dimension. Also, since Ω is L-lipschitz, we can conclude that the image set of a closed ball having radius r and centre $\boldsymbol{u} \in [0,1]^\alpha$ would be a subset of the closed ball having centre $\Omega(\boldsymbol{u})$ and radius $L \times r$.

The range of Ω is then a subset of the union of the image sets off all the closed balls defined around S. The volume of this set is upper bounded by the sum of the volumes of the individual image balls, each having volume $\frac{c}{\epsilon^\beta}$ where c is a constant having value $\frac{(L)^\beta(\alpha\pi)^{\frac{\beta}{2}}}{\Gamma(\frac{\beta}{2}+1)}$. Therefore,

$$\text{vol(R)} \leq |S| \times \frac{c}{\epsilon^\beta} = \frac{c}{\epsilon^{\beta-\alpha}}. \tag{3}$$

The final quantity of Eq. 3 can be made arbitrarily small by choosing ϵ appropriately. Since the Lebesgue measure of a closed ball is same as its volume, the range of Ω, R has measure 0 in $\mathbb{R}^\beta$. □

Since f, and g are Lipschitz, $g \circ f$ must have a range with Lebesgue measure 0 as a consequence of Lemma 2. Now we show that as a consequence of the range of $g \circ f$ (call it $\mathcal{R}$) having measure 0, the cross-entropy between Π and Ψ goes to infinity.

Lemma 2: If Π and Ψ are two distributions as defined in Sec.3.1 such that the support of the latter has a 0 Lebesgue measure, then $\mathcal{H}(\Pi, \Psi)$ grows to be arbitrarily large.

Proof: Ψ can be equivalently expressed as:

$$\Psi(\boldsymbol{z}) = \begin{cases} \widetilde{\Psi}(\widetilde{\boldsymbol{z}}) & \text{if } \exists\, \widetilde{\boldsymbol{z}}^4 \in \widetilde{\mathcal{Z}} \text{ s.t. } g(f(\widetilde{\boldsymbol{z}})) = \boldsymbol{z}, \\ 0 & \text{otherwise} \end{cases} \tag{4}$$

Define $\mathbb{I}_\mathcal{R}$ as the indicator function of $\mathcal{R}$, i.e.

$$\mathbb{I}_\mathcal{R}(\boldsymbol{z}) = \begin{cases} 1 & \text{if } \exists\, \widetilde{\boldsymbol{z}} \in \widetilde{\mathcal{Z}} \text{ s.t. } g(f(\widetilde{\boldsymbol{z}})) = \boldsymbol{z}, \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

Since $\mathcal{R}$ has measure 0 (Lemma 2), we have

$$\int_{\mathbb{R}^m} \mathbb{I}_\mathcal{R}(\boldsymbol{z}) d\boldsymbol{z} = 0 \tag{6}$$

Further, since $\mathbb{I}_\mathcal{R}$ is identically 1 in the support of Ψ,

$$\Psi(\boldsymbol{z}) = \Psi(\boldsymbol{z})\mathbb{I}_\mathcal{R}(\boldsymbol{z}) \tag{7}$$

Next, consider the cross-entropy between Π and Ψ:

$$\begin{aligned} \mathcal{H}(\Pi, \Psi) &= \int_\mathcal{Z} \Pi(\boldsymbol{z})(-\log(\Psi(\boldsymbol{z})))d\boldsymbol{z} \\ &\geq \int_{\mathcal{Z}-\mathcal{R}} \Pi(\boldsymbol{z})(-\log(\Psi(\boldsymbol{z})\mathbb{I}_\mathcal{R}(\boldsymbol{z})))d\boldsymbol{z} \\ &\geq \varrho \int_{\mathcal{Z}-\mathcal{R}} \Pi(\boldsymbol{z}) d\boldsymbol{z} \end{aligned} \tag{8}$$

[4]Note that in general, $\widetilde{\boldsymbol{z}}$ is not unique, and if multiple such $\widetilde{\boldsymbol{z}}$ exist, we have to sum(or perhaps integrate) $\widetilde{\Psi}$ over all such $\widetilde{\boldsymbol{z}}$

for any arbitrarily large positive real ϱ. This holds true because $\mathbb{I}_\mathcal{R}$ is identically 0 over the domain of integration. Further,

$$\begin{aligned} \int_{\mathcal{Z}-\mathcal{R}} \Pi(\boldsymbol{z}) &\geq \int_\mathcal{Z} \Pi(\boldsymbol{z}) - \int_\mathcal{R} \Pi(\boldsymbol{z}) \\ &= 1 - \int_{\mathbb{R}^m} \Pi(\boldsymbol{z})\mathbb{I}_\mathcal{R}(\boldsymbol{z}) d\boldsymbol{z} \\ &\geq 1 - \max_{\mathbb{R}^m}(\Pi(\boldsymbol{z})) \int_{\mathbb{R}^m} \mathbb{I}_\mathcal{R}(\boldsymbol{z}) d\boldsymbol{z} \\ &= 1 \end{aligned} \tag{9}$$

Combining 8 and 9, the required cross-entropy is lower bounded by an arbitrarily large quantity ϱ. □

Thus Lemma 2 contradicts R2 required for good generation when $m > n$. Therefore, to ensure good generation neither $m > n$ nor $m < n$ can be true. Thus, the only possibility is $m = n$. This concludes Theorem 1. □

One can ensure good generation, by satisfying both R1 and R2 via a trivial solution in the form of $g' = f$ with an appropriate g and making $m = n$. However, since neither n nor f is known, one needs a practical method to ensure m approaches n which is described in the next section.

4 MaskAAE (MAAE)

4.1 MODEL DESCRIPTION

Our premise in section 3.2 demands a pair of deterministic Encoder and Decoder networks satisfying R1 and R2, to ensure good quality generation. AE-models with deterministic E_κ and D_ψ networks, such as Adversarial Auto-Encoder (AAE) (Makhzani et al. (2016)) and Wasserstein Auto-Encoder (WAE) (Tolstikhin et al. (2018)) implement R1 by approximating norm-based losses and R2 through an adversarial training mechanism under metrics such as JS-Divergence or Wasserstein distance. However, most of the time, the choice of the latent dimensionality is ad hoc and there is no mechanism to get rid of the excess latent dimensions that is critical for good-quality generation as demanded by Theorem 1. Therefore, in this section, we take the ideas presented in Section 3, and propose an architectural modification on models such as AAE/WAE, such that being initialized with a large enough estimated latent space dimension the model would learn a binary-mask automatically discovering the right number of latent dimensions required.

Specifically, we propose the following modifications in the AAE-like architecture (Makhzani et al. (2016); Tolstikhin et al. (2018)), which contain an additional component called Discriminator (H_ζ) that is used to match

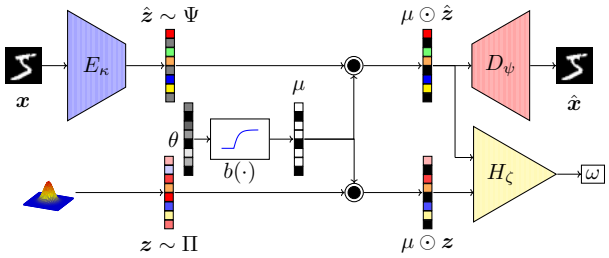


Figure 3: Block Diagram of MaskAAE. It consists of an encoder, E_κ, a decoder, D_ψ, and a discriminator H_ζ as in AAE. A new layer called mask, μ is introduced at the end of the encoder to suppress spurious latent dimensions. The prior also gets multiplied with the same mask vector before going into the Discriminator to ensure prior matching (R2).

$\Psi(\boldsymbol{z})$ and $\Pi(\boldsymbol{z})$ via adversarial learning. Our model, called the MaskAAE is detailed in figure 3.

1. We introduce a trainable mask layer, $\mu \in \{0,1\}^m$, just after the final layer of the Encoder network.

2. Before passing the encoded representation, $\hat{\boldsymbol{z}}$ of an input image $\boldsymbol{x}$ to the decoder network (D_ψ) and the Discriminator network (H_ζ) a Hadamard product is performed between $\hat{\boldsymbol{z}}$ and μ.

3. A Hadamard product is performed between the prior sample, $\boldsymbol{z} \sim \Pi(\boldsymbol{z})$ and the same mask μ as in item (1), before passing it as an input to the discriminator network H_ζ to ensure R2.

4. During inference, the prior samples are multiplied with the learned mask before giving as input to the Decoder (D_ψ) network which serves the generator.

Intuitively, masking of both the encoded latent vector and prior with a same binary mask allows us to work only with a subset of dimensions in the latent space. This means that even though m (the initial assumed latent dimensionality) may be greater than n, mask (if learned properly) reduces the encoded latent space to $\mathcal{R}^n$. This will in-turn facilitate better matching of $\Psi(\boldsymbol{z})$ and $\Pi(\boldsymbol{z})$ (R2) required for better generation.

4.2 TRAINING MaskAAE

MaskAAE is trained exactly similarly as one would train an AAE/WAE but with the addition of a loss term to train the mask layer. Here, we provide the details of the mask-loss only. For a complete description of other AAE/WAE based training loss terms refer to the supplementary.

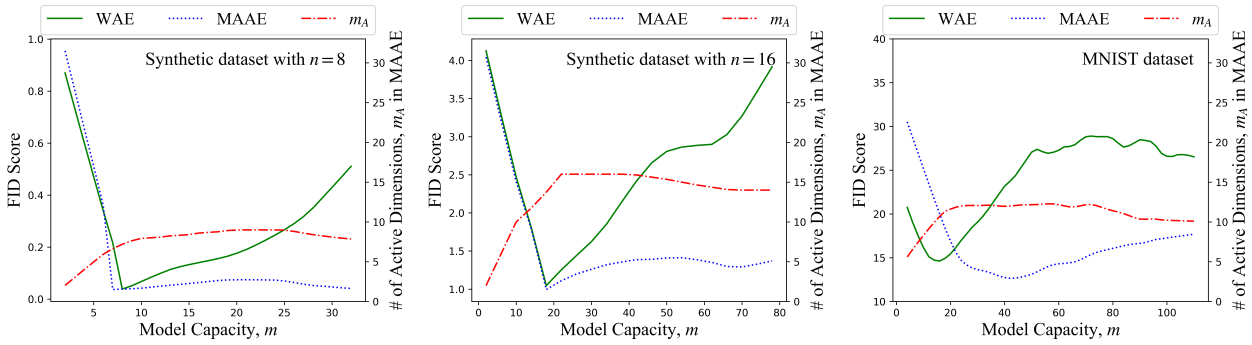
Although, the mask by definition is a binary-valued vector, to facilitate gradient flow during training, we relax it to be continuous valued while penalizing it for deviation from either 0 or 1. Specifically, we parameterize μ using a vector $\theta \in \mathbb{R}^m$ such that $\mu = b(\theta)$ where, $b(\theta) = \max(0, 1 - e^{-\theta})$. θ is initialized by drawing samples from $\mathcal{U}[0, a]$, where $a \in \mathbb{Z}^+$. Intuitively, this parameterization bounds μ in the range $[0, 1)$. Since the mask layer affects both the requirements R1 and R2, it is trained so as to minimize both the norm-based reconstruction error (first term in Eq. 10) and divergence metrics such as JS-divergence or Wasserstein's distance, between the masked prior distribution and the masked encoded latent distribution (second term in Eq. 10). Finally, a polynomial regularizer (third term in Eq. 10) is also added on μ so that any deviation from $\{0, 1\}$ is penalized. Therefore, the final objective function for the mask layer, L_{mask} consists of three terms as below.

$$L_{mask} = \frac{\lambda_1}{s} \sum_{i=1}^{s} ||\boldsymbol{x}^{(i)} - D_\psi(\mu \odot E_\kappa(\boldsymbol{x}^{(i)}))|| + \lambda_2(1+\omega)^2 + \lambda_3 \sum_{j=1}^{m} |\mu_j(\mu_j - 1)| \tag{10}$$

where, $\omega = \frac{1}{s}\sum_i H_\zeta(\mu \odot \boldsymbol{z}^{(i)}) - \frac{1}{s}\sum_i H_\zeta(\mu \odot E_\kappa(\boldsymbol{x}^{(i)}))$ is the Wasserstein's distance, s denotes batch size, and the weights $(\lambda_1, \lambda_2, \lambda_3)$ of different loss terms are hyperparameters. The training algorithm, and the architectures for E_κ , D_ψ and H_ζ are available in the supplementary.

5 EXPERIMENTS AND RESULTS

We divide our experiments into two parts: (a) Synthetic, and (b) Real. In synthetic experiments, we control the data generation process, with a known number of true latent dimensions. Hence, we can compare the performance of our proposed model for several true latent dimensions, and examine whether our method can discover the true number of latent dimensions. This also helps us validate some of the theoretical claims made in Section 3. On the other hand, the objective of the experiments with real datasets is to examine whether our masking based approach can result in a better generation quality as compared to the state-of-the-art AE-based models. We would also like to understand the behaviour of the number of dimensions which are masked in this case (though the true latent dimension may not be known). We also analysed linear and ternary search over a range on the size of the latent space as naïve alternatives. We found them to be computationally prohibitive, taking at least an order of magnitude more time compared to our approach. Refer to supplement Sec. 8 for details.



(a) (b) (c)

Figure 4: (a) and (b) shows FID score for WAE and MAAE and active dimension in a trained MAAE model with varying model capacity, m for synthetic dataset of true latent dimensions, $n = 8$ and $n = 16$, m_A represents the number of unmasked latent dimensions in the trained model and (c) shows the same plots for MNIST dataset.

5.1 SYNTHETIC EXPERIMENTS

In the following description, we will use n to denote the true latent dimension, and m to denote the assumed latent dimension (or model capacity) in line with the notation used earlier in the paper. Assuming that data is generated according to the generation process described in Section 3, we are interested in answering the following questions: (a) Given sufficient model capacity (i.e, $m \geq n$ and sufficiently powerful E_κ, D_ψ and H_ζ), can MAAE discover the true number of latent dimensions? (b) How is the quality of the data generated by MAAE for different values of m?

Ideally, we would expect that whenever $m \geq n$, MAAE masks $(m-n)$ number of dimensions. Further, we would expect that the performance of MAAE is independent of the value of m, whenever $m \geq n$. For each value of m that we experimented with, we trained an equivalent WAE model with exactly same architecture for E_κ , D_ψ and H_ζ as in MAAE without the mask layer. We would expect the performance of the WAE model to deteriorate whenever $m \neq n$ if our theory were to hold correct.

In line with our assumed data generation process, the data for our synthetic experiments is generated as below:

- Sample $\tilde{\boldsymbol{z}} \sim \mathcal{N}(\mu_s, \Sigma_s)$, where the mean $\mu_s \in \mathbb{R}^n$ was fixed to be zero and $\Sigma_s \in \mathbb{R}^{n \times n}$ represents the diagonal co-variance matrix (isotropic Gaussian).
- Compute $\boldsymbol{x} = f(\tilde{\boldsymbol{z}})$, where f is a non-linear function computed using a two-layer fully connected neural network with k units in each layer, $d >> n$ output units, and using leaky ReLU as the non-linearity (refer to the supplement for more details). The weights of these networks are randomly fixed and k was taken as 128.

We set $n = 8$ and 16, and varied m in the range of $[2, 32]$ and $[2, 78]$ with step size 2, for $n = 8$ and $n = 16$ respectively. We use the standard Fréchet Inception Distance (FID) [5] (Heusel et al. (2017)) score between generated and real images to validate the quality of the generated data, because FID has been shown to correlate well the human visual perception and also sensitive to artifacts such as mode collapse (Lucic et al. (2018); Sajjadi et al. (2018)). Figure 4 (a) and (b) presents our results on synthetic data. On X-axis, we plot m and Y-axis (left) plots the FID score comparing MAAE and WAE for different values of m. Y-axis (right) plots the number of active dimensions discovered by our algorithm. It is seen that both MAAE and WAE, achieve the best FID score when $m = n$. But whereas the performance for WAE deteriorates with increasing m, MAAE retains the optimal FID score independent of the value of m. Further, in each case, we get very close to the true number of latent dimensions, even with different values of m (as long as $m > 8$ or 16, respectively). Table 3 of the supplementary material presents the variation of log-likelihood scores for generated data with model capacity (m) for WAE and MaskAEE for synthetic dataset $(n = 16)$; this exhibits a similar behaviour. These results clearly validate our theoretical claims, and also the fact that MAAE is capable of offering good quality generation in practice.

5.2 REAL EXPERIMENTS

Next, we examine the behavior of MAAE on real-world datasets. The true latent data dimensions (n) is unknown for real datasets. However, the behaviour can still be analyzed as the estimated latent dimension (m) is varied. We experiment with the following four image datasets: (a) MNIST (Lecun (2010)) (b) Fashion MNIST (Xiao et al.

[5] We compute the Fréchet Distance between the real and the generated data directly for synthetic experiments. As synthetic data is low-dimensional, computation of Inception Net embedding is not required.

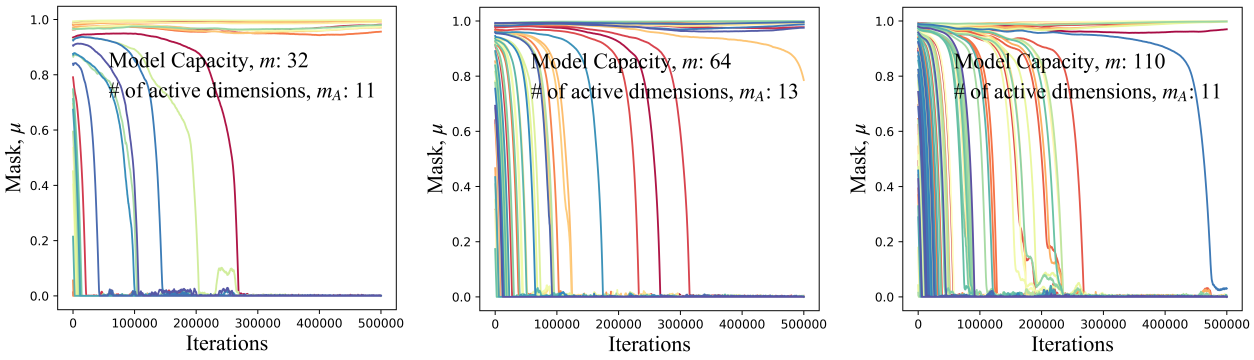


Figure 5: Behaviour of mask in MAAE with different model capacities, m for MNIST dataset. m, in figure (a), (b), and (c) are 32, 64, and 110, respectively. Dimensions active after training are m_A are 11, 13, and 11 respectively.

(a) (b) (c) (d)

Figure 6: Randomly generated images of (a) MNIST, (b) Fashion MNIST, (c) CelebA, and (d) CIFAR-10 datasets.

(2017)) (c) CIFAR-10 (Krizhevsky (2009)) (d) CelebA (Liu et al. (2015)) with standard test/train splits.

In our first set of experiments, we perform an analysis similar to the one done in the case of synthetic data, for the MNIST dataset. Specifically, we varied the estimated latent dimension (model capacity m) for MNIST from 10 to 110, and analyzed the FID score, as well as the true dimensionality as discovered by the model. For comparison, we also did the same experiment using the WAE model. Figure 4 (c) shows the results. As in the case of synthetic data, we observe a U-shape behavior for the WAE model, with the lowest value achieved at $m = 13$. This validates our thesis that the best performance is achieved at a specific value of latent dimension, which is around 13 in this case. Further, looking at MAAE curve, we notice that the performance (FID score) more or less stabilizes for $m \geq 16$. In addition, the true latent dimension discovered also stabilizes around $10 - 13$ irrespective of m, without compromising much on the generation quality. Note that the same network architecture was used at all points of Figure 4. These observations are in line with the expected behavior of MAAE, and the fact that it can indeed mask the spurious dimensions to achieve good generation quality.

Figure 5 shows the behaviour of mask for model capacity $m = 32, 64$ and 110 on MNIST dataset. Interestingly, in each case, we are able to discover almost the same number of unmasked dimensions, independent of the starting point. It is also observed that the Wasserstein distance is minimized at the point where the mask reaches the optimal point (we refer to the supplementary material for the plots).

Table 1: FID scores for generated images from different AE-based generative models (Lower is better).

	MNIST	Fashion	CIFAR-10	CelebA
VAE (cross-entr.)	16.6	43.6	106.0	53.3
VAE (fixed variance)	52.0	84.6	160.5	55.9
VAE (learned variance)	54.5	60.0	76.7	60.5
VAE + Flow	54.8	62.1	81.2	65.7
WAE-MMD	115.0	101.7	80.9	62.9
WAE-GAN	12.4	31.5	93.1	66.5
2-Stage VAE	12.6	29.3	72.9	44.4
MAAE	**10.5**	**28.4**	**71.9**	**40.5**

Finally, to measure generation quality, we present the FID scores of MAAE in Table 1 along with several state-of-the-art AE-based models mentioned in Sec. 2. Our approach achieves the best FID score on all the datasets compared to the state-of-the-art AE based generative models. Performance of MAAE is also comparable to that of GANs listed in Lucic et al. (2018), despite using a simple reconstruction loss and an isotropic unimodal Gaussian prior. Figure 6 presents 100 randomly selected MAAE-generated samples for each dataset. The better FID scores of MAAE can be attributed to better distribution matching in the latent space between $\Psi(\boldsymbol{z})$

and $\Pi(\boldsymbol{z})$. But a quantative comparison of distributional match is not straight forward as MAAE might mask out some of the latent dimensions resulting in a dimensionality mismatch among the latent space in different models, thus rendering the usual metrics unsuitable. We therefore, calculate the averaged off-diagonal normalized absolute co-variance[6] (NAC) of the encoded latent vectors and report it in Table 2 (Refer supp. for full co-variance matrix). Since $\Pi(\boldsymbol{z})$ is assumed to be an isotropic Gaussian, ideally NAC should be zero and any deviation from zero indicates a mismatch. We use only the unmasked latent dimensions of MAAE for NAC computation, to avoid underestimation by considering the unused dimension. Note that for the same model capacity, MAAE has lesser NAC than the corresponding WAE indicating better distribution matching in the latent space. These results clearly demonstrate that not only MAAE can achieve the best FID scores on various datasets, it also serves as a first step in discovering the underlying latent structure for a given dataset.

Table 2: Average off-diagonal covariance NAC for both WAE and MAAE. m_A represents the number of unmasked latent dimensions in the trained model. It is seen that MAAE has lower NAC values indicating lesser deviation of $\Psi(\boldsymbol{z})$ from $\Pi(\boldsymbol{z})$ as compared to a WAE.

Dataset	Model Capacity	WAE		MAAE	
		m_A	NAC	m_A	NAC
Synthetic_8	16	16	0.040	9	**0.030**
Synthetic_{16}	32	32	0.031	16	**0.013**
MNIST	64	64	0.027	13	**0.020**
FMNIST	128	128	0.025	40	**0.019**
CIFAR-10	256	256	0.017	120	**0.013**
CelebA	256	256	0.046	77	**0.039**

6 DISCUSSION AND CONCLUSION

Despite demonstrating its pragmatic success, we critically analyze the possible deviations of the practical cases from the presented analysis. More often than not, the naturally occurring data contains some noise superimposed onto the actual image. Thus, theoretically one can argue that this noise can be utilized to minimize the divergence between the distributions. Practically, however, this noise has a very low amplitude, so it can only work for a few extra dimensions, giving a slight overestimate of n. Further, in practice, not all latent dimensions contribute equally to the data generation. Since the objective of our model is to ignore noise dimensions, it may at times end up throwing away meaningful data dimensions which do not contribute significantly. This can lead to a slight underestimate of n (which is occasionally observed during experimentation). Finally, neural networks, however deep, can represent only a certain level of complexity in a function which is simultaneous advantageous and otherwise. It is good because while we have shown that certain losses cannot be made zero for $m \neq n$, universal approximators can bring them arbitrarily close to zero, which is practically the same thing. Due to their limitation, however, we end up getting a U-curve. It is a disadvantageous because even when $m \geq n$, the encoder and decoder networks might be unable to learn the appropriate functions, and for $m \leq n$, the Discriminator fails to make distributions apart. This implies that instead of discovering the exact same number of dimensions every time, we might get a range of values near the true latent dimension. Also, the severity of this problem is likely to increase with the complexity of the dataset (again corroborated by the experiments).

To conclude, in this work, we have taken a step towards constructing an optimal latent space for improving the generation quality of Auto-Encoder based neural generative model. We have argued that, under the assumption two-step generative process, the optimal latent space for the AE-model is one where its dimensionality matches with that of the latent space of the generative process. Further, we have proposed a practical method to arrive at this optimal dimensionality from an arbitrary point by masking the 'spurious' dimensions in AE-based generative models. Finally, we have shown the effectiveness of our method in improving the generation quality using several experiments on synthetic and real datasets.

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[6]Refer supplementary material for mathematical formula.

[7]`http://supercomputing.iitd.ac.in`

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