## Imperial College of Science, Technology and Medicine Department of Computing

## On the Feasibility of Using Fully-Convolutional Variational Autoencoders to Advance Deep Symbolic Reinforcement Learning

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## Acknowledgements

I would like to express (whatever feelings I have) to:

- My supervisor
- My second supervisor
- Other researchers
- My family and friends

### Dedication

Dedication here.

'Quote text here.'

Guy Quoted

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## Chapter 1

## Introduction

### 1.1 Motivation

A long term goal of artificial intelligence (AI) is the development of artificial general intelligence (AGI). Since the field's inception in the 1950s, it has swung between hype and breakthroughs, followed by disappointment and reduced funding, known as AI winters [9]. During the first period of hype from the 50s to the early 70s, Marvin Minsky made the following prediction: [4]

"In from three to eight years we will have a machine with the general intelligence of an average human being." - Marvin Minsky, 1970

This prediction was clearly not realised, and the first AI winter would shortly follow.

Symbolic AI was developed during this winter, which encodes knowledge as human-readable rules and facts, making it easy to comprehend chains of actions and abstract relationships [14]. For instance, given the unary relations red and strawberry, and the binary relation bigger, we can say that A is the smallest red strawberry by writing

red(A) strawberry(A) ∀B bigger(B, A)

But given the unary relations yellow and banana we could also write that A is the third biggest yellow strawberry, or a red banana, and so on. We can see that the rules and facts in symbolic logic can be endlessly recombined and extended. This allows for the manipulation of high-level abstract concepts, which is key to AGI [6].

However, symbolic AI has a major philosophical problem: the facts and rules are only meaningful to the human writing them; their meaning is not intrinsic to the system itself. This is known as the *symbol grounding problem*.

Today we find ourselves in yet another period of hype and exciting breakthroughs not afflicted by the symbol grounding problem. Reinforcement learning (RL) has become a prominent area of research, with many considering it fundemental for AGI [7], as have deep neural networks. Recently, deep reinforcement learning (DRL) systems have achieved impressive feats, including mastering a wide range of Atari 2600 games to a superhuman level using only raw pixels and score as input, and the board game Go [12, 16].



Figure 1.1: May 1997: Gary Kasparov makes his first move against IBM's Deep Blue. Deep Blue would later emerge the victor in the best of six games; the first time a reigning world chess champion is defeated by a computer. [15]



Figure 1.2: March 2016: Lee Sedol, one of the greatest modern Go players, plays his first move of game three against AlphaGo. AlphaGo won four of five games. This feat was considered by many to be a decade away. [13]

Though DRL systems are not afflicted by the same problems as symbolic AI, they have a number of drawbacks of their own. Namely, they are: [6]

1. Slow to learn. Neural networks require large data sets and are therefore slow to learn.

1.1. Motivation 3

2. Unable to transfer past experience. They often fail to perform well on tasks very

similar to those they have mastered.

3. Unable to reason abstractly. They fail to exploit statistical regularities in the data.

4. Hard to reason about. It's often difficult to extract a comprehensible chain of reasons

for why a deep neural network operated in the way it did.

Deep symbolic reinforcement learning (DSRL) is a marrying of DRL and symbolic AI; a recent

advance which overcomes the symbol grounding problem and the drawbacks associated with

DRL [6]. That is, DSRL systems overcome the symbol grounding problem, and are:

1. **Fast to learn**. Large data sets are not necessary.

2. Able to transfer past experience. Symbolic AI lends itself to multiple processes

associated with high-level reasoning, including transfer learning.

3. Able to reason abstractly. The agent is able to exploit statistical regularities in the

training data by using high-level processes like planning or causal reasoning.

4. Easy to reason about. Since the front end uses symbolic AI, its knowledge is encoded

as human-readble facts and rules, making the extraction of comprehensible chains of logic

much easier.

An overview of DSRL is shown in Figure 1.3. The neural back end takes a high-dimensional

input and outputs a symbolic representation. This symbolic representation is then fed to the

symbolic front end, whose role is action selection. The agent then acts on the environment

and obtains a reward and the sensory input of the next time step. As the neural back end

learns how to represent the raw input data in a compositionally structured representation in

an unsupervised manner, and the symbolic front end learns to select the action with maximum

expected reward over time, the system as a whole learns end-to-end.

TODO: Finish description of DSRL

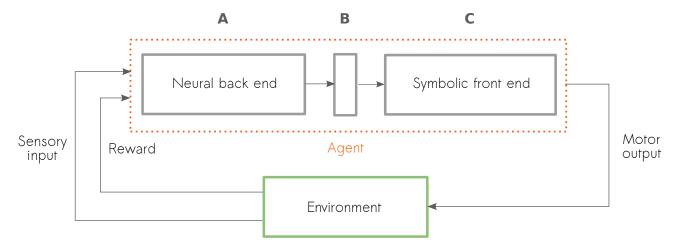


Figure 1.3: Overview of deep symbolic reinforcement learning system architecture. **A**: The neural back end maps high-dimensional raw input data to a compositionally structured symbolic representation. **B**: The compositionally structured symbolic representation. **C**: Reinforcement learning of mapping from symbolic representation to action with maximum expected reward over time. *Source: Garnelo et al.* [6].

### 1.2 Objectives

We'll use the image in Figure 1.4 as an example of a high-dimensional input to the neural back end. This world consists of only two shapes (circle and square) and four spaces occupied by at most one shape (top left, top right, bottom left and bottom right). The neural back end maps this raw high-dimensional input to a low-dimensional symbolic representation, shown in Table ??.

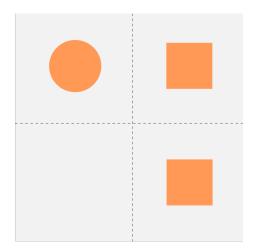


Figure 1.4: A toy example of a raw high-dimensional input.

How this is done will be explained in Chapter 2, but as for now we can just take it as fact that the current method doesn't scale. That is, for very simple scenes, as in Figure ..., This is done 1.3. Contributions 5

Type	Location
1	[0, 0]
2	[0, 1]
2	[1, 1]

Table 1.1: Low-dimensional symbolic representation

by passing the high-dimensional input through a series of convolutional layers and extracting the activation spectra in the latent space. These spectra are then used to classify the

relies on the unsupervised extraction of disentangled features, allowing for transfer learning and high-level cognitive processes. However, the unsupervised extraction of features from a wide range of scenes is still a challenge in AI research [?]. Fortunately methods are getting better, and the first unsupervised scalable model  $\beta$ -VAE was developed recently.

TODO: Finish objectives

### 1.3 Contributions

Contributions here.

## Chapter 2

## **Background Theory**

### 2.1 Introduction

We will cover how deep symbolic reinforcement learning extracts symbolic representations from raw input data, which will motivate a discussion of loss functions and the introduction of autoencoders. Seeing the limitations of the current approach in extracting symbolic representations, we can appreciate the recent development of  $\beta$ -VAE, a variant of the variational autoencoder used to learn disentangled representations. Finally, we can conclude by mentioning less technical matters, such as libraries and hardware used.

### 2.2 Arithmetic in Neural Networks

#### 2.2.1 Neurons

#### 2.2.2 Activation Functions

#### 2.2.3 Convolutions

#### 2.2.4 Deconvolutions

### 2.2.5 Pooling and Up-Sampling

### 2.3 Loss functions

The idea of image reconstruction plays a vital role throughout this project. Although it's possible to qualitatively compare the original to its reconstruction, it's important to be able to quantify the difference, which lends itself to automation. The loss function will quantify how similar two images are.

To compare loss functions, we'll use the MNIST data set. MNIST is a collection of 70,000 black-and-white images of handwritten digits, with 60,000 in the training set containing and 10,000 in the test set. These images will be represented as vectors without loss of generality.

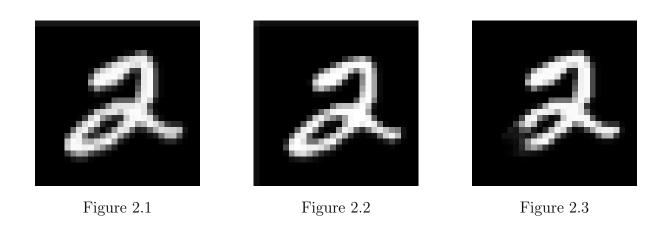
#### 2.3.1 Euclidean Distance

The Euclidean distance between two vectors  $\boldsymbol{x}$  and  $\boldsymbol{y}$  is defined by

$$\sqrt{\sum_{i} (x_i - y_i)^2}$$

where  $x_i$  and  $y_i$  are the  $i^{th}$  components of  $\boldsymbol{x}$  and  $\boldsymbol{y}$  respectively.

Euclidean distance is an intuitive measure of the distance between two points in space. Unfortunately, this doesn't also translate to visual similarity, as illustrated by Doersch et al. [5]. Figure 2.1 is a digit drawn from the MNIST dataset, and Figures 2.3 and 2.2 are attempted reconstructions. Of the reconstructions, Figure 2.2 looks most like the original, but Figure 2.3 is closer in space.



This leads to an alternative measure, binary cross-entropy, which gives a much better quantification of how visually similar two images are.

### 2.3.2 Binary Cross-Entropy

Consider a single black-and-white pixel with probability p(0) = c of being 0 and p(1) = 1 - c of being 1. Here p(x) is a probability distribution over the possible pixel values  $x \in \{0, 1\}$ . Suppose a given model tries to learn the distribution described by p(x), and says that the pixel has probability  $q(0) = \hat{c}$  of being 0 and  $q(1) = 1 - \hat{c}$  of being 1. The model is perfect if it learns the true distribution, that is, if q(x) = p(x) for  $x \in \{0, 1\}$ . We'd like to quantify how similar the distributions p and q are.

This is done by computing the binary cross-entropy between p and q, which is defined by

$$H(p,q) = -c \log \hat{c} - (1-c) \log(1-\hat{c})$$

To see how we may use this as a similarity measure among images, consider a  $1 \times 1$  image.

Normalising this image yields a pixel value in the interval [0, 1], which may now be interpreted as a probability, corresponding to c above. In the normalised reconstructed image, the pixel value corresponds to  $\hat{c}$ . We simply compute the binary cross-entropy to measure the similarity of these two distributions, and in turn, the similarity of the images themselves! (Note: we could have also assigned the probabilities to 1 - y and  $1 - \hat{y}$  by symmetry of binary cross-entropy).

For images larger than  $1 \times 1$ , we may take the component-wise binary cross-entropy, then, for example, average the components. How the component-wise binary cross-entropies are combined to give a score single floating point number is the choice of the designer and will vary from problem to problem.

### 2.4 Autoencoders

An autoencoder is a neural network that learns a compression algorithm for its input data in an unsupervised manner [11]. This is achieved by placing constraints on a hidden layer, called the latent space, and setting the target values to the input values, effectively learning the identity function. Since the network is trying to reconstruct the original input from the constrained latent space, over time the latent space corresponds to a meaningful compression of the network's input.

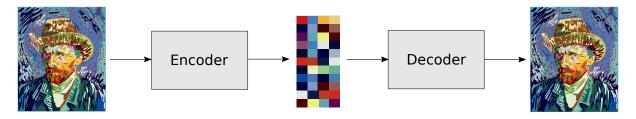


Figure 2.4: A black-box description of an autoencoder. The autoencoder learns the identity function, and in turn, the encoder and decoder learn suitable encoding and decoding algorithms respectively.

As before, we will use the MNIST data set to compare architectures. Unless specified in the example, the Adam optimiser is used with a learning rate of 1e - 4, the batch size is 1 and the loss function is binary cross-entropy. Intermediate layers use the ReLU activation function, while the final layer uses sigmoid.

### 2.4.1 Fully-Connected Autoencoders

In dense feed-forward neural networks we may place a constraint on the latent space by reducing the number of neurons, as shown in Figure 2.5. Images must be flattened into vectors to be fed as input. Consequently, any spatial information is destroyed in dense feed-forward neural networks.

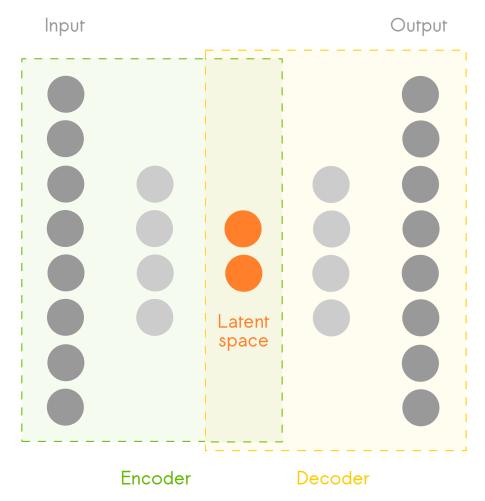


Figure 2.5: An example architecture of a fully-connected autoencoder. The latent space is constrained by having fewer neurons than the input and output layers.

An example architecture is given in Table 2.1, which was trained on MNIST. Despite the latent space being  $\sim 4\%$  of the size of the input space, the network is capable of producing realistic reconstructions. For verification, a collection of samples from the dataset and their corresponding reconstructions are shown in Figure 2.6.

Layer Type	Output Shape
InputLayer	(1, 28, 28)
Flatten	(784,)
Dense	(32,)
Dense	(784,)
Reshape	(1, 28, 28)

Table 2.1: A simple fully-connected autoencoder with one hidden layer. After 15 epochs, the validation score was recorded to be 71.94.

### 2.4.2 Fully-Convolutional Autoencoders

In fully-convolutional feed-forward neural networks, we may place a constraint on the latent space by reducing the number and/or size of the filters, as shown in Figure 2.8. To compare the fully-convolutional autoencoder to the fully-connected, we'll train the architecture in Table 2.2 on MNIST. As before, we'll compare the reconstructions to the originals, which can be found in Figure 2.7.

Layer Type	Output Shape
InputLayer	(1, 28, 28)
Conv2D	(32, 28, 28)
MaxPooling2D	(32, 14, 14)
Conv2D	(4, 14, 14)
MaxPooling2D	(4, 7, 7)
UpSampling2D	(4, 14, 14)
Conv2DTranspose	(32, 14, 14)
UpSampling2D	(32, 28, 28)
Conv2DTranspose	(1, 28, 28)

Table 2.2: A simple fully-convolutional autoencoder with 2D convolutions and max pooling, plus the corresponding deconvolutional layers. After 15 epochs, the validation score was recorded to be 64.89.

Convolutional layers have been shown to be effective in tasks with images as input [10, 18, 17]. This is because spatial information is preserved in convolutional layers, and the number of trainable parameters is far less in a convolutional layer than it is in a fully connected layer. Convolutional layers will be used from here on as we'll be using images as input.

#### 2.4.3 Variational Autoencoders

The variational autoencoder is central to this project, and we'll therefore dedicate a considerable amount of time exploring it. First we'll precisely define the problems the variational autoencoder solves, after which we may develop its loss function and detail its implementation. This section will conclude by developing an intution of the theory covered by way of examples.

#### Introduction: A Probabilistic Perspective

Let  $X = \{x^{(i)}\}_{i=1}^N$  be the data set of N independent and identically distributed samples of the variable  $\boldsymbol{x}$ . (X may be a data set of images, for instance). Let us assume that these samples are generated by a random process with parameters  $\boldsymbol{\theta}^*$  involving an unobserved latent variable  $\boldsymbol{z}$  in the following way:

```
Algorithm 1 Generate data set X

1: for i = 1 \rightarrow N do

2: \mathbf{z}^{(i)} \sim p_{\theta^*}(\mathbf{z}) // Sample from true prior

3: \mathbf{x}^{(i)} \sim p_{\theta^*}(\mathbf{x}|\mathbf{z}^{(i)}) // Sample from true conditional

4: Append \mathbf{x}^{(i)} to X

5: end for
```

We only observe the data set X in this process. The parameters  $\boldsymbol{\theta}^*$  and latent variables  $Z = \{\boldsymbol{z}^{(i)}\}_{i=1}^N$  are unknown to us. Let us assume that the prior  $p_{\boldsymbol{\theta}^*}(\boldsymbol{z})$  and conditional  $p_{\boldsymbol{\theta}^*}(\boldsymbol{x}|\boldsymbol{z})$  are parameterised by the distributions  $p_{\boldsymbol{\theta}}(\boldsymbol{z})$  and  $p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})$  respectively. In this context, the variational autoencoder provides [8]:

- 1. ML or MAP estimation for the parameters  $\boldsymbol{\theta}$
- 2. An approximation of the latent variable  $\boldsymbol{z}^{(i)}$  given  $\boldsymbol{x}^{(i)}$  and set of parameters  $\boldsymbol{\theta}$
- 3. Approximate marginal inference of the variable  $\boldsymbol{x}$

#### Overcoming the Intractable Posterior

The variational autoencoder solves the problems above by approximate inference of the latent variable z. Exact inference is not possible, and to see this we may use Bayes' theorem to find an expression for the posterior:

$$p_{\theta}(\boldsymbol{z}|\boldsymbol{x}) = \frac{p_{\theta}(\boldsymbol{x}|\boldsymbol{z})p_{\theta}(\boldsymbol{z})}{p_{\theta}(\boldsymbol{x})}$$

The marginal likelihood

$$p_{m{ heta}}(m{x}) = \int p_{m{ heta}}(m{z}) p_{m{ heta}}(m{x}|m{z}) dm{z}$$

involves an exponential-time integral over every combination of the latent variable z, and is therefore computationally intractable [8]. Instead, we define an approximation  $q_{\phi}(z|x)$  to the intractable posterior. Since  $q_{\phi}(z|x)$  gives a distribution over the possible latent variables z that generated the given data point x, it is known as the probabilistic decoder. By the same reasoning,  $p_{\theta}(x|z)$  is known as the probabilistic decoder.

#### Finding a Suitable Loss Function: the ELBO

The variational autoencoers's ability to learn the generative parameters  $\theta^*$  relies on how closley  $q_{\phi}(\boldsymbol{z}|\boldsymbol{x})$  approximates  $p_{\theta}(\boldsymbol{z}|\boldsymbol{x})$ . In the interest of training a model, this difference will be quantified. For this we use the KL divergence

$$D_{KL}(q_{\phi}(\boldsymbol{z}|\boldsymbol{x})||p_{\theta}(\boldsymbol{z}|\boldsymbol{x})) = \mathbf{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[ \log_{e} \frac{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}{p_{\theta}(\boldsymbol{z}|\boldsymbol{x})} \right]$$

which measures how much information is lost when we represent  $p_{\theta}(\boldsymbol{z}|\boldsymbol{x})$  with  $q_{\phi}(\boldsymbol{z}|\boldsymbol{x})$  (measured in nats) [3]. Using the KL divergence, our problem now amounts to the optimisation problem [?]:

$$\boldsymbol{\theta}^*, \boldsymbol{\phi}^* = \arg\min_{\boldsymbol{\theta}^*, \boldsymbol{\phi}^*} D_{KL}(q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})||p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x}))$$
(2.1)

To see how we can start to minimise the KL divergence, we'll start by rewriting it in a different form:

$$D_{KL}(q_{\phi}(\boldsymbol{z}|\boldsymbol{x})||p_{\theta}(\boldsymbol{z}|\boldsymbol{x})) = \mathbf{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[ \log_{e} \frac{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}{p_{\theta}(\boldsymbol{z}|\boldsymbol{x})} \right]$$

$$= \mathbf{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[ \log_{e} q_{\phi}(\boldsymbol{z}|\boldsymbol{x}) \right] - \mathbf{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[ \log_{e} p_{\theta}(\boldsymbol{z}|\boldsymbol{x}) \right]$$

$$= \mathbf{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[ \log_{e} q_{\phi}(\boldsymbol{z}|\boldsymbol{x}) \right] - \mathbf{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[ \log_{e} p_{\theta}(\boldsymbol{z},\boldsymbol{x}) \right] + \mathbf{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[ \log_{e} p_{\theta}(\boldsymbol{x}) \right]$$

$$= \mathbf{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[ \log_{e} \frac{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}{p_{\theta}(\boldsymbol{z},\boldsymbol{x})} \right] + \log_{e} p_{\theta}(\boldsymbol{x})$$

$$(2.2)$$

Here we see that the KL divergence depends on the intractable marginal likelihood  $p_{\theta}(x)$ ! There's no way we can minimise it if we can't write down  $p_{\theta}(x)$ . However, we can get around this: we'll minimise the KL divergence, but not directly. Instead, we try to find a quantity which we can maximise, and show that in turn this minimises the KL divergence. The trick is not obvious, but is simply done by finding a lower bound on the log marginal likelihood.

Using Jensen's inequality

$$f(\mathbf{E}[X]) \ge \mathbf{E}[f(X)]$$

we can write down a lower bound on the log marginal likelihood:

$$\log_{e} p_{\theta}(\boldsymbol{x}) = \log_{e} \int p_{\theta}(\boldsymbol{x}, \boldsymbol{z}) d\boldsymbol{z}$$

$$= \log_{e} \int p_{\theta}(\boldsymbol{x}, \boldsymbol{z}) \frac{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} d\boldsymbol{z}$$

$$= \log_{e} \mathbf{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[ \frac{p_{\theta}(\boldsymbol{x}, \boldsymbol{z})}{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \right]$$

$$\geq \mathbf{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[ \log_{e} \frac{p_{\theta}(\boldsymbol{x}, \boldsymbol{z})}{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \right]$$

$$:= \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \boldsymbol{x})$$

$$(2.3)$$

Expression (2.3) is called the ELBO (short for expected lower bound) [2, 8].

How does the ELBO help us with minimising the KL divergence? First recall the alternative

form of the KL divergence written in Equation (2.2):

$$D_{KL}(q_{\phi}(\boldsymbol{z}|\boldsymbol{x})||p_{\theta}(\boldsymbol{z}|\boldsymbol{x})) = \mathbf{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[ \log_{e} \frac{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}{p_{\theta}(\boldsymbol{z},\boldsymbol{x})} \right] + \log_{e} p_{\theta}(\boldsymbol{x})$$

Writing this in terms of the ELBO we have:

$$D_{KL}(q_{\phi}(\boldsymbol{z}|\boldsymbol{x})||p_{\theta}(\boldsymbol{z}|\boldsymbol{x})) = -\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \boldsymbol{x}) + \log_{e} p_{\theta}(\boldsymbol{x})$$

Since the KL divergence is the negative of the ELBO up to an additive constant (with respect to q), minimising the KL divergence is equivalent to maximising the ELBO [1]. Now we may make a revision to our original optimisaiton problem (2.1). Our problem is now written as:

$$\boldsymbol{\theta}^*, \boldsymbol{\phi}^* = \arg \max_{\boldsymbol{\theta}^*, \boldsymbol{\phi}^*} \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \boldsymbol{x})$$
 (2.4)

#### Writing the ELBO in Closed-Form

We've found that we can maximise the ELBO to minimise the KL divergence between the approximation  $q_{\phi}(\boldsymbol{z}|\boldsymbol{x})$  and the intractable posterior  $p_{\theta}(\boldsymbol{z}|\boldsymbol{x})$ . The ELBO may be written as follows:

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \boldsymbol{x}) = \mathbf{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})} \left[ \log_e \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})} \right]$$
(2.5)

$$= -\mathbf{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[ \log_e \frac{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}{p_{\theta}(\boldsymbol{x},\boldsymbol{z})} \right]$$
 (2.6)

$$= -\mathbf{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[ \log_e \frac{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}{p_{\theta}(\boldsymbol{x}|\boldsymbol{z})p_{\theta}(\boldsymbol{z})} \right]$$
(2.7)

$$= -\mathbf{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[ \log_e \frac{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}{p_{\theta}(\boldsymbol{z})} \right] + \mathbf{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[ \log_e p_{\theta}(\boldsymbol{x}|\boldsymbol{z}) \right]$$
(2.8)

$$= -D_{KL}(q_{\phi}(\boldsymbol{z}|\boldsymbol{x})||p_{\theta}(\boldsymbol{z})) + \mathbf{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}[\log p_{\theta}(\boldsymbol{x}|\boldsymbol{z})]$$
(2.9)

Thus for a single data point  $x^{(i)}$ , the *ELBO* becomes:

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \boldsymbol{x}^{(i)}) = -D_{KL}(q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})||p_{\boldsymbol{\theta}}(\boldsymbol{z})) + \mathbf{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})} \left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z})\right]$$
(2.10)

With some assumptions and a bit of work, we're finally in a position to write the ELBO in closed-form. The first term is the KL divergence between the probabilistic encoder and the prior. To make our lives simpler, we can choose the prior to be the isotropic multivariate Gaussian:

$$p_{\theta}(z) = \mathcal{N}(0, I) \tag{2.11}$$

We will also assume that the posterior is a k-dimensional Gaussian with diagonal covariance

$$p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x}^{(i)}) = \mathcal{N}(\boldsymbol{\mu}^{(i)}, \boldsymbol{\sigma}^{2(i)}\boldsymbol{I})$$
(2.12)

where  $\boldsymbol{\mu}^{(i)}$  and  $\boldsymbol{\sigma}^{(i)}$  are the mean and standard deviation (respectively) for data point  $\boldsymbol{x}^{(i)}$ . With these two assumptions, and the KL divergence for k-dimensional Gaussians,

$$D_{KL}(\mathcal{N}_0||\mathcal{N}_1) = \frac{1}{2} \left[ \operatorname{tr}(\boldsymbol{\Sigma}_1^{-1} \boldsymbol{\Sigma}_0) + (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0)^T \boldsymbol{\Sigma}_1^{-1} (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0) - k + \ln \left( \frac{\det \boldsymbol{\Sigma}_1}{\det \boldsymbol{\Sigma}_0} \right) \right]$$
(2.13)

we may write the first term in closed form:

$$D_{KL}(q_{\phi}(\boldsymbol{z}|\boldsymbol{x}^{(i)})||p_{\theta}(\boldsymbol{z})) = \frac{1}{2} \left[ \sum_{i=1}^{k} \sigma_{j}^{2(i)} + \sum_{j=1}^{k} \mu_{j}^{2(i)} - k - \ln \prod_{j=1}^{k} \sigma_{j}^{2(i)} \right]$$
(2.14)

Now we turn our attention to the second term of the ELBO:

$$\mathbf{E}_{q_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x}^{(i)})} \left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}|\boldsymbol{z})\right] \tag{2.15}$$

Luckily maximising terms like this is encountered regularly in statistics, and is known as maximum likelihood estimation. This can be taken to be the reconstruction loss as we defined it in the non-variational autoencoders earlier.

#### Implementing the Variational Autoencoder

In summary, to solve the original problems specified in the introduction, we



Figure 2.6: A collection of images from the MNIST data set and their respective reconstructions using the fully-connected autoencoder specified in Table 2.1. The original MNIST images are in odd columns, and their reconstructions to their immediate right.



Figure 2.7: A collection of images from the MNIST data set and their respective reconstructions using the fully-convolutional autoencoder specified in Table 2.2. The original MNIST images are in odd columns, and their reconstructions to their immediate right.



Figure 2.8: An example architecture of a fully-convolutional autoencoder. The latent space is constrained by reducing the number and/or size of the filters.

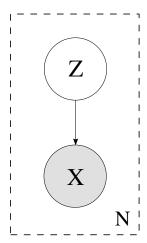


Figure 2.9: An example architecture of a fully-convolutional autoencoder. The latent space is constrained by reducing the number and/or size of the filters.

# Chapter 3

## Conclusion

## 3.1 Summary of Thesis Achievements

Summary.

## 3.2 Applications

Applications.

### 3.3 Future Work

Future Work.

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