A moment-matching metric for latent variable generative models

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Abstract

It is difficult to assess the quality of a fitted model when facing unsupervised learning problems. Latent variable models, such as variational autoencoders and Gaussian mixture models, are often trained with likelihood-based approaches. In the scope of Goodhart's law, when a metric becomes a target it ceases to be a good metric and therefore we should not use likelihood to assess the quality of the fit of these models. The solution we propose is a new metric for model comparison or regularization that relies on moments. The key idea to study the difference between the data moments and the model moments using a matrix norm, such as the Frobenius norm. We show how to use this new metric for model comparison and then for regularization. We show that our proposed metric is faster to compute and has a smaller variance than the commonly used procedure of drawing samples from the fitted distribution. We conclude this article with a proof of concept for both applications and we discuss future work.

Keywords : Moment estimators, Latent Variable models, Gaussian Mixture Models, Variational Auto-Encoders, Frobenius norm

1 Introduction

When fitting supervised models, statisticians and computer scientists alike have come up with a variety of metrics in order to evaluate the quality of their predictions, from simple mean-squared error to general loss functions. However, in the context of unsupervised learning there is no direct measure of success and it can be difficult to assess the validity of the fitted model [12].

Assume an unsupervised learning context where we have a data set $S = \{\mathbf{x}_1, ..., \mathbf{x}_N\}$ and the abstract goal of capturing the distribution $p(\mathbf{x})$. One way to train such model is to assume a distribution and then maximize the likelihood of the data set with respect to the distribution parameters. Then the trained models are assessed and compared using the likelihood as well. Goodhart's law [10, 27] states that *when a measure becomes a target, it ceases to be a good measure* and thus we should not strictly rely on the likelihood to evaluate models that were trained using the likelihood.

In this article we propose a new way to assess the quality of the fit of a large family of unsupervised models with respect to our abstract goal of capturing the distribution $p(\mathbf{x})$. In other words, we propose a way to measure if estimated distribution $\hat{p}(x)$ resembles the observed distribution $p_S(x)$. More precisely, we offer a diagnostic technique for parametric latent variable models such as Variational AutoEncoders (VAEs) [15, 16] and Gaussian Mixture Models (GMMs). Our proposed metric evaluates the quality of the *fitted model*; we compare the learned parameters of the unsupervised model with the observed data distribution the model is trying to capture. We do so by building two distinct moment estimators. The main purpose of such metric is to provide a way to compare the fit of multiple models from different families by assessing how well these models captured the first two moments of the data. Though capturing the first and second moment of a data set is not a sufficient condition to claim the trained model has captured the data distribution it certainly is a necessary condition under some assumption we discuss later.

In statistics and machine learning, Goodhart's law is often compared with the concept of overfitting. One popular way to circumvent model overfitting has been regularization. Consequently, we offer a second perspective on our new metric; it can be used for regularization. Our metric favours simple models such as a simple Gaus-

sian distribution, thus it can be easily integrated in the optimization procedure as a regularize.

The technique we propose is fast to compute, works for a wide range of models and is built upon a rigorous mathematical formulation. It provides a new way to compare multiple models or regularize them and behaves similarly to previously used heuristic techniques.

In the next section, we establish the family of latent variable models suited for this metric. After we discuss related work in section 3, we discuss the moments estimators used in section 4. In section 5, we present our metric and its implementation and next we demonstrate how it performs on simple examples in section 6. We then introduce the framework for the application of our metric for regularization in section 7 and we demonstrate how it behaves as a regularizer in section 8. Finally, we discuss the limitations of our approach in section 9 before some concluding remarks in section 10.

2 Latent variable generative models

In this section we define the family of Latent variable generative models (LVGMs).

Assume we have a data set $S = \{\mathbf{x}_1, ..., \mathbf{x}_N\}$ consisting of N observations of a D-dimensional variable $\mathbf{x}$. Assume $\mathbf{x} \in \mathcal{X}$ which is D-dimensional. We want to estimate the distribution of the random variable $\mathbf{x}$ but it is *too complicated* to be captured by a simple distribution. Latent variable models suppose there exist an unobserved latent variable, say $\mathbf{z}$, that has a direct influence on the distribution of $\mathbf{x}$

$$p(\mathbf{x}) = \int_z p(\mathbf{x}|z)p(\mathbf{z})dz, \tag{1}$$

where we assume $\mathbf{z} \in \mathcal{Z}$ which is M-dimensional. The model proposed by equation (1) is quite general but allows relatively complex marginal distributions over observed variables $\mathbf{x}$ to be expressed in terms of more tractable conditional distributions $p(\mathbf{x}|z)$ [7]. Similarly, it leads to a tractable joint distribution as well

$$p(\mathbf{x}, \mathbf{z}) = p(\mathbf{z})p(\mathbf{x}|z), \tag{2}$$

and this is quite often represented using a simple graph as seen in Figure 1.

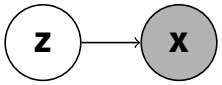


Figure 1: Graphical representation of latent variables models with joint distribution $p(\mathbf{x}, \mathbf{z}) = p(\mathbf{z})p(\mathbf{x}|z)$.

These models are *generative models* because learning $p(\mathbf{x}, \mathbf{z}) = p(\mathbf{z})p(\mathbf{x}|z)$ allows us to generate new samples of $\mathbf{x}$ using ancestral sampling. What makes this model probabilistic is that the mapping from $\mathbf{z}$ to $\mathbf{x}$ is not a deterministic function $f : \mathcal{Z} \to \mathcal{X}$ but instead a *probabilistic mapping* from $\mathcal{Z}$ to Θ, where Θ is the parameter space of $p_\theta(\mathbf{x}|z)$; $\theta \in \Theta$. We call $p_\theta(\mathbf{x}|z)$ the emission distribution or observation distribution interchangeably.

When training or fitting such models, we train the function $f : \mathcal{Z} \to \Theta$ to maximize the likelihood of the data set $\mathcal{S}$ under the model of equation (1). This mapping f explains the effect of $\mathbf{z}$ on $\mathbf{x}$ and is at the centre of latent variable models. Learning this function f is the main challenge of training latent variable models and the Expectation-Maximization algorithm (EM) or variational inference are commonly used strategies to learn this function. In most cases, $p(\mathbf{z})$ is assumed to be known and fixed but in some cases the parameters of $p(\mathbf{z})$ are estimated as well.

Usually $p_\theta(\mathbf{x}|z)$ is a simple parametric distribution and the latent variable increases the complexity of $p_\theta(\mathbf{x})$. Additionally, the function f can take many forms, from simple linear combination to neural network functions. We use $f(\mathbf{z})$ interchangeably with f or the *distribution parameters* it outputs directly.

Let us introduce a simple example. Assume the emission distribution is Poisson: $p_\theta(\mathbf{x}|z) = \text{Poisson}(\lambda)$ then $f : \mathcal{Z} \to \mathbb{R}^+$ because $\theta = \lambda \in \mathbb{R}^+$ and we use $f(\mathbf{z})$ and $\lambda(\mathbf{z})$ interchangeably. If there exist a simple mapping from the parameters of the distribution to its expectation and its variance, we also use them interchangeably. For the Poisson example, $\mathbf{E}_x[\mathbf{x}|\mathbf{z}] = \lambda(\mathbf{z})$ and $\mathbf{Var}_x[\mathbf{x}|\mathbf{z}] = \lambda(\mathbf{z})$.

One important detail to bring up is that the moments are only meaningful for a certain family of emission distributions. For the application of our metric, we will consider the family of emission distribution for which the moment generating function exists.

2.1 Probabilistic Principal Component Analysis

The Probabilistic Principal Component Analysis (pPCA) [29, 7] is a member of the LVGM family we just described where $p(\mathbf{z})$ is assumed to be a normal distribution $N(0, I)$. We also assume the emission distribution to be Normal: $p(\mathbf{x}|\mathbf{z}) = N(W\mathbf{z} + b, I\sigma^2)$. In this formulation, we see that $f : \mathbb{R}_M \to \mathbb{R}_D$ is a linear function that maps the latent variable $\mathbf{z}$ to $\mathbf{E}_x[\mathbf{x}|\mathbf{z}]$: $\mathbf{E}_x[\mathbf{x}|\mathbf{z}] = \mu(\mathbf{z}) = W\mathbf{z} + b$. Outside of estimating W and b as part of f, the model also estimates the parameter σ^2 though it is not a function of z. However it is a function of D and M, the dimension of $\mathcal{X}$ and $\mathcal{Z}$.

The parameters of pPCA can be obtained analytically as the solution of a direct maximization of the likelihood or with the EM algorithm.

2.2 Variational AutoEncoders

The VAE is also a member of the LVGM family. It is assumed that $\mathbf{z}$ is a continuous variable where $p(\mathbf{z})$ is assumed to be $N(0, I)$ in the introductory papers [15, 16]. $p(\mathbf{x}|\mathbf{z})$ can be any parametric distribution where $f(\mathbf{z})$ outputs the parameters of this distribution. For instance, if $p(\mathbf{x}|\mathbf{z})$ is normal then $f(\mathbf{z})$ will output a mean and a variance parameter, $f : \mathbb{R}_M \to \mathbb{R}_D \times \mathbb{R}^+_{(D,D)}$.

One novelty of VAEs is that the function f proposed is much more flexible than a linear combination; it is a neural network. In turn, this makes the posterior distribution $p(\mathbf{z}|\mathbf{x})$ intractable and prevents the model from being fitted by the EM algorithm. The solution proposed is to assume a variational distribution $q(\mathbf{z}|\mathbf{x})$ and optimize the likelihood by maximizing the Evidence Lower BOund (ELBO) [7, 15], a lower bound of the observed-data log-likelihood.

2.3 Gaussian Mixture Models

For a GMM with K-components we define $\mathbf{z}$ as a k-class categorical variable, $\mathbf{z} \in \{1, ..., K\} = \mathcal{Z}$, $p(\mathbf{z})$ is a categorical distribution where $\pi_j = p(\mathbf{z} = j)$, and $\sum_{j=1}^{K} \pi_j = 1$. Finally, setting $p(\mathbf{x}|z = j) = N(\mu_j, \Sigma_j)$ leads to a GMM:

$$p(\mathbf{x}) = \sum_{j=1}^{K} \pi_j p(\mathbf{x}|z = j). \tag{3}$$

In this situation, f maps the latent variable to a pair of *distribution parameters*, μ and Σ, $f : \{1, ..., K\} \to \mathbb{R}_D \times \mathbb{R}^+_{D \times D}$. In this particular case $\mathbf{E}_x[\mathbf{x}|\mathbf{z}] = f_1(\mathbf{z})$ where f_1 is the *first* output of $f(\mathbf{z})$ or simply $\mu(\mathbf{z})$ and $\mathbf{Var}_x[\mathbf{x}|\mathbf{z}] = f_2(\mathbf{z}) = \Sigma(\mathbf{z})$.

The GMM is a special case of LVGM where we also estimate the parameters $\{\pi_j : j \in 1, ...K\}$ of $p(\mathbf{z})$, identifiable up to a permutation. A GMM is usually trained with the EM algorithm.

3 Related Works

In this article, we propose a metric to evaluate the goodness-of-fit of the family of latent variable models defined in section 2 and in this section we discuss some common alternatives. When proposing new LVGMs researchers rely either on the likelihood of the data under the fitted model or a heuristic analysis of generated data points [15, 19, 14, 31, 30]. To evaluate the performance of the models, both those techniques have their fair share of problems which we discuss in this section. The metric we propose is an alternative to those techniques.

A problem with evaluating models with the likelihood is that a high likelihood does not necessarily mean that the proposed model captured the distribution of the observed data. For instance, Bishop et al. [7] demonstrate that for GMMs it is possible to have a likelihood be infinite (∞) by setting the mean of one component to be exactly one of the observed points, say $\mathbf{x}_i$, and then pushing the variance of that component to 0, thus the likelihood of $\mathbf{x}_i$ under that particular component will be infinite. Similarly, Zhao et al. [31] built a toy example where the ELBO (a lower bound of the log-likelihood) would converge to infinity.

Another commonly employed strategy is to generate new observations and try to determine if they look like real data with a simple visual inspection, this is a technique used by many authors [15, 19, 14, 16, 31, 30]. A weakness of visual inspection is that it is subjective, it incentivizes cherry-picking of results and it is not a rigorous means of comparing models.

Comparing data moments with model moments have been proposed in the past but only for training purposes [3, 4, 8, 19, 23]. Anandkumar [3, 4] proposes efficient

ways to code and optimize latent variable models by comparing the true data set with a sample generated from the model. Podosinnikova [23] approaches this topic very thoroughly in their thesis where they also discuss the use of moment-generating function estimators. What we propose here is different; we propose a metric. Even though we discuss the possibility of using our metric for optimization in later sections we believe there already exists a rich literature that discusses new ways of optimizing latent variable models but few publications that address the lack of evaluation metrics.

4 Moment estimators

In this section we define two different moment estimators for the first and the second moment. Our goal is to build different estimators that contain different information. To begin, we define moment estimators for the data set, we call those Data Estimators (DE). Then, we define another set of moment estimators that represent the distribution captured by the LVGM, we call those Forward Model Estimators (FME).

4.1 Second moment

We build two different estimators of the same quantity, the second moment. One uses observed data while the other uses the proposed generative model. What makes the proposed FME different is that we do not sample new data points from the LVGM but instead rely on a simple probability identity to build the FME.

To do so, let us introduce the well-know Law of Total Variance

$$\mathbf{Var}_x(\mathbf{x}) = \mathbf{E}_z[\mathbf{Var}_x(\mathbf{x}|\mathbf{z})] + \mathbf{Var}_z[\mathbf{E}_x(\mathbf{x}|\mathbf{z})], \tag{4}$$

and notice the second term is

$$\mathbf{Var}_z[\mathbf{E}_x(\mathbf{x}|\mathbf{z})] = \mathbf{E}_z[\mathbf{E}_x(\mathbf{x}|\mathbf{z})^2] - (\mathbf{E}_z[\mathbf{E}_x(\mathbf{x}|\mathbf{z})])^2 \tag{5}$$

$$= \mathbf{E}_z[\mathbf{E}_x(\mathbf{x}|\mathbf{z})^2] - (\mathbf{E}_x[\mathbf{x}])^2. \tag{6}$$

We combine and reorganize both equations

$$\mathbf{Var}_x(\mathbf{x}) + (\mathbf{E}_x[\mathbf{x}])^2 = \mathbf{E}_z[\mathbf{Var}_x(\mathbf{x}|\mathbf{z})] + \mathbf{E}_z[\mathbf{E}_x(\mathbf{x}|\mathbf{z})^2]. \tag{7}$$

We have reorganized both terms in this particular way because the left-hand side of equation (7) is independent of the latent variables and can be estimated from S independently from the choice of model while the right-hand side contains information about both the expectation and the variance of the generative model. Additionally, notice the left-hand side is actually $\mathbf{E}_x[\mathbf{x}^2]$, the second moment of $\mathbf{x}$ and thus our work here consists of comparing two different estimators of $\mathbf{E}_x[\mathbf{x}^2]$ which we introduce next. The left-hand side of equation (7) can be estimated using the observed data

$$\mathbf{Var}_x(\mathbf{x}) + (\mathbf{E}_x[\mathbf{x}])^2 \approx \frac{\sum_{i=1}^{n}(\mathbf{x}_i - \bar{\mathbf{x}})^T(\mathbf{x}_i - \bar{x})}{n-1} + \bar{\mathbf{x}}^T\bar{\mathbf{x}} := \text{DE}, \tag{8}$$

where $\bar{\mathbf{x}}$ is the mean vector. The right-hand side of equation (7) can be estimated using the proposed generative model through a Monte Carlo sample of $p_\theta(z)$ and using both $\mathbf{Var}_x(\mathbf{x}|\mathbf{z})$ and $\mathbf{E}_x(\mathbf{x}|\mathbf{z})$.

$$\mathbf{E}_z[\mathbf{Var}_x(\mathbf{x}|\mathbf{z}) + \mathbf{E}_x(\mathbf{x}|\mathbf{z})^2] = \int_z (\mathbf{Var}_x(X|Z=z) + \mathbf{E}_x(\mathbf{z}|\mathbf{z}=z)^2)p(z)dz \tag{9}$$

$$\approx \frac{1}{m}\sum_{i=1}^{m}\left[\mathbf{Var}_x(\mathbf{x}|\mathbf{z}=z_i) + \mathbf{E}_x(\mathbf{x}|\mathbf{z}=z_i)^T\mathbf{E}_x(\mathbf{x}|\mathbf{z}=z_i)\right] := \text{FME}, \tag{10}$$

where $z_i \sim p(\mathbf{z})$, and $\mathbf{E}_x(\mathbf{x}|\mathbf{z}=z_i)$ and $\mathbf{Var}_x(\mathbf{x}|\mathbf{z}=z_i)$ are expressed as functions of $f(z_i)$. Thus this estimator relies on both components of the fitted LVGM: $p(\mathbf{z})$ and $f(\mathbf{z})$. This is the forward model estimates (FME). Notice that this estimator does not require we sample from $p_\theta(x|z)$ and directly uses the estimated parameters of the emission distribution. It is faster to sample a large amount of z than sample a large amount of x because traditionally $M << D$. Additionally, this is a rather simple Monte Carlo sample and it is unbiased [25].

Thus it follows from equation (7) that

$$(\mathbf{Var}_x(\mathbf{x}) + (\mathbf{E}_x[\mathbf{x}])^2) - (\mathbf{E}_z[\mathbf{Var}_x(\mathbf{x}|\mathbf{z})] + \mathbf{E}_z[\mathbf{E}_x(\mathbf{x}|\mathbf{z})^2]) = 0, \tag{11}$$

and since both DE and FME are unbiased estimators of the second moment then consequently, the gap between those two estimators reflects how the LVGM captured the second moment of the data set; the bigger the gap is, the poorer the fit is. Thus, we propose to analyse the following moment estimator gap

$$\text{DE} - \text{FME}, \tag{12}$$

which is a matrix of dimension $D \times D$.

4.2 First moment

We have a similar result for the first moment

$$\mathbf{E}_x[\mathbf{x}] = \mathbf{E}_z[\mathbf{E}_x(\mathbf{x}|\mathbf{z})], \tag{13}$$

where we estimate the left-hand side with $\bar{x}$ (DE) and the right-hand side with $\frac{1}{m}\sum_{i=1}^{m}\mathbf{E}_x(\mathbf{x}|\mathbf{z} = z_i)$ where $z_i \sim p_\theta(z)$ (FME). However, to get a complete picture of the fitted LGVM proficiency at estimating the distribution of the observed-data we proposed looking at the gap between moment estimators for both the first and the second moment.

4.3 Additional justifications

For any generative model, it is always possible to generate a new sample of G points say $S_{LVGM} = \{\tilde{x_1}, ..., \tilde{x_G}\}$ and a simple model estimator for the first and second moment would be to simply compute $\frac{1}{G}\sum_{i=1}^{G}(\tilde{x_i})$ for the first moment and similarly $\frac{1}{G}\sum_{i=1}^{G}(\tilde{x_i}\tilde{x_i}^T)$, let us call those *sample estimators* (SE). These estimators could replace both FMEs defined previously as they also reflect the distribution learned by the LVGM. Conceptually, the SEs are simple and easy to use and thus we want to justify why our estimators (FMEs) are *better*.

To begin, FMEs are faster to compute by a slight margin. In order to draw the same sample size for the Monte Carlo estimates, say m sample, we need m sample for the FMEs. However, for the SEs have to draw twice as many samples ($2m$), since we must sample from $p(\mathbf{z})$ m times and then from $p(\mathbf{x}|\mathbf{z})$ an additional m times. However, more importantly, $M << D$, this means that not only we FME requires half as many samples, but they are samples from a much lower dimension distribution which further increases the difference in computational cost between the FME and the SE.

Next, our estimator has a smaller variance for both the first and the second moment. A complete proof is located in the appendices.

Finally, we proceeded with a simulation that demonstrates which estimators is closer to the true LVGM moments. For simple models, such as GMMs, we can compute analytically $\mathbf{E}_z[\mathbf{Var}_x(\mathbf{x}|\mathbf{z}) + \mathbf{E}_x(\mathbf{x}|\mathbf{z})^2]$, the LVGM second moment. We compared the gap between the true LVGM second moment and the FME to the gap between the true LVGM second moment and the SE and plot both against m the number of Monte Carlo

samples. We can see in figure 2 that the estimator we proposed (FME) is overall closer to the true LVGM second moment than the SE while being faster to compute.

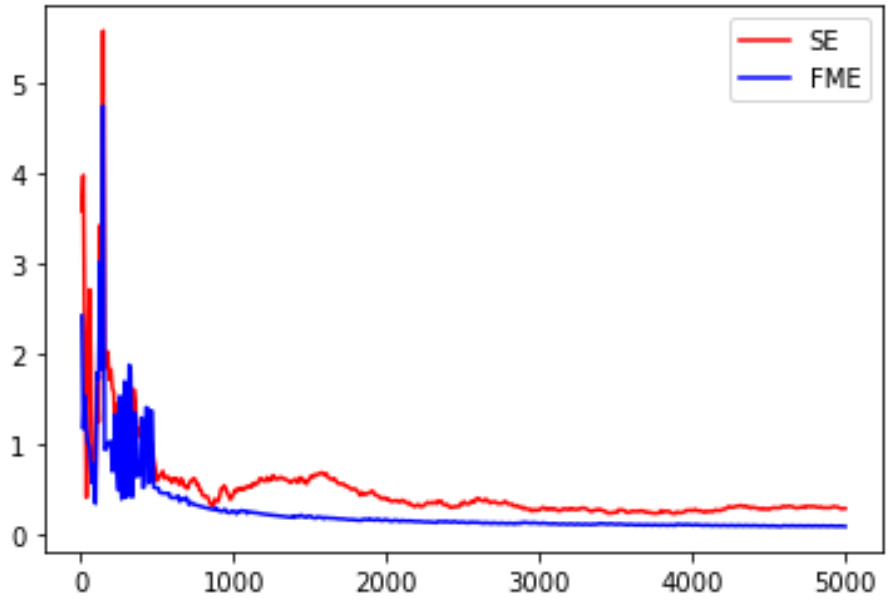


Figure 2: The evolution of both gap plotted against m. This gap is computed using the Frobenius norm as justified in section 5.

5 MEGA: a new metric for comparing models

For latent variable models as defined in section 2 we assess the ability of the model to capture the moment of the data set S by comparing the DE with the FME. Since we are looking at the difference between two different moment estimators of the same value, we named this metric the Moment Estimators Gap (MEGA). We study the difference between our two second moment estimators and we refer to this matrix as 2MEGA. Similarly, we refer to the vector representing the first moment estimator gap as 1MEGA.

5.1 Selecting a matrix norm

In order to make the MEGA tangible and comparable we propose to use a matrix norm of the MEGA as our metric. There exist a wide range of possible candidates, let us introduce a few and justify our finale choice.

We want to use a norm that looks at the global properties of the matrix and fortunately Rigollet [24] introduces and studies the behaviour of well-established matrix norms. To begin we use norms inspired by vector norms. Given the vector v, assume $|v|_q$ is the following vector norm

$$|v|_q = (\sum_i |v_i|^q)^{(1/q)}, \tag{14}$$

and given the matrix M, its matrix equivalent is $|M|_q$

$$|M|_q = (\sum_{ij} |M_{ij}|^q)^{(1/q)}. \tag{15}$$

When $q = 2$, this is a special case call the Frobenius norm

$$|M|_2 = |M|_F = (\sum_{ij} |M_{ij}|^2)^{(1/2)} = \sqrt{\text{Tr}(M^T M)}, \tag{16}$$

where Tr is the trace operator that sums the elements of the diagonal of the input matrix.

This norm is also a member of the Schatten q-norms (for $q = 2$) which is a family of matrix norms defined as the vector norm of Equation 14 for the singular values of the matrix. Since we work with second moment estimators, our matrix M is a squared matrix (dimension $m \times m$) and symmetric and thus the singular values of M are equal to its eigenvalues. We identify the vector of eigenvalues as λ. Consequently, the Schatten q-norm for matrix M is $||M||_q = |\lambda|_q$.

Another member of this family is considered, when $q = \infty$ we define $||M||_\infty = \lambda_{max} = ||M||_{op}$ and this is referred to as the operator norm.

In random matrix theory and in matrix estimation, these two norms appear frequently and are consequently well known in the statistical research community. For instance, in covariance matrix estimation it is possible, under *mild* assumptions, to bound the operator norm of the difference between the true covariance matrix and simple estimators [24]. Because of the popularity and the known properties of both the Frobenius norm and the operator norm, they are both legitimate options to measure the MEGA.

The bigger the 2MEGA is, the further away our model second moment is from the data second moment. However, one can perceive the Frobenius norm as the length

of the hypotenuse of a multidimensional triangle whose sides are given by the eigenvectors of the matrix while the operator norm is the length of the longest cathetus of the same multidimensional triangle. For that reason and for computational reasons expressed in the next section, we prefer MEGA-F and this will serve as our metric in the sections to come. In other words, the metric we propose to evaluate the quality of the fit for the second moment is

$$2\text{MEGA-F} = |2\text{MEGA}|_F = |\text{DE-FME}|_F. \tag{17}$$

Additionally, if we also consider 1MEGA, we can then again simply use the Frobenius norm (the vector q-norm with $q = 2$) on the vector 1MEGA

$$1\text{MEGA-F} = |1\text{MEGA}|_2. \tag{18}$$

5.2 Implementation of the selected norm

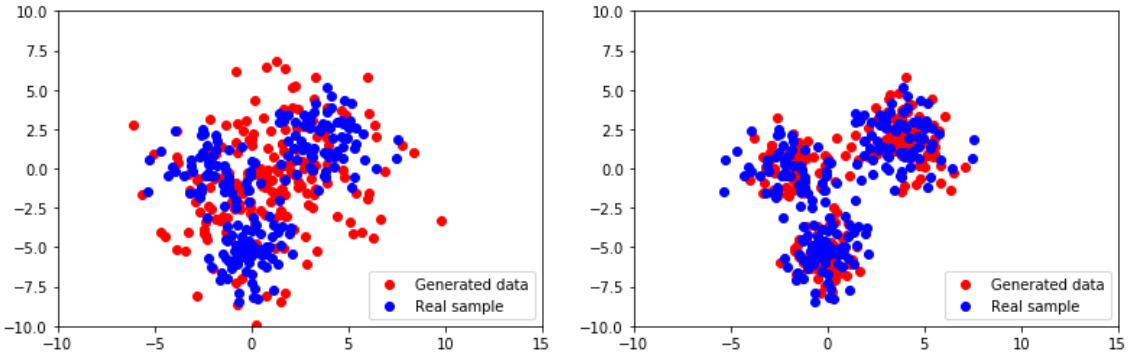
Implementing the Frobenius norm is quite straight forward. To compute to Frobenius norm, we need square of the MEGA , m^2 operations, and then sum its diagonal which results in $m^2 + m$ operations. The largest eigenvalue of a matrix can be estimated with the von Mises iteration [21], where each of the p iterations will require m^2 operations resulting in pm^2 operations in total. Consequently, because we can implement an exact computation of the Frobenius norm and because it is computationally faster (as soon as $p \geq 2$) we strictly consider the Frobenius norm for the rest of this article. However, there could be some merit to exploring the operator norm as well in future work.

We implemented the vector Frobenius norm and the matrix Frobenius norm in Python using the NumPy library [11] and using the Pytoch library [22]. We also implemented a MEGA function that takes as input a sample of $\mathbf{Var}_x(\mathbf{x}|\mathbf{z})$ and $\mathbf{E}_x(\mathbf{x}|\mathbf{z})$ alongside the data set S and returns 1MEGA-F and 2MEGA-F. These implementations are publicly available on the author's GitHub [5].

6 Experiments : comparing models

Now that we established the metric, let us use it to compare two distributions $\hat{p}(x)$ learned from two different models.

For this demonstration we use simple 2-dimensional observations. We demonstrated that large MEGAs are associated with poor fit when visualizing generated data from LVGMs. In other words, our metric is concordant with the currently used techniques but it provides more precise quantification of the mismatch.



(a) Model 1 (b) Model 2

Figure 3: Three-cluster data set

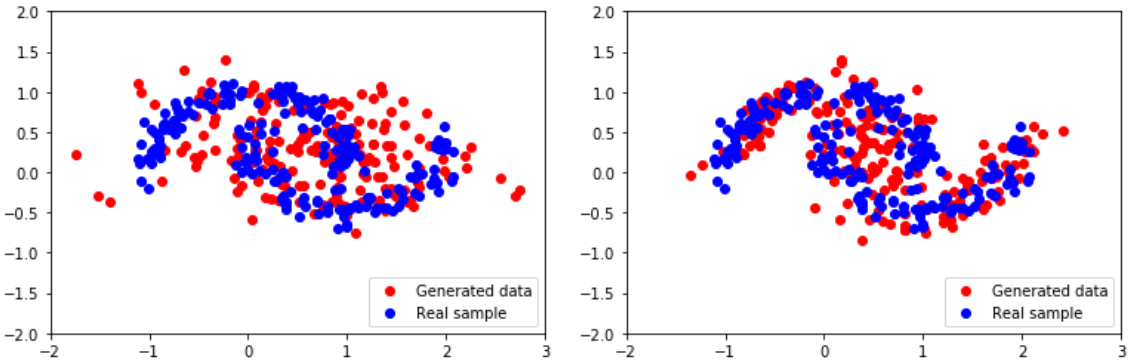
	Model 1	Model 2
1MEGA-F	0.08100187	0.02810075
2MEGA-F	1.9527672	0.320804925

Table 1: MEGA for both model when trained on the three-cluster data set.

Figure 3 contains both the training observations (in blue) and generated data points (in red) from both tested LVGM models, Model 1 and Model 2. By looking at Figure 3, Model 2 seems to have a better fit, mostly because it seems like it captures the true variance much better.

We computed 1MEGA-F and 2MEGA-F for both trained distributions, the results are containing in Table 1. The results agree with our intuitive visualisation of the situation. Though the distribution learned by fitting Model 2 has a first moment that matches better than training observations than the distribution learning by fitting Model 1, this difference is much more drastic when comparing the second moment of both trained distributions according to our metric.

We have repeated this small demonstration with a second data set as illustrate in figure 4.



(a) Model 1 (b) Model 2

Figure 4: Moon data sets

	Model 1	Model 2
1MEGA-F	0.01490262	0.00728456
2MEGA-F	0.07236395	0.00862108

Table 2: MEGA for both model when trained on the moon data set.

We observe similar results using the moon data set as illustrated in Figure 4 and table 2; the MEGA metric favours the model that visually looks better.

7 MEGA for regularization

As we previously mentioned, based on the principle of Goodhart's Law, we proposed to use the proposed metrics 1MEGA-F and 2MEGA-F to compare complex LVGMs such as IAF-VAEs [17] or NVAEs[30]. In section 3 we discussed some issues with the likelihood as an evaluation metric in some special cases. Additionally, it is unfair to use likelihood as a metric to compare two models when one is trained using a likelihood approach and the other is not.

However, if this metric has some merit when comparing model, why could we not simply included in the optimization process ? In this section we address the effect of incorporating MEGA as part of the optimization process.

Because the likelihood and the moments reflect different aspects of the distri-

bution $p(\mathbf{x})$ then incorporating MEGA as part of the optimization process for models trained by maximum likelihood acts as regularization.

This is easy to see for models with Gaussian emission distribution such as GMMs and VAEs. To simplify the explanation we will focus on the GMM case for now. When fitting a single Gaussian distribution with maximum likelihood, we set its parameters μ and σ to the data mean and the data standard error and thus a single Gaussian performs very well according to MEGAs. As we increase the number of components k in a GMM, we increase its likelihood but we also increase its MEGA. This means that we can use the MEGA as a model selection (or regularization metric) to fit GMM in place of alternatives such as AIC and BIC in order to get a model that balances likelihood and moment matching.

One way to do so is to select the model that maximizes:

$$\text{ll}(S) - \alpha(\text{1MEGA-F} + \sqrt{\text{2MEGA-F}}), \tag{19}$$

where $\text{ll}(S)$ is the log-likelihood of the data under the fitted model and α is a hyper-parameter that we manually fixed in the experiments of section 8. Basically in this particular case, the α parameters interpolated between maximum-likelihood and moment estimator. Additionally, we can draw an entire regularization path for different values of α, similar to what is produced when using Lasso [28, 26, 9].

Similarly, we can use a MEGA term in the objective function while training a VAE. Our proposed metric could again serve as regularization in order to ensure the VAE model captures those moments by maximizing:

$$\mathbf{E}_q[\ln p(\mathbf{x}|\mathbf{z})] - KL(q(\mathbf{z}|\mathbf{x})|p(\mathbf{z})) - \alpha(\text{1MEGA-F} + \sqrt{\text{2MEGA-F}}). \tag{20}$$

Arguments have been made in the past [16, 14] that the KL divergence term serves as a regularizer and that adding a β parameter can provide a way to adjust the strength of the regularization. Adding a MEGA term to the ELBO should provide a different type of regularization. The KL divergence term provides regularization for the distribution $q(\mathbf{z}|\mathbf{x})$ and the MEGA term provides regularization for $p(\mathbf{x})$:

$$\underbrace{\mathbf{E}_q[\ln p(\mathbf{x}|\mathbf{z})]}_{\text{Reconstruction error}} - \underbrace{\beta KL(q(\mathbf{z}|\mathbf{x})|p(\mathbf{z}))}_{\text{Regularization for } q(\mathbf{z}|\mathbf{x})} - \underbrace{\alpha(\text{1MEGA-F} + \sqrt{\text{2MEGA-F}})}_{\text{Regularization for } p(\mathbf{x})}. \tag{21}$$

As previously demonstrated [6], tunning a VAE to obtain both good reconstruction and generative performances is difficult. For instance, when using the β-VAE [14, 13] we can make the hyper-parameter β arbitrary small and obtain close to perfect reconstruction but this leads to poor generative performance due to the distribution $q(z)$ used for training being widely different from $p(z)$ used for generation. The additional term we add to the VAE objective function should help with generative perspective of VAEs.

Thus, to understand the benefits of integrating this additional term to the objective function we have to understand how different it is from the first term. The first term measure the reconstruction error because the likelihood $p(x|z)$ is computed on latent variable z sampled from $q(z|x)$. In contrast, the MEGA penalty term evaluate the first and second moment of $p(x)$ independently from $q(z|x)$ but rather based on the generative model where $p(x) = \int_z p(\mathbf{X}|z)p(\mathbf{Z})dz$. We believe this additional constraint in the objective function should lead to samples that matches the true distribution of $p(x)$ more closely.

8 Experiments: regularization

As discussed in section 7 another way to integrate such metric in a workflow is to regularize LVGMs with Gaussian observation distributions. In the following experiments, we explore the use of our proposed metric as a regularizer for GMMs and VAEs.

8.1 Regularizer for GMMs

For GMMs, increasing the number of components increases the likelihood and thus it is necessary to regularize this model; we cannot simply select the ideal number of components based on the likelihood alone. We have generated a simple data set from a 3-component GMM. Figure 5 is a scatter of the simulated data, by looking at the figure we would like the model selection procedure to settle on three components.

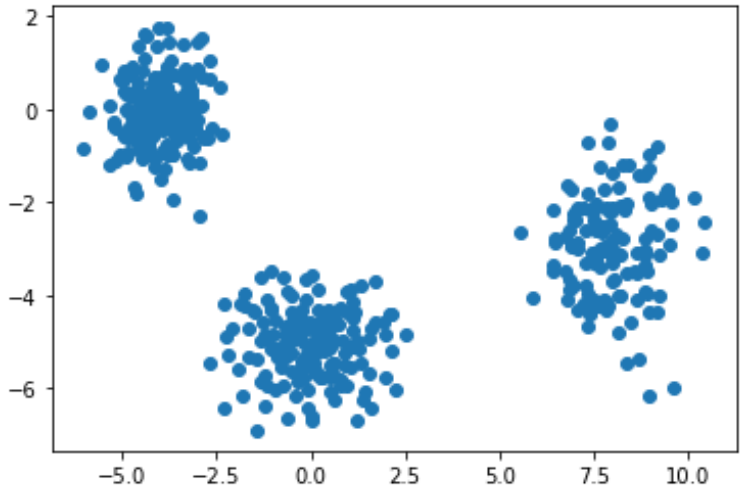


Figure 5: Scatter plot of the simulated data set.

The Akaike Information Criteria (AIC) [2, 1] is a well-establish penalized likelihood function that can be used to select the number of components in a GMM. The AIC can be expressed as

$$\text{AIC} = 2p - 2\ln(L), \tag{22}$$

where L is the likelihood of the model, and p is the number of parameters ($p = 2k$ in the GMM case). In equation 22 we see a natural tradeoff; $-2\ln(L)$ goes down as we increase the number of components but $2p$ goes up. To select the right GMM model, we can fit multiple GMM with various number of components and we select the model that minimizes the AIC.

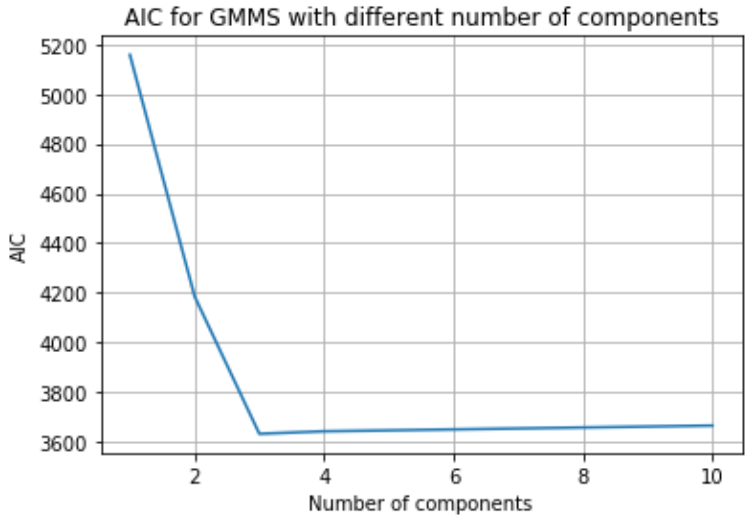


Figure 6: AIC plotted against the number of components for trained GMM models (lower is better).

Based on Figure 6, the AIC is minimized at $k = 3$ which is concordant the model used to generate the data.

Next, we use our MEGA-penalized likelihood function described in equation 19 to select the number of components.

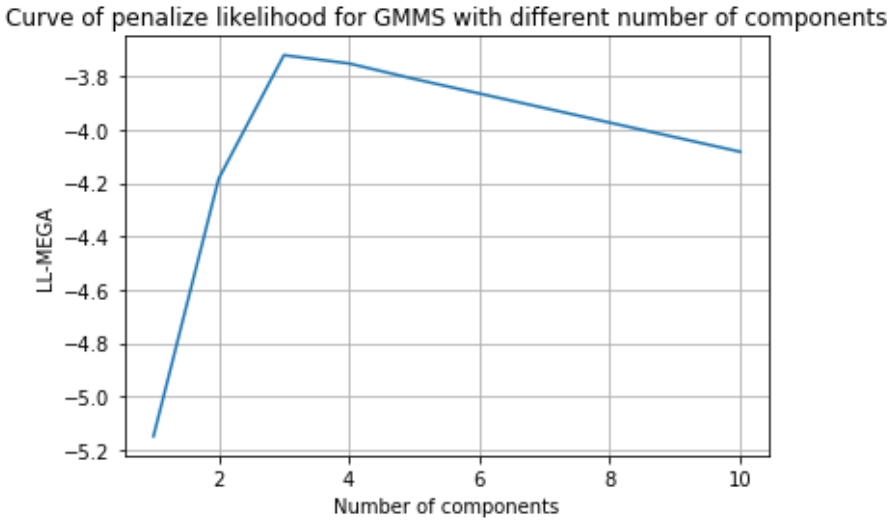


Figure 7: MEGA-penalized likelihood plotted against the number of components for trained GMM models (higher is better)

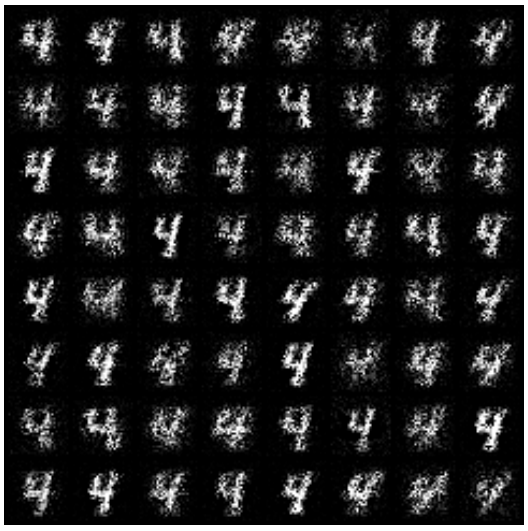
As observed above, when using our proposed metric for GMM regularization we also obtain a function that favours 3 components, which is concordant with both the model used to generate the data and the AIC. However, in this instance the flexibility given by the hyper-parameter α is both a benefit and a drawback. Using the hyper-parameter, we can easily adjust how strong we want the penalty to be but on the flip side there are no automated ways to adjust it. As previously mentioned, we can build a regularization path for different values of α leading to a sequence of possible models from which the user can select one.

8.2 Regularizer for VAEs

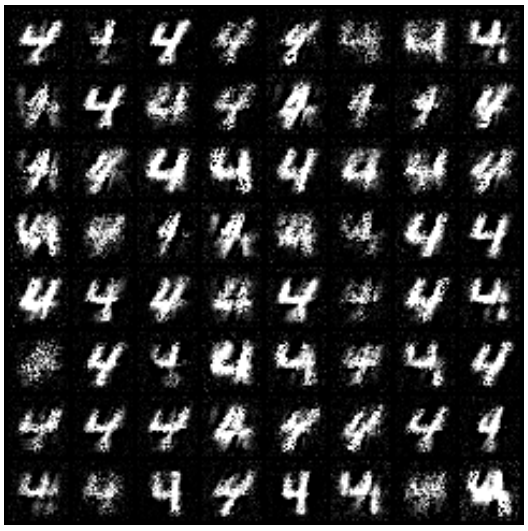
Finally we experiment with using MEGA as a regularization for VAEs. Now that we used MEGA as part of the objective function we can no longer use it to assess the quality of the samples so we are forced to visually inspect samples and their parameters.

We run this demonstration on a subset of the MNIST data set [18] that contains only the digit four. We have experimented with a wide range of parameters α and β, as defined in equation 21 and fixed the hyper-parameters to the values leading to the more realistic-looking images.

Figures 8,9 and 10 illustrate our results. The images on in the left column were produced by a VAE trained without MEGA and the right one with MEGA. We have included images of a sample, its mean and its standard deviation.



(a) Model train without MEGA



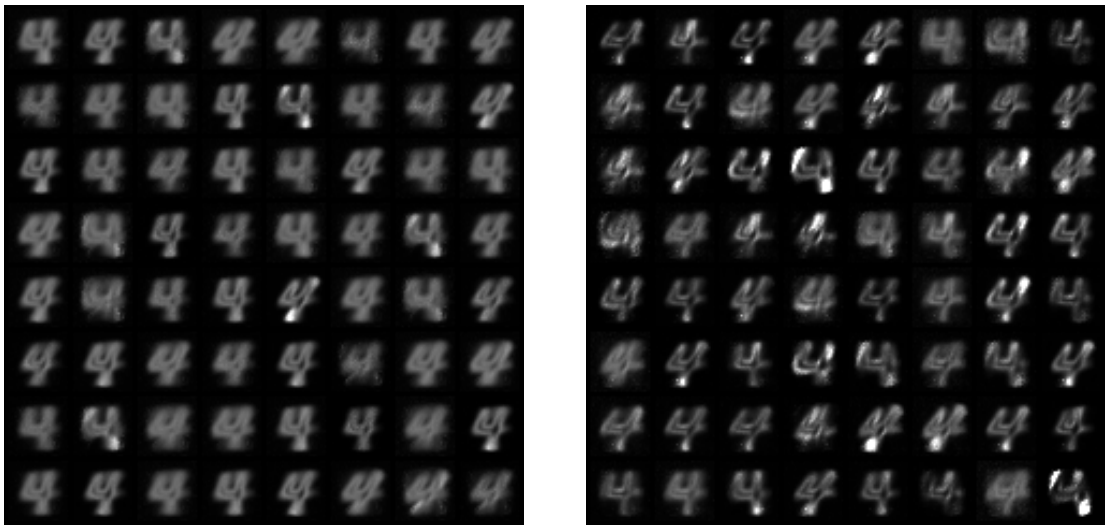
(b) Model train with MEGA

Figure 8: A sample of 64 images from $p_\theta(\mathbf{X}\|\mathbf{Z}) = N(\mu(\mathbf{Z}), \sigma(\mathbf{Z}))$ where $\mathbf{Z} \sim N(0, 1)$.

(a) Model train without MEGA

(b) Model train with MEGA

Figure 9: The 64 sampled mean of the images: $\mu(\mathbf{Z})$ where $\mathbf{Z} \sim N(0, 1)$.



(a) Model train without MEGA

(b) Model train with MEGA

Figure 10: The 64 sampled standard deviation for each pixel of the images: $\sigma(\mathbf{z})$ where $\mathbf{z} \sim N(0, 1)$. For those images, the whiter the pixel is the larger the standard deviation of that pixel is.

The samples are still grainy, and this is due to the pixel-independence assumption of the simple VAE which only learns individual pixel variance and not a full-covariance matrix. However, the images generated by a VAE trained with the MEGA penalty seems to have sharper edges; the contrast between the white of the digit and the black of the exterior is bigger. This is noticeable in all three figures but mostly in figure 10. It seems like the MEGA penalty changes rather drastically $\sigma(\mathbf{z})$, the variance of the observed distribution. Both the exterior of the digit and the inner part of the digit are darker than the model trained without MEGA. The model trained with MEGA perceives the contour and extremities of the digit as the location with higher variability which is not as prevalent for the model trained without MEGA.

We also notice a bigger variability in the shapes of fours that we are able to generate, mostly visible in figures 8 and 9. The lack of variability in the left column is most likely caused by posterior collapse [20, 6], a common problem when using β-VAEs that the MEGA penalty seems to counteract.

9 Discussion

As a comparative metric, MEGA is fast to compute and easy to interpret. The larger 1MEGA is, the larger is the gap between the first moment of trained distribution $p(x)$ and the empirical first moment of the data set S. Similarly, the larger 2MEGA is, the larger the gap is for the second moment. This can give us a quick and easy to compare and evaluate the quality of fitted models.

However, there are still some limitations to this approach. The most obvious is that the formulation we propose only allow us to quickly evaluate the gap for the first two moments. This leads to an incomplete comparison of the learned and empirical distribution which can create some problems in niche cases. A example of this problem is the high performance of the simple Gaussian distribution. Usually, when fitting a Gaussian distribution to a data set we set the parameters μ and σ to be the empirical mean and the empirical, thus the Gaussian mixture with a single component shows very good results (low MEGA).

Fortunately, we have designed this metric for complex latent variable model and there are no reasons to use it when assessing the fit of a single Gaussian. Additionally, other comparative strategies discussed in section 3 can still be used in parallel of our proposed one.

We also want to point out that if a trained distribution has low MEGA but bad-looking generated samples this still provides us with insightful information. It indicates that the problem is in the LVGM distribution's higher moments and our metric was able to provide us with that information very quickly.

For regularization applications, we were able to successfully used MEGA with two different LVGMs, GMMs and VAEs. Though in both these cases we managed to achieve good results, selecting the appropriate constraint using the hyper-parameters was not an easy task and had to be done heuristically. This is certainly a weakness that should be addressed in future work.

Let us now discuss some of ongoing work. We are currently working on a generalization of MEGA. We want to extend our metric not only to higher moments of $\mathbf{x}$ but to any functions $g(\mathbf{x})$. This would not only allow us to compare the skewness of the

trained model compared to the data but also more complicated properties of distributions such as multimodality. This generalized MEGA would provide a more complete evaluation of models than the currently proposed metric.

Because we believe our theoretical arguments to be quite solid, the experiments above are a quick showcase of possible applications of the MEGA metric, they serve as a proof of concept rather than exhaustive tests. However, some components of our experiments were done heuristically and more thorough test should be done to broaden our understanding of the possible applications of our metric.

10 Conclusion

In this article we have introduced a fairly simple, easy and computationally fast way to check the generative model's distribution of a large class of LVGMs. This metric, MEGA, evaluates the gap between the LVGM distribution first and second moment and the training (or validation) data set first and second moment.

The premise of the proposed metric is theoretically simple and quite intuitive. Both the DE and the FME are unbiased estimators of both the first and the second moment and if a gap exists between them then the LVGM distribution does not match key aspects of the data distribution.

To support our theoretical arguments, we have demonstrated how to use this metric for two different purposes. First, as an evaluation metric that can replace the more heuristics approaches that rely on eyeballing generated samples. Second, since this metric is currently available for the first two moments, it favours a simple model, such a single Gaussian, and thus can be used as regularization for models such as GMMs and VAEs.

However, we believe we have only scratched the surface of all of the applications and ways to incorporate these moment-gap-based metrics in model fitting and model selection pipelines. We hope to make further progress in this direction in future work. Another future work direction is to extend these moment gap estimators to sequential LVGMs, such as Hidden Markov Models and State-Space Models. Finally, the biggest improvement we could work on is to extend the moment estimators to higher moments; this would make the evaluation metrics much more valuable.

Nonetheless, we believe this work is a first step in data-driven automated model selection and we hope it inspires similar contributions.

Ackowledgement

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Appendices

Proof that the FME has small variance than the SE

First moment

For the SE, we first sample $z_1, ...z_m$, a set of m latent variables where $z \sim p(\mathbf{z})$ then sample $x_1, ..., x_m$ with $x_i \sim p(\mathbf{x}|\mathbf{z}_i)$; this implies that $x \sim p(\mathbf{x}|\mathbf{z})p(\mathbf{z}) = p(\mathbf{x})$. Then, the SE for the first moment is $\frac{1}{m}\sum_{i=1}^{m}\mathbf{x}_i$.

$$\mathbf{Var}_x(\text{SE}) = \mathbf{Var}_x\left(\frac{\sum_{i=1}^{m} x_i}{m}\right) = \frac{1}{m^2}\sum_{i=1}^{m}\mathbf{Var}_x(x_i) = \frac{\mathbf{Var}_x(\mathbf{x})}{m}. \tag{23}$$

When building our FME, we sample $z_1, ...z_m$, a set of m latent variables where $z \sim p(\mathbf{z})$ and then compute $\frac{1}{m}\sum_{i=1}^{m}\mathbf{E}_x(\mathbf{x}|\mathbf{z} = z_i)$.

$$\mathbf{Var}_z(\text{FME}) = \mathbf{Var}_z\left(\frac{\sum_{i=1}^{m}\mathbf{E}_x(\mathbf{x}|z_i)}{m}\right) = \frac{1}{m^2}\sum_{i=1}^{m}\mathbf{Var}_z(\mathbf{E}_x(\mathbf{x}|z_i)) = \frac{\mathbf{Var}_z[\mathbf{E}_x(\mathbf{x}|z_i)]}{m}. \tag{24}$$

Then using the Law of Total Variance we have that:

$$
\begin{aligned}
\mathbf{Var}_x(\mathbf{x}) &= \mathbf{E}_z[\mathbf{Var}_x(\mathbf{x}|\mathbf{z})] + \mathbf{Var}_z[\mathbf{E}_x(\mathbf{x}|\mathbf{z})] \\
&\geq \mathbf{Var}_z[\mathbf{E}_x(\mathbf{x}|\mathbf{z})] \\
\Rightarrow \frac{\mathbf{Var}_x(\mathbf{x})}{m} &\geq \frac{\mathbf{Var}_z[\mathbf{E}_x(\mathbf{x}|z_i)]}{m} \\
\Rightarrow \mathbf{Var}(\text{SE}) &\geq \mathbf{Var}(\text{FME}),
\end{aligned} \tag{25}
$$

and thus our FME has lower variance than the commonly used alternative.

Second moment

For the SE, we first sample $z_1, \ldots z_m$, a set of m latent variables where $z \sim p(\mathbf{z})$ then sample $x_1, \ldots, x_m$ with $x_i \sim p(\mathbf{x}|\mathbf{z}_i)$; this implies that $x \sim p(\mathbf{x}|\mathbf{z})p(\mathbf{z}) = p(\mathbf{x})$. Then, the SE for the second moment is $\frac{1}{m}\sum_{i=1}^{m}\mathbf{x}_i^2$.

$$
\mathbf{Var}_x(\text{SE}) = \mathbf{Var}_x\left(\frac{\sum_{i=1}^{m} x_i^2}{m}\right) = \frac{\mathbf{Var}_x(\mathbf{x}^2)}{m}. \tag{26}
$$

When building our FME, we sample $z_1, \ldots z_m$, a set of m latent variables where $z \sim p(\mathbf{z})$ and then compute $\frac{1}{m}\sum_{i=1}^{m}\left(\mathbf{Var}_x(\mathbf{x}|\mathbf{z}=z_i) + [\mathbf{E}_x(\mathbf{x}|\mathbf{z}=z_i)]^2\right)$.

$$
\begin{aligned}
\mathbf{Var}_z(\text{FME}) &= \mathbf{Var}_z\left(\frac{\sum_{i=1}^{m}\left(\mathbf{Var}_x(\mathbf{x}|\mathbf{z}=z_i) + [\mathbf{E}_x(\mathbf{x}|\mathbf{z}=z_i)]^2\right)}{m}\right) \\
&= \frac{\mathbf{Var}_z\left(\mathbf{Var}_x(\mathbf{x}|\mathbf{z}=z_i) + [\mathbf{E}_x(\mathbf{x}|\mathbf{z}=z_i)]^2\right)}{m}.
\end{aligned} \tag{27}
$$

Now let's take a closer look at the numerator of equation (27).

$$
\begin{aligned}
\mathbf{Var}_z\left(\mathbf{Var}_x(\mathbf{x}|\mathbf{z}=z_i) + [\mathbf{E}_x(\mathbf{x}|\mathbf{z}=z_i)]^2\right) &= \mathbf{Var}_z\left(\mathbf{E}_x[\mathbf{x}^2|\mathbf{z}] - \mathbf{E}_x[\mathbf{x}|\mathbf{z}]^2 + \mathbf{E}_x[\mathbf{x}|\mathbf{z}]^2\right) \\
&= \mathbf{Var}_z\left(\mathbf{E}_x[\mathbf{x}^2|\mathbf{z}] - \mathbf{E}_x[\mathbf{x}|\mathbf{z}]^2 + \mathbf{E}_x[\mathbf{x}|\mathbf{z}]^2\right) \\
&= \mathbf{Var}_z\left(\mathbf{E}_x[\mathbf{x}^2|\mathbf{z}]\right) \\
&= \mathbf{E}_z\left(\mathbf{E}_x[\mathbf{x}^2|\mathbf{z}]^2\right) - \mathbf{E}_z\left(\mathbf{E}_x[\mathbf{x}^2|\mathbf{z}]\right)^2 \\
&= \mathbf{E}_z\left(\mathbf{E}_x[\mathbf{x}^2|\mathbf{z}]^2\right) - \mathbf{E}_x\left(\mathbf{x}^2\right)^2 \\
\Rightarrow \mathbf{Var}(\text{FEM}) &= \frac{\mathbf{E}_z\left(\mathbf{E}_x[\mathbf{x}^2|\mathbf{z}]^2\right) - \mathbf{E}_x\left(\mathbf{x}^2\right)^2}{m}
\end{aligned} \tag{28}
$$

Finally, let us apply the Law of Total Variance to $\mathbf{x}^2$:

$$\begin{aligned}
\mathbf{Var}_x(\mathbf{x}^2) &= \mathbf{E}_z(\mathbf{Var}_x[\mathbf{x}^2|\mathbf{z}]) + \mathbf{Var}_z(\mathbf{E}_x[\mathbf{x}^2|\mathbf{z}]) \\
&= \mathbf{E}_z(\mathbf{Var}_x[\mathbf{x}^2|\mathbf{z}]) + \mathbf{E}_z\left(\mathbf{E}_x[\mathbf{x}^2|\mathbf{z}]^2\right) - \mathbf{E}_z(\mathbf{E}_x[\mathbf{x}^2|\mathbf{z}])^2 \\
&= \mathbf{E}_z(\mathbf{Var}_x[\mathbf{x}^2|\mathbf{z}]) + \mathbf{E}_z\left(\mathbf{E}_x[\mathbf{x}^2|\mathbf{z}]^2\right) - \mathbf{E}_x[\mathbf{x}^2]^2 \qquad (29) \\
\Rightarrow \mathbf{Var}_x(\mathbf{x}^2) &\geq \mathbf{E}_z\left(\mathbf{E}_x[\mathbf{x}^2|\mathbf{z}]^2\right) - \mathbf{E}_x[\mathbf{x}^2]^2 \\
\Rightarrow \frac{\mathbf{Var}_x(\mathbf{x}^2)}{m} &\geq \frac{\mathbf{E}_z\left(\mathbf{E}_x[\mathbf{x}^2|\mathbf{z}]^2\right) - \mathbf{E}_x[\mathbf{x}^2]^2}{m} \\
\Rightarrow \mathbf{Var}(\text{SE}) &\geq \mathbf{Var}(\text{FME})
\end{aligned}$$

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