Machine Learning and Differential Equations

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Abstract

In this report we will discuss the theory required to understand variational auto-encoders and generative latent time-series models. Variational auto-encoders are a probabilistic approach of auto-encoders that aims to overcome the irregularities that appears in the latent space. This probabilistic approach allows for generation of new data, and we demonstrate this ability by producing unseen handwritten digits. We then look at generative latent time-series models, which is an adaptation of variational auto-encoders, that aims to extrapolate time-series data by introducing a time-dependence to the latent variable.

Contents

1 Introduction

In this report, we will discuss the theory required to understand variational autoencoders [2] and generative latent time-series models [3], and explore their applications in tackling the following problems:

1. Generation of new data: Suppose that we are given the dataset, $\boldsymbol{\mathcal{D}}$ which contains N independent data points. Then we aim to artificially generate data points that look like they came from the dataset $\boldsymbol{\mathcal{D}}$.

2. Extrapolation of time-series data: Suppose that we observe a system at discrete times $t_0, \ldots, t_N$. Then, given these observations, we would like to predict the system's state at the future times $t_{N+1}, \ldots, t_M$.

These problems are very appealing to tackle, as we can train a model on sensitive medical data and produce new data without effecting the privacy of the patient. Whilst, extrapolation of time-series data can be used for forecasting ECG data to predict heart attacks.

To understand the theory required for variational autoencoders and generative latent time-series models, we will split the report into four main parts:

1. Background Theory

2. Variational Autoencoders

3. Neural Ordinary Differential Equations

4. Generative Latent Time-series Models

In the first part, we introduce the statistical and machine learning theory necessary to understanding variational autoencoders and generative latent time-series models. Whilst in the second part, we will introduce variational autoencoders, and demonstrate how they can be used to generate new data by producing unseen handwritten digits. Following that, we introduced neural ordinary differential equations, which we will use as a black-box approach for learning the forcing function of an ordinary differential equation. Finally, we will use the theory of variational autoencoders and neural ordinary differential equations, to define generative latent time-series models and show how they can be used to extrapolate time-series data.

2 Statistics

Whilst this report will not focus heavily on the statistical side of machine learning, it is important that we recap some key statistical theory as it will provide motivation and deepen our understanding to what we discuss later.

2.1 Marginal Likelihood

In this section we will introduce some important machinery that will help us quantify how "good" a model is at approximating the observed distribution of our data. This is extremely useful as having a model that describes the distribution of our data can help us understand underlying mechanisms at play.

We first start by framing the general problem that we would like to solve. Suppose that we have the dataset $\boldsymbol{X} = (\boldsymbol{x}^{(i)})_{i=1}^{N}$ with $\boldsymbol{x}^{(i)} \in \mathbb{R}^n$. Then given a parametric distribution, $p_\theta(\cdot)$, we want to find the parameter $\boldsymbol{\theta}^*$ such that the distribution $p_{\boldsymbol{\theta}^*}(\cdot)$, closely approximates the observed distribution of the data $\boldsymbol{X}$. This idea is demonstrated in Figure. 1, where by changing the value of $\boldsymbol{\theta}$ for the parametric distribution, $p_{\boldsymbol{\theta}}(\cdot) = \mathcal{N}(\boldsymbol{\theta}, 0.1)$, changes how well its PDF approximates the observed distribution of the data.

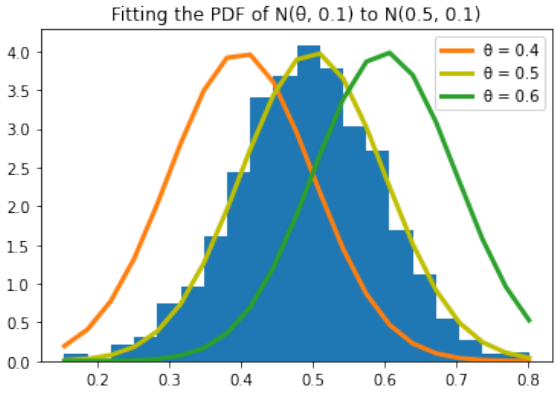


Figure 1: Fitting the PDF of $\mathcal{N}(\boldsymbol{\theta}, 0.1)$ to 1000 samples of $\mathcal{N}(0.5, 0.1)$ with different values of $\boldsymbol{\theta}$ (i.e $\boldsymbol{\theta} = 0.4, 0.5, 0.6$). [4]

As alluded to above with with the above, we define how "good" a parametric distribution is at approximating the distribution of our data, by how likely it is to observe our data given our parametric distribution.

Definition 2.1 (Likelihood function [5])**.** Given a sample $\boldsymbol{x}^{(i)}$ from the data set $\boldsymbol{X}$, and a parametric distribution $p_{\boldsymbol{\theta}}(\cdot)$, then likelihood function $\hat{L}$ is defined as,

$$\hat{L}(\boldsymbol{\theta}, \boldsymbol{x}^{(i)}) = p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) \tag{1}$$

Therefore, given the sample $\boldsymbol{x}^{(i)}$, the likelihood function, $\hat{L}(\boldsymbol{\theta}, \boldsymbol{x}^{(i)})$, tells us how likely we would be to obtain that sample given the model parameter $\boldsymbol{\theta}$.

Moreover, by assuming that our dataset $\boldsymbol{X}$ is made up of N independent and identically distributed random variables, we define the joint likelihood function as the following,

$$\hat{L}(\boldsymbol{\theta}, \boldsymbol{X}) = \prod_{i=1}^{N} p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) \tag{2}$$

Now that we have the machinery to measure how likely it is to observe our data given the model parameter $\boldsymbol{\theta}$. We want to find the value of $\boldsymbol{\theta}$ that maximises the likelihood of observing our data.

Definition 2.2. (Maximum likelihood estimator [5]) Given the data set $\boldsymbol{X}$, and the parametric distribution $p_{\boldsymbol{\theta}}(\cdot)$, then the maximum likelihood estimate (MLE) is a value of $\boldsymbol{\theta}$ that maximises the likelihood function $\hat{L}(\boldsymbol{\theta}, \boldsymbol{X})$.

$$\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta}}{\operatorname{argmax}}\, \hat{L}(\boldsymbol{\theta}, \boldsymbol{X}) = \underset{\theta}{\operatorname{argmax}} \prod_{i=1}^{N} p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})$$

Up to now we are have only dealt with models that are fully-observed as we are able to compute the maximum likelihood estimator directly from our data. Now we suppose that our model depends on variables which we can not observe, and which are therefore not explicitly represented in the dataset. These variables are what we refer to as latent variables, and which we will denote by $\boldsymbol{z}$. Hence, to compute the likelihood as a function of $\boldsymbol{\theta}$ over our observed data, we define the marginal likelihood.

Definition 2.3. (Marginal likelihood)

Given the joint parametric probability distribution $p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z})$ over the observed and latent variables, we define the marginal likelihood as the following,

$$p_{\boldsymbol{\theta}}(\boldsymbol{x}) = \int_{\Omega_{\boldsymbol{z}}} p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z}) d\boldsymbol{z}$$

Where $\Omega_{\boldsymbol{z}}$ is the domain of the latent variable $\boldsymbol{z}$.

Remark. By using Bayes' Rule, we can express the marginal likelihood in terms the distributions, $p_{\boldsymbol{\theta}}(\boldsymbol{z})$ and $p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})$.

$$p_{\boldsymbol{\theta}}(\boldsymbol{x}) = \int_{\Omega_{\boldsymbol{z}}} p_{\boldsymbol{\theta}}(\boldsymbol{z}) p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z}) d\boldsymbol{z}$$

Hence, the marginal likelihood can thought as "getting rid of what is unknown". Thus, given $p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z})$, in principle we can work out maximum likelihood estimator $\boldsymbol{\theta}^*$, as $p_{\boldsymbol{\theta}}(\boldsymbol{x})$ only contains variables which are observed. We will see later in Section 4.2.3 that the integral in Definition 2.3 is intractable. Hence, we can not find the maximum likelihood parameter $\boldsymbol{\theta}^*$ directly. Therefore, we require some clever tricks to overcome this limitation.

2.2 Kullback–Leibler Divergence

We will now define the Kullback–Leibler Divergence, which measures how well the probability distribution p approximates the probability distribution q. This will be an important tool we will use in Section 4.2.4, as we are unable to observe a distribution directly. Therefore will use a parametric distribution to approximation the unobserved distribution, and hence we aim to minimise differences between them.

Definition 2.4 (Kullback–Leibler Divergence)**.** Let p and q be two probability distributions densities, then the Kullback–Leibler Divergence D_{KL} is defined by,

$$D_{\mathrm{KL}}(p||q) = \int_{\Omega_{\boldsymbol{x}}} p(x) \log\left(\frac{p(x)}{q(x)}\right) dx \tag{3}$$

Remark. By Gibbs' inequality (Appendix 1), $D_{\mathrm{KL}} \geq 0$ and we have equality iff $p \equiv q$.

2.2.1 Important Example

To illustrate this definition, we will compute the KL divergence of two Gaussians. This calculation will be important in Section 4.2.4, as we need to know the negative Kullback–Leibler Divergence between the two multivariate Gaussian distributions, $q_{\boldsymbol{\theta}}(\cdot) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\sigma}^2\boldsymbol{I})$ and, $p(\cdot) = \mathcal{N}(\mathbf{0}, \boldsymbol{I})$, where $\boldsymbol{\mu}, \boldsymbol{\sigma}^2, \mathbf{0} \in \mathbb{R}^m$ and $\boldsymbol{I}$ is the m by m identity matrix.

To achieve this we firstly compute the two integrals,

$$\begin{aligned}\int q_{\boldsymbol{\theta}}(\boldsymbol{z}) \log p(\boldsymbol{z}) d\boldsymbol{z} &= \int \mathcal{N}(\boldsymbol{z}; \boldsymbol{\mu}, \boldsymbol{\sigma}^2\boldsymbol{I}) \log \mathcal{N}(\boldsymbol{z}; \mathbf{0}, \boldsymbol{I}) d\boldsymbol{z} \\ &= -\frac{m}{2}\log(2\pi) - \frac{1}{2}\sum_{j=1}^{m}(\boldsymbol{\mu}_j^2 + \boldsymbol{\sigma}_j^2)\end{aligned}$$

and,

$$\begin{aligned}\int q_{\boldsymbol{\theta}}(\boldsymbol{z}) \log q_{\boldsymbol{\theta}}(\boldsymbol{z}) d\boldsymbol{z} &= \int \mathcal{N}(\boldsymbol{z}; \boldsymbol{\mu}, \boldsymbol{\sigma}^2\boldsymbol{I}) \log \mathcal{N}(\boldsymbol{z}; \boldsymbol{\mu}, \boldsymbol{\sigma}^2\boldsymbol{I}) d\boldsymbol{z} \\ &= -\frac{m}{2}\log(2\pi) - \frac{1}{2}\sum_{j=1}^{m}(1 + \log \boldsymbol{\sigma}_j^2)\end{aligned}$$

Therefore, by combining these results and get the following,

$$\begin{aligned}-D_{\mathrm{KL}}(q_{\boldsymbol{\phi}}(\cdot)|||p_{\boldsymbol{\theta}}(\cdot)) &= -\int q_{\boldsymbol{\phi}}(\boldsymbol{z}) \log\left(\frac{q_{\boldsymbol{\phi}}(\boldsymbol{z})}{p_{\boldsymbol{\theta}}(\boldsymbol{z})}\right) d\boldsymbol{z} \\ &= \int q_{\boldsymbol{\phi}}(\boldsymbol{z})(\log p_{\boldsymbol{\theta}}(\boldsymbol{z}) - \log q_{\boldsymbol{\phi}}(\boldsymbol{z})) d\boldsymbol{z} \\ &= \frac{1}{2}\sum_{j=1}^{m}(1 + \log(\boldsymbol{\sigma}_j^2) - \boldsymbol{\mu}_j^2 - \boldsymbol{\sigma}_j^2)\end{aligned}$$

3 Machine Learning Basics

Throughout this section we will introduce the basics of machine learning and explain how they can be used to solve modelling and prediction problems. We will start by stating some terminology that we will use throughout this section. Suppose that we were given the sets $\boldsymbol{X} = \{\boldsymbol{x}^{(i)}\}_{i=1}^{N}$ and $\boldsymbol{Y} = \{\boldsymbol{y}^{(i)}\}_{i=1}^{N}$, and we want to predict $\boldsymbol{y}^{(i)}$ given $\boldsymbol{x}^{(i)}$, then we term $\boldsymbol{X}$ our dataset and $\boldsymbol{Y}$ our observations.

3.1 Parametric models

As we described in the previous chapter, a parametric model is any model that is parameterised. These parameters are quantity that we can control and are used to describe what "features we can tune" in our model. This ability allows us to produce different model dynamics that we can use to find the parameters that best predicts our observations.

It is important to note that we have left the definition of a parametric model very open and loosely defined. This is on purpose as throughout this paper a parametric model may take a form of probability distributions, neural networks or functions.

3.2 Loss Function

A loss function is a way of describing how well our parametric model performs on given data point and is defined as the following,

$$L(\cdot, \cdot) : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$$

Where the inputs of the loss function is our parametric model, $p_{\boldsymbol{\theta}}$ evaluated at the data point $\boldsymbol{x}^{(i)} \in \boldsymbol{X}$ and the corresponding observation, $\boldsymbol{y}^{(i)} \in \boldsymbol{Y}$ (i.e $L(p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}), \boldsymbol{y}^{(i)})$). Therefore, if our parametric model closely predicts observation $\boldsymbol{y}^{(i)}$ given the data point $\boldsymbol{x}^{(i)}$, $L(p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}), \boldsymbol{y}^{(i)})$ will be small.

To demonstrate this point, suppose that our data came from the function, $f(x) = 2x + 1$, and our parametric model $f_{\boldsymbol{\theta}}(x) = \theta_0 + \theta_1 x + \theta_2 x^2$, takes the form $f_{\boldsymbol{\theta}}(x) = 2x + 4$. By choosing the loss function to be the squared error between the true observation and our parametric model prediction (i.e $L(f(x), f_{\boldsymbol{\theta}}) = ||f(x) - f_{\boldsymbol{\theta}}(x)||^2$), we see that our loss function is 9 given a data point, $x \in \mathbb{R}$.

As we alluded to above, suppose that our dataset consists of multiply data points, $\boldsymbol{X} = \{\boldsymbol{x}^{(i)}\}_{i=1}^{N}$ and $\boldsymbol{Y} = \{\boldsymbol{y}^{(i)}\}_{i=1}^{N}$, respectively. We define the total loss of our model given $\boldsymbol{X}$ and $\boldsymbol{Y}$, as the following,

$$E(\boldsymbol{\theta}) = \sum_{i=1}^{N} L(\boldsymbol{y}^{(i)}, p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})) \tag{4}$$

Where $p_{\boldsymbol{\theta}}$ is a parametric model, parameterized by $\boldsymbol{\theta}$. This quantity allows us to understand how our model performs on the total data set, as our model might model well certain observations and poorly on others.

3.3 Gradient Descent

Now that we have the total loss function $E(\boldsymbol{\theta})$, for the parametric model $p_{\boldsymbol{\theta}}$, we want to find the value of $\boldsymbol{\theta}$ that minimises $E(\boldsymbol{\theta})$ (i.e $\theta^* = \text{argmin}_{\boldsymbol{\theta}} E(\boldsymbol{\theta})$). We do this by introducing an iterative approach to find the local mimima of $E(\boldsymbol{\theta})$, as solving for $\partial E(\boldsymbol{\theta})/\partial \boldsymbol{\theta} = \mathbf{0}$ for θ is too computationally complex. We start by initialising the parameter $\boldsymbol{\theta}_0$ to a random values and follow the procedure,

$$\begin{aligned} \boldsymbol{v}_n &= \eta_n \nabla_{\boldsymbol{\theta}} E(\boldsymbol{\theta}) \\ \boldsymbol{\theta}_{n+1} &= \boldsymbol{\theta}_n - \boldsymbol{v}_n \end{aligned}$$

Where $\nabla_{\boldsymbol{\theta}} E(\boldsymbol{\theta})$ is the derivative of $E(\boldsymbol{\theta})$ with respect to $\boldsymbol{\theta}$ and η_n is the learning rate at step n. The learning rate η_n, describes how big of a step in the direction $-\nabla_{\boldsymbol{\theta}} E(\boldsymbol{\theta})$ that we will take. We take steps in the direction of $-\nabla_{\boldsymbol{\theta}} E(\boldsymbol{\theta})$ as $\nabla_{\boldsymbol{\theta}} E(\boldsymbol{\theta})$ gives us the direction of maximal increase of $E(\boldsymbol{\theta})$; Therefore by going in inverse direction, we will go towards the minimum of $E(\boldsymbol{\theta})$. It is important that we get the value of η_n correct, as if it is too small the algorithm will take too long and if we take too big of a step it will over shoot the minimum. This effect is demonstrated in Figure. 2, as choosing different values of the learning rate can cause various effects when finding the minima. This procedure is normally terminated when the values $\boldsymbol{\theta}_{n+1}$ and $\boldsymbol{\theta}_n$ differ within a tolerance that we choose (i.e $||\boldsymbol{\theta}_{n+1} - \boldsymbol{\theta}_n||^2 < \varepsilon$ with $\varepsilon \ll 1$).

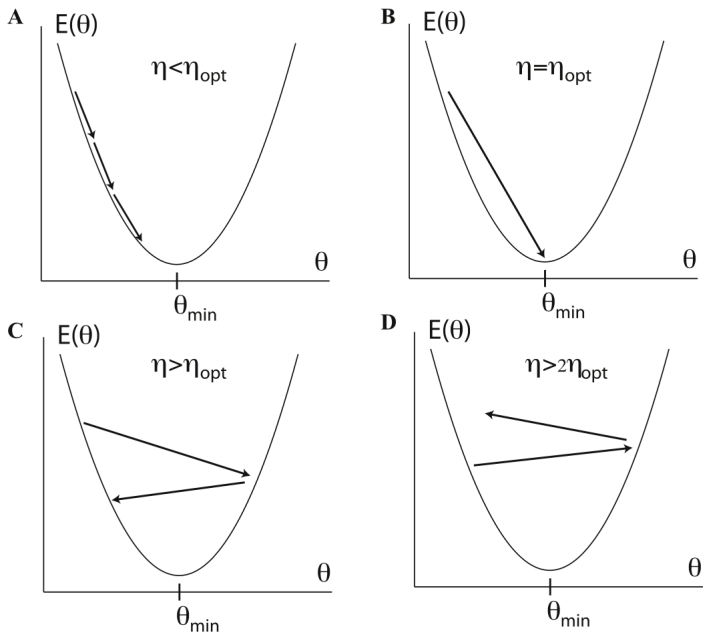


Figure 2: Effect of learning rate on convergence. For a one dimensional quadratic potential, one can show that there exists four different qualitative behaviours for gradient descent (GD) as a function of the learning rate η depending on the relationship between η and $\eta_{\text{opt}} = [\partial^2_{\boldsymbol{\theta}} E(\boldsymbol{\theta})]^{-1}$. (a) For $\eta < \eta_{\text{opt}}$, GD converges to the minimum. (b) For $\eta = \eta_{\text{opt}}$, GD converges in a single step. (c) For $\eta_{\text{opt}} < \eta < 2\eta_{\text{opt}}$, GD oscillates around the minima and eventually converges. (d) For $\eta > 2\eta_{\text{opt}}$, GD moves away from the minima. ([6], p.15)

3.4 Training

Up to now we have only dealt with fitting a model to a given data set. However one of the main advantages of modelling data comes from its ability to model data that we have not seen before. To ensure that our model preforms well at modelling new data, we split our data into two sets, $\boldsymbol{X}_{\text{train}}$ and $\boldsymbol{X}_{\text{test}}$, with corresponding $\boldsymbol{Y}_{\text{train}}$ and $\boldsymbol{Y}_{\text{test}}$ respectively. This splitting allows us to train our model using $\boldsymbol{X}_{\text{train}}$ and $\boldsymbol{Y}_{\text{train}}$ then test the performance of our model on data that it has has not seen before (i.e $\boldsymbol{X}_{\text{test}}$ and $\boldsymbol{Y}_{\text{test}}$). We measure this performance by defining the in-sample error $E_{\text{in}} = E(\boldsymbol{\theta}|\boldsymbol{X}_{\text{train}}, \boldsymbol{Y}_{\text{train}})$ and out-of-sample error $E_{\text{out}} = E(\boldsymbol{\theta}|\boldsymbol{X}_{\text{test}}, \boldsymbol{Y}_{\text{test}})$. Therefore, if the difference between the in-sample error E_{in}, is much smaller than out-of-sample error E_{out}, we know that we over-fitted our model, as it performs poorly at modelling new data.

The out-of-sample error E_{out}, will naturally decrease as the number of data points increase. This is due to there being less sampling noise that appears in the data, and our model tending to its true distribution. As the model tends to its true distribution, the in-sample and out-of-sample error must therefore converge to the same value. This is termed the "bias" of our model. The bias tells us how good of a model we have if we had infinite data points. However, since in practical applications we only have a finite amount of data points, it is better to minimise the out-of-sample error E_{out} rather than the bias, (as we are unable to measure it) as this will lead to a model has better predicting abilities. This is due to the fact that the difference between E_{in} and E_{out} is the same as fitting and predicting new data.

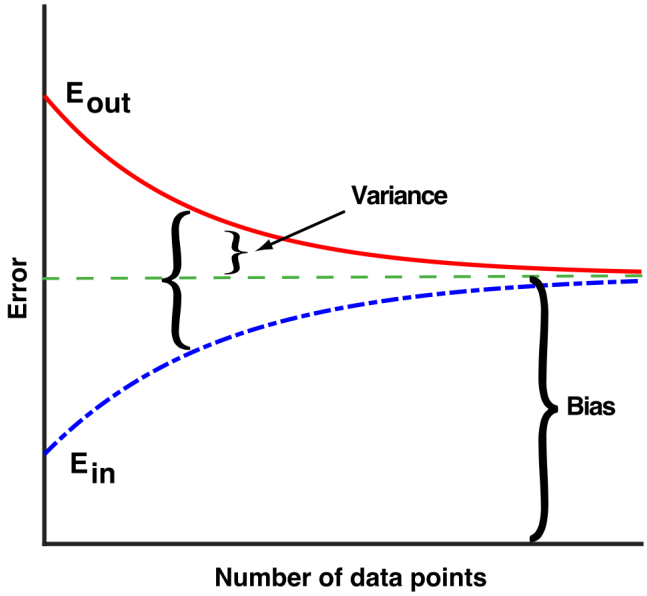


Figure 3: Schematic of typical in-sample and out-of-sample error as a function of training set size. The typical in-sample or training error, E_{in}, out-of-sample or generalisation error, E_{out}, bias, variance, and difference of errors as a function of the number of training data points. ([6], p.11)

Figure. 4, shows that the out-of-sample error E_{out} is a function of "model complexity". Where model complexity describes how many parameters the model has. This supports the idea of over-fitting that we discussed above. As we expect increas-

ing the number of parameters in our model we over-fit our model to the training data and hence, perform poorly at predicting new data. This is due to there being a finite amount of data points, even though increasing the model complexity will lead to a smaller bias due to a smaller in-sample error. Therefore it is a more favourable to choose a model with smaller variance than a less-biased model with large variance.

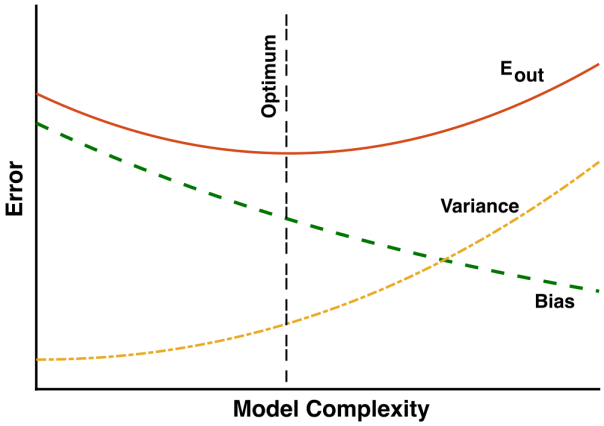


Figure 4: Bias–Variance tradeoff and model complexity. This schematic shows the typical out-of-sample error E_{out} as function of the model complexity for a training dataset of fixed size. ([6], p.12)

3.5 Stochastic Gradient Descent

Another way that we might control over-fitting is the use of epochs and batches when doing gradient descent. Epochs are the number of times that we use the whole training data $\boldsymbol{X}_{\text{train}}$ and $\boldsymbol{Y}_{\text{train}}$ in training. Whilst batches randomly splits up the training data $\boldsymbol{X}_{\text{train}}$ into smaller training data sets that we minimise the total cost over. This idea allows us to make more evenly space jumps and hence not over-fit out data.

To demonstrate this idea suppose we we have a training data set consisting of 100 data points, and apply five epochs of batch sizes 25. Therefore we use the total data set five times, and each round of epoch contrasting of four evaluations of the training algorithm on the data set,

$$E^i_{\text{in}} = E(\boldsymbol{\theta}|\boldsymbol{X}^i_{\text{train}}, \boldsymbol{Y}^i_{\text{train}}), \quad \boldsymbol{X}^i_{\text{train}} = \sum_{j=25i+1}^{25(i+1)} \boldsymbol{x}^{(j)}, \quad \boldsymbol{Y}^i_{\text{train}} = \sum_{j=25i+1}^{25(i+1)} \boldsymbol{y}^{(j)}, \quad i \in \{0,1,2,3\}$$

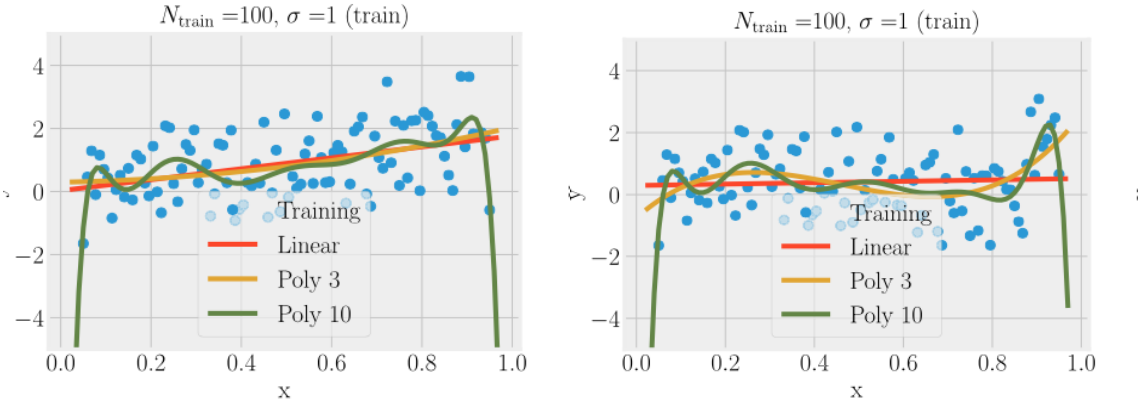
3.6 Theory Example

We will now combine the theory that we have introduced into a small example to demonstrate how each part plays a key role of solving a one-dimensional modelling problem. Suppose that our data was generated by drawing samples from the equation

$$y^{(i)} = f(x^{(i)}) + \eta^{(i)}$$

Where $f(\cdot)$ is some fixed function $f : \mathbb{R} \to \mathbb{R}$ and $\eta^{(i)}$ is some Guassian noise (i.e $\eta^{(i)} \sim \mathcal{N}(0, \sigma^2)$). Then we will try to model our data $y^{(i)}$ by using the parametric functions, which are polynomials of order one, three and, 10 denoted $f_{\boldsymbol{\theta}_1}, f_{\boldsymbol{\theta}_3}$, and $f_{\boldsymbol{\theta}_{10}}$, respectively. Where each parametric function tries to learn the value of $\boldsymbol{\theta}_i$ that best fits $f_{\boldsymbol{\theta}_i}$ to our data. Finally we choose the squared error loss function to measure this difference and minimise over,

$$\begin{aligned}
\boldsymbol{\theta}_i^* &= \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, E(\boldsymbol{\theta}_i) \\
&= \underset{\boldsymbol{\theta}}{\operatorname{argmin}} \sum_{i=1}^{N} L(y^{(i)}, f_{\boldsymbol{\theta}_i}(x^{(i)})) \\
&= \underset{\boldsymbol{\theta}}{\operatorname{argmin}} \sum_{i=1}^{N} ||y^{(i)} - f_{\boldsymbol{\theta}_i}(x^{(i)})||^2
\end{aligned}$$



(a) (b)

Figure 5: Fitting the tree parametric function to 100 noisy data points ($\sigma = 1$) in the range $x \in [0, 1]$ that were generated from a the functions (a) $f(x) = 2x$ and (b) $f(x) = 2x - 10x^5 + 15x^{10}$. ([6], p.8)

3.7 Neural Networks Architecture

Deep neural networks consist of layers highly interconnected nodes, where the output of a layer is the input of the next. This architecture forms a very dense network that is defined as the following,

$$\boldsymbol{a}^l = \boldsymbol{\sigma}(\boldsymbol{W}^l \boldsymbol{a}^{l-1} + \boldsymbol{b}^l) =: \boldsymbol{\sigma}(\boldsymbol{z}^l), \qquad l \in \{1, \dots, L\}, \qquad L \in \mathbb{N} \tag{5}$$

$$n_l \in \mathbb{N}, \qquad \boldsymbol{a}^l \in \mathbb{R}^{n_l}, \qquad l \in \{0, \dots, L\} \tag{6}$$

$$\boldsymbol{W}^l \in \mathbb{R}^{n_l \times n_{l-1}}, \qquad \boldsymbol{b}^l \in \mathbb{R}^{n_l}, \qquad l \in \{1, \dots, L\} \tag{7}$$

Where l is referred to as the layer of our network and we refer to $\boldsymbol{a}^l$ as an activation layer. This is because this quantity represents how much "activation" each neuron/node gets when it is fed into the next layer. $\boldsymbol{W}^l$ is the weight matrix, as it represents how much weight each neuron of the previous activation layer has on the

next layer (i.e by the matrix-multiplication $\boldsymbol{W}^l\boldsymbol{a}^{l-1}$). $\boldsymbol{b}^l$ is the bias (or bias vector) as it shifts the each value of $\boldsymbol{W}^l\boldsymbol{a}^{l-1}$ either to the left (upwards) or right (downwards). Finally, $\boldsymbol{\sigma}(\cdot)$ is refereed to as the activation function, as it outputs how much "activation" is carried on to the next layer. Since, $\boldsymbol{W}^l$ and $\boldsymbol{b}^l$ are not explicitly defined, a neural network can be thought of as a parametric model, parameterised by $\boldsymbol{W}^l$ and $\boldsymbol{b}^l$. Therefore we are apply all the theory we have just introduced to them. This is not the only way we can define neural networks, as they can come in many of forms such as, Recurrent Neural Networks [7], which tries to learn the temporal natural of our data and Convolutional Neural Networks [8] which can be used for imaging classification.

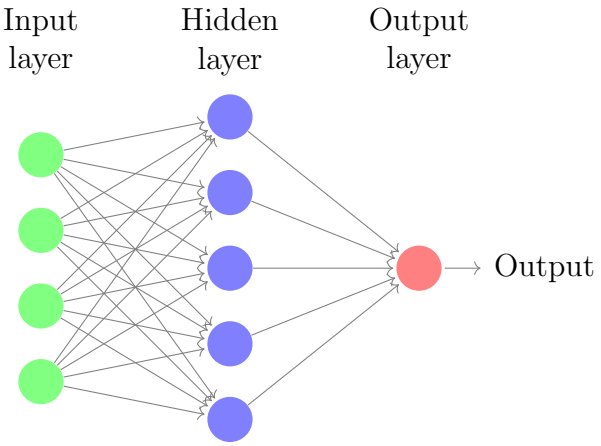


Figure 6: A deep neural network with an input dimension of 4 ($n_0 = 4$) , a hidden state of dimension of 5 ($n_1 = 5$), and an output dimension of 1 ($n_2 = 1$).

3.8 Backpropagation Algorithm

The backpropagation algorithm for a deep neural network allows us take gradients with respect to the weights and biases to find the minima of the loss function, C (as a neural network can be thought of as a parametric distribution). Since the loss function depends on the output layer of our neural network, we define the error at the j-th neuron of the output layer, as the following,

$$\boldsymbol{\Delta}_j^L = \frac{\partial C}{\partial \boldsymbol{z}_j^L} \tag{8}$$

Where L denotes the output layer of our neural network, defined in (5). Moreover, as the error of our output indirectly depends on the previous layers of our network, we can generalise (8), to get the error at the j-th neuron on the l-th layer, $\boldsymbol{\Delta}_j^l$, as the change in the loss function with respect to $\boldsymbol{z}_j^l$.

$$\boldsymbol{\Delta}_j^l = \frac{\partial C}{\partial \boldsymbol{z}_j^l} = \frac{\partial C}{\partial \boldsymbol{a}_j^l}\frac{\partial \boldsymbol{a}_j^l}{\partial \boldsymbol{z}_j^l} = \frac{\partial C}{\partial \boldsymbol{a}_j^l}\boldsymbol{\sigma}'(\boldsymbol{z}_j^l) \tag{9}$$

Where $\boldsymbol{\sigma}'(\boldsymbol{z}_j^l)$ is the derivative of the activation function $\boldsymbol{\sigma}(\cdot)$, evaluated at $\boldsymbol{z}_j^l$, where it is important to note that the dimension of the activation function's derivative may change per layer.

By noting that $\partial \boldsymbol{b}_j^l / \partial \boldsymbol{z}_j^l = \mathbf{1}$, we are able to express the loss function with respect to the bias $\boldsymbol{b}_j^l$ as $\boldsymbol{\Delta}_j^l$,

$$\frac{\partial C}{\partial \boldsymbol{b}_j^l} = \frac{\partial C}{\partial \boldsymbol{b}_j^l}\frac{\partial \boldsymbol{b}_j^l}{\partial \boldsymbol{z}_j^l} = \frac{\partial C}{\partial \boldsymbol{z}_j^l} = \boldsymbol{\Delta}_j^l \tag{10}$$

Hence by using the chain rule again, we are able to express the error at the l-th layer in terms of the $l+1$-th layer. This is because error can be thought of as being carried forward through the neural network.

$$\boldsymbol{\Delta}_j^l = \frac{\partial C}{\partial \boldsymbol{z}_j^l} = \sum_k \frac{\partial C}{\partial \boldsymbol{z}_k^{l+1}}\frac{\partial \boldsymbol{z}_k^{l+1}}{\partial \boldsymbol{z}_j^l} \tag{11}$$

$$= \sum_k \boldsymbol{\Delta}_l^{k+1}\frac{\partial \boldsymbol{z}_k^{l+1}}{\partial \boldsymbol{z}_j^l} = \left(\sum_k \boldsymbol{\Delta}_k^{l+1}\boldsymbol{W}_{kj}^{l+1}\right)\boldsymbol{\sigma}(\boldsymbol{z}_j^l) \tag{12}$$

Finally, we derive the derivative of the loss function with respect to the weight $\boldsymbol{W}_{jk}^l$,

$$\frac{\partial C}{\partial \boldsymbol{W}_{jk}^l} = \frac{\partial C}{\partial \boldsymbol{z}_j^l}\frac{\partial \boldsymbol{z}_j^l}{\partial \boldsymbol{W}_{jk}^l} = \boldsymbol{\Delta}_j^l \boldsymbol{a}_k^{l-1} \tag{13}$$

Algorithm 1 Backpropagation algorithm ([6] p.55)

1. **Feedforward**: Start with the first layer, exploit the feed-forward architecture through (5) to compute $\boldsymbol{z}^l$ and $\boldsymbol{a}^l$ for each subsequent layer.
2. **Error at output layer**: Calculate the error of the output layer using (9).
3. **"Backpropagate" the error**: We now use (12) to propagate the error backwards and calculate $\boldsymbol{\Delta}_j^l$ for all the layers.
4. **Calculate gradient**: Now use (10) and (13) to calculate $\frac{\partial C}{\partial \boldsymbol{b}_j^l}$ and $\frac{\partial C}{\partial \boldsymbol{W}_{jk}^l}$.

3.9 Generative Modelling

Generative modelling is a way that we can produce new data. It does this by learning the joint probability $p(\boldsymbol{X}, \boldsymbol{Y})$ or just $p(\boldsymbol{X})$ if there are no observations $\boldsymbol{Y}$ given. Therefore by sampling from its learned distribution, we are also producing samples which would of likely came from our test data $\boldsymbol{X}$.

4 Variational Autoencoders

4.1 Autoencoder

Before we understand variational autoencoders (VAEs), we firstly must understand their primitive cousin, autoencoders. Autoencoders encapsulate the idea that data can be expressed by a small number of key features, whilst the rest is noise. For example, if you were to communicate the key ideas of a face to someone, the main features would be the position and shape of the eyes, mouth, and nose, whilst the rest of the details like facial hair and piercings are noise.

This feature selection process is expressed formally by performing dimensional reduction to the input data. This can be done in various ways and we will refer to this action as the Encoder. We will also term the output of the Encoder the feature/latent space, as it expresses the key features that make up our input data. The autoencoder then projects the output of the Encoder back to the space containing the data, and we will refer to this operation as the Decoder. As we have assumed that our data can be represented by a small number of features, the aim is to minimise the difference between our input and reconstructed data. We will use the squared error loss function to quantify how accurate our autoencoder is at reconstructing the input data. To summarise, we have the following model,

$$\text{(Encoder)}\ \ \phi_{\mathrm{E}} : \mathbb{R}^n \to \mathbb{R}^m, \quad \text{(Decoder)}\ \ \phi_{\mathrm{D}} : \mathbb{R}^m \to \mathbb{R}^n, \quad m \ll n,\ \ m, n \in \mathbb{N}$$

$$\text{(L2 loss function)}\ \ L = ||\boldsymbol{x} - \hat{\boldsymbol{x}}||^2 = ||\boldsymbol{x} - \phi_{\mathrm{D}}(\phi_{\mathrm{E}}(\boldsymbol{x}))||^2$$

As we alluded to earlier, both the Encoder and Decoder can take many forms with the simplest case being linear maps. However in this paper we will only look at them being neural networks. Therefore, the autoencoder can be thought of as a single neural network, as it is just a combination of two smaller neural networks sequentially. By ensuring that $m \ll n$, our architecture creates a bottleneck for the data, allowing the key features to be used for the reconstruction. Hence, by performing gradient descent, we are able to find the parameters that minimise the loss function for our data.

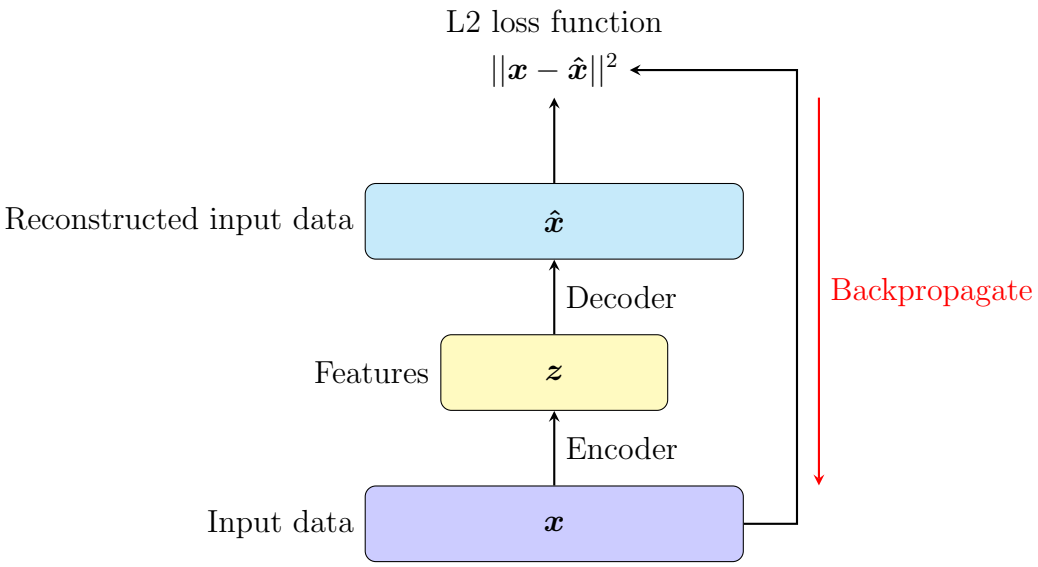


Figure 7: Training model for an autoencoder

However, this approach leads to the limitation that two points close in the feature space, may not necessary correspond to two similar points in data space. This renders the autoencoder model useless for generative modelling, as we want points that are close in feature space to be mapped to points close in data space because we expect them to have "similar qualities".

4.2 Variational Autoencoders

4.2.1 Motivation

Variational autoencoders are a probabilistic approach of autoencoders that aims to overcome the irregularity that appears between the feature and data space in autoencoders. This is achieved by mapping our input data to a distribution over the feature space rather than to a single point, we then sample from a decoder distribution to get our reconstructed input data. This procedure allows us to introduce regularisation at the time of training to prevent overfitting and ensures that our feature spaces has good properties for generative modelling.

Putting together the model described above, the variational autoencoder evaluated at the point $\boldsymbol{x}$ takes the form:

1. Our input data $\boldsymbol{x}$ is encoded as a distribution $p_{\boldsymbol{\theta}}(\cdot|\boldsymbol{x})$ in feature space.
2. We then sample the point $\boldsymbol{z}$ from the distribution $p_{\boldsymbol{\theta}}(\cdot|\boldsymbol{x})$.
3. Then $\boldsymbol{z}$ is decoded into the distribution $p_{\boldsymbol{\theta}}(\cdot|\boldsymbol{z})$.
4. Finally, $\hat{\boldsymbol{x}}$ is then drawn from the decoder distribution $p_{\boldsymbol{\theta}}(\cdot|\boldsymbol{z})$.

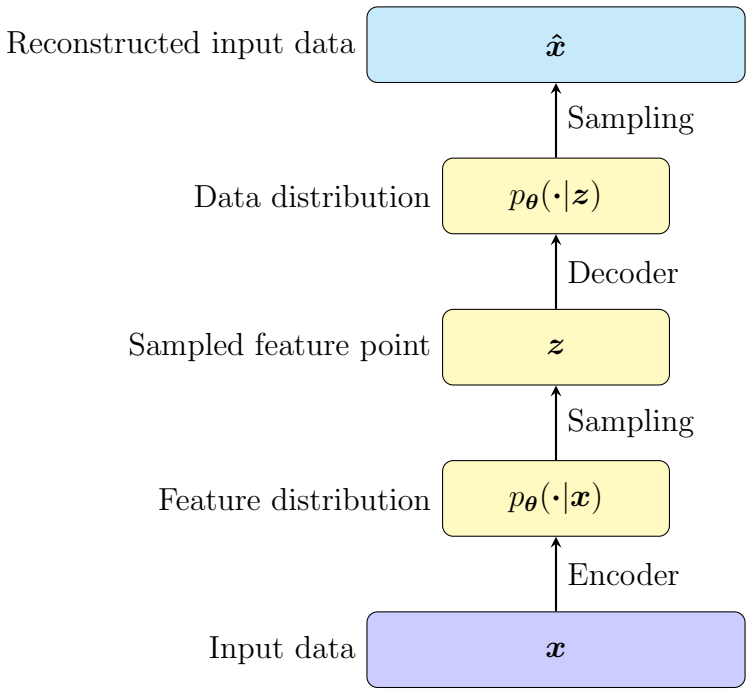


Figure 8: Graphical representation of a variational autoencoder evaluated at the point $\boldsymbol{x}$.

4.2.2 Probabilistic Framework

To support the above claims, we will create a probabilistic framework. Variational autoencoders build off the assumption that our dataset $\boldsymbol{\mathcal{D}} = \{\boldsymbol{x}^{(i)}\}_{i=1}^{N}$, was generated by N independent samples of an unchanging underlying distribution. Where each sample $\boldsymbol{x}^{(i)}$, was generated from some random process that involves the continuous unobserved latent random variable $\boldsymbol{z}^{(i)}$. This process happens in two distinct steps:

1. The value $\boldsymbol{z}^{(i)}$ is generated from some prior distribution $p_{\boldsymbol{\theta}^*}(\boldsymbol{z})$
2. Then $\boldsymbol{x}^{(i)}$ is generated from some conditional distribution $p_{\boldsymbol{\theta}^*}(\boldsymbol{x}|\boldsymbol{z}^{(i)})$

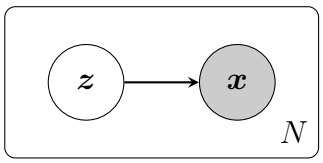


Figure 9: Probabilistic graphical model for our data generation process

Where $\boldsymbol{\theta}^*$, are the true parameters of the parametric families of differentiable distributions, $p_{\boldsymbol{\theta}}(\boldsymbol{z})$ and $p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})$. This in turn allows us to define the joint parametric distribution $p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z})$, as $p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z}) = p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})p_{\boldsymbol{\theta}}(\boldsymbol{z})$.

4.2.3 The Problem With This Approach

Therefore by using the the joint parametric distribution above $p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z}) = p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})p_{\boldsymbol{\theta}}(\boldsymbol{z})$, the marginal likelihood is defined as the following,

$$p_{\boldsymbol{\theta}}(\boldsymbol{x}) = \int_{\Omega_{\boldsymbol{z}}} p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z}) dz = \int_{\Omega_{\boldsymbol{z}}} p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})p_{\boldsymbol{\theta}}(\boldsymbol{z})\, d\boldsymbol{z}$$

So in principle we are able find the optimal parameter $\boldsymbol{\theta}^*$ by applying GD to the likelihood given data set. However, due to integral being intractable as it does not have an analytical solution or an efficient estimator, we are unable take derivative with respect to the parameter $\boldsymbol{\theta}$ and find $\boldsymbol{\theta}^*$ that maximises $p_{\boldsymbol{\theta}}(\boldsymbol{x})$.

The intractability of $p_{\boldsymbol{\theta}}(\boldsymbol{x})$, is related to the intractability of the unobserved posterior distribution $p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x})$, by the relationship,

$$p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x}) = \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z})}{p_{\boldsymbol{\theta}}(\boldsymbol{x})} = \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})p_{\boldsymbol{\theta}}(\boldsymbol{z})}{\int_{\Omega_{\boldsymbol{z}}} p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})p_{\boldsymbol{\theta}}(\boldsymbol{z})\, d\boldsymbol{z}}$$

Therefore, if we have a tractable $p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x})$ (or $p_{\boldsymbol{\theta}}(\boldsymbol{x})$ respectably) this will lead to a tractable $p_{\boldsymbol{\theta}}(\boldsymbol{x})$ (or $p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x})$ respectably), as $p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z})$ is tractable due to it being modelled as the product of two known parametric distributions.

4.2.4 Overcoming This Problem

To overcome this problem we try to approximate the true unobserved posterior distribution $p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x})$ by using the encoder model $q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})$, parameterised by $\boldsymbol{\phi}$. We aim to finding the value for $\boldsymbol{\phi}$ such that the distribution $q_{\boldsymbol{\phi}^*}(\boldsymbol{z}|\boldsymbol{x})$, closely approximates the true intractable posterior $p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x})$. This is also equivalent to solving the minimisation problem,

$$\boldsymbol{\phi}^* = \underset{\boldsymbol{\phi}}{\operatorname{argmin}}\, D_{\mathrm{KL}}(q_{\boldsymbol{\phi}}(\cdot|\boldsymbol{x})||p_{\boldsymbol{\theta}}(\cdot|\boldsymbol{x})). \tag{14}$$

Since we have assumed that each data point $\boldsymbol{x}^{(i)}$ are independent, the total marginal likelihood is the sum of the individual likelihoods. Hence, by using our encoder model, we will compute the following marginal likelihood,

$$\begin{aligned}
\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) &= \mathbb{E}_{\boldsymbol{z}\sim q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})}[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})] \quad (\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) \text{ does not depend on } \boldsymbol{z}) \\
&= \mathbb{E}_{\boldsymbol{z}}\left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z})p_{\boldsymbol{\theta}}(\boldsymbol{z})}{p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})}\right] \quad \text{(Bayes' Rule twice)} \\
&= \mathbb{E}_{\boldsymbol{z}}\left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z})p_{\boldsymbol{\theta}}(\boldsymbol{z})}{p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})}\frac{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})}{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})}\right] \quad \text{(Multiplication by 1)} \\
&= \mathbb{E}_{\boldsymbol{z}}[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z})] - \mathbb{E}_{\boldsymbol{z}}\left[\log \frac{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})}{p_{\boldsymbol{\theta}}(\boldsymbol{z})}\right] + \mathbb{E}_{\boldsymbol{z}}\left[\log \frac{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})}{p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})}\right] \quad \text{(Logs)} \\
&= \underbrace{\mathbb{E}_{\boldsymbol{z}}[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z})] - D_{KL}(q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})||p_{\boldsymbol{\theta}}(\boldsymbol{z}))}_{\mathcal{L}(\boldsymbol{x}^{(i)};\boldsymbol{\theta},\boldsymbol{\phi})} + \underbrace{D_{KL}(q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})||p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x}^{(i)}))}_{\geq 0}
\end{aligned}$$

The true intractable posterior $p_\theta(\boldsymbol{z}|\boldsymbol{x})$ still appears in the last term of the marginal likelihood. However, we are able to use the fact that the Kullback–Leibler divergence is non-negative and zero if and only if $q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})$ equals the true posterior, and obtain an evidence lower bound (ELBO), $\mathcal{L}(\boldsymbol{x}^{(i)};\boldsymbol{\theta},\boldsymbol{\phi})$, for our marginal likelihood.

$$\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) \geq \mathcal{L}(\boldsymbol{x}^{(i)};\boldsymbol{\theta},\boldsymbol{\phi}) = \mathbb{E}_{\boldsymbol{z}}[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z})] - D_{KL}(q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})||p_{\boldsymbol{\theta}}(\boldsymbol{z}))$$

Hence, we aim to maximise $\mathcal{L}(\boldsymbol{x}^{(i)};\boldsymbol{\theta},\boldsymbol{\phi})$ through gradient descent and obtain the optimal parameters $\boldsymbol{\theta}^*$ and $\boldsymbol{\phi}^*$ that maximises the evidence lower bound.

$$\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) \geq \mathcal{L}(\boldsymbol{x}^{(i)};\boldsymbol{\theta}^*,\boldsymbol{\phi}^*) \geq \mathcal{L}(\boldsymbol{x}^{(i)};\boldsymbol{\theta},\boldsymbol{\phi})$$

We will now look at the terms in $\mathcal{L}(\boldsymbol{x}^{(i)};\boldsymbol{\theta},\boldsymbol{\phi})$, as it will allow us to understand what the ELBO is maximising for:

$\mathbb{E}_{\boldsymbol{z}}[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z})]$, can be thought of as how well the model has done at reconstructing the input data. Therefore maximising for $\boldsymbol{\theta}$ will give use a good reconstruction of our input data.

$D_{KL}(q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})||p_{\boldsymbol{\theta}}(\boldsymbol{z}))$, can be thought of as regularising $\boldsymbol{\phi}$ such that $q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})$ approximate the distribution $p_{\boldsymbol{\theta}}(\boldsymbol{z})$. It is not entirely obvious that this will yield the correct $q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})$ that we set out to obtain. However, if we fix $\boldsymbol{\theta}$ and think about finding the value of $\boldsymbol{\phi}$ that minimises the KL-divergence between $q_{\boldsymbol{\phi}}(\cdot|\boldsymbol{x})$ and $p_{\boldsymbol{\theta}}(\cdot|\boldsymbol{x})$, we get the following,

$$
\begin{aligned}
\boldsymbol{\phi}^* &= \underset{\boldsymbol{\phi}}{\operatorname{argmin}} \left(D_{KL}(q_{\boldsymbol{\phi}}(\cdot|\boldsymbol{x}^{(i)})||p_{\boldsymbol{\theta}}(\cdot|\boldsymbol{x}^{(i)}))\right) \text{ (Using the notation } \mathbb{E}_z(\cdot) \equiv \mathbb{E}_{\boldsymbol{z}\sim q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})}(\cdot)) \\
&= \underset{\boldsymbol{\phi}}{\operatorname{argmin}} \left(\mathbb{E}_{\boldsymbol{z}}[\log q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})] - \mathbb{E}_{\boldsymbol{z}}[\log p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})]\right) \quad \text{(Logs)} \\
&= \underset{\boldsymbol{\phi}}{\operatorname{argmin}} \left(\mathbb{E}_{\boldsymbol{z}}[\log q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})] - \mathbb{E}_{\boldsymbol{z}}\left[\frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z})p_{\boldsymbol{\theta}}(\boldsymbol{z})}{p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})}\right]\right) \quad \text{(Bayes' Rule twice)} \\
&= \underset{\boldsymbol{\phi}}{\operatorname{argmin}} \left(\mathbb{E}_{\boldsymbol{z}}[\log q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})] - \mathbb{E}_{\boldsymbol{z}}[\log p_{\boldsymbol{\theta}}(\boldsymbol{z})] - \mathbb{E}_{\boldsymbol{z}}[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z})] + \mathbb{E}_{\boldsymbol{z}}[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})]\right) \text{ (Logs)}
\end{aligned}
$$

Since, $\mathbb{E}_{\boldsymbol{z}}[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})]$ is independent of $\boldsymbol{\phi}$, we can remove it without effecting the argmin.

$$
\begin{aligned}
&= \underset{\boldsymbol{\phi}}{\operatorname{argmin}} \left(\mathbb{E}_{\boldsymbol{z}}[\log q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})] - \mathbb{E}_{\boldsymbol{z}}[\log p_{\boldsymbol{\theta}}(\boldsymbol{z})] - \mathbb{E}_{\boldsymbol{z}}[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z})]\right) \\
&= \underset{\boldsymbol{\phi}}{\operatorname{argmax}} \left(-\mathbb{E}_{\boldsymbol{z}}[\log q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})] + \mathbb{E}_{\boldsymbol{z}}[\log p_{\boldsymbol{\theta}}(\boldsymbol{z})] + \mathbb{E}_{\boldsymbol{z}}[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z})]\right) \text{ (argmin to argmax)} \\
&= \underset{\boldsymbol{\phi}}{\operatorname{argmax}} \left(\mathbb{E}_{\boldsymbol{z}}[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z})] - D_{KL}(q_{\boldsymbol{\phi}}(\cdot|\boldsymbol{x}^{(i)})||p_{\boldsymbol{\theta}}(\cdot))\right) \quad (D_{\text{KL}} \text{ definition})
\end{aligned}
$$

Hence, we arrive at the same expression as $\mathcal{L}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}, \boldsymbol{\phi})$. Therefore, maximising $\mathcal{L}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}, \boldsymbol{\phi})$ for $\boldsymbol{\phi}$ will produce the correct $\boldsymbol{\phi}*$.

Therefore, by maximising $\mathcal{L}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}, \boldsymbol{\phi})$, we have the maximal trade-off between good reconstruction of our input data and $q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})$ approximating the true intractable posterior, $p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x})$.

4.2.5 Reparameterization Trick

Now that we have a computable lower bound for the marginal likelihood, we want to differentiate $\mathcal{L}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}, \boldsymbol{\phi})$ with respect to $\boldsymbol{\theta}$ and $\boldsymbol{\phi}$ to find their optimal parameters $\boldsymbol{\theta}^*$ and $\boldsymbol{\phi}^*$, such that $\mathcal{L}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}^*, \boldsymbol{\phi}^*) \geq \mathcal{L}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}, \boldsymbol{\phi})$. However, we are unable to take the derivative of $p_{\boldsymbol{\theta}}(\cdot|\boldsymbol{z})$ as depends on a random and non-deterministic sample $\boldsymbol{z} \sim q_{\boldsymbol{\phi}}(\cdot|\boldsymbol{x}^{(i)})$. We overcome this by choosing our encoder model $q_{\boldsymbol{\phi}}(\cdot|\boldsymbol{x}^{(i)})$ under certain conditions (explained below) such that we are able to reparameterise the random variable $\boldsymbol{z}$, as a differentiable transformation function $g_{\boldsymbol{\phi}}(\boldsymbol{\varepsilon}, \boldsymbol{x}^{(i)})$, where $\boldsymbol{\varepsilon}$ is some auxiliary noise.

$$
\boldsymbol{z} = g_{\boldsymbol{\phi}}(\boldsymbol{\varepsilon}, \boldsymbol{x}^{(i)}), \qquad \boldsymbol{\varepsilon} \sim p(\boldsymbol{\varepsilon}) \tag{15}
$$

We will now state the conditions where we can choose a differentiable transformation $g_{\boldsymbol{\phi}}(\boldsymbol{\varepsilon}, \boldsymbol{x}^{(i)})$ and auxiliary variable $\boldsymbol{\varepsilon} \sim p(\boldsymbol{\varepsilon})$ to replace $\boldsymbol{z} \sim q_{\boldsymbol{\phi}}(\cdot|\boldsymbol{x})$ for $\boldsymbol{z} = g_{\boldsymbol{\phi}}(\boldsymbol{\varepsilon}, \boldsymbol{x}^{(i)})$. [2]

1. $q_{\boldsymbol{\phi}}(\cdot|\boldsymbol{x})$ has a tractable inverse CDF. In this case, let $\varepsilon \sim \mathcal{U}(\boldsymbol{0}, \boldsymbol{I})$, and let $g_{\boldsymbol{\phi}}(\boldsymbol{\varepsilon}, \boldsymbol{x})$ be the inverse CDF of $q_{\boldsymbol{\phi}}(\cdot|\boldsymbol{x})$. Examples: Exponential, Cauchy, Logistic, Rayleigh, Pareto, Weibull, Reciprocal, Gompertz, Gumbel and Erlang distributions.

2. $q_{\boldsymbol{\phi}}(\cdot|\boldsymbol{x})$ is from any "location-scale" family of distributions. In this we can choose the standard distribution (with location = 0, scale = 1) as the auxiliary variable $\boldsymbol{\varepsilon}$, and then let $g_{\boldsymbol{\phi}}(\boldsymbol{\varepsilon}, \boldsymbol{x}) = \text{location} + \text{scale} \times \boldsymbol{\varepsilon}$. Examples: Laplace, Elliptical, Student's t, Logistic, Uniform, Triangular and Gaussian distributions.

3. $q_{\boldsymbol{\phi}}(\cdot|\boldsymbol{x})$ is a composition of random variables as different transformations of auxiliary variables. Then we take $g_{\boldsymbol{\phi}}(\boldsymbol{\varepsilon}, \boldsymbol{x})$ their composition of the above reparmeterizations. Examples: Log-Normal (exponentiation of normally distributed variable), Gamma (a sum over exponentially distributed variables), Dirichlet (weighted sum of Gamma variates), Beta, Chi-Squared, and F distributions.

Hence, by using the reparameterization (15), we are able to form a Monte Carlo estimate of expectation for the function $\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z})$ with respect to our encoder model $q_{\boldsymbol{\phi}}(\cdot|\boldsymbol{x}^{(i)})$, as the following,

$$\mathbb{E}_{\boldsymbol{z}\sim q_{\boldsymbol{\phi}}(\cdot|\boldsymbol{x}^{(i)})}[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z})] = \mathbb{E}_{\boldsymbol{\varepsilon}\sim p(\boldsymbol{\varepsilon})}[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|g_{\boldsymbol{\phi}}(\boldsymbol{\varepsilon}, \boldsymbol{x}^{(i)}))] \tag{16}$$

$$\simeq \frac{1}{L}\sum_{l=1}^{L} \log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|g_{\boldsymbol{\phi}}(\boldsymbol{\varepsilon}^{(l)}, \boldsymbol{x}^{(i)})), \quad \boldsymbol{\varepsilon}^{(l)} \sim p(\boldsymbol{\varepsilon}) \tag{17}$$

Now applying the method above to our ELBO, we obtain a differentiable estimator $\mathcal{L}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}, \boldsymbol{\phi}) \simeq \tilde{\mathcal{L}}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}, \boldsymbol{\phi})$.

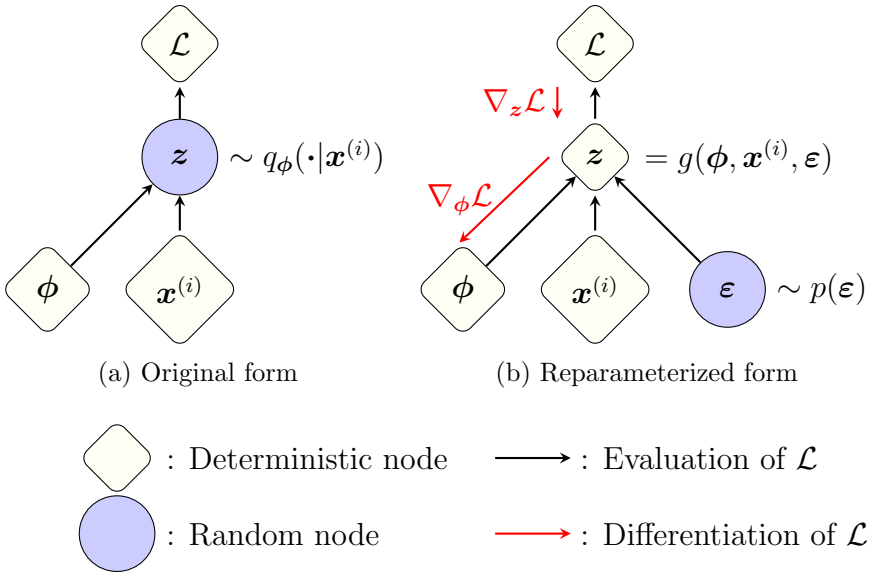
$$\tilde{\mathcal{L}}(\boldsymbol{x}^{(i)}, \boldsymbol{\theta}, \boldsymbol{\phi}) = \frac{1}{L}\sum_{l=1}^{L} \log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z}^{(i,l)}) - D_{KL}(q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})||p_{\boldsymbol{\theta}}(\boldsymbol{z})) \tag{18}$$

$$\text{where} \quad \boldsymbol{z}^{(i,l)} = g_{\boldsymbol{\phi}}(\boldsymbol{\varepsilon}^{(i,l)}, \boldsymbol{x}^{(i)}), \quad \text{and} \quad \boldsymbol{\varepsilon}^{(l)} \sim p(\boldsymbol{\varepsilon})$$

Now suppose our dateset $\boldsymbol{X}$ consisting of N data points. We are able to preformed minibatch training to the above result, to get the following approximation of $\mathcal{L}$,

$$\mathcal{L}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}, \boldsymbol{\phi}) \simeq \tilde{\mathcal{L}}^{M}(\boldsymbol{X}^{M}; \boldsymbol{\theta}, \boldsymbol{\phi}) = \frac{N}{M}\sum_{i=1}^{M} \tilde{\mathcal{L}}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}, \boldsymbol{\phi})$$

Where, $X^M = (\boldsymbol{x}^{(i)})_{i=1}^{M}$ are M randomly chosen data points from our training data $\boldsymbol{X}$. If we perform minibatch training with M is large enough (i.e. $M = 100$), we are able to set $L = 1$ in (18). As experiments show that there is no significant performance decrease by taking a single sample [2]. This allows us to save time training as we don't have to perform multiple samples for each data point, decreasing the complexity of training.



(a) Original form (b) Reparameterized form

(c) Figure Key

Figure 10: Illustration of the reparameterization trick used to get a differentiable $\mathcal{L}$ w.r.t $\boldsymbol{\phi}$. ([9], p.22)

4.3 Gaussian VAE Example

We will now demonstrate this reparameterization trick, by assuming that the prior distribution over the latent variables, is given by an isotropic multivariate Gaussian $p_{\boldsymbol{\theta}}(\boldsymbol{z}) = \mathcal{N}(\boldsymbol{z}; \boldsymbol{0}, \boldsymbol{I})$ and our true posterior $p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x})$ is a multivariate Gaussian. Therefore, we will approximate the true posterior $p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x})$ with a multivariate parametric Gaussian model that has a diagonal covariance, $q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\sigma}^2 I)$. Where $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}^2$ are function of $\boldsymbol{\phi}$. We chose a diagonal covariance structure to promote the latent variables learning unique generalise features.

Since our parametric model $q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})$ is a "location-scale" distribution, we will use the following reparameterisation,

$$\boldsymbol{z} = g_{\boldsymbol{\phi}}(\boldsymbol{x}, \boldsymbol{\varepsilon}) = \boldsymbol{\mu} + \boldsymbol{\sigma} \odot \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$$

Where $\odot$ is element-wise multiplication. Therefore, by using the calculation that we carried out in Section 2.2, we obtain the following approximation for $\tilde{\mathcal{L}}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}, \boldsymbol{\phi})$,

$$\tilde{\mathcal{L}}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}, \boldsymbol{\phi}) \simeq \frac{1}{2}\sum_{j=1}^{m}(1 + \log((\boldsymbol{\sigma}_j^{(i)})^2) - (\boldsymbol{\mu}_j^{(i)})^2 - (\boldsymbol{\sigma}_j^{(i)})^2) + \frac{1}{L}\sum_{l=1}^{L}\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z}^{(i,l)})$$

$$\text{where} \quad \boldsymbol{z}^{(i,l)} = \boldsymbol{\mu}^{(i)} + \boldsymbol{\sigma}^{(i)} \odot \boldsymbol{\varepsilon}^{(l)}, \quad \boldsymbol{\varepsilon}^{(l)} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I}) \tag{19}$$

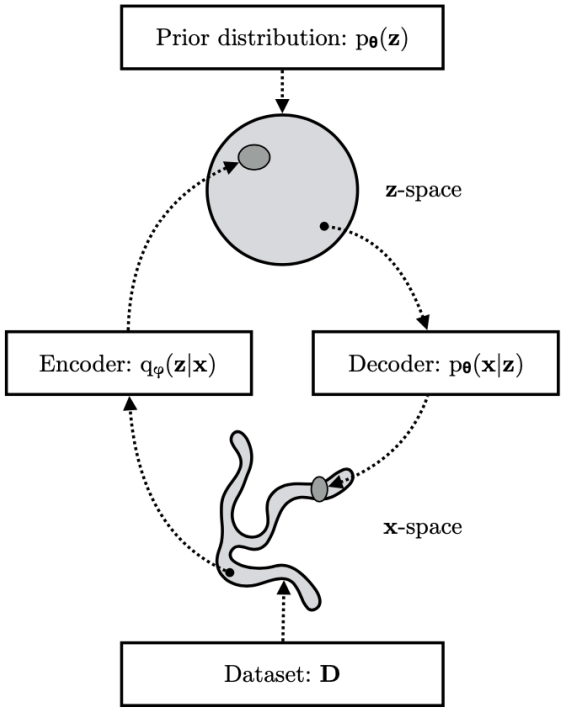


Figure 11: A VAE learns the mappings between our observed data space which its distribution which is typically complicated, and a feature space, whose distribution can be relatively simple (such as Gaussian, as in this figure). ([9], p.17)

4.4 Application of VAE to MNIST Dataset

In this section we will show how a variation autoencoder trained on the MNIST data set [10], can be used to generate new images of handwritten digits. To demonstrate this, we start by following the same set up as the previous section. Suppose, that the prior over the latent variables is given by an isotropic multivariate Gaussian $p_{\boldsymbol{\theta}}(\boldsymbol{z}) = \mathcal{N}(\mathbf{0}, \boldsymbol{I})$ and our true posterior $p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x})$, is a multivariate Gaussian. Therefore, to approximate the true posterior $p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x})$, we will use a multivariate parametric Gaussian model that has a diagonal covariance (i.e $q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\sigma}^2 I)$ where $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}^2$ are functions of $\boldsymbol{\phi}$). Therefore by using the result from the previous section, $\tilde{\mathcal{L}}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}, \boldsymbol{\phi})$ takes the form,

$$\tilde{\mathcal{L}}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}, \boldsymbol{\phi}) \simeq \frac{1}{2}\sum_{j=1}^{m}(1 + \log((\boldsymbol{\sigma}_j^{(i)})^2) - (\boldsymbol{\mu}_j^{(i)})^2 - (\boldsymbol{\sigma}_j^{(i)})^2) + \frac{1}{L}\sum_{l=1}^{L}\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z}^{(i,l)})$$

$$\text{where} \quad \boldsymbol{z}^{(i,l)} = \boldsymbol{\mu}^{(i)} + \boldsymbol{\sigma}^{(i)} \odot \boldsymbol{\varepsilon}^{(l)}, \quad \boldsymbol{\varepsilon}^{(l)} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})$$

To produce the $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}$ that will be used in $q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})$, we define $\text{EncoderNeuralNet}_{\boldsymbol{\phi}}$ that encodes a data point $\boldsymbol{x}^{(i)}$, into a $\boldsymbol{\mu}$ and a $\boldsymbol{\sigma}$. The $\text{EncoderNeuralNet}_{\boldsymbol{\phi}}$ is a CNN takes the data point $\boldsymbol{x}^{(i)}$, (which are a 28×28 matrix) and outputs the encoded $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}$.

To be able to make a complete model for training, we will also make the additional assumption that $p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})$ is a multivariate parametric Gaussian of the form, $p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z}) = \mathcal{N}(\hat{\boldsymbol{x}}^{(i)}, \sigma_2 \boldsymbol{I})$. Where $\hat{\boldsymbol{x}}^{(i)} = \text{DecoderNeuralNet}_{\boldsymbol{\theta}}(\boldsymbol{z}^{(i,l)})$ is the mean and

σ_2 is the variance of our data. The DecoderNeuralNet$_{\boldsymbol{\theta}}$ up-scaling CNN that takes in the sampled point $\boldsymbol{z}^{(i,l)}$ and produces a mean $\hat{\boldsymbol{x}}^{(i)}$. Formally, we should learn the parameter σ_2. However, we will simplify our problem by setting it to one (i.e $\sigma_2 = 1$). Therefore, as $p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z}^{(i,l)})$ is a multivariate Gaussian of mean $\hat{\boldsymbol{x}}^{(i)}$ and variance 1, $\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z}^{(i,l)})$ is given by,

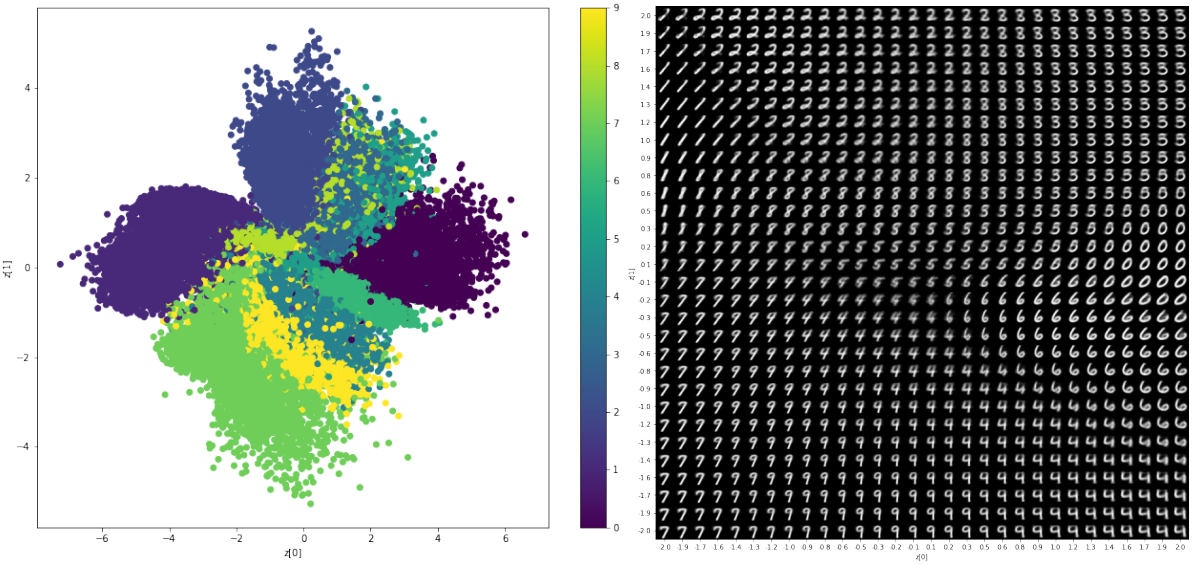
$$\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z}^{(i,l)}) = -\frac{1}{2}||\boldsymbol{x}^{(i)} - \hat{\boldsymbol{x}}^{(i)}||^2 + C$$

Where C is a constant. Moreover, as we are planning on using batch training in our training procedure, we can simplify the expression for $\tilde{\mathcal{L}}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}, \boldsymbol{\phi})$ further, as we can set $L = 1$. Therefore, by applying the above adaptations, $\tilde{\mathcal{L}}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}, \boldsymbol{\phi})$ is now expressed as the following,

$$\begin{aligned}
\tilde{\mathcal{L}}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}, \boldsymbol{\phi}) &\simeq \frac{1}{2}\sum_{j=1}^{m}(1 + \log((\boldsymbol{\sigma}_j^{(i)})^2) - (\boldsymbol{\mu}_j^{(i)})^2 - (\boldsymbol{\sigma}_j^{(i)})^2) + \log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z}^{(i)}) \\
&= \frac{1}{2}\sum_{j=1}^{m}(1 + \log((\boldsymbol{\sigma}_j^{(i)})^2) - (\boldsymbol{\mu}_j^{(i)})^2 - (\boldsymbol{\sigma}_j^{(i)})^2) - \frac{1}{2}||\boldsymbol{x}^{(i)} - \hat{\boldsymbol{x}}^{(i)}||^2 + C
\end{aligned}$$

$$\text{where} \quad \boldsymbol{z}^{(i)} = \boldsymbol{\mu}^{(i)} + \boldsymbol{\sigma}^{(i)} \odot \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$$

After training the full model of the VAE (described in Figure. 13), with 70,000 samples of hand written digits, using batch sizes of 128, and 30 epochs. We obtain the following figures that describes the behaviour of the latent to data space.



(a) (b)

Figure 12: (a) Density distribution of MNIST digits in 2-dimensional latent space. (b) Data space mapping that corresponds to the density distribution of MNIST digits in 2-dimensional latent space (i.e the mapping of latent a latent point in data space). [4]

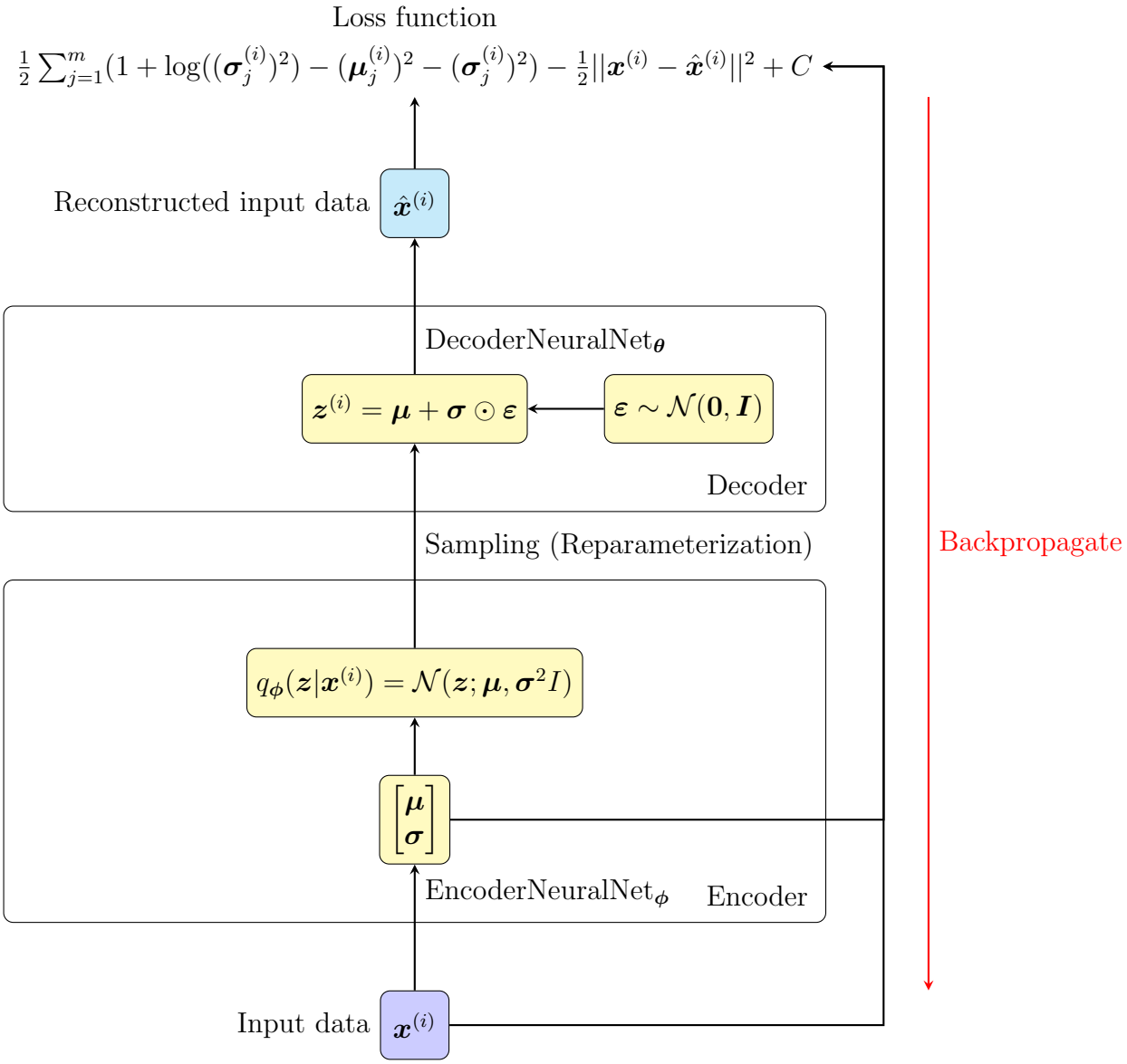


Figure 13: Trainable variational autoencoder

We are able to see from Figure. 12, that the VAE regularised the latent space which provided good properties for generative modelling. This was in turn due to the choice of using a Gaussian centred at the origin with variance one, as our prior distribution. This forced the KL divergence term in the ELBO to be small if the encoder model is well-behaved, (i.e. if it is a relatively smooth distribution which is small far away from the origin). Thus, the KL term regularises the VAE. We can see this effect in Figure. 12 (a), as most of the MNIST digits get regularised close to the origin.

5 Neural Ordinary Differential Equations

We will now introduce the final piece of the background knowledge required before we introduce generative latent time-series models in the next chapter. As the title of the chapter may suggest, we will be looking at the combination of neural networks and

ordinary differential equations (ODEs). The reason for studying this architecture is because in the next chapter we are going to be looking at modelling time series data with the use of VAE. However, we have only looked at VAEs without a time dependency and therefore the Neural ODE architecture will be used to help us close that gap.

5.1 Motivation

Many models in machine learning can be described as discrete transformations of hidden states, and can be expressed by the following relationship,

$$\boldsymbol{z}_{t+1} = \boldsymbol{z}_t + \boldsymbol{\phi}(\boldsymbol{z}_t, \boldsymbol{\theta}_t), \qquad t \in \{0, \dots, T\}, \;\; \boldsymbol{z}_t \in \mathbb{R}^m, \;\; \boldsymbol{\phi}(\cdot, \boldsymbol{\theta}_t) : \mathbb{R}^m \to \mathbb{R}^m \tag{20}$$

Where t is the depth of the network and $\boldsymbol{\theta}_t$ parameterizes the network at depth t. This relationship closely resembles the forward Euler method for solving ordinary differential equations for discrete time steps, $t \in \{0, \dots, T\}$. Therefore, analogously we can think of the network at depth t, representing the network at time t.

Hence, with the idea that (20) is the solution of the forward Euler method for solving an ODE at discrete layers $\{0, \dots, T\}$, we can hypothesise that $\boldsymbol{z}(t)$ is continuous and governed by,

$$\frac{d\boldsymbol{z}(t)}{dt} = \boldsymbol{f}(\boldsymbol{z}(t), t, \boldsymbol{\theta}), \qquad \boldsymbol{z}(0) = \boldsymbol{z}_0 \tag{21}$$

Where $\boldsymbol{f} : \mathbb{R}^m \to \mathbb{R}^m$ is a neural network, parameterized by $\boldsymbol{\theta}$. This can always be achieved as we can ensure by our choice of $\boldsymbol{\theta}$ that (20) holds (i.e $\boldsymbol{f}(\boldsymbol{z}(t), t, \boldsymbol{\theta}) = \phi(\boldsymbol{z}_t, \boldsymbol{\theta}_t), \forall t \in \{0, \dots, T\}$) .

Thus, we can think of the layers of our network in the continuous sense. Therefore, given an initial state of the network $\boldsymbol{z}_0$, we can solve (21) forwards to obtain the network's value at an arbitrary layer. This solution is unique and can always be achieved by treating the ODE solver as a black-box.

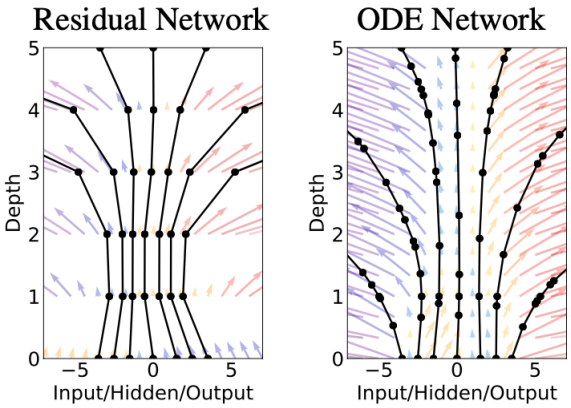


Figure 14: Left: A Residual network defines a discrete sequence of finite transformations. Right: An ODE network defines a vector field, of continuously state transforms. [3]

5.1.1 Toy Circular Dynamics Example

Since we are able to make the analogous link between layer depth of our network and time, we will show how neural ODEs can be used as a black-box approach for learning a forcing function of an ODE. We will use this idea to try and learn a continuous function of time. To achieve this, we will frame our problem using (21) and find the value of $\boldsymbol{\theta}$ that minimises the difference between $\boldsymbol{z}(t)$ and the true solution.

We will make life easier for ourselves. We will try to learn a continuous function of time that we know its form as an initial value problem,

$$\dot{\boldsymbol{x}}(t) = \frac{d}{dt}\begin{bmatrix} x(t) \\ y(t) \end{bmatrix} = \begin{bmatrix} -y(t) \\ x(t) \end{bmatrix} =: \boldsymbol{f}(\boldsymbol{x}(t)), \quad \boldsymbol{x}(0) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad t \in [0, 2\pi] \tag{22}$$

We start by noticing the following relationship,

$$\ddot{x}(t) = -\dot{y} = -x(t), \qquad x(0) = 1$$

Therefore, by the symmetry of our problem, we obtain,

$$\ddot{y}(t) = -y(t), \qquad y(0) = 0$$

Hence, the unique solution to our initial value problem is given by,

$$\boldsymbol{x}(t) = \begin{bmatrix} \cos(t) \\ \sin(t) \end{bmatrix}, \qquad t \in [0, 2\pi] \tag{23}$$

To learn the correct $\boldsymbol{z}(t)$, we will use the affine function, $\boldsymbol{f}_\theta : \mathbb{R}^2 \to \mathbb{R}^2$ as our model.

$$\dot{\boldsymbol{z}}(t) = \frac{d}{dt}\begin{bmatrix} x(t) \\ y(t) \end{bmatrix} = \boldsymbol{f}_\theta(\boldsymbol{z}(t)) \coloneqq \begin{bmatrix} \theta_1 & \theta_2 \\ \theta_3 & \theta_4 \end{bmatrix}\begin{bmatrix} x(t) \\ y(t) \end{bmatrix} + \begin{bmatrix} \theta_5 \\ \theta_6 \end{bmatrix}, \boldsymbol{z}(0) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, t \in [0, 2\pi] \tag{24}$$

Since we have the explicit form of the continuous function that we want to model (given by (23)), we will artificially simulate data points for our problem. This is done by randomly sampling a stopping time t_{stop} from $\mathcal{U}(0, 2\pi)$ (i.e $t_{\text{stop}} \sim \mathcal{U}(0, 2\pi)$) and using (23) to calculated the true value of the solution at that time. After doing this procedure 12,800 times, we have a large enough data set that we can use for training. To form a prediction from our network, we will use the fourth-order Runge–Kutta (RK4) method to integrate (24) forward in time to t_{stop}. Then we will use the squared error between our prediction and the true solution to quantify how well our prediction is. Finally, as the RK4 integration discretised the ODE, $\text{RK4}((1,0)^T, \boldsymbol{f}_\theta, 0, t_{\text{stop}})$, can be through of a parametric function of $\boldsymbol{\theta}$ (as it is discrete transformation and compositions of the forcing function $\boldsymbol{f}_\theta$) and therefore, we are able to take its derivative with respect to $\boldsymbol{\theta}$. Hence, we are able to compute the derviate of the loss function with respect to $\boldsymbol{\theta}$,

$$\begin{aligned} \text{L2 loss function } L &= ||\boldsymbol{x}_{\text{stop}} - \boldsymbol{z}_{\text{stop}}||^2 \\ &= ||\boldsymbol{x}_{\text{stop}} - \text{RK4}((1,0)^T, \boldsymbol{f}_\theta, 0, t_{\text{stop}})||^2 \\ \implies \frac{\partial L}{\partial \boldsymbol{\theta}} &= \frac{\partial ||\boldsymbol{x}_{\text{stop}} - \text{RK4}((1,0)^T, \boldsymbol{f}_\theta, 0, t_{\text{stop}})||^2}{\partial \boldsymbol{\theta}} \end{aligned}$$

We demonstrate this whole training process by the following figure,

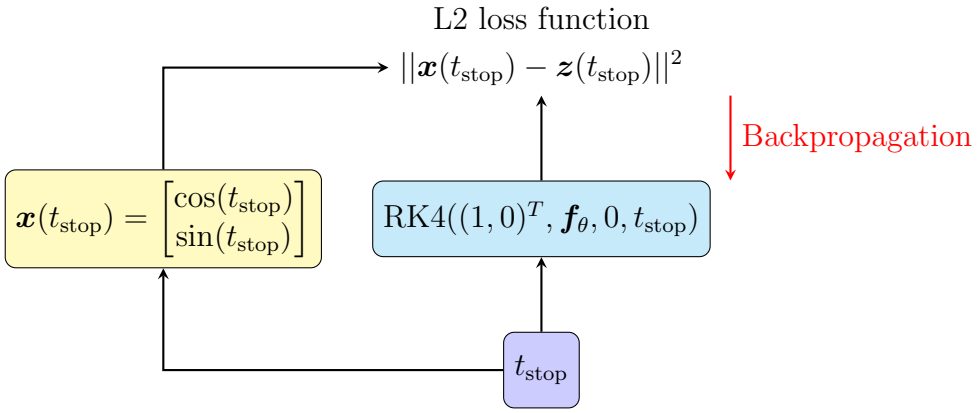


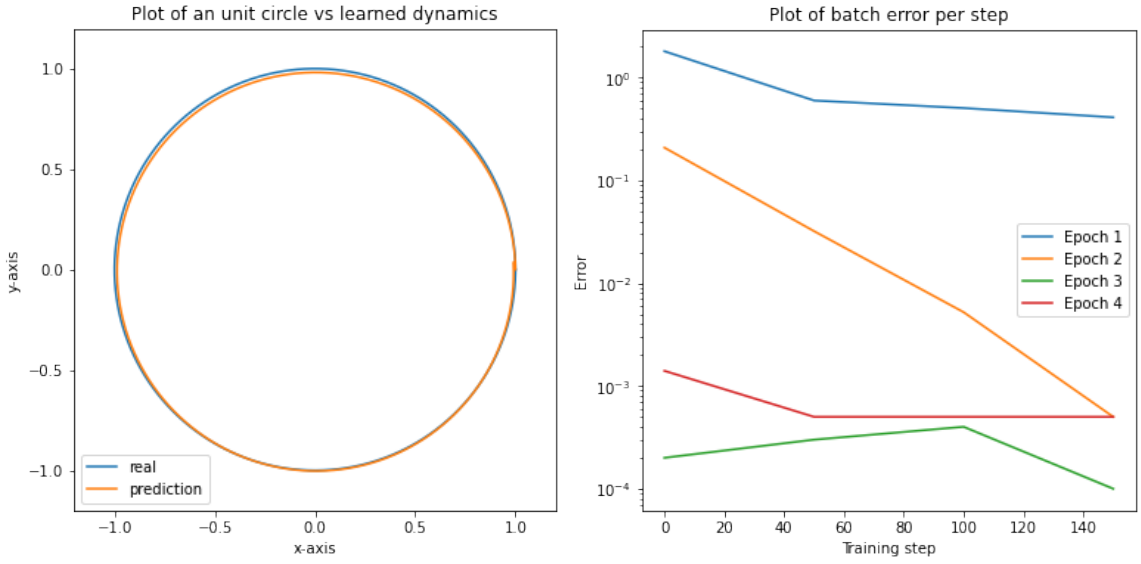
Figure 15: Training model for learning (23) using (24) and RK4 integration.

After training using the process described in Figure. (15), with 12,800 sample points, batch sizes of 64, and 4 epochs, we get the following forcing function,

$$\boldsymbol{f_\theta}(\boldsymbol{z}(t)) = \begin{bmatrix}-0.00 & 1.01\\ -1.01 & 0.00\end{bmatrix}\begin{bmatrix}x(t)\\ y(t)\end{bmatrix} + \begin{bmatrix}-0.01\\ -0.00\end{bmatrix} \approx \begin{bmatrix}y(t)\\ -x(t)\end{bmatrix}$$

Due to the symmetrical nature of our ODE example we still get same set of equations to solve,

$$\ddot{x}(t) = \dot{y}(t) = -x(t), \quad x(0) = 1, \quad \text{and} \quad \ddot{y}(t) = -y(t), \quad y(0) = 0$$



(a) (b)

Figure 16: (a) Plot of the networks learnt trajectory $\boldsymbol{z}(t)$ (orange) vs the true solution's trajectory $\boldsymbol{x}(t)$ (blue) to the problem (22). (b) Plot of the every 50th batch error over four epochs (converge to an error of 0.5×10^{-3}). [4]

5.2 Formalisation and Improvements

Like we did in our toy example (5.1.1), the native approach for training (21) is to apply backpropagation through the black-box solver. This works due to the block-box solver discretising the ODE, allowing us to take the derivative with respect to the parameters. However, this leads to high memory cost and introduces additional numerical error. This is because the black-box solver can be thought of as discrete transformation and compositions of the forcing function. As this procedure will be done a lot, this causes the derivative with respect to the parameters to be expensive, as they appear in each layer of the compositions. Hence, we seek to find a better solution to overcome this problem. We achieve this by deriving an expression for the derivative of the loss function with respect to the model parameters, that involves solving an ODE backward through the layers. This is a more appealing approach as modern ODE solvers allow for the problem to scale linearly with size. We can also control the tolerance of our solution, allowing for the ability to dictate how accurate our training is. Thus, helping us prevent over-fitting.

To make understanding the theory more digestible, we will impose the following simplification to our problem. We will only consider the network as being evaluated at two discrete points, t_0 and t_1, and we will look at minimising the loss produced over that interval. This simplification does not cause any initiations to our theory, as we can extend this theory to multiple observations (i.e minimising the loss function over $t_0, \ldots, t_N$ observations) and is shown at the end of Appendix 2.2.

We will now define the scalar loss function $L : \mathbb{R}^m \to \mathbb{R}$, that we alluded to above, where the input is the output of our black-box solver.

$$L(\boldsymbol{z}(t_1)) = L\left(\boldsymbol{z}(t_0) + \int_{t_0}^{t_1} \boldsymbol{f}(\boldsymbol{z}(t), t, \theta)dt\right) = L(\text{ODESolve}(\boldsymbol{z}(t_0), \boldsymbol{f}, t_0, t_1, \theta))$$

We aim to find the value of $\boldsymbol{\theta}$ that minimises L, as this will provide us with a model that captures the dynamics of our data closely. To obtain this we firstly define the adjoint, which is gradient of L with respect to the hidden state $\boldsymbol{z}(t)$,

$$\boldsymbol{a}(t) = \frac{\partial L}{\partial \boldsymbol{z}(t)} \tag{25}$$

It is important to remember that t is the layer depth and it is now continuous, so this holds for all $t \geq 0$.

We show in Appendix 2.1, that the derivative of the adjoint with respect to the layer is given by,

$$\frac{d\boldsymbol{a}^T(t)}{dt} = -\boldsymbol{a}^T \frac{\partial \boldsymbol{f}(\boldsymbol{z}(t), \theta, t)}{\partial \boldsymbol{z}} \tag{26}$$

Since this does not tell use how L changes with respect to the parameters $\boldsymbol{\theta}$ and t. We define the augmented state $\boldsymbol{z}_{\text{aug}}(t)$, to allow us to do so.

$$\boldsymbol{z}_{\text{aug}}(t) = \begin{bmatrix} \boldsymbol{z}(t) \\ \theta \\ t \end{bmatrix}$$

We now derive the new dynamical system,

$$\frac{d\boldsymbol{z}_{\text{aug}}(t)}{dt} = \boldsymbol{f}_{aug}([\boldsymbol{z}, \theta, t]) := \begin{bmatrix} \boldsymbol{f}([\boldsymbol{z}, \theta, t]) \\ \boldsymbol{0} \\ 1 \end{bmatrix}$$

$$\boldsymbol{a}_{\text{aug}}(t) := \begin{bmatrix} \boldsymbol{a} \\ \boldsymbol{a}_\theta \\ \boldsymbol{a}_t \end{bmatrix}(t), \quad \boldsymbol{a}_\theta(t) := \frac{dL}{d\theta(t)}, \quad \boldsymbol{a}_t(t) := \frac{dL}{dt(t)}$$

Therefore, we are able to use (26) on our new dynamics to obtain,

$$\frac{d\boldsymbol{a}_{\text{aug}}^T(t)}{dt} = -\boldsymbol{a}_{\text{aug}}^T \frac{\partial \boldsymbol{f}_{\text{aug}}}{\partial[\boldsymbol{z}, \theta, t]} \tag{27}$$

Thus, by the calculating (27) (which is shown in Appendix 2.2), we obtain the derivative of $\boldsymbol{a}_\theta(t)$ with respect to the layer,

$$\frac{d\boldsymbol{a}_\theta^T(t)}{dt} = \frac{d}{dt}\left(\frac{dL^T}{d\theta}\right) = -\boldsymbol{a}^T \frac{\partial \boldsymbol{f}(\boldsymbol{z}(t), \theta, t)}{\partial \theta}$$

Hence, by integrating this expression with backwards over the layers and assuming that $\boldsymbol{a}_\theta(t_1) = \boldsymbol{0}$ (explained in the Appendix 2.2), we achieved what we set out to obtain,

$$\frac{dL^T}{d\theta} = -\int_{t_1}^{t_0} \boldsymbol{a}^T(t) \frac{\partial \boldsymbol{f}(\boldsymbol{z}(t), \theta, t)}{\partial \theta} dt \tag{28}$$

To understand why we integrate backwards over the layers, we draw parallels from the discrete case. As the loss function depends of the output of the network (or in our case at t_1), we backpropgrate the error through the network updating the model parameters as we go. This is the same idea in the continuous case by integrating from t_1 to t_0 (i.e from the output to the input of our network) allowing us to compute the overall sensitivity of the model parameters.

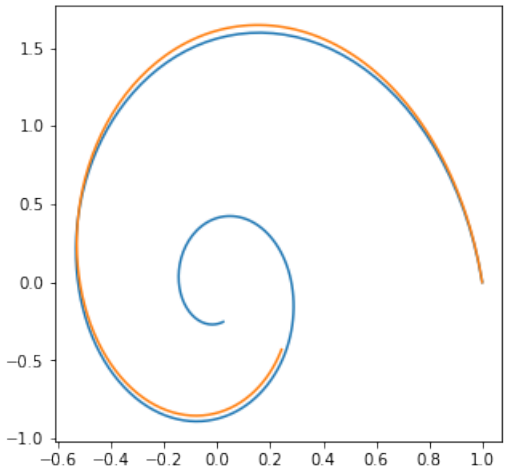


Figure 17: Plot of the networks learnt trajectory (orange) vs the true solution's trajectory (blue) using the adjoint sensitivity method to compute the gradients. [4]

6 Generative Latent Time-series Models

We will now use the theory established throughout this report to develop a generative approach to model continuous time series-data. We first start by framing the general problem that we would like to solve. Suppose that we observe a system at discrete times $t_0, \ldots, t_N$, which we will denote by $\boldsymbol{x}_{t_0}, \ldots, \boldsymbol{x}_{t_N}$, respectively. Then, given these observations, we would like to predict the system's state at the future times $t_{N+1}, \ldots, t_M$.

6.1 Model

Generative latent time-series models builds of the assumption that the observed data $\boldsymbol{x}_{t_0}, \ldots, \boldsymbol{x}_{t_N}$ was created from a random process that involves a continuous unobserved time dependent latent random variable $\boldsymbol{z}$. This process is described by the following sampling procedure,

$$\boldsymbol{z}_{t_0} \sim p_{\boldsymbol{\theta}^*}(\boldsymbol{z}) \tag{29}$$

$$\boldsymbol{z}_{t_0}, \ldots, \boldsymbol{z}_{t_N} = \text{ODESolve}(\boldsymbol{z}_{t_0}, \boldsymbol{f}_{\boldsymbol{\theta}^*}, t_0, \ldots, t_N) \tag{30}$$

$$\text{draw each } \boldsymbol{x}_{t_i} \sim p_{\boldsymbol{\theta}^*}(\boldsymbol{x}|\boldsymbol{z}_{t_i}) \tag{31}$$

Where $\boldsymbol{\theta}^*$ are the true parameters of the parametric forcing function $\boldsymbol{f}_\theta$ (that describes how the latent variables evolves with time) and the parametric differentiable distributions, $p_{\boldsymbol{\theta}}(\boldsymbol{z})$ and $p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})$. To ensure that our trajectory in latent space is uniquely defined, we make the assumption that the parametric forcing function, $\boldsymbol{f}_{\boldsymbol{\theta}}$ is a time-invariant function (i.e $\boldsymbol{f}_{\boldsymbol{\theta}}(\boldsymbol{z}(t), t) = \boldsymbol{f}_\theta(\boldsymbol{z}(t))$). This sampling procedure can be thought of as adding the dimension of time to the data creation process described in Section 4.2.2.

With the above data creation process in mind, we now make the following adaptations to the variational autoencoder model described in Figure. 8:

1. Instead of conditioning over a single observation for the posterior distribution, we now condition over all $N+1$ observations. Therefore the true posterior is given by, $p_{\boldsymbol{\theta}}(\cdot|\boldsymbol{x}_{t_0}, \ldots, \boldsymbol{x}_{t_N})$.

2. After we sample from the posterior distribution (i.e $\boldsymbol{z}_{t_0} \sim p_{\boldsymbol{\theta}}(\cdot|\boldsymbol{x}_{t_0}, \ldots, \boldsymbol{x}_{t_N})$), we now integrate the equation,

$$\frac{d\boldsymbol{z}(t)}{dt} = \boldsymbol{f}_{\boldsymbol{\theta}}(\boldsymbol{z}(t)), \quad \boldsymbol{z}(t_0) = \boldsymbol{z}_{t_0}$$

   forwards in time, to obtain $\boldsymbol{z}_{t_0}, \ldots, \boldsymbol{z}_{t_N}$ (i.e $\boldsymbol{z}_{t_1}, \ldots, \boldsymbol{z}_{t_N} = \text{ODESolve}(\boldsymbol{z}_{t_0}, \boldsymbol{f}_{\boldsymbol{\theta}}, t_0, \ldots, t_N)$).

3. Finally instead of sampling from a single point to get the reconstructed input data, we now sample from each $p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z}_{t_i})$, to get our to get our reconstructed input data at time t_i (i.e $\hat{\boldsymbol{x}}_{t_i} \sim p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z}_{t_i})$).

Therefore, to extrapolation of time-series data, $\boldsymbol{x}_{t_0}, \ldots, \boldsymbol{x}_{t_N}$. We first encode our observations, into the posterior distribution, where we then sample $\boldsymbol{z}_{t_0}$. Then we integrate our forcing function $f_{\boldsymbol{\theta}}$ forwards, in time, to the times $t_{N+1}, \ldots, t_M$, where we then decode our feature points (i.e $\hat{\boldsymbol{x}}_{t_i} \sim p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z}_{t_i})$ for $i \in \{N+1, \ldots, M\}$).

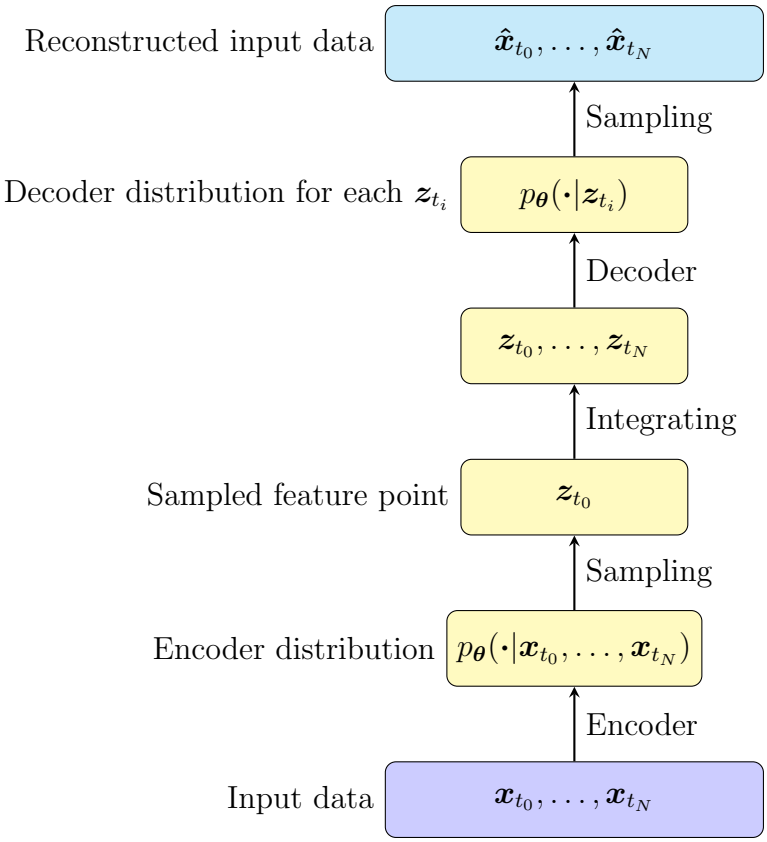


Figure 18: Graphical representation of the adaptive variational autoencoder evaluated at the points $\boldsymbol{x}_{t_0}, \ldots, \boldsymbol{x}_{t_N}$.

6.2 Bi-directional Spiral Example

In this section we will show how the adaptive version of the variational autoencoder can be used to extrapolate time-series data of bi-directional spirals. We start off by assuming that prior over the latent variables is given by an isotropic multivariate Gaussian $p_{\boldsymbol{\theta}}(\boldsymbol{z}) = \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$ and our true posterior $p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x}_{t_1}, , \boldsymbol{x}_{t_N})$, is a multivariate Gaussian. Therefore, we will approximate the true posterior $p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x}_{t_1}, \ldots, \boldsymbol{x}_{t_N})$, by a multivariate parametric Gaussian model that has a diagonal covariance (i.e $q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}_{t_1}, \ldots, \boldsymbol{x}_{t_N}) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\sigma}^2 I)$ where $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}^2$ are functions of $\boldsymbol{\phi}$). To produce the $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}$ that will be used in $q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}_{t_1}, \ldots, \boldsymbol{x}_{t_N})$, we define EncoderNeuralNet$_{\boldsymbol{\phi}}$ that encodes the observations, $\boldsymbol{x}_{t_0}, \ldots, \boldsymbol{x}_{t_N}$, into $\boldsymbol{\mu}$ and a $\boldsymbol{\sigma}$. The EncoderNeuralNet$_{\boldsymbol{\phi}}$ is a RNN that takes the input $\boldsymbol{x}_{t_1}, \ldots, \boldsymbol{x}_{t_N}$ and outputs the encoded $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}$ that is used in $q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}_{t_1}, \ldots, \boldsymbol{x}_{t_N})$.

Hence, to be able to have a complete model for training, we will make the additional assumption that the decoder distribution, $p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z}_{t_i})$, is a multivariate parametric Gaussian of the form, $p_{\boldsymbol{\theta}}(\cdot|\boldsymbol{z}_{t_i}) = \mathcal{N}(\hat{\boldsymbol{x}}_{t_i}, \sigma_2 \boldsymbol{I})$. Where $\hat{\boldsymbol{x}}_{t_i} = \text{DecoderNeuralNet}_{\boldsymbol{\theta}}(\boldsymbol{z}_{t_i})$ is the mean and σ_2 is the variance of our data. The DecoderNeuralNet$_{\boldsymbol{\theta}}$ is a NN that takes in the point $\boldsymbol{z}_{t_i}$ and produces the mean $\hat{\boldsymbol{x}}_{t_i}$. Therefore our ELBO takes the form,

$$\tilde{\mathcal{L}}(\boldsymbol{x}_{t_0}, , \boldsymbol{x}_{t_N}; \boldsymbol{\theta}, \boldsymbol{\phi}) \simeq \frac{1}{2} \sum_{j=1}^{m} (1 + \log((\boldsymbol{\sigma}_j)^2) - (\boldsymbol{\mu}_j)^2 - (\boldsymbol{\sigma}_j)^2) - \frac{1}{2\sigma_2} \sum_{i=0}^{N} ||\boldsymbol{x}_{t_i} - \hat{\boldsymbol{x}}_{t_i}||^2 + C$$

Where $\boldsymbol{z}_{t_0} = \boldsymbol{\mu} + \boldsymbol{\sigma} \odot \boldsymbol{\varepsilon}$, $\boldsymbol{\varepsilon} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})$ and C is a constant. We include the sum i from 0 to N in the ELBO, because we take samples from distributions $p_{\boldsymbol{\theta}}(\cdot|\boldsymbol{z}_{t_0}), \ldots, p_{\boldsymbol{\theta}}(\cdot|\boldsymbol{z}_{t_N})$. Hence, whole processes is described by the following figure,

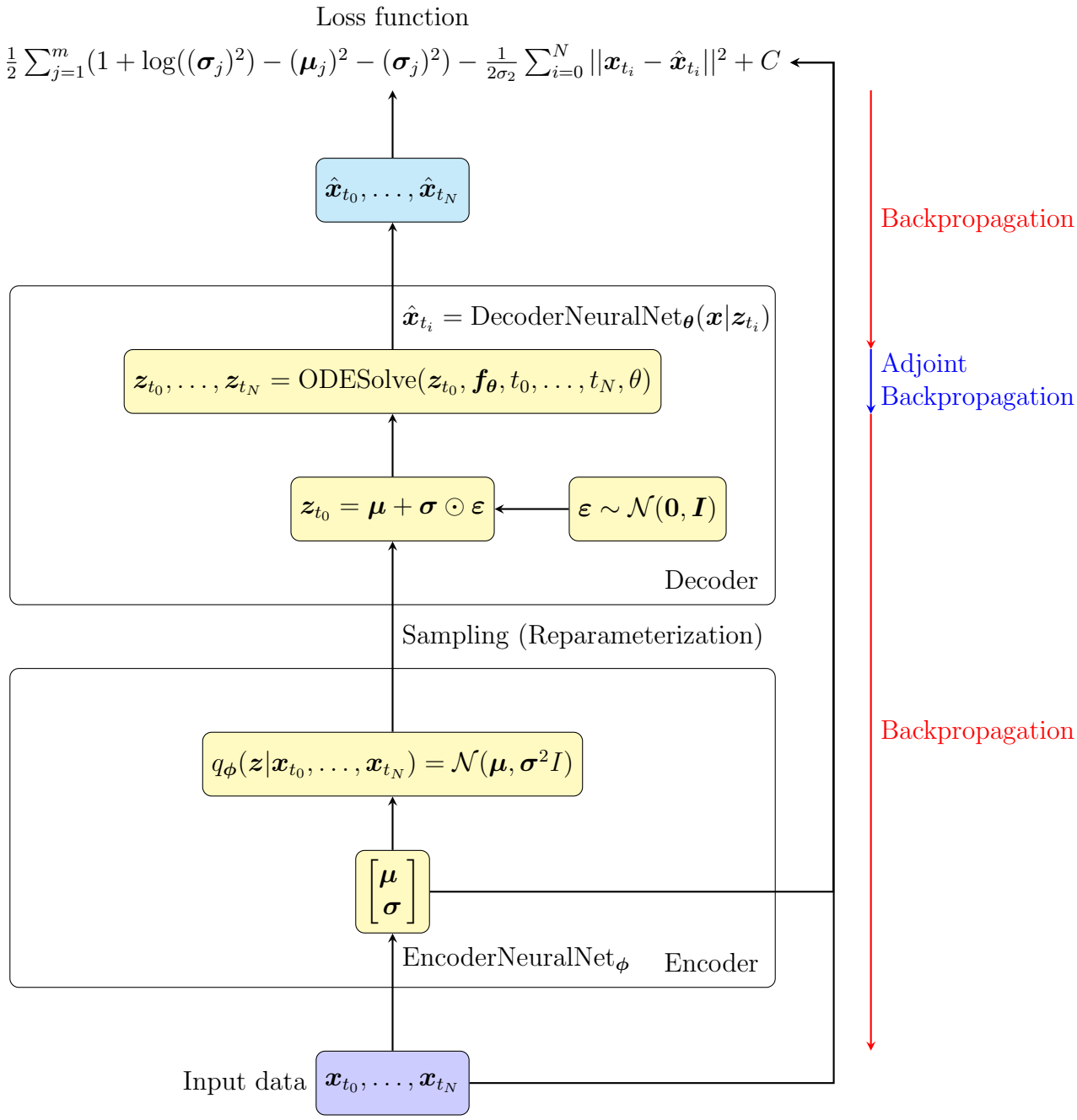
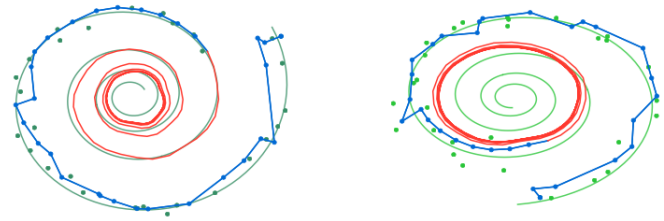


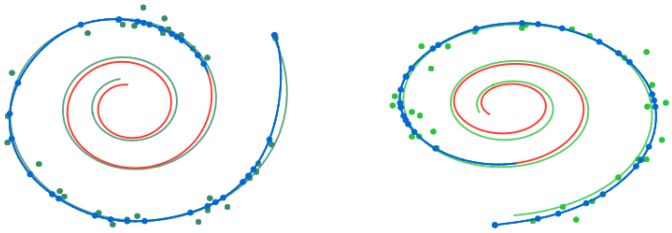
Figure 19: Trainable generative latent time-series model

By training the above model (over a 4-dimensional latent space) on 1000 2-dimensional spirals (half clockwise and half anti-clockwise), each starting at a different point and each spiral consisting of 100 observation that are equally-spaced (i.e $\boldsymbol{x}_{t_0}, \ldots, \boldsymbol{x}_{99}$). Where f_θ and $p_{\boldsymbol{\theta}}(\boldsymbol{x}_{\boldsymbol{t_i}}|\boldsymbol{z}_{t_i})$ describe by a two different one-hidden-layer NNs with 20 hidden units, and encoder network is a RNN with 25 hidden units. [3] shows in Figure. 20, that generative latent time-series models performs better at modelling the spiral dynamics of the observed spirals and produced close extrapolations dynamics. While the baseline RNN with 25 hidden units, trained to

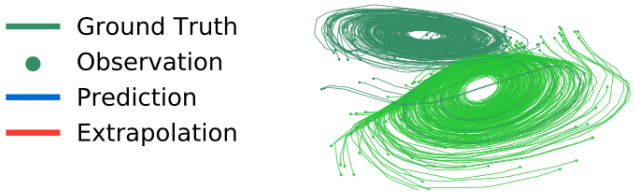
minimise negative Gaussian log-likelihood, overfit the training data by producing a "saw-tooth" effect and preformed poorly at extrapolating the dynamics, as it forms closed loops.



(a) Recurrent Neural Network



(b) Latent Neural Ordinary Differential Equation



(c) Latent Trajectories

Figure 20: (a): Reconstruction and extrapolation of spirals with irregular time points by a recurrent neural network. (b): Reconstructions and extrapoations by a latent neural ODE. Blue curve shows model prediction. Red shows extrapolation. (c) A projection of inferred 4-dimensional latent ODE trajectories onto their first two dimensions. Color indicates the direction of the corresponding trajectory. The model has learned latent dynamics which distinguishes the two directions.[3]

7 Conclusion

This report set out to discuss variational autoencoders and generative latent time-series models, and explore their applications in tackling the following problems:

1. Generation of new data: Suppose that we are given the dataset, $\boldsymbol{\mathcal{D}}$ which contains N independent data points. Then we aim to artificially generate data points that look like they came from the dataset $\boldsymbol{\mathcal{D}}$.

2. Extrapolation of time-series data: Suppose that we observe a system at discrete times $t_0, \ldots, t_N$. Then, given these observations, we would like to predict the system's state at the future times $t_{N+1}, \ldots, t_M$.

We tackled the generation of new data problem, by introducing variational autoencoders, that overcame the irregularity that appears in the latent space of autoencoders, which allowed for good properties when generative modelling. We then demonstrated this ability by training a variational autoencoder model on the MNIST dataset and produced unseen handwritten digits (Figure. 12 (b)).

Following that, we introduced neural ordinary differential equations and derived an expression for the derivative of the loss function with respect to the model parameters, that involves solving an ODE backward through the layers. Where we shown a coded example of this application, by learning the dynamics of a spiral, in Figure. 17.

Finally we combined the theory established throughout the paper by introducing generative latent time-series model aimed to tackle extrapolation of time-series data. However, due to time limitation, we were unable reproduce the bi-directional spiral example given in [3] of the generative latent time-series models or apply the theory to model more challenging datasets.

Appendix A

Gibbs' Inequality and Derivations

1 Gibbs' Inequality [1]

Let $p = \{p_1, \ldots, p_k\}$ and $q = \{q_1, \ldots, q_k\}$ be two arbitrary discrete probability distributions, then Gibbs' inequality states that,

$$-\sum_{i=1}^{k} p_i \log p_i \leq -\sum_{i=1}^{k} p_i \log q_i$$

and equality if and only if,

$$p_i = q_i, \;\; i \in \{1, \ldots, k\}$$

2 Adjoint and Augmented Dynamics Derivations

We will now expand upon the derivations given in Neural Ordinary Differential Equations paper [3] to include details that were omitted from the original paper.

2.1 Adjoint Derivation

In this section we will prove the statement claimed in Section 5.2, that the layer derivative of $\boldsymbol{a}(t)$ is given by,

$$\frac{d\boldsymbol{a}^T(t)}{dt} = -\boldsymbol{a}^T(t)\frac{\partial \boldsymbol{f}(\boldsymbol{z}(t), t, \theta)}{\partial \boldsymbol{z}(t)}. \tag{A.1}$$

It is important to remember that t is the layer depth and is now continuous.

We start by drawing parallels from a general (discrete) neural network. We use the fact that the gradient of the loss function with respect to the hidden layer $\boldsymbol{z}_t$, can be expressed in terms of the next layer $\boldsymbol{z}_{t+1}$,

$$\frac{dL}{d\boldsymbol{z}_t} = \frac{dL}{d\boldsymbol{z}_{t+1}}\frac{d\boldsymbol{z}_{t+1}}{d\boldsymbol{z}_t}$$

We now generalise this approach to a neural network with continuous hidden states, by first defining $\boldsymbol{z}(t+\varepsilon)$, as the following,

$$\boldsymbol{z}(t+\varepsilon) = \int_t^{t+\varepsilon} \boldsymbol{f}(\boldsymbol{z}(t), t, \theta)dt + \boldsymbol{z}(t) =: T_\varepsilon(\boldsymbol{z}(t), t), \quad \varepsilon > 0.$$

Hence, by applying the chain rule, we are able to express the gradient of the loss function with respect to the continuous hidden state $\boldsymbol{z}(t)$, in terms of gradients that include, $\boldsymbol{z}(t+\varepsilon)$.

$$\frac{dL^T}{d\boldsymbol{z}(t)} = \frac{dL^T}{d\boldsymbol{z}(t+\varepsilon)}\frac{d\boldsymbol{z}(t+\varepsilon)}{d\boldsymbol{z}(t)} \quad \text{or} \quad \boldsymbol{a}^T(t) = \boldsymbol{a}^T(t+\varepsilon)\frac{\partial T_\varepsilon(\boldsymbol{z}(t),t)}{\partial \boldsymbol{z}(t)} \tag{A.2}$$

Thus, we have the required machinery to prove (A.1),

$$\begin{aligned}
\frac{d\boldsymbol{a}^T(t)}{dt} &= \lim_{\varepsilon\to 0^+} \frac{\boldsymbol{a}^T(t+\varepsilon) - \boldsymbol{a}(t)^T}{\varepsilon} && \text{(Derivative definition)} \\
&= \lim_{\varepsilon\to 0^+} \frac{\boldsymbol{a}^T(t+\varepsilon) - \boldsymbol{a}^T(t+\varepsilon)\frac{\partial}{\partial \boldsymbol{z}(t)}T_\varepsilon(\boldsymbol{z}(t))}{\varepsilon} && \text{(Using (A.2))} \\
&\text{Now by expanding } T_\varepsilon(\boldsymbol{z}(t)) \text{ around } \boldsymbol{z}(t), \text{ we get,} \\
&= \lim_{\varepsilon\to 0^+} \frac{\boldsymbol{a}^T(t+\varepsilon) - \boldsymbol{a}^T(t+\varepsilon)\frac{\partial}{\partial \boldsymbol{z}(t)}(\boldsymbol{z}(t) + \varepsilon \boldsymbol{f}(\boldsymbol{z}(t),t,\theta) + \mathcal{O}(\varepsilon^2))}{\varepsilon} \\
&= \lim_{\varepsilon\to 0^+} \frac{\boldsymbol{a}^T(t+\varepsilon) - \boldsymbol{a}^T(t+\varepsilon)\left(I + \varepsilon\frac{\partial \boldsymbol{f}(\boldsymbol{z}(t),t,\theta)}{\partial \boldsymbol{z}(t)} + \mathcal{O}(\varepsilon^2)\right)}{\varepsilon} && \text{(Applying the derivative)} \\
&= \lim_{\varepsilon\to 0^+} \frac{-\varepsilon \boldsymbol{a}^T(t+\varepsilon)\frac{\partial \boldsymbol{f}(\boldsymbol{z}(t),t,\theta)}{\partial \boldsymbol{z}(t)} + \mathcal{O}(\varepsilon^2)}{\varepsilon} && \text{(Expanding bracket)} \\
&= \lim_{\varepsilon\to 0^+} -\boldsymbol{a}^T(t+\varepsilon)\frac{\partial \boldsymbol{f}(\boldsymbol{z}(t),t,\theta)}{\partial \boldsymbol{z}(t)} + \mathcal{O}(\varepsilon) && \text{(Cancelling terms)} \\
&= -\boldsymbol{a}^T(t)\frac{\partial \boldsymbol{f}(\boldsymbol{z}(t),t,\theta)}{\partial \boldsymbol{z}(t)} && \text{(Taking limit)}
\end{aligned}$$

Hence, we have arrived at what we set out to prove, that the layer derivative of $\boldsymbol{a}(t)$ is given by,

$$\frac{d\boldsymbol{a}^T(t)}{dt} = -\boldsymbol{a}^T(t)\frac{\partial \boldsymbol{f}(\boldsymbol{z}(t),t,\theta)}{\partial \boldsymbol{z}(t)}$$

2.2 Augmented Dynamics

By assuming that the model parameters $\boldsymbol{\theta}$ is layer invariant, we are able to generalise (26), to obtain the gradient of L with respect to $\boldsymbol{\theta}$ and t respectively.

To achieve this, we introduce the augmented state dynamics for our system. Which is defined as the following,

$$\frac{d\boldsymbol{z}_{\text{aug}}(t)}{dt} = \frac{d}{dt}\begin{bmatrix}\boldsymbol{z}\\ \theta \\ t\end{bmatrix}(t) = \boldsymbol{f}_{\text{aug}}([\boldsymbol{z},\theta,t]) := \begin{bmatrix}\boldsymbol{f}([\boldsymbol{z},\theta,t])\\ \boldsymbol{0} \\ 1\end{bmatrix} \tag{A.3}$$

$$\boldsymbol{a}_{\text{aug}}(t) := \begin{bmatrix}\boldsymbol{a}\\ \boldsymbol{a}_\theta \\ \boldsymbol{a}_t\end{bmatrix}(t), \quad \boldsymbol{a}_\theta(t) := \frac{dL}{d\theta(t)}, \quad \boldsymbol{a}_t(t) := \frac{dL}{dt(t)} \tag{A.4}$$

$$\frac{\partial \boldsymbol{f}_{\text{aug}}}{\partial[\boldsymbol{z}, \theta, t]} = \begin{bmatrix} \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{z}} & \frac{\partial \boldsymbol{f}}{\partial \theta} & \frac{\partial \boldsymbol{f}}{\partial t} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix}(t) \tag{A.5}$$

Where each $\mathbf{0}$ is a matrix of zeroes with the appropriate dimensions.

Therefore, by applying (A.1) to our augmented system, we can understand how the augmented adjoint changes with respect to the layer,

$$\begin{aligned} \frac{d\boldsymbol{a}_{\text{aug}}^T(t)}{dt} &= -\begin{bmatrix} \boldsymbol{a}^T(t) & \boldsymbol{a}_\theta^T(t) & \boldsymbol{a}_t^T(t) \end{bmatrix} \frac{\partial \boldsymbol{f}_{\text{aug}}}{\partial[\boldsymbol{z}, \theta, t]}(t) \\ &= -\begin{bmatrix} \boldsymbol{a}^T \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{z}} & \boldsymbol{a}^T \frac{\partial \boldsymbol{f}}{\partial \theta} & \boldsymbol{a}^T \frac{\partial \boldsymbol{f}}{\partial t} \end{bmatrix}(t) \end{aligned} \tag{A.6}$$

Thus, by looking at the second element of equation (A.6), we get the following relationship,

$$\frac{d\boldsymbol{a}_\theta^T(t)}{dt} = \frac{d}{dt}\left(\frac{dL^T}{d\theta}\right) = \boldsymbol{a}^T(t)\frac{\partial \boldsymbol{f}}{\partial \theta}$$

Therefore, by integrating backwards over the layers and setting the adjoint of θ at time t_1 to zero as it has not "accumulated" any error yet. We obtain the overall sensitivity of the model parameters,

$$\implies \frac{dL^T}{d\theta} = \boldsymbol{a}_\theta^T(t_0) = -\int_{t_1}^{t_0} \boldsymbol{a}^T(t)\frac{\partial \boldsymbol{f}(\boldsymbol{z}(t), \theta, t)}{\partial \theta} dt$$

Finally, we can work out expressions for the derivative of L with respect to the times t_0 and t_1, respectively. To derive the expression at t_1, we apply the chain rule to get,

$$\frac{\partial L^T}{\partial t_N} = \frac{\partial L^T}{\partial \boldsymbol{z}(t)}\frac{d\boldsymbol{z}(t)}{dt}\Big|_{t=t_N} = \boldsymbol{a}^T(t_N)\boldsymbol{f}(\boldsymbol{z}(t_N), \theta, t) \tag{A.7}$$

Hence, by using the final term in equation (A.6), and integrating backwards over the layers, we get,

$$\implies \frac{\partial L^T}{\partial t_0} = \boldsymbol{a}_t^T(t_0) = \boldsymbol{a}_t^T(t_1) - \int_{t_1}^{t_0} \boldsymbol{a}^T(t)\frac{\partial \boldsymbol{f}(\boldsymbol{z}(t), \theta, t)}{\partial t} dt \tag{A.8}$$

Up to now we have only considered our loss function L depends between t_0 and t_1. However, if we wanted to evaluate the ODE at multiple observations $t_0, \ldots, t_N$ (and therefore our loss function depends on $t_0, \ldots, t_N$), we would adapt the above process by iterating the process over the intervals, $[t_{N-1}, t_N], [t_{N-2}, t_{N-1}], \ldots$, accumulating the overall sensitivity of the model parameters from each interval.

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