List of topics to cover

With section titles and brief explantions.

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Abstract

punkt. punkt.

Declaration

punkt. punkt.

Acknowledgement

punkt.[8] punkt. bip/bop/boop **XxZzYyWw**$\mathbb{Z}$ so-so–so—so

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Introduction

punkt. *punkt*, *punkt*.

Chapter 2

Notations and definitions, preliminary concepts

2.1 Tensors, shape, axis, dimension

In machine learning one often encounters data structures that have multi-dimensional *shape* which we call *tensors*. For example a 28 over 28 color image can be represented as a 3-dimensional shape $(28, 28, 3)$ representing pixel's height, width, and rgb color "channel". This creates some confusion as to what one means by dimensions. For example a vector $\mathbf{x} \in \mathbb{R}^5$ is represented as a 1 dimensional shape but it has 5 *dimensions in total*. Similarly the color image has a 3 dimensional shape but it has $28 \cdot 28 \cdot 3$ dimensions in total. It has 3 *axes*, whose respective sizes are 28, 28, and 3.

A (real valued) *tensor* is an element of a tensor product space, for example the color image described above, $\mathbf{x} \in \mathbb{R}^{28\times 28\times 3} \triangleq \mathbb{R}^{28} \otimes \mathbb{R}^{28} \otimes \mathbb{R}^3$. A *tensor* has 0 or more axes and it generalizes scalar, vector, matrix and higher dimensional shaped entities.

In Pytorch [15] terminology dimension is used for the number of axes but I think it is inconsistent with the way dimension is used in mathematics with regards to vectors.

Definition 2.1. A *scalar* $x \in \mathbb{R}$ is an element of the (real) field. It has 0 *dimensions*, 0 *axes* and *shape* $(,)$.

A *vector* $\mathbf{x} \in \mathbb{R}^n$ has n dimensions, 1 axis, and shape $(n,)$.

A matrix $\mathbf{X} \in \mathbb{R}^{m\times n}$ has mn dimensions (in total), 2 axes, and shape of (m, n). Its first and second axes are said to be of sizes m and n respectively.

A tensor $\mathbf{x} \in \mathbb{R}^{n_1\times\cdots\times n_k}$ has $\prod_1^k n_i$ dimensions, k axes, and shape $(n_1, \ldots, n_k)$. Its i's axis is said to be of size n_i.

In practice a tensor $\mathbf{x} \in \mathbb{R}^{n_1\times\cdots\times n_k}$ is represented as a k dimensional array. We call its first axis the *row axis* or alternatively when we want to emphasize that this is a collection of several tensors, the *batch axis*. The tensor $\mathbf{x}_i = \mathbf{x}[i]$, which is the $k-1$ dimensional sub-array with the first coordinate held fixed, is called the *i'th row* of $\mathbf{x}$. Sometimes we want to represent a tensor $\mathbf{x}$ as a collections of tensors. For example it can represent a collection of several images. Each "row" then represents an image tensor.

It may be that our data set comes not as one tensor but in several tensors. For example we might have a tensor $\mathbf{x}$ representing an ordered set of images, and a tensor $\mathbf{y}$ which represents the category of each image. Because they have different shapes they don't fit together in one tensor. However since they refer to the same entities (images) their first axes have equal sizes. We use the notation $(\mathbf{x}, \mathbf{y})$ to denote the matching pairs of image/category, implicitly requiring them to have equally sized first axes.

If $\mathbf{x}, \mathbf{y}$ have the same number of axes and their respective axes sizes are equal on all but the last axis then we can concatenate them by "stacking" $\mathbf{y}$ on top of $\mathbf{x}$ along the last axis.

Definition 2.2. If $\mathbf{x}$ is a tensor, $\mathbf{x}_i$ represents the i'th "row" of $\mathbf{x}$, and $\mathbf{x} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ is the *row representation* or *batch representation* of $\mathbf{x}$.

Definition 2.3. Let $\mathbf{x}, \mathbf{y}$ be tensors whose first axes have equal dimensions, n. Then $(\mathbf{x}, \mathbf{y})$ is the set of ordered pairs $(\mathbf{x}, \mathbf{y}) \triangleq \{(\mathbf{x}_i, \mathbf{y}_i) : i = 1 \ldots n\}$.

Definition 2.4. If $\mathbf{x}, \mathbf{y}$ have the same number of axes and equal dimension on all but their last axis, the $(\mathbf{x}|\mathbf{y})$ is their concatenation on the last axis.

2.2 samples, batches, mean-sum rule

We distinguish between two types of tensors depending on what they represents. Let $\mathbf{x} \in \mathbb{R}^{m \times n \times l}$ be a tensor. If we say that $\mathbf{x}$ is a *sample* or a *data point* it means it is a single sample from our data set. If we say that it is a *batch*, then it represent a collection of m samples. In this case the first axis is the batch axis and the rest of the axes are the sample axes.

As a rule the default reduction is summation over sample axes and mean over the batch axes. For example if $\mathbf{x}$ is a sample, then $\|\mathbf{x}\|_1 = \sum_i \sum_j \sum_k |x_{i,j,k}|$ because it has no batch axis. If $\mathbf{x}$ is a batch, then we take the mean over the first axis: $\|\mathbf{x}\|_1 = \frac{1}{m} \sum_i \|\mathbf{x}_i\|_1 = \frac{1}{m} \sum_i \sum_j \sum_k |x_{i,j,k}|$.

The reason that we do that is that for batches, we want batches of different sizes to be comparable so it is straight forward to take mean. For the other axes, as we will see in the case of VAE we use the ELBO function where we have to sum over the sample axes.

2.3 Matrices and vectors

The type of data we work with in this paper can be represented as vectors. For example images of shape (h, w, c) can be flattened into a single axis shape $(h \cdot w \cdot c,)$ vector.

Throughout this paper (modulo typing errors) we use capital bold math Latin or Greek letters $(\boldsymbol{X}, \boldsymbol{\Sigma})$ to represent matrices. To stress that we talk about matrices rather than vectors we show product $(\times)$ in the dimension, i.e $\boldsymbol{X} \in \mathbb{R}^{m \times n}$. Although technically the matrix–space is the tensor product $\mathbb{R}^m \otimes \mathbb{R}^n$.

Bold small math letters $(\boldsymbol{x})$ represent usually row vectors, but in cases where it makes sense may also represent matrices such as a batch of several vectors (each row is a different data point). In few occasions it makes sense to let it represent both a matrix and a vector,

for example, $\boldsymbol{\sigma}$ may represent both the covariance matrix and the variance vector of a diagonal Gaussian distribution. Non-bold math letters $(x, \sigma, \dots)$ may represent scalar or vectors in some cases and hopefully it is clear from the context or explicitly stated.

Since we are only dealing with real matrices the transpose and the conjugation operators are the same ($A^T = A^*$) but over $\mathbb{C}$ conjugation is usually the "natural" operation and we use it to indicate that some property is still valid over $\mathbb{C}$ with conjugation.

Sometimes matrices are given in row/column/block notations inside brackets where the elements are concatenated in a way that makes positional sense. For example both $(\mathbf{x}, \mathbf{y})$ and $(\mathbf{x}|\mathbf{y})$ represent a matrix with 2 **columns**.

As mentioned usually just $\mathbf{x}$ means a column vector and $\mathbf{x}^T$ means a row vector but sometimes in matrix notation $\mathbf{x}$ represents a row when it makes sense. We use **curly** brackets to indicate the **row** representations of a matrix. For example $\{\mathbf{x}, \mathbf{y}\}$ represents a matrix whose **rows** are $\mathbf{x}$ and $\mathbf{y}$ (as row vectors), which alternatively could be represented as $(\mathbf{x}, \mathbf{y})^T$ (and symmetrically $(\mathbf{x}, \mathbf{y}) = \{\mathbf{x}, \mathbf{y}\}^T$).

$(\mathbf{X}, \mathbf{Y})$ or $(\mathbf{X}|\mathbf{Y})$ represent concatenation of two matrices along the second axis (concatenation of rows) which implicitly means they have the same number of rows. $\{\mathbf{X}, \mathbf{Y}\}$ represents concatenation along the first axis (concatenation of columns) which implies they must have equal number of columns.

Zero–blocks are indicated with 0 or are simply left as voids. For example $\begin{pmatrix} \boldsymbol{A} & \boldsymbol{B} \\ \mathbf{0} & \boldsymbol{D} \end{pmatrix}$, $\begin{pmatrix} \boldsymbol{A} & \boldsymbol{B} \\ & \boldsymbol{D} \end{pmatrix}$ both represent block notation of the same upper–triangular matrix.

Definition 2.5. Let $\mathbf{X} = \{\mathbf{x}_1, \dots \mathbf{x}_m\} \in \mathbb{R}^{m \times n}$ be a matrix in **row** notation. Then its *squared Frobenius norm* is

$$\|X\|_F^2 \triangleq \operatorname{trace}(\mathbf{X}\mathbf{X}^*) = \sum_{i=1}^{m} \|\mathbf{x}_i\|_2^2 = \sum_{i=1}^{m} \sum_{j=1}^{n} x_{ij}^2 \tag{2.1}$$

2.4 Functions and maps

Functions are usually understood to be scalar, namely $f : \mathbb{R}^n \to \mathbb{R}$ while maps are more general $g : \mathbb{R}^n \to \mathbb{R}^m$. When we say that a map (or function) $\phi : \mathbb{R}^n \to \mathbb{R}^m$ is *parameterized*, it implicitly means that ϕ has additional variables which we treat as parameters $\phi_{\mathbf{w}}(\mathbf{x}) = \phi(\mathbf{x}, \mathbf{w})$ where $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{w}$ is the parameter set which we don't always specify its domain and we may not always subscript ϕ with it. The parameterized map ϕ itself may be identified with its parameter set and then both are designated with ϕ.

In the context of neural networks, when we say *linear* map, we actually mean an *affine* map. An affine map $f(x_1 \dots x_n)$ can always be represented as a linear map with one extra variable which is held fixed $x_0 \equiv 1$: $f(x_0, \dots x_n) = b + a_1 x_1 + \dots a_n x_n$. We call b the *bias* of the linear map f.

2.5 Data types

we assume that the input data unless otherwise stated is real-valued matrix. Rows represent *samples* and columns represent *variables*. We assume that each raw is a realization of a random vector. If we have N rows, then the corresponding N random vectors are assumed to be independent. So depending on the context, when we say observation, or row, we may mean the actual observed values, or to the random vector which was realized by said observation.

We deal with two kinds of datasets in this thesis. One of them is Single cell RNAseq data. This kind of data represents gene expression levels in individual cells, where rows represent cells and columns represent genes. So if we see a reading of 0.5 in row 2 column 4 in means that in cell 2 gene 4 has normalized expression of 0.5.

The other kind of data is images. For example the MNIST data set contains greyscale 28×28 images of hand written digits. We still think of such data set as a matrix. The first axis always represents the samples, so each "row" represent an image. The rest of the axes represent the image. Alternatively we can also flatten the images into one axis and think of an image as a row vector of $28 * 28$ dimensions.

There could possibly be additional data matrices with information about class or conditions. We use *one-hot encoding* to represent such information. For example in the case of the MNIST dataset every image also comes with a label which indicates what digit it is. Since there are 10 digits (0 to 9) the class matrix is going to have 10 columns and each row is a one-hot vector indicating the digit of the corresponding image.

Definition 2.6. A *data matrix* is a real–valued matrix $\boldsymbol{X} \in \mathbb{R}^{N \times n}$ which represents a set of N n-dimensional data points. The N rows are also called *observations* and the n columns are *variables*.

Definition 2.7. A *class matrix*, or also a *condition matrix* $\boldsymbol{C} \in \mathbb{R}^{\mathbb{N} \times c}$ is a real matrix which represents one-hot encoding of c classes or conditions over N samples. For example if sample i has class j, then $(\forall k \in 1, \ldots, c)\boldsymbol{C}[i, k] = \delta_{jk}$.

We say that that $\boldsymbol{C}$ is a *class probability matrix* or a *relaxed class matrix* (same with condition) if instead of being one-hot its rows are distributions—each row is non-negative and sums up to 1.

Usually if the input data includes class/condition information, it comes as a class matrix (pure one-hot) but the output (the prediction) is naturally probabilistic and hence is relaxed.

2.5.1 Input set and target set

Our data may come in several, two or more matrices. Sometimes the data is paired into the input data $\mathbf{X}$ and the target data $\mathbf{Y}$, representing for example, samples from some unknown function $f(\mathbf{x}) = \mathbf{y}$ that we want to "learn". For example in an image classification task,$\mathbf{X}$ may be a set of images, and $\mathbf{Y}$ is their labels. Implicitly $\mathbf{X}, \mathbf{Y}$ must have the same number of rows. And when we speak about paired input/target $\mathbf{x}, \mathbf{y}$ it means some $(\mathbf{x}, \mathbf{y}) \in (\mathbf{X}, \mathbf{Y})$ and $\mathbf{x}, \mathbf{y}$ belong to the same sample (same row number).

2.5.2 Probabilistic interpretation of the data

Suppose that we have a data matrix $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$. We think of $\mathbf{X}$ as a set of N independent samples, all drawn from the same data distribution $\mathbf{x} \sim p(\mathbf{x})$. We think of $\mathbf{x}_i$ as a realization of a random vector which we also denote with $\mathbf{x}_i$. The random vectors $\mathbf{x}_i$ are independent replications of a random vector $\mathbf{x}$. This is another motivation why we take mean for the batch dimension because then $\|\mathbf{X}\| = \frac{1}{N}\sum_1^N \|\mathbf{x}_i\| \approx \mathbf{E}[\|\mathbf{x}\|]$.

2.6 Linear algebra preliminary: SVD and PCA

In the following state some facts and bring without proof what are the singular value decomposition and the principle components of a matrix. For a full proof see [18].

Let $\boldsymbol{X} \in \mathbb{R}^{N\times n}$ be a real-valued matrix representing N samples of some n-dimensional data points and let $r = \operatorname{rank}(\boldsymbol{X}) \leq \min(n, N)$.

$\mathbf{X}\mathbf{X}^*$ and $\mathbf{X}^*\mathbf{X}$ are both symmetric and positive semi-definite. Their eigenvalues are non-negative, and they both have the same positive eigenvalues, exactly r such, which we mark $s_1^2 \geq s_2^2 \geq \ldots s_r^2 > 0$. The values $s_1 \ldots s_r$ are called the *singular values* of $\boldsymbol{X}$.

Let $\boldsymbol{S} = \begin{pmatrix} s_1 & & & \\ & s_2 & & \\ & & \ddots & \\ & & & s_r \end{pmatrix} \in \mathbb{R}^{r\times r}$

Let $\boldsymbol{U} = (\boldsymbol{u}_1|\ldots|\boldsymbol{u}_N) \in \mathbb{R}^{N\times N}$ be the (column) right eigenvectors of $\mathbf{X}\mathbf{X}^*$ sorted by their eigenvalues. Then $\boldsymbol{U} = (\boldsymbol{U}_r, \boldsymbol{U}_k)$ where $\boldsymbol{U}_r = (\boldsymbol{u}_1|\ldots|\boldsymbol{u}_r) \in \mathbb{R}^{N\times r}$ are the first r eigenvectors corresponding to the non-zero eigenvalues, and $\boldsymbol{U}_k$ are the eigenvectors corresponding to the $N - r$ 0-eigenvalues. Similarly let $\boldsymbol{V} = (\boldsymbol{V}_r, \boldsymbol{V}_k) \in \mathbb{R}^{n\times n}$ be the (column) right eigenvectors of $\mathbf{X}^*\mathbf{X}$, sorted by the eigenvalues, where $\boldsymbol{V}_r = (\boldsymbol{v}_1|\ldots|\boldsymbol{v}_r) \in \mathbb{R}^{n\times r}$ are the firs r eigenvalues and $\boldsymbol{V}_k$ are the $n - r$ null-eigenvectors.

The critical observations is that $\boldsymbol{V}_r = \boldsymbol{X}^*\boldsymbol{U}_r S^{-1}$ and then $\boldsymbol{U}_r^*\mathbf{X}\boldsymbol{V}_r = S$.

The *singular value decomposition (SVD)* of $\mathbf{X}$ is

$$\mathbf{X} = \boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^* \tag{2.2}$$

where $\boldsymbol{D} = \begin{pmatrix} \boldsymbol{S} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \in \mathbb{R}^{N\times n}$ is diagonal.

$\boldsymbol{V}_r$ are called the *(right) principal components* of $\mathbf{X}$. Note that $\boldsymbol{V}_r^*\boldsymbol{V}_r = \boldsymbol{I}_r$ and that $\mathbf{X} = \mathbf{X}\boldsymbol{V}_r\boldsymbol{V}_r^* = (\mathbf{X}\boldsymbol{V}_r)\boldsymbol{V}_r^T$. If one looks at the second expression, it means that the each row of $\mathbf{X}$ is spanned by the orthogonal basis $\boldsymbol{V}_r^T$ (because the other vectors of $\boldsymbol{V}$ are in $\ker(\mathbf{X})$.

More generally For every $l \leq r$, let $\boldsymbol{V}_l \in \mathbb{R}^{N\times l}$ be the first l components, Then $\mathbf{X}\boldsymbol{V}_l\boldsymbol{V}_l^T$ is as close as we can get to $\mathbf{X}$ within an l-dimensional subspace of R^n, and $\boldsymbol{V}_l$ minimizes

$$\boldsymbol{V}_l = \text{argmin}_{\mathbf{W}}\{\|\mathbf{X} - \mathbf{X}\boldsymbol{W}\boldsymbol{W}^T\|_F^2 \quad : \quad \boldsymbol{W} \in \mathbb{R}^{n\times l}, \boldsymbol{W}^T\boldsymbol{W} = \boldsymbol{I}_l\} \tag{2.3}$$

Where $\|\cdot\|_F^2$ is simply the sum of squares of the matrix' entries.

If we consider the more general minimization problems:

$$\min_{\boldsymbol{E},\boldsymbol{D}}\{\|\mathbf{X} - \mathbf{X}\boldsymbol{E}\boldsymbol{D}\|_F^2 \quad : \quad \boldsymbol{E}, \boldsymbol{D^T} \in \mathbb{R}^{n\times l}, \} \tag{2.4}$$

$$\min_{\mathbf{W}}\{\|\mathbf{X} - \mathbf{X}\boldsymbol{W}\boldsymbol{W}^\dagger\|_F^2 \quad : \quad \boldsymbol{W} \in \mathbb{R}^{n\times l}, \} \tag{2.5}$$

It can be shown [14] that the last two problems 2.4, 2.5 are equivalent and that for any solution E, D it must hold that $\boldsymbol{D} = \boldsymbol{E}^\dagger$. ($\boldsymbol{D}$ is the Moore–Penrose generalized inverse of $\boldsymbol{E}$). Moreover, $\boldsymbol{V}_l$ still minimizes the general problem 2.4 and for every solution $\boldsymbol{W}$, it must hold that $\text{span}\{\boldsymbol{W}\} = \text{span}\{\boldsymbol{V}_l\}$ (but it isn't necessarily an orthogonal matrix).

Chapter 3

Neural networks

We briefly discuss here some of the basics of neural network to provide clarity and motivation. Mostly based on [13].

3.1 Universal families of parameterized maps

If we take an expression such as $f_{a,b}(x) = ax + b$, if we hold (a, b) fixed on specific values, then we get a linear function on x. Every assignment of (a, b) defines a different linear function and in fact every linear function on one dimension can be uniquely described by these a and b. So we can say that $\{f_{a,b}\}_{a,b\in\mathbb{R}}$ is a *parameterization* of the class of all real linear functions on one variable. The distinction between what are the variables and what are the parameters is somewhat arbitrary and in the end, $f_{a,b}(x)$ is just another way to represent a 3-variable function $f(a, b, x)$. As we mentioned 2.4 sometimes we don't specify the parameters and we identify the parametrize map f with its parameter set as this set uniquely determines f.

The way we parameterize a function is important. Usually given a parameterized map $\phi(\mathbf{x})$ we want ϕ to be differentiable in its parameters so that $\frac{\partial}{\partial \mathbf{w}}\phi$ exits for every parameter $\mathbf{w}$.

We call a class $\mathcal{F}$ of parameterized functions *universal* if every continuous function can be uniformly approximated (inside a bounded domain) by a function of that class. The class of all linear functions is not universal. But taking "any function" g is too general. What we actually want is a class of parameterized functions that is:

- as simple as possible to construct
- differentiable in both the parameters as well as the variables
- can uniformly approximate any continuous function in a bounded domain given sufficiently large set of parameters (i.e. is universal).

Still these requirements are not enough. For example, the class of multivariate polynomials can uniformly approximate any function. However it may not be a good idea to try to learn very complicated high dimensional data using polynomial representation. One

reason is that the number of terms (monomials) grows very rapidly with the dimension and the degree of the polynomials: for n dimensions and m degrees there are something like $\binom{m+n}{m}$ monomial terms.

We want a universal class of simpler functions, that are almost as simple as linear, and yet that suits well for statistical learning. For example we want to be able to represent complicated functions with relatively few parameters. One such class of functions is the feed forward neural networks, which is the class of functions that are comprised from "neurons".

3.2 Neurons

Inspired from biology, a *neuron* is a many–to–one ($\mathbb{R}^n \to \mathbb{R}$) parameterized function which "integrates" the input with a linear, or affine (see remark 2.4) function, and then applies a non-linear scalar function, which we call an *activation function*. In a sense it is the simplest function that is not linear. Moreover we only need one type of non-linear activation, e.g sigmoid, to construct arbitrarily complex neural networks. A degree 2 polynomial would be considered "less simple" because it applies multiple non-linear multi-variable functions $x_i x_j \dots$.

Definition 3.1. An *activation function* $\sigma : \mathbb{R} \to \mathbb{R}$ is any one of the following functions: $x \mapsto 1$ (constant), $x \mapsto x$ (identity) $x \mapsto \frac{e^x}{1+e^x}$ (sigmoid), and $x \mapsto \max(0, x)$ (ReLU).

σ can be applied on tensors by element-wise application. For example If $\mathbf{x} = (x_1, \dots x_n) \in \mathbb{R}^n$ then $\sigma(\mathbf{x})$ is the element-wise application $\sigma(\mathbf{x}) \triangleq (\sigma(x_1), \dots, \sigma(x_n))$.

In the official definition we narrowed it down to just 4 kinds but in general there are plenty of other activation functions. Also note that these functions have no parameters.

Definition 3.2. Let $\sigma : \mathbb{R} \to \mathbb{R}$ be an activation function and let $f_{\mathbf{w}} : \mathbb{R}^n \to \mathbb{R}$ be a *parameterized* linear function. A *neuron* ν is the parameterized function $\nu = \nu_{\mathbf{w}} \triangleq \sigma \circ f_{\mathbf{w}}$.

The parameters $\mathbf{w}$ are called the *weights* of the neuron ν.

. Here the bias b is explicitly shown but usually it is not depicted. In the left the variable names are explicitly shown, while in the right they are not.

Figure 3.1: Two graphical descriptions of the neuron $\sigma(w_1 x_1 + w_2 x_2 + b)$

Connecting many neurons together can create powerful parameterized functions which we call neural networks. In feed forward networks the information only goes in one direction (no feedback) and as we will see it means the network is a directed acyclic graph.

Definition 3.3. A *feed forward neural network (NN)*is a **parameterized** map ϕ recursively defined follows:

1. Activation functions (1, *id*, and σ) are NNs which are called the *elementary neurons* and they have no parameters ($\mathbf{w} = \emptyset$).

2. neurons are NNs

3. If $\psi : \mathbb{R}^n \to \mathbb{R}^m$ is a parameterized linear map then it is a NN.

4. If $\psi : R^n \to \mathbb{R}^m$ and $\rho : \mathbb{R}^m \to \mathbb{R}^l$ are NNs and their parameter sets are disjoint then $\phi = \rho \circ \psi$ is a NN.

5. if $\nu : \mathbb{R}^n \to \mathbb{R}^m$ is a NN and if $\psi_i : \mathbb{R}^{k_i} \to \mathbb{R}^{n_i}, i = 1 \dots l$ are NNs, such that $\sum_1^l n_i = n$ and if the parameter set of ν is disjoint from the combined parameters of the ψ_i's then $\phi = \nu(\psi_1, \dots, \psi_n)$ is a NN .

The parameter set $\mathbf{w}$ is called the *weights* of ϕ. Often we don't distinguish between the network ϕ and its weights, and we identify both as ϕ.

In the definition we made the range and domain to be the entire $\mathbb{R}^n$ but it is not necessary, we just need for the composition to be valid.

Feed forward neural network are depicted as a directed acyclic graph where every node (with its incoming edges) corresponds to a neuron. You can think of figure 3.1 left as depicting the neuron "component" in a network, while figure 3.1 right shows a neural network description of single neuron, comprised from elementary neurons.

If rule 5 of the definition 3.3 is not used in the construction of ϕ, then the resulting network is hierarchical. Its graph can be partitioned into *levels* $l_0, l_1 \dots$ and there are only directed edges between two consecutive levels $l_i \to l_{i+1}$ (see figure 3.2).

The label inside the neuron describes its activation function. In the diagrams, we let σ represent the sigmoid function. We represent the identity function either by the name of the variable (x_1, y etc.) it acts on or simple by *id*. We let the label 1 represent the constant function. We need the constant function because with it we can represent any affine map as a linear map with the first input always clamped to 1. But connecting 1 to every (non-input level) neuron would clutter the graph so it is not shown in most diagrams but still implicitly assumed. A directed edge between neurons means that the output of the neuron at the tail is multiplied by the edge weight and assigned to the input variable of the neuron it connects to. A Node's output is therefore only dependent on the output of its direct ancestral nodes (plus the bias which is usually not shown). Input-level neurons (sources) have no incoming edges and they represent the beginning of the computation. Output neurons (sinks) have no outgoing edges and their output is the final result of the computation.

It turns out [13] that the feed forward neural networks with a single type of non-linear activation (e.g. sigmoid) and a single hidden layer are "universal"; Which means that any continuous function f can be uniformly approximated by a feed forward neural network with a single hidden layer and Sigmoid as the non-linear activation function. More precisely, let $B \subseteq \mathbb{R}^n$ be a bounded domain. Let $f : B \to \mathbb{R}^m$ be continuous, and let $\epsilon \in (0, 1)$. Then there is a feed forward neural network with a single hidden layer $\phi = \phi_{\mathbf{w}}$ and there is some value assignment for the parameters $\mathbf{w}$ such that $(\forall \mathbf{x} \in B)\|\phi(\mathbf{x}) - f(\mathbf{x})\|_2 < \epsilon$. The size of that single hidden layer (the number of parameters) depends on f and ϵ.

In the definitions we only used linear maps to grow the network. There are other

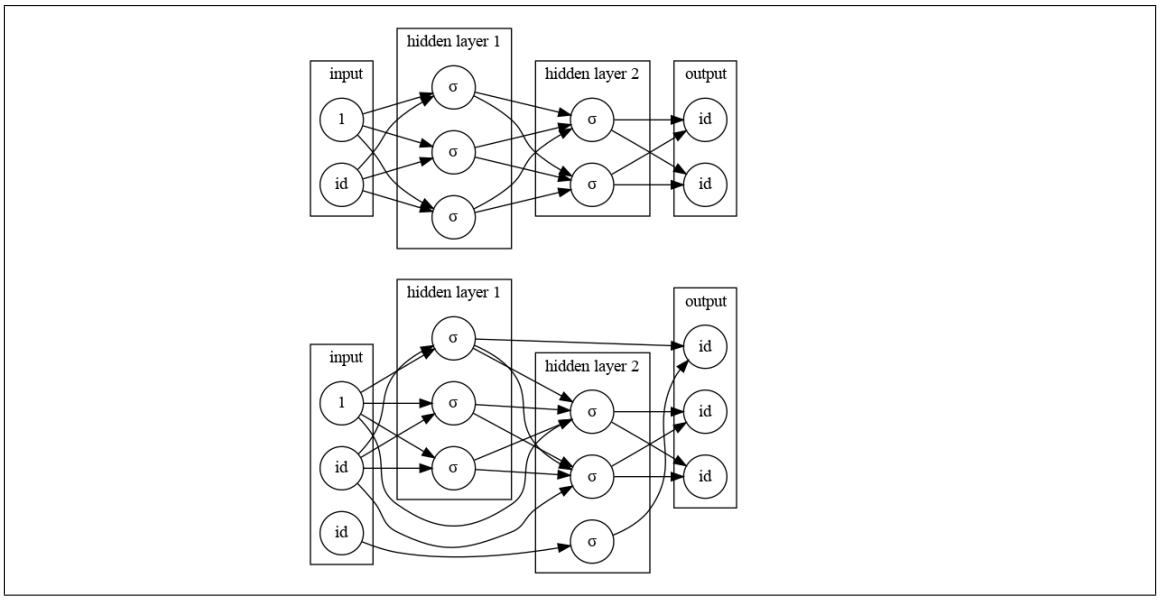


Figure 3.2: The network in the top didn't use rule 5 3.3 in the construction. It is strictly hierarchical and there are only edges between nodes of two consecutive layers. The one on the bottom is more general.

types of maps which are used, most commonly are convolutions but the principles and the graphical description remain essentially the same.

There are additional types of parameterized functions which are used "within the layer" such as batch normalization but we won't get into that as this is not a thesis about neural networks per se.

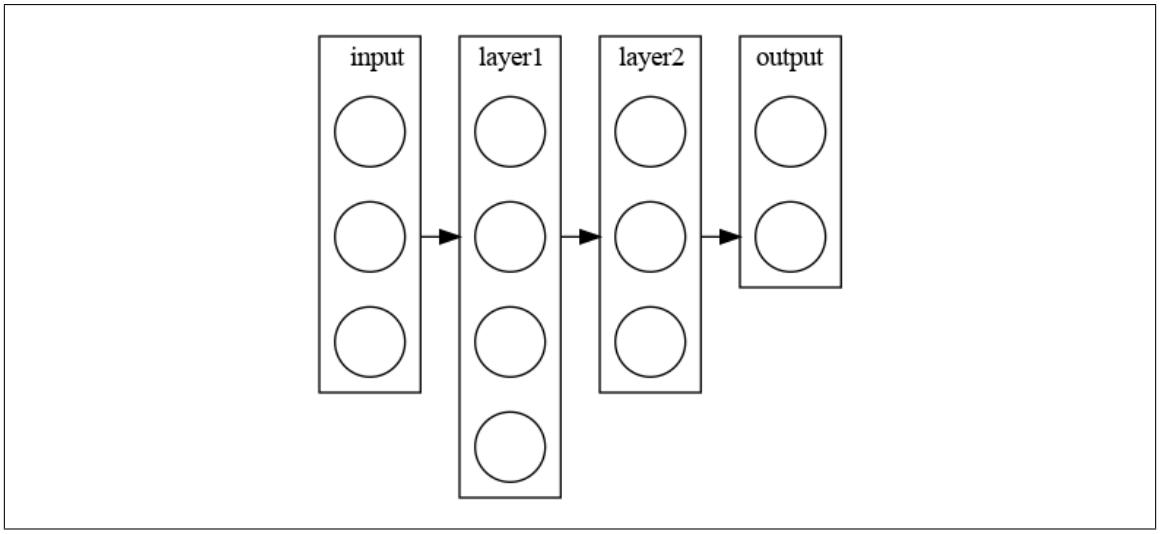


Figure 3.3: A graph of a hierarchical feed forward neural network where the connections are abstracted. Edges between layers may represent in this case a fully connected layer (every neuron has incoming edges from all neurons of the previous layer) but it could also be used for describing a convolution.

As figure 3.2 shows, The input layer is the where the input ($\mathbf{x}$) is "fed in" and the output layer is the final result of the evaluation $\phi(\mathbf{x})$. We call all the layers (or neurons) that are not in the input level or the output level "hidden" because we don't usually know what is the input/output value in these.

3.3 Loss functions

In the claim about neural networks being "universal" in terms of approximating function $f(\mathbf{x}) = \mathbf{y}$ with neural network $\phi(\mathbf{x})$. We stated specifically convergence in terms of l_2 norm $\|\phi(\mathbf{x}) - \mathbf{y}\|_2$, but the claim holds in theory and in practice with other types of "distance-like" functions which we call loss functions.

Moreover we usually don't know what is the function f which we try to approximate. Rather we are given paired samples of input/target $(\mathbf{x}, \mathbf{y})$ and we try to minimize the total error.

Definition 3.4. Let $\phi : \mathbb{R}^n \to \mathbb{R}^m$ be a neural network. A *loss function* is a differentiable function $\mathcal{L} : \mathbb{R}^m \oplus \mathbb{R}^m \to \mathbb{R}$. With "distance-like quality".

Typically the loss function is additive on the dimension, meaning it has the form $(\forall \mathbf{y}, \mathbf{z} \in \mathbb{R}^m)\mathcal{L}(\mathbf{y}, \mathbf{z})) = \sum_{i=1}^{m} \psi(y_i, z_i))$

Let $\mathbf{X} \in \mathbb{R}^{N \times n}, \mathbf{Y} \in \mathbb{R}^{N \times m}$ be the input and the target set and let $(\mathbf{x}, \mathbf{y})$ be a paired input/target. We use the loss function $\mathcal{L}$ as the target function for the minimization problem, $\min_{\mathbf{w}} \sum_{(\mathbf{x},\mathbf{y})} \mathcal{L}(\phi(\mathbf{x}), \mathbf{y})$ where the sum goes over all paires (N rows) (input, target).

For example $\mathcal{L}(\mathbf{y}, \mathbf{z})) = \|\mathbf{y} - \mathbf{z}\|_2^2 = \sum_i |y_i - z_i|^2$ is a one such loss function (the square error).

So far we defined ϕ and $\mathcal{L}$ on single input/target data points $\mathbf{x}$ and $\mathbf{y}$. But we are interested in minimizing the total error $\mathcal{L}(\phi(\mathbf{X}), \mathbf{Y})$. So first we need to state how these functions operate on sets of samples (matrices) rather than on data points (vectors).

Usually evaluation over the entire dataset is infeasible. Instead computation is performed on batches, which are relatively small chunks of the data.

Definition 3.5. Let $\boldsymbol{X} \in \mathbb{R}^{N \times n}$ be a data matrix. A *batch* $\boldsymbol{x} \in \mathbb{R}^{b \times n}$ is any subset of b rows of $\boldsymbol{X}$ (Note that in this case $\mathbf{x}$ represents a matrix).

Batch $\mathbf{x} = \{\mathbf{x}_1, \dots \mathbf{x}_b\} \in \mathbb{R}^{b \times n}$ (row notation) represents a subset of b samples out of the total of N samples in the dataset. Extending ϕ to operate on batches is trivial. $\phi(\mathbf{x}) = \{\phi(\mathbf{x}_i)\}$ is the matrix where ϕ is applied on the rows of the batch. Given an input batch $\mathbf{x}$ and corresponding target batch of $\mathbf{y}$, We extend the loss function to batches by averaging over the batch: $\mathcal{L}(\phi(\mathbf{x}), \mathbf{y}) \triangleq \frac{1}{b} \sum_{i=1}^{b} \mathcal{L}(\phi(\mathbf{x}_i), \mathbf{y}_i)$

Definition 3.6. Let ϕ be a neural network as defined in 3.3 and let $\mathcal{L}$ its associated loss function as defined in 3.4—over vectors. Let $\mathbf{x} = \{\mathbf{x}_1, \dots, \mathbf{x}_b\} \in \mathbb{R}^{b \times n}$ be a b-batch (in row notation) , and let $\mathbf{y} = \{\mathbf{y}_1, \dots, \mathbf{y}_b\} \in \mathbb{R}^{b \times m}$ be a corresponding target batch. Then ϕ and $\mathcal{L}$ *extended* over batches are:

$$\phi(\boldsymbol{x}) \triangleq \{\phi(\boldsymbol{x}_i)\}_{i=1}^{b} \in \mathbb{R}^{b \times m} \tag{3.1}$$

$$\mathcal{L}(\phi(\mathbf{x}), \mathbf{y}) \triangleq \frac{1}{b} \sum_{i=1}^{b} \mathcal{L}(\phi(\mathbf{x}_i), \mathbf{y}_i) \in \mathbb{R} \tag{3.2}$$

If $\mathcal{L}$ is the square error function $\|\cdot\|_2^2$ on vectors, then its extension to batches is $\frac{1}{b}\|\cdot\|_F^2$. The reason why we sum and don't average over the dimensions will be cleared later when we get into variational inference.

There is also a probabilistic way to interpret the total loss. We assume that the data points $\mathbf{X}, \mathbf{Y}$ were randomly and independently sampled from the unknown data distribution $p(\mathbf{x}, \mathbf{y})$. Then equation 3.2 can be reformulated as the expected loss [1]:

$$\mathcal{L}(\phi(\mathbf{X}), \mathbf{Y}) \approx \mathrm{E}_{\mathbf{x},\mathbf{y}\sim P(\mathbf{x},\mathbf{y})}\mathcal{L}(\phi(\mathbf{x}), \mathbf{y}) \tag{3.3}$$

3.4 Training

This is just a brief explanation of the basic principals. Training deep networks is a big subject which has many challenges and obstacles and a lot of heuristics are used.

Training the neural network ϕ_w means finding the weights that minimize the loss function applied on the training input/target paired sets $\mathbf{X}, \mathbf{Y}$, in other words minimizing $\min_w(\mathcal{L}(\phi_w(\mathbf{X}), \mathbf{Y})$. Usually we can't compute efficiently ϕ and $\mathcal{L}$ over the entire sets because N is too large, therefore we use batches.

Definition 3.7. Let ϕ_ω be a neural network and $\mathcal{L}$ its associated loss function. And let $(\mathbf{X}, \mathbf{Y})$ be our *training set* consisting of the data matrix $\mathbf{X}$ and $\mathbf{Y}$ the corresponding target matrix. Then *Training* of ϕ_ω with respect to $\mathcal{L}, \mathbf{X}$ means algorithmically approximating the minimization problem:

$$\min_\omega \mathcal{L}(\phi_\omega(\mathbf{X}), \mathbf{Y}) \tag{3.4}$$

During a *training step* the network is applied on a batch $(\mathbf{x}, \mathbf{y})$. Then the loss function is applied on the output of the network and a gradient (with relation to the weights) is taken using the efficient backpropagation algorithm [13]. The gradient is used for the weight update rule, which varies depending on the specific training algorithm. Typical training algorithms are SGD (stochastic gradient decent) and Adam [5], which is the one used throughout this work.

We only need to define the network, the loss function and the specific training algorithm. The rest (derivation, weight update etc.) is taken care for us by the backend of the software (Pytorch [15]) and can be regarded as a black box.

3.4.1 Training, validation and testing data sets

The data is partitioned into disjoint sets. The training set is used for the training of the model. The testing set is used for the final performance assessment. Sometimes a third subset, the validation set is used for tuning and tweaking the model during training. The point is that the model "doesn't know" the validation data because the weights are only trained on the training set, but the hyper-parameters are optimized based on the validation set. For example the validation set can be used for early stopping during the training. We didn't use a validation subset in our tests. Finally the assessment is performed on the testing set which was completely held out during the training and hyper-parameter tuning.

3.4.2 Un/Supervised learning

In unsupervised learning one seeks to "learn" or infer the target set $\mathbf{Y}$ (for example category information) from $\mathbf{X}$ without seeing $\mathbf{Y}$ during training. For example in the case of MNIST we want to teach the model to distinguish 10 categories of images corresponding to the 10 digits, without having access to the digit tags in the training set.

Supervised learning means the $\mathbf{Y}$ target information is fully accessible (every image is tagged with the digit it represents). This is a much simpler classification task.

Semisupervised learning is the hybrid case of both, where the training set includes a small portion of known paired input/targets $(\mathbf{x}, \mathbf{y})$ while for the rest of the training set we only have $\mathbf{x}$ input and need to infer $\mathbf{y}$. Semisupervised learning tasks often arise in natural situations. For example there may be a large image data set where only a portion of the images have been manually tagged.

3.5 Autoencoders

The basic type of an autoencoder which we informally call "vanilla" autoencoder is a neural network that tries to "learn" the identity function. Though it sounds pointless on a first thought, the point is how we construct this network. An autoencoder consists of two neural networks. An encoder network maps the input into a lower dimensional so called "latent space", and a decoder network maps the latent space back into the high dimensional input layer. In the case of the vanilla autoencoder the target for the loss function is the same as the input $\mathbf{Y} = \mathbf{X}$.

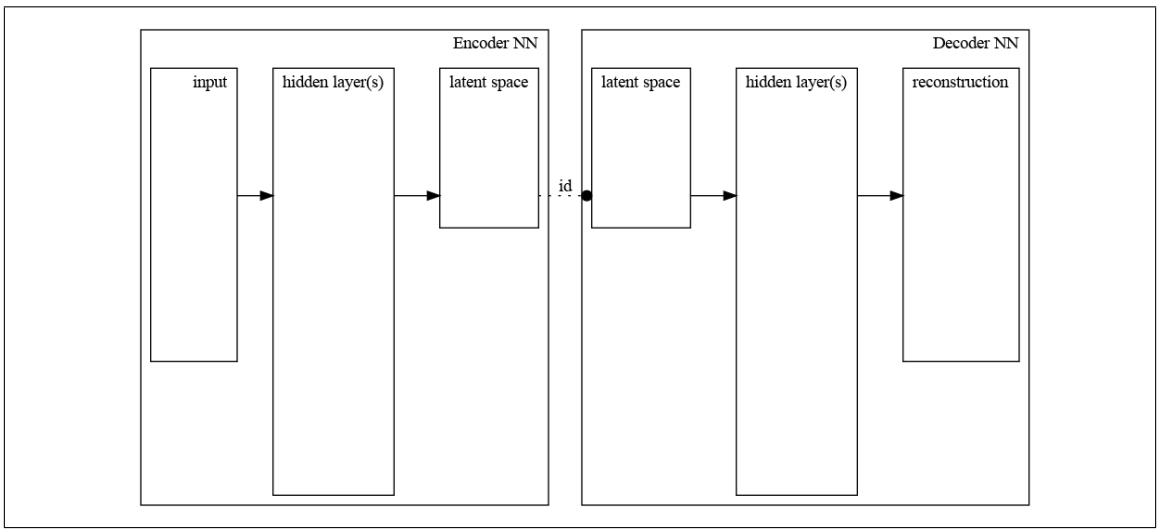


Figure 3.4: A graphic description of a "vanilla" autoencoder.

Definition 3.8. An *Autoencoder* (AE) is a pair (ϕ, ψ) of feed forward neural networks $\psi : \mathbb{R}^n \to \mathbb{R}^m, \nu : \mathbb{R}^m \to \mathbb{R}^n$.

ψ is called the *encoder* network, and ν is called the *decoder* network and the composition $\phi = \nu \circ \psi$ is called the *autoencoding network*.

We call $\mathbb{R}^m$ or more genrally the domain of the decoder, *the latent space*, and $\mathbb{R}^n$ (or more generally the domain of the encoder) is called *the observed space*.

Given a batch $\mathbf{x} \in \mathbb{R}^{b \times n}$ we call $\mathbf{z} = \psi(\mathbf{x}) \in \mathbb{R}^{b \times m}$ the *latent representation* of $\mathbf{x}$ or the *encoding* of $\mathbf{x}$.

While the definition as is given is symmetric, it is assumed that $n > m$, and therefore ψ represents dimensional reduction (in other words encoding) of the data and ν represents expansion back to original space (decoding).

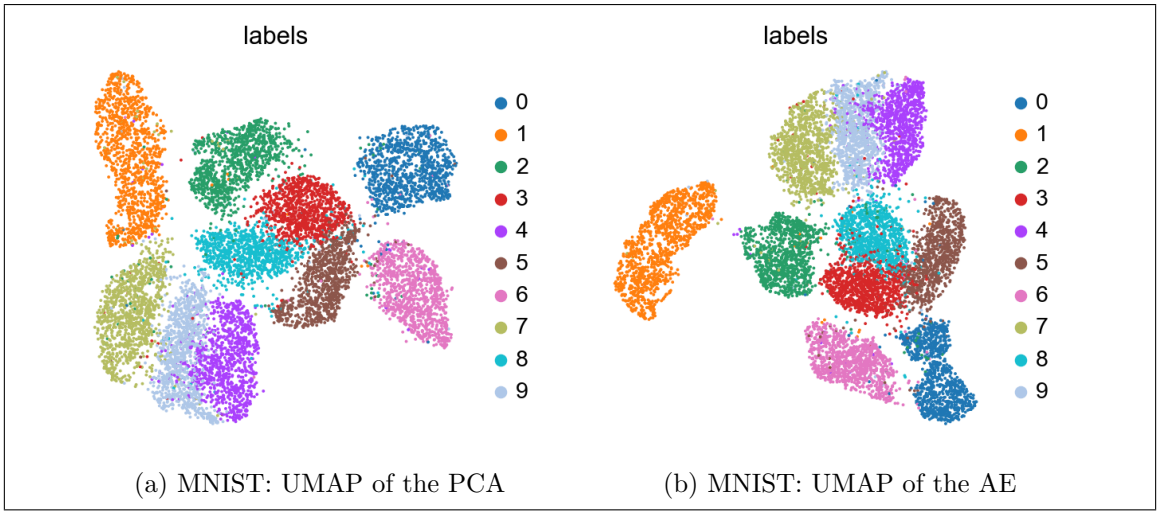
The idea here is that the original high dimensional data can be embedded in a low dimensional space by the encoder. The decoder then can reconstruct the original data from the embedding.

There are many variations of autoencoders. For example a "denoising" autoencoder is essentially that same model but it receives a "noisy" version of the input and tries to reconstruct the original clean version. We informally call the type of autoencoder of definition 3.8 which aims to learn the identity function on the original input, and which is using the square error loss function, a "vanilla" autoencoder.

3.5.1 Relation between PCA and AE

For **centered** data, where every variable (column of $\boldsymbol{X}$) has a sample mean of 0, the first $k \leq \text{rank}(\boldsymbol{X})$ principle components $\boldsymbol{P}$ are the solution for equation 2.3; Whereas a **linear** autoencoder solves equation 2.5. As mentioned, it must hold that $E = D^{\dagger}$ (the encoder must be the Moore-Penrose inverse of the decoder).

A linear autoencoder with the square error loss function is almost equivalent to PCA [14]; At the optimum, a bottleneck space of dimension k is spanned by the first k principle components of the input $\boldsymbol{X}$. In general, an AE can be seen a PCA-like, but non-linear method for dimensionality reduction.



(a) MNIST: UMAP of the PCA (b) MNIST: UMAP of the AE

Figure 3.5: PCA (l) compared with "vanilla" autoencoder (r) on the MNIST dataset

Figure 3.5 shows on the left a UMAP [12] of the principle components of the testing subset of MNIST (images of hand written digits). On the left we see a UMAP of the latent space encoded by the encoder of a "vanilla" autoencoder with the square error loss function. The autoencoder was trained on the training set and didn't "see" the testing images during training. The results appear quite similar.

Chapter 4

Variational inference and variational autoencoders

4.1 Variational Inference

Here we briefly explain the idea behind variational inference and introduce the ELBO which is the loss function we'll use throughout this text. For more details see [1].

We treat the data matrix as a set of independent observations (its rows) $\boldsymbol{X} = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$ which we try to explain by a probabilistic model. Each row $\mathbf{x}_i$ is considered a realization of a random vector, which we also denote by $\mathbf{x}_i$ (as explained in the notation section) and similarly $\mathbf{X}$ represents both the set of r.vs as well as the realization.

We assume that the $\boldsymbol{x}_i$'s are independent and identically distributes (i.i.d) random vectors with some distribution function $\mathbf{x} \sim p(\mathbf{x})$ and therefore for the entire dataset it holds that $p(\boldsymbol{X}) = \prod p(\boldsymbol{x}_i)$.

Definition 4.1. Let $\boldsymbol{X} \in \mathbb{R}^{N \times n}$ be a data matrix and let $\{\boldsymbol{x}_i\}_1^n$ be its rows, which we assume to be i.i.d with some (unknown) distribution $\mathbf{x} \sim p(\boldsymbol{x})$. Then $\log p(\boldsymbol{X}) = \sum_1^N \log p(\boldsymbol{x}_i)$ is called the *log evidence* of our data.

$\frac{1}{N} \log p(\mathbf{X})$ is the *mean log evidence* (remember the mean-sum rule for data sets and batches 2.2).

An observation r.v $\boldsymbol{x}$ is high dimensional however we have some reason to believe that behind the scenes there is some hidden (latent), smaller dimensional random vector $\mathbf{z}$ that generates it. In other words we think that $\mathbf{x}$ is conditioned on $\mathbf{z}$ and we can speak of the joint distribution $p(\mathbf{x}, \mathbf{z}) = p(\mathbf{x}|\mathbf{z})p(\mathbf{z})$. And again $\mathbf{x}_i$ only depends on $\mathbf{z}_i$ so everything factors nicely, e.g. $p(\mathbf{X}|\mathbf{Z}) = \prod_i p(\mathbf{x}_i|\mathbf{z}_i)$.

Suppose that we have a fully Bayesian model. In this case there are no parameters because the parameters are themselves stochastic variables with some suitable priors. We can therefore pack all the latent variables and stochastic parameters into one latent "meta variable" $\mathbf{z}$, which is some multidimensional r.v and which is possibly composed of several simpler r.vs (for example a categorical and a normal r.vs). We similarly pack all the observed variables into one meta variable $\boldsymbol{x}$. Together we have a distribution $p(\boldsymbol{x}, \boldsymbol{z})$ and the working assumption is that it is easy to factorize $p(\boldsymbol{x}, \boldsymbol{z}) = p(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})$, however $p(\boldsymbol{z}|\boldsymbol{x})$

is intractable and $p(\boldsymbol{x})$ is unknown.

We are being Bayesian here so we consider $\boldsymbol{X} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \dots\}$ to be a constant set of observations and we want to best explain $p(\boldsymbol{X})$ by finding as high as possible lower bound for it (or rather to $\log p(\boldsymbol{X})$, the *log evidence*). A second goal is to approximate the intractable $p(\boldsymbol{z}|\boldsymbol{x})$ by some simpler distribution $q(\boldsymbol{z})$ taken from some family of distributions.

Definition 4.2. Let $\boldsymbol{x}, \boldsymbol{z}$ be random variables with joint distribution $p(\boldsymbol{x}, \boldsymbol{z})$ and let $q(\boldsymbol{z})$ be any distribution. Let $(\mathbf{X}, \mathbf{Z}) = \{(\mathbf{x}_1, \mathbf{z}_1), \dots, (\mathbf{x}_N, \mathbf{z}_N)\}$ be N independent replications of $(\mathbf{x}, \mathbf{z})$. The *evidence lower bound (ELBO)* with respect to p, q is:

$$-\mathcal{L}(q, p, \mathbf{x}) \triangleq \int \log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q(\boldsymbol{z})} dq(\boldsymbol{z}) \tag{4.1}$$

$$-\mathcal{L}(q, p) \triangleq -\mathcal{L}(q, p, \mathbf{X}) = \frac{1}{N} \sum_{1}^{N} (-\mathcal{L}(q, p, \mathbf{x}_i) \tag{4.2}$$

$$\approx \mathbf{E}_{\mathbf{x}}[-\mathcal{L}(q, p, \mathbf{x})] \tag{4.3}$$

Equation 4.2 is no longer treated as a function of $\mathbf{X}$ because it is taken over all of our data which we think of as a constant. The reason that we mark the ELBO with $-\mathcal{L}$ is because we use the minus ELBO, $\mathcal{L}$, as the loss function for VAEs.

The following equation shows that the *ELBO* is a lower bound for the *mean log evidence*. (using Jensen's inequality)

$$\begin{aligned}
\frac{1}{N} \log p(\boldsymbol{X}) &= \frac{1}{N} \log \int p(\boldsymbol{X}, \boldsymbol{Z}) d\boldsymbol{Z} = \frac{1}{N} \log \int \frac{p(\boldsymbol{X}, \boldsymbol{Z})}{q(\boldsymbol{Z})} q(\boldsymbol{Z}) d\boldsymbol{Z} \\
&= \frac{1}{N} \log \int \frac{p(\boldsymbol{X}, \boldsymbol{Z})}{q(\boldsymbol{Z})} dq(\boldsymbol{Z}) \geq \frac{1}{N} \int \log \frac{p(\boldsymbol{X}, \boldsymbol{Z})}{q(\boldsymbol{Z})} dq(\boldsymbol{Z}) \\
&= \frac{1}{N} \int \sum_{1}^{N} \log \frac{p(\mathbf{x}_i, \mathbf{z}_i)}{q(\mathbf{z}_i)} dq(\mathbf{z}_i) \\
&= \frac{1}{N} \sum_{1}^{N} -\mathcal{L}(q, p, \mathbf{x}_i) = -\mathcal{L}(q, p, X) \triangleq -\mathcal{L}(q, p)
\end{aligned} \tag{4.4}$$

In equation 4.4 we found a lower bound $-\mathcal{L}(q, p)$ for the mean log evidence $\log p(\boldsymbol{X})/N$, the *ELBO*. Whatever distribution q we put in ELBO will not be greater than the real log evidence so we are looking for the q which **maximizes** it.

Now we show that maximizing the ELBO actually obtains the mean log evidence and it is equivalent to minimizing $KL(q(\boldsymbol{Z}) \| p(\boldsymbol{Z}|\boldsymbol{X}))$:

$$\begin{aligned}
-\mathcal{L}(q, p, \mathbf{x}) &\triangleq \int \log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q(\boldsymbol{z})} dq(\boldsymbol{z}) = \int \log \frac{p(\boldsymbol{z}|\boldsymbol{x}) p(\boldsymbol{x})}{q(\boldsymbol{z})} dq(\boldsymbol{z}) \\
&= \int \log p(\boldsymbol{x}) dq(\boldsymbol{z}) - \int \log \frac{q(\boldsymbol{z})}{p(\boldsymbol{z}|\boldsymbol{x})} dq(\boldsymbol{z}) = \log p(\boldsymbol{x}) - KL(q(\boldsymbol{z}) \| p(\boldsymbol{z}|\boldsymbol{x}))
\end{aligned} \tag{4.5}$$

We can rewrite equation 4.5 as:

$$\log p(\boldsymbol{x}) = -\mathcal{L}(q, p, \mathbf{x}) - KL(q(\boldsymbol{z}) \| p(\boldsymbol{z}|\boldsymbol{x})) \tag{4.6}$$

Equation 4.6 shows that the ELBO minus the kl-divergence are constant and equal the log evidence. Therefore minimizing the kl-divergence (which is always non-negative) simultaneously maximizes the ELBO and vicer-versa.

4.2 Variational Autoencoder

4.2.1 Adding parameters

Our models will not be fully Bayesian, but rather parametrized. Suppose that the p distribution over $\mathbf{x}, \mathbf{z}$ belongs to some parametrized family of distributions $p_\theta(\mathbf{x})$ and the q distribution over $\mathbf{z}$ belongs to another family $q_\phi(\mathbf{z})$. In a fully Bayesian model we would make θ and ϕ stochastic parameters and give them appropriate prior distributions, but with the VAE we leave them as parameters that we determine with neural network as will shortly be explained.

For any θ and any ϕ, the equations from the previous chapter hold also in the parametrize form, i.e $\log p_\theta(\mathbf{x}) = -\mathcal{L}(q_\phi, p_\theta, \mathbf{x}) - KL(q_\phi(\mathbf{z})\|p_\theta(\mathbf{z}|\mathbf{x}))$.

We assume that we can only approach the "real" distribution using θ from below $\log p(\mathbf{x}) \geq \log p_\theta(\mathbf{x})$. So together with equation 4.4 we have

$$(\forall\theta, \phi) \log p(\mathbf{x}) \geq \log p_\theta(\mathbf{x}) \geq -\mathcal{L}(q_\phi.p_\theta, \mathbf{x}) = \int \frac{p_\theta(\mathbf{x}, \mathbf{z})}{q_\phi(\mathbf{z})} dq_\phi(\mathbf{z}) \tag{4.7}$$

And from equation 4.6 we again see that by finding the parameters ϕ, θ that maximize the ELBO we approach the real log evidence as much as we can within the limits of the parametrized family of distributions we use.

4.2.2 Rearranging the ELBO

Equations 4.4 and 4.5 were defined for any distribution $q(\mathbf{z})$ and in particular we are allowed to plug in a conditioned distribution $q(\mathbf{z}|\mathbf{x})$. That implies the existence of $q(\mathbf{z}, \mathbf{x})$ and $q(\mathbf{x})$ but we actually don't care about them. We condition everything on $\mathbf{x}$ but $\mathbf{x}$ is treated as a given constant from a Bayesian view point and we only want to somehow make $q(\mathbf{z}|\mathbf{x})$ to closely approximate $p(\mathbf{z}|\mathbf{x})$.

A second thing we need to achieve is to express the -ELBO in terms of $p(\mathbf{x}|\mathbf{z})$ and $q(\mathbf{z}|\mathbf{x})$ rather than the joint distribution. To that end we need also the prior $p(\mathbf{z})$.

$$\begin{aligned}
\mathcal{L}(q, p, \mathbf{x}) &\triangleq \int -\log \frac{p(\mathbf{x}, \mathbf{z})}{q(\mathbf{z}|\mathbf{x})} dq(\mathbf{z}|\mathbf{x}) = \int -\log \frac{p(\mathbf{x}|\mathbf{z})p(\mathbf{z})}{q(\mathbf{z}|\mathbf{x})} dq(\mathbf{z}|\mathbf{x}) \\
&= \int -\log p(\mathbf{x}|\mathbf{z}) dq(\mathbf{z}|\mathbf{x}) + \int \log \frac{q(\mathbf{z}|\mathbf{x})}{p(\mathbf{z})} dq(\mathbf{z}|\mathbf{x}) \\
&= \int -\log p(\mathbf{x}|\mathbf{z}) dq(\mathbf{z}|\mathbf{x}) + KL(q(\mathbf{z}|\mathbf{x})\|p(\mathbf{z}))
\end{aligned} \tag{4.8}$$

So to sum it up, if we want to maximize the log evidence $\log p(\mathbf{X})$ it suffices to minimize

$\mathcal{L}(q,p)$ and equation 4.8 shows that this means finding the balance between making the term $\int \log p(\mathbf{X}|\mathbf{Z})dq(\mathbf{Z}|\mathbf{X})$ (which we call the reconstruction term) large as possible, and making the KL-term small. The KL term is seen as a regularization term.

4.2.3 Using neural networks for the parametrization

In this text we deal with variational autoencoders (VAE). A VAE is a neural network which is used to define and optimize the parameters ϕ and θ which define $p_\theta(\mathbf{x}|\mathbf{z})$ and $q_\phi(\mathbf{z}|\mathbf{x})$ and we train the network to maximize equation 4.8.

Specifically the encoder part of the network is a feed forward neural network $f_\theta(\mathbf{z})$ which is used to define the distribution $p_\theta(x|z)$. For example, we can assume that p_θ is a family of multivariate Gaussians and in this case $f_\theta(z) = (\mu(z), \Sigma(z))$. Meaning the encoder maps z to the location vector and covariance matrix. The parameter θ in this case are the weights of the encoder neural network.

The decoder network is similarly defined as neural network $g_\phi(\mathbf{x})$ which maps $\mathbf{x}$ into the parameters defining the family $q_\phi(\mathbf{z})$. Here too ϕ represent the weights of the decoder.

For the prior $p(\mathbf{z})$ we set some fixed prior distribution.

Note that the encoder network (similarly the decoder) is used to define a distribution over $\mathbf{z} \in \mathbb{R}^m$, but the encoder itself maps into some other space. For example, to define a normal one Gaussian distribution (so over $\mathbf{z} \in \mathbb{R}$, the encoder maps into $\mathbb{R}^2$, and its output creates $\mu, \sigma\mathbb{R}$ which are used to define the Gaussian distribution $\mathcal{N}(\mathbf{z}; \mu, \sigma)$. We also need to make sure that the range of the network obeys to the constraints of the parameters. For example the variance must be non-negative. Alternatively we can use transformations to remove constraints. For example instead of letting the network specify the variance. we let it specify the log-variance.

Definition 4.3. Let $\{p_\theta\}_{\theta\in\Theta}$ be a parameterized family of distributions over $\mathbb{R}^n$ and let $\{q_\phi\}_{\phi\in\Phi}$ be a family of distributions over $\mathbb{R}^m$. Where Θ and Φ are real domains (i.e $\Theta \subseteq \mathbb{R}^k \dots$).

A *variational autoencoder (VAE)* consists of a pair (E, D) of neural networks, $E : \mathbb{R}^n \to \Phi$ and $D : \mathbb{R}^m \to \Theta$ and some fixed distribution $p \in \Phi$.

We call $\mathbb{R}^m$ or more genrally the distribution space of the decoder, *the latent space*, and $\mathbb{R}^n$ (or more generally the distribution space of the encoder) is called *the observed space*. p is called *the prior distribution of the latent space*.

An autoencoder works deterministically, where the encoder maps the input $\mathbf{x} \mapsto \mathbf{z}$ and the decoder then maps the latent space $\mathbf{z} \mapsto \hat{\mathbf{x}}$ to the reconstruction. A VAE does basically the same thing but non-deterministically. It maps $\mathbf{x}$ into a distribution over $\mathbf{z}$: $\mathbf{x} \mapsto q(\mathbf{z}|\mathbf{x}) = q_{\phi(\mathbf{x})}(\mathbf{z})$ and it maps $\mathbf{z}$ into a distribution over $\mathbf{x}$: $\mathbf{z} \mapsto p(\mathbf{x}|\mathbf{z}) = p_{\theta(\mathbf{z})}(\mathbf{x})$.

The loss function associated with a VAE is minus ELBO. This means training the VAE maximizes equation 4.8 and therefore also the log evidence.

To give a concrete example lets say that the distribution family for q_ϕ is the diagonal normal distribution. We can set the parameter domains $\Phi = \mathbb{R}^m \oplus \mathbb{R}^m$. The means can be any real vector, but the variances are non-negative. We can either restrict the encoder

to be non-negative on the variance-domain, or we can agree to use the log-variance as the second parameter, which is then unconstrained.

We identify $q(\mathbf{z}|\mathbf{x})$ with the encoder but technically what it means is that the encoder network maps $\mathbf{x}$ into the distribution parameters $E(\mathbf{x}) = \phi(\mathbf{x}) \in \Phi$; in the case we use diagonal normal distribution $\phi(\mathbf{x}) = (\mu(\mathbf{x}), \sigma(\mathbf{x}))$. Thus we defined a distribution over $\mathbf{z}$ by using $\mathbf{x}$ to map into the parameter domain: $q(\mathbf{z}|\mathbf{x}) = q_{\phi(\mathbf{x})}(\mathbf{z})$

Similarly we call $p(\mathbf{x}|\mathbf{z})$ the decoder although it is technically the distribution defined by the decoder. $D(\mathbf{z}) = \theta(\mathbf{z})$: $p(\mathbf{x}|\mathbf{z}) = p_\theta(\mathbf{x})$

4.2.4 Mean field approximation

Usually we treat the dimensions of $\mathbf{x}$, $\mathbf{z}$ etc. as independent. That means if $\mathbf{x} = (x_1, \ldots, x_n)$ is a r.v. in $\mathbb{R}^n$ we assume that the x_i are independent and therefore $P(\mathbf{x}) = \prod_1^n p_i(x_i)$.

Specifically the mean fields approximation of a multivariate Gaussian $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$ is a diagonal Gaussian distribution $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\sigma}) \triangleq \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\sigma}\boldsymbol{I})$. Mean field approximation simplifies the implementation and speeds up the computation and has been the standard practice since the beginning of VAEs [8].

4.2.5 Computing the ELBO

It may not be immediately clear how to how to compute the integral in the ELBO function. Recall that given an input $\mathbf{x} \in \mathbb{R}^n$, The loss function is

$$\mathcal{L}(p, q, \mathbf{x}) = \int -\log \frac{p(\mathbf{x}|\mathbf{z})p(\mathbf{z})}{q(\mathbf{z}|\mathbf{x})} dq(\mathbf{z}|\mathbf{x}) = \int -\log p(\mathbf{x}|\mathbf{z}) dq(\mathbf{z}|\mathbf{x}) + \int \log \frac{q(\mathbf{z}|\mathbf{x})}{p(\mathbf{z})} dq(\mathbf{z}|\mathbf{x}) \tag{4.9}$$

Given concrete input $\mathbf{x} \in \mathbb{R}^n$, the decoder specifies a distribution over $\mathbf{z} \in \mathbb{R}^m$ rather then a concrete deterministic point: $\mathbf{z} \sim q(\mathbf{z}|\mathbf{x})$. Suppose that we draw one concrete sample $\mathbf{z} \in \mathbb{R}^m$ taken from that distribution. Now that we have the concrete input $\mathbf{x}$ and a concrete $\mathbf{z}$ we can compute $\log q(\mathbf{z}|\mathbf{x})$ as well as the prior $p(z)$. Remember that the decoder takes $\mathbf{z}$ and produces a distribution $p(\mathbf{x}|\mathbf{z})$. With a concrete $\mathbf{z}$, and $\mathbf{x}$ we can also compute $\log p(\mathbf{x}|\mathbf{z})$ So once we draw a specific sample $\mathbf{z}$ we can compute everything inside the integral.

In fact what we have done is already a form of Monte Carlo integration. More generally, instead of drawing just one concrete sample $\mathbf{z}$, we draw k samples $\mathbf{z}_i \sim q(\mathbf{z}|\mathbf{x})$ per input $\mathbf{x}$, and take the average. Then we have

$$\begin{aligned}\mathcal{L}(p,q,\mathbf{x}) &= \int -\log \frac{p(\mathbf{x}|\mathbf{z})p(\mathbf{z})}{q(\mathbf{z}|\mathbf{x})} dq(\mathbf{z}|\mathbf{x}) \\ &= \int -\log p(\mathbf{x}|\mathbf{z}) dq(\mathbf{z}|\mathbf{x}) + \int \log \frac{q(\mathbf{z}|\mathbf{x})}{p(\mathbf{z})} dq(\mathbf{z}|\mathbf{x}) \\ &\approx \frac{1}{k}\sum_{i=1}^{k}[-\log p(\mathbf{x}|\mathbf{z}_i) + \log \frac{q(\mathbf{z}_i|\mathbf{x})}{p(\mathbf{z}_i)}]\end{aligned} \tag{4.10}$$

In practice we take just one ($k = 1$) sample z for each input data point x. Remember that we are working on batches and computing an average loss over batches so for a given batch we are taking many samples $\mathbf{z}$. Experimental data shows that taking larger samples usually brings little benefit [7].

Reparameterization trick

The loss function is computed by using Monte Carlo integration, which requires taking samples $\mathbf{z} \sim q(\mathbf{z}|\mathbf{z})$. But the loss function needs to be differentiable with respect to the model's parameters which are the encoder's weights ϕ and the decoder's weights θ. There is a method, "the reparameterization trick" which uses some random noise which allows to express the sample $\mathbf{z} = h_\phi(\epsilon, \mathbf{x})$ as a deterministic smooth function of the parameters given random noise ϵ [8].

For example in the "vanilla" VAE, $\mathbf{z}$ is sampled from diagonal Gaussian distribution $\phi(\mathbf{x}) = (\mu(\mathbf{x}), \sigma(\mathbf{x}))$. Sampling $\mathbf{z} \sim \mathcal{N}(\mu(\mathbf{x}), \sigma(\mathbf{x}))$ is equivalent to sampling standard normal noise $\epsilon \sim \mathcal{N}(0, 1)$ and taking $\mathbf{z} = \mu(\mathbf{x}) + \sigma(\mathbf{x}) \cdot \epsilon$. Most other types of distributions (Dirichlet, Negative Binomial, etc.) can be sampled using the reparameterization trick as deterministic, differentiable transformation of Gaussian or uniform random noise and in Pytorch, this feature is built into the distribution object types.

4.2.6 Using the decoder for data generation

Suppose that we have a vanilla auto encoder (ϕ, ψ) and suppose that we want to generate synthetic data set that looks similar to the original data. We need to choose points $\mathbf{z} \in \mathbb{R}^m$ from the latent space and project back to observed space $\psi(\mathbf{z}) \in \mathbb{R}^n$. The question is then how to sample these $\mathbf{z}$? It's not immediately clear how to do this because we don't know what is the distribution in the latent space.

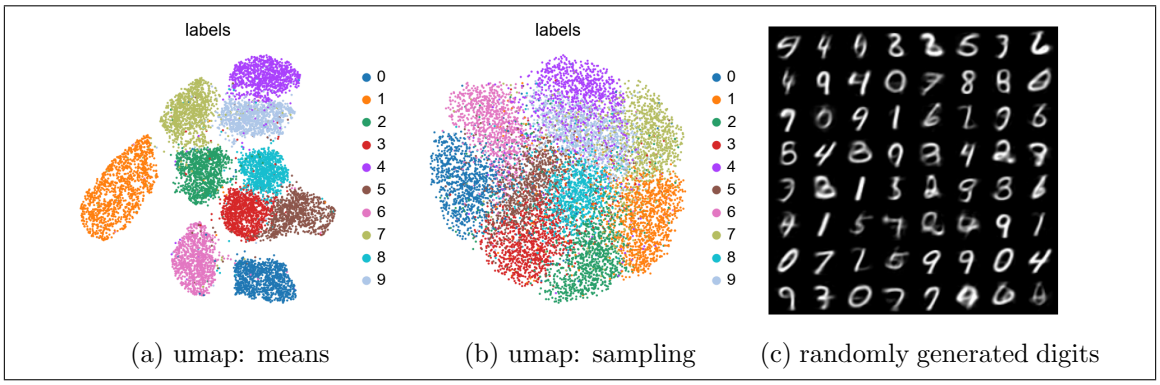
If we use a VAE instead, we know that $\mathbf{z}$ should have a distribution that is pretty close to the prior $p(\mathbf{z})$, which we can easily sample from. Given a VAE (E, D, p), synthetic data samples can be generated as follows: sample $\mathbf{z} \sim p(\mathbf{z})$. Then given the samples in the latent space, sample from the decoder distribution $\mathbf{x} \sim D(\mathbf{z})$, in the observed space. Figure 4.1c shows randomly generated digits which were created in such process.

4.2.7 Encoding data in the latest space with a VAE

Unlike a vanilla autoencoder, a VAE doesn't deterministically encode input $\mathbf{x}$ but rather maps it to a distribution $q(\mathbf{z}|\mathbf{x})$. We can use the distribution's mean $\mu(\mathbf{x})$ as the encoding.

Given observation $\mathbf{x}$, we can deterministically encode $\mathbf{x}$ into the latent space by taking the mean: $\mathbf{x} \mapsto \mathbf{E}[E(\mathbf{x})]$. Since $q(\mathbf{x}|\mathbf{z})$ is some kind of parameterized distribution for example $\mathcal{N}(\mathbf{z} : \mu(\mathbf{x}), \sigma(\mathbf{x}))$ the mean is a known parameter of the distribution so we don't need to estimate it. See for example in figure 4.1a.

Alternatively we can deliberately add stockanticity to the encoding by non-deterministically drawing $\mathbf{z} \sim q(\mathbf{z}|\mathbf{x})$ from the encoder distribution, as is dones in figure 4.1b.



(a) umap: means (b) umap: sampling (c) randomly generated digits

Figure 4.1: "vanilla" VAE trained on MNIST. The first two images show UMAP plot of the latent space $\mathbf{z}$. In (a) we take the mean of the distribution $p(\mathbf{z}|\mathbf{x})$ while in (b) a random sample from the distribution is used. Third plot shows random digits generated by sampling $z \sim p(\mathbf{z}|\mathbf{x})$ and projecting back to the observed space $\mathbf{x}$ by the decoder.

4.2.8 Choosing the distribution types

This is another topic that can get arbitrarily complex.

Recall that our loss function in the case that we take just one sample $\mathbf{z}$ for input $\mathbf{x}$ is:

$$\begin{aligned} \mathcal{L}(p, q, \mathbf{x}) &= (-\int \log p(\mathbf{x}|\mathbf{z}) dq) + KL(q(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z})) \\ &\approx -\log p(\mathbf{x}|\mathbf{z}) + \log \frac{\log q(\mathbf{z}|\mathbf{x})}{p(\mathbf{z})} \end{aligned} \tag{4.11}$$

The left term is called the reconstruction error and the right term is called the regularization term or the kl-term.

Lets suppose that we just want to use diagonal Gaussian distributions (which is a type of mean field approximation). The advantage is that it is easy to compute them because we just sum over the dimensions:

$$\log \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\sigma}) = \sum_{1}^{n} \log \mathcal{N}(x_i; \mu_i, \sigma_i) \tag{4.12}$$

The dimension of the latent space is a significant hyper parameter of the VAE model. Since we sum over the dimensions rather than averaging, the larger we let the dimension of the latent space $\mathbf{z}$ it can have an effect of upscaling the importance of the kl-term relative to the reconstruction. Moreover the dimension should also be appropriate in terms of the "real" dimensionality of the data.

In the case of the vanilla VAE we choose $p(\mathbf{z}) = \mathcal{N}(\mathbf{z}; 0, 1)$ (diagonal Gaussian standard normal) for the prior and $q(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mathbf{z}; \boldsymbol{\mu}(\mathbf{x}), \boldsymbol{\sigma}(\mathbf{x}))$ for the encoder. There is a closed form formula for KL-divergence between two diagonal Gaussians so in this case we don't need to use Monte Carlo integration for the KL-term (we show it in one dimensions and for k dimension in the diagonal case we sum over the dimensions:

$$KL(\mathcal{N}(;\mu_1,\sigma_1)\|\mathcal{N}(;\mu_2,\sigma_2)) = -\frac{1}{2} + \log\frac{\sigma_2}{\sigma_1} + \frac{\sigma_1^2 + (\mu_1-\mu_2)^2}{2\sigma_2^2} \tag{4.13}$$

The reconstruction term is more tricky. Lets say we still want some sort of Gaussian diagonal distribution for $\mathbf{x}$, so $p(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}(\mathbf{z}), \boldsymbol{\sigma}(\mathbf{z}))$. If we allow the decoder to create arbitrarily small variances, then the decoder will stop being stochastic and it becomes deterministic. The decoder will also be able to pinpoint the sources in the latent space. As a result the encoding becomes meaning-less and the encoded data will tend to be arbitrarily spread in the latent space without meaningful clusters. In addition there is a problem of numerical instability because the distribution function can become arbitrarily large and the reconstruction loss might approach $-\infty$.

A common approach is to use a fixed variance of 1, because then the reconstruction term becomes square error loss. $p(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}(\mathbf{z}), 1))$.

Another approach, σ-VAE [17], is to let the variance be a trainable parameter but not a function of $\mathbf{z}$. $p(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}(\mathbf{z}), \boldsymbol{\sigma})$. In this case as well in my experiments at least, if σ is allowed to be too small we sometimes get similar issues of numerical stability, non-stochastic decoder and meaningless encoding in the latent space.

4.2.9 VAE as a generalization of AE

Suppose that we take a σ-VAE as described above, and suppose that we hold σ fixed.

So the decoder is $p(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}; \mu(\mathbf{z}), \sigma)$ where $\mu(z)$ is a a function of $\mathbf{z}$ the decoder neural network. The decoder is $q(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mathbf{z}; \mu(\mathbf{x}), \sigma(\mathbf{x}))$ For the kl-term we use the analytical solution and for the reconstruction error we use Monte Carlo integration with one sample. We can assume that the KL term is uniformly (with respect to $\mathbf{x}$) bounded by some constant M. We could also make sure that the encoder map is bounded but normally there is no reason for the encoder to take the mean or the variance to infinity during training as it would just increase the loss.

Our -ELBO loss function is:

$$\begin{aligned}\mathcal{L}(p,q,\mathbf{x}) &= -\log\mathcal{N}(\mathbf{x}; \mu(\mathbf{z}), \sigma) + KL(q(\mathbf{z}|\mathbf{x})\|p(\mathbf{z})) \\ &= \frac{1}{2}\|\frac{x-\mu(\mathbf{z})}{\sigma}\|^2 + \log\sigma + KL(q(\mathbf{z}|\mathbf{x})\|p(\mathbf{z}))\end{aligned} \tag{4.14}$$

Minimizing $\mathcal{L}(p,q,\mathbf{x})$ in equation 4.14 is equivalent to minimizing $\sigma\mathcal{L}(p,q,\mathbf{x})$, and if we let $\sigma \to 0$ we get:

$$\begin{aligned}\lim_{\sigma\to 0}\mathcal{L}(p,q,\mathbf{x})\sigma &= \lim_{\sigma\to 0}[-\log\mathcal{N}(\mathbf{x}; \mu(\mathbf{z}), \sigma)\sigma + \sigma KL(q(\mathbf{z}|\mathbf{x})\|p(\mathbf{z}))] \\ = \lim_{\sigma\to 0}[\frac{1}{2}\|x-\mu(\mathbf{z})\|^2 + \sigma\log\sigma + \sigma KL(q(\mathbf{z}|\mathbf{x})\|p(\mathbf{z}))] &= \frac{1}{2}\|x-\mu(\mathbf{z})\|^2\end{aligned} \tag{4.15}$$

So if we set σ be arbitrary small, $p(\mathbf{x}|\mathbf{z})$ become almost point mass and the KL term loses significance, effectively removing the constraint from the encoder. As a result the encoder itself will also become point mass in order to minimize the reconstruction term and disregarding the constraint on its distribution. Thus the VAE becomes essentially a vanilla auto encoder at the limit.

4.2.10 Graphical representation

It is both convenient as well as informative to include a graphical description of our probabilistic models by way of modified plate diagrams which describes both the generative model (p distribution) and the inference model (q) on the same graph.

Definition 4.4. A *modified plate diagram* describes the factorization of two probabilistic models with respectively distributions p and q, according to the following scheme.

Round or oval nodes represent *random variables*, *rectangular or square* nodes represent *hyperparameters* or stochastic parameters, and *arrows* represent dependency.

Solid arrows with pointed arrowhead represent the dependencies of the p distribution. *Dotted arrows with round arrowheads* represent the dependencies of the q distribution. In order to describe a legal distribution the subgraph of just the pointed (and of just round) arrows must form a DAG.

Plate represents the packing of N i.i.d random vectors.

Shaded nodes represent known values. Shaded oval or round nodes are called *observations* or *observed variables*. Clear oval nodes are called *latent* variables.

Shaded square or rectangular nodes represent fixed hyperparameters of the model. Clear square or rectangular nodes represent stochastic parameters of the model.

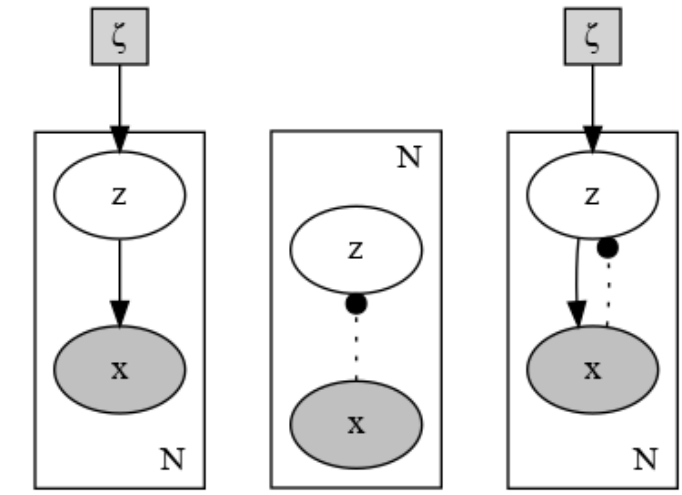
Figure 4.2 is a modified plate diagram of the VAE model. We use doted arrows with round arrowhead to represent the inference model (encoder network), and regular arrows for the generative model (decoder network) so the combined diagram describes the two networks together.

The squared ζ node represent some *fixed hyperparameter* which describes the prior distribution of $p(\mathbf{z}) := p(\mathbf{z}|\zeta)$. It is possible to make ζ a non-fixed stochastic parameter but in the case of this vanilla VAE I don't think it has any advantage and don't know of anyone who does that.

The generative model therefore factors as: $p(\mathbf{x}, \mathbf{z}) = p(\mathbf{x}|\mathbf{z})p(\mathbf{z}|\zeta) = p(\mathbf{x}|\mathbf{z})p(\mathbf{z})$. The inference model in this case is just $q(\mathbf{z}|\mathbf{x})$.

Note that the graphical model has no assumption about the specific types of distributions involved (Gaussian, Dirichlet or whatever ...) and that is left for the actual implementation.

In the case of a "vanilla" VAE (E, D, p), We use mean field approximation for p and q with Gaussian distributions. We set the prior $p(\mathbf{z})$ to be diagonal standard Gaussian $p(\mathbf{z}) \sim \mathcal{N}(;\mathbf{0}, \mathbf{1})$. And $p(\mathbf{z}|\mathbf{x}) \sim \mathcal{N}(; D(\mathbf{z}))$ is a diagonal Gaussian, where the decoder determines its means and variances $D(\mathbf{z}) = (\boldsymbol{\mu}(\mathbf{z}), \boldsymbol{\sigma}(\mathbf{z}))$, And similarly $q(\mathbf{z}|\mathbf{x}) \sim \mathcal{N}(; E(\mathbf{x}))$.



(a) generative model ($p(x, z)$) (b) inference model ($q(z|x)$) (c) the combined graphical model

Figure 4.2: VAE graphical model

4.3 Expanding the VAE model

If we look at figure 4.2 it looks very simple, but it also pretty much forces us to choose a simple type of distribution family (e.g diagonal Gaussians in the case of the vanilla VAE). Recall that That $\mathbf{z}$ packs up all the latent variables and the stochastic parameters and $\mathbf{x}$ packs up all the observed variables.

We can describe a more complex distribution by unpacking them and describe the dependencies between them. This is done in the following way:

1. Define the set of observed random vectors $\mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_k$, and the set of latent random vectors and stochastic parameters $\mathbf{z}_1, \ldots \mathbf{z}_l$.
2. Specify how to factor the generative model $p(\mathbf{x}_1, \ldots, \mathbf{x}_k|\mathbf{z}_1 \ldots, \mathbf{z}_l)$
3. Specify how to factor the inference model $q(\mathbf{z}_1 \ldots \mathbf{z}_l|\mathbf{x}1, \ldots \mathbf{x}_k)$
4. Choose appropriate priors $p(\mathbf{z}_i)$ and
5. Choose appropriate distribution families for the $\mathbf{x}_i$ and $\mathbf{z}_i$, and choose priors $p(\mathbf{z}_i)$.

4.3.1 Example: CVAE

Suppose that we have data that carries both numerical and categorical data $(\mathbf{X}, C)$. For example suppose that $\mathbf{X}$ represent a set of images (as flattened vectors), and C represents the object types shown in the images. Moreover lets assume that we have k types of categories and that the data is balanced so we have k/N samples from each category. We have just specified our observed variables $\mathbf{x}, c$. We will have one latent variable $\mathbf{z}$ (remember it is actually a vector but we call them variables...). The idea here is that because we have different categories, we will have some type of a mixture of distributions.

Lets specify the generative model $p(\mathbf{x}, \mathbf{z}, c)$. We can factor it "arbitrarily" however the choice may make a significant difference on the result. In this case there aren't too many ways to factor. We can factor as $p(\mathbf{x}, \mathbf{z}, c) = p(\mathbf{x}|\mathbf{z}, c)p(\mathbf{z}|c)p(c)$ which mean $\mathbf{x}$ is directly dependent on both $\mathbf{z}$ and c. If we use this factorization then we concatenate $\mathbf{z}$ and c for computing the decoder's reconstruction $p(\mathbf{x}|\mathbf{z}, c)$. But suppose we assume that $\mathbf{x}$ and c are conditionally independent given $\mathbf{z}$, so we may set $p(\mathbf{x}, \mathbf{z}, c) = p(\mathbf{x}|\mathbf{z})p(\mathbf{z}|c)p(c)$. We call $p(\mathbf{z}|c)$ a "learned prior" of $\mathbf{z}$ since it is not fixed like in the VAE case but rather the decoder maps the categorical c into some distribution.

As for the inference model (encoder), given the observation $\mathbf{x}$ and c it will determine our only latent variable $\mathbf{z}$, in other words $q(\mathbf{z}|\mathbf{x}, c)$ is the inference model without anything further to factorize. Conditioning in c is done here as well by concatenating the inputs $\mathbf{x}$ and c.

Since our data is balanced, we use uniform prior $p(c) = \frac{1}{k}$.

The generative process (decoder) is therefore as follows:

- draw a category $c \sim Cat(\frac{1}{k})$.
- draw $\mathbf{z} \sim p(\mathbf{z}|c)$.
- draw $\mathbf{x} \sim p(\mathbf{x}|\mathbf{z})$.
- the resulting factorization of p is: $p(\mathbf{x}, \mathbf{z}, c) = p(\mathbf{x}|\mathbf{z})p(\mathbf{z}|c)\frac{1}{k}$.

Remember that the loss function is still the minus ELBO, which according to our factorization becomes:

$$\begin{aligned} \mathcal{L}(p, q, \mathbf{x}, c) &= \int -\log \frac{p(\mathbf{x}, c, \mathbf{z})}{q(\mathbf{z}|\mathbf{x}, c)} dq \\ &= \int -\log \frac{p(\mathbf{x}|\mathbf{z})p(\mathbf{z}|c)p(c)}{q(\mathbf{z}|\mathbf{x}, c)} dq \\ &= \int -\log p(\mathbf{x}|\mathbf{z}) dq + \int \log \frac{q(\mathbf{z}|\mathbf{x}, c)}{p(\mathbf{z}|c)} dq + \log(k) \\ &= \int -\log p(\mathbf{x}|\mathbf{z}) dq + KL(q(\mathbf{z}|\mathbf{x}, c) \| p(\mathbf{z}|c)) + \text{const} \end{aligned} \tag{4.16}$$

Since the $\mathbf{z}$ prior depends on the category, $p(\mathbf{z}|c)$, it should be some sort of "blobs" mixture type of distribution. The inference model is just $q(\mathbf{z}|\mathbf{x}, c)$. The regularization kl-term tries to impose $q(\mathbf{z}|\mathbf{x}, c)$ to be close to $p(\mathbf{z}|c)$, so if all works well $q(\mathbf{z}|\mathbf{x}, c)$ should look like a mixture distribution ("blobs").

Now for concrete choice of distribution families: $p(c)$ is already chosen for us as uniform categorical. For the rest we again use diagonal Gaussians. $p(\mathbf{z}|c)$ will be parametrized by an encoder network taking only the categorical information. Essentially this network will map each category into some "blob" around some centroid in the latent space. $p(\mathbf{x}|\mathbf{z})$ describes how given $\mathbf{z}$ it defines a diagonal normal distribution with fixed (or restricted) variance back in the observed space like the decoder network in the vanilla case. $q(\mathbf{z}|\mathbf{x}, c)$ means that in this case the encoder takes as input both $\mathbf{x}$ and c and defines a diagonal Gaussian in the latent space. The difference is that with this model after we train it, the encoder will encode a mixture distribution in $\mathbf{z}$, we will get several blobs in the latent space corresponding to the classes.

From equation 4.16, we can ignore the constant and see that the reconstruction term that will make sure the decoder reconstruct the image in our example, while the kl-term imposes a mixture distribution in the latent space.

Finally there are circumstances that we use CVAE to "forget" the categories rather then to encode them by setting a fixed prior $p(\mathbf{z}|c) \equiv p(\mathbf{z})$. An example for such use-case is for batch effect reduction. In cases where for example, there are several batches of data of the same type and but from different experiments. We expect any differences in the data of the same entity are a result of technical differences (different measuring tools etc.) rather than reflecting true differences between the entity of interest. In this case we can use a CVAE model with fixed prior to reduce the batch effect.

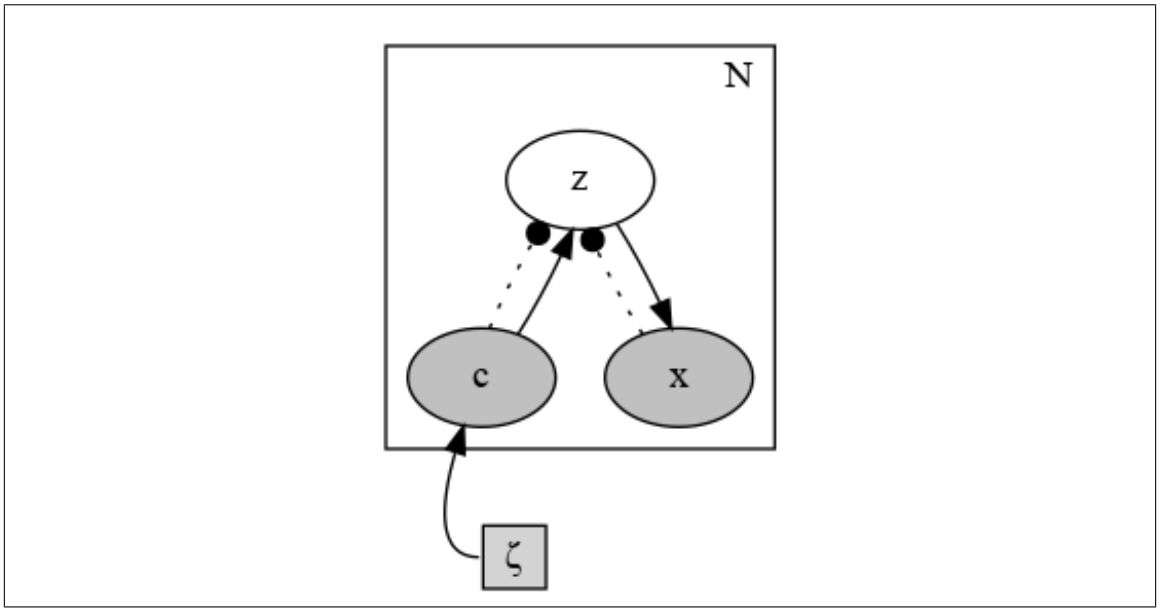
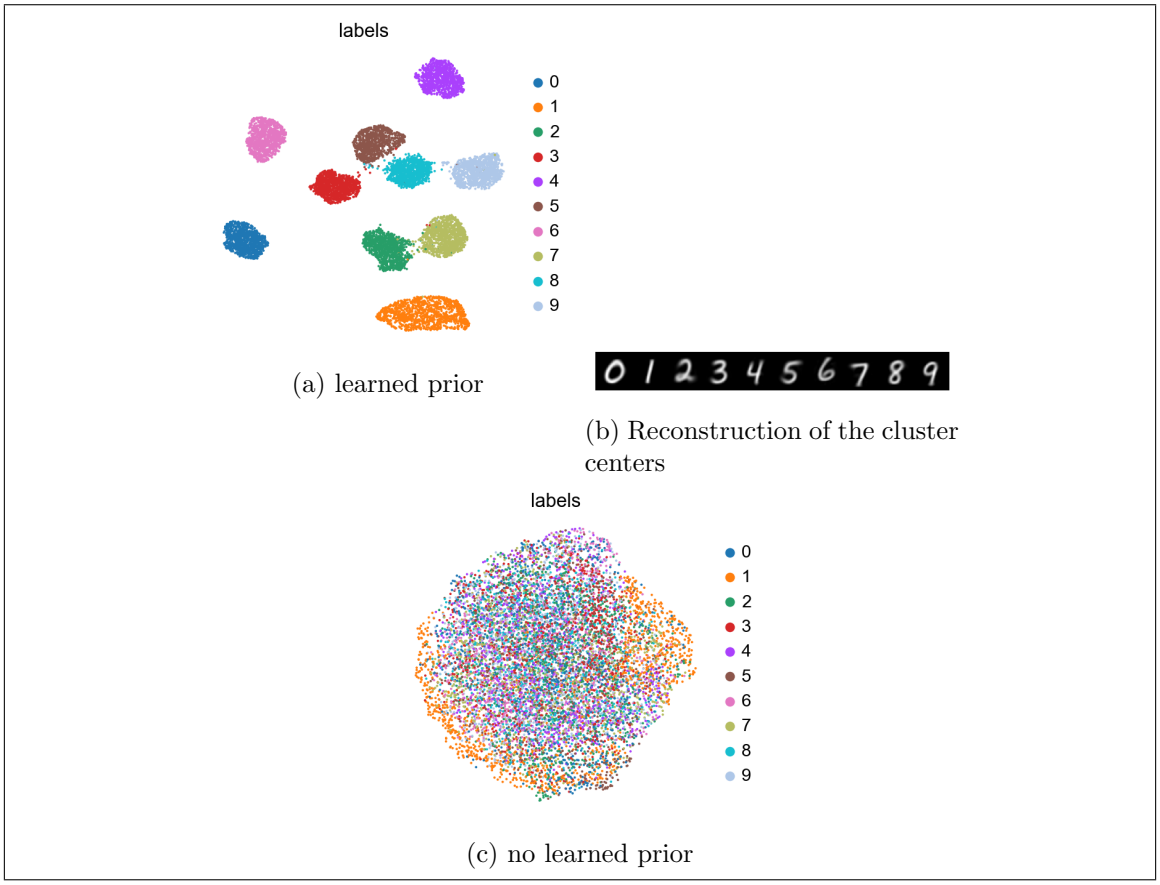


Figure 4.3: Graphical model of the CVAE with a learned prior $p(\mathbf{z}|c)$. as usual the solid arrows depict the inference model (encoder) and the dotted ones the generative model (decoder)

Figure 4.4 shows in the left a umap plot of the latent space for the CVAE model which we described first, on the MNIST data set. It uses the learned prior $p(\mathbf{z}|c)$ and $\mathbf{x}$ and c are conditionally independent given $\mathbf{z}$. The middle image shows the reconstruction of the clusters centers (the means of $p(\mathbf{z}|c)$). In this model the encoder completely separates the categories in the latent representation, resulting in distinct blobs. The right image is the CVAE described last, the one which "forgets" the category, with fixed prior $p(\mathbf{z}|c) = p(\mathbf{z}) = \mathcal{N}(\mathbf{z}; 0, 1)$. In this model $\mathbf{x}$ is not conditionally independent from c, but instead it is directly dependent on both $\mathbf{z}$ and c ($p(\mathbf{x}|\mathbf{z}, c)$). The result is an encoding which mixes a lot of the categories in the latent space but we can still notice some clustering.



(a) learned prior

(b) Reconstruction of the cluster centers

(c) no learned prior

Figure 4.4: CVAE, different use cases

Chapter 5

Gaussian mixture model VAEs

5.1 Motivation

Suppose that we have data of type $(\mathbf{x}, \mathbf{y})$ which like in the CVAE case has numerical and categorical information, but unlike in the CVAE section we don't have access to the categories $\mathbf{y}$, only to $\mathbf{x}$. We are looking for a model that can partition $\mathbf{X}$ according to the true categories. This is a task of unsupervised learning which is much harder then classifying data with known targets $\mathbf{Y}$.

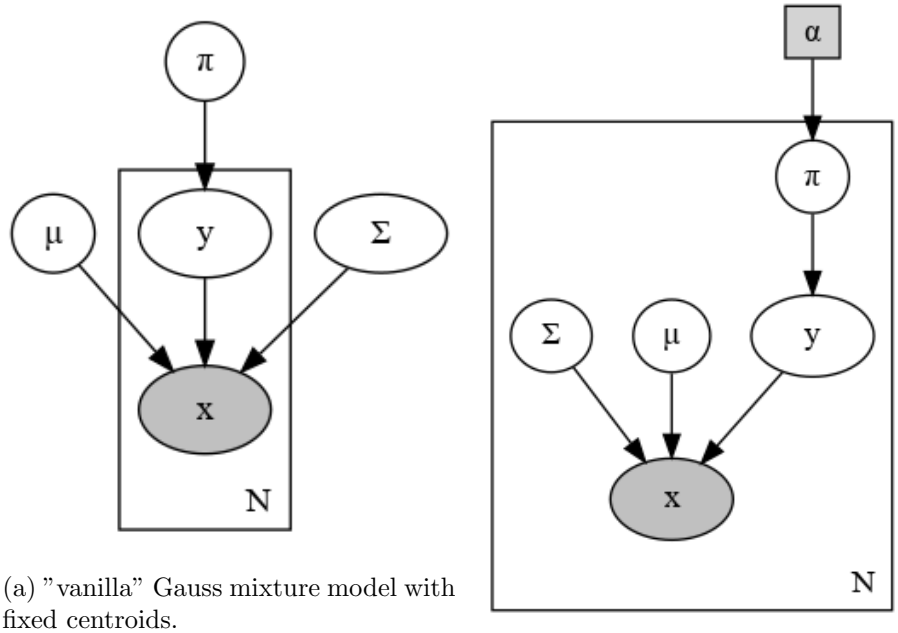
The original data has a complex distribution. Not only is it high dimensional, but because the data belongs to distinct categories, it is natural to assume that $\mathbf{x}$ comes from a mixture distribution.

We want to create some mixture distribution, where a latent categorical random variable $\mathbf{y}$ functions as the component selector. We could try to directly create the mixture $p(\mathbf{x}|\mathbf{z}, \mathbf{y})$ in the $\mathbf{x}$ space, as the M2 model in [9]. The other option, following the Gaussian mixture model proposed by Dilokthanakul et.al [2] and which base our model is to create a mixture prior distribution $p(\mathbf{z}|\mathbf{w}, \mathbf{y})$ on the lower dimensional latent $\mathbf{z}$ space.

There are several advantages to doing this. For once we are interested in dimensionality reduction and not just in unsupervised classification. If we create a mixture distribution in the latent space $\mathbf{z}$ we can then further analyse it (by clustering algorithms for example) and plot it, for example with UMAP. A second reason is that it may be easier to create a mixture Gaussian on the simpler, lower dimensional space $\mathbf{z}$ rather than on the high dimensional $\mathbf{x}$ space where the data occupies a complex hyper-surface.

Figure 5.1a describes the usual Gaussian mixture model [1]. The components' centroids, $\boldsymbol{\mu} = (\boldsymbol{\mu}_1, \dots \boldsymbol{\mu}_k)$, its covariances, $\boldsymbol{\Sigma}$, and the categorical selection distribution π, are outside the plate. It means we draw the centroids, variances, and the categorical distribution once, and use them for all the samples inside the plate. That constraints each category to be distributed around some fixed center which is pretty restrictive and perhaps too much so. By moving the random vectors inside the plate (figure 5.1b), we create a much more flexible distribution.

Another issue with the original mixture model, if we try to base a VAE model on it, is that it imposes a "bad categorical prior" on $\mathbf{y}$. We usually set $p(\mathbf{y}) \sim \text{Cat}(\pi)$ and $\pi = \frac{1}{k}$ assuming the data is balanced. The problem is that we want the inference model (the



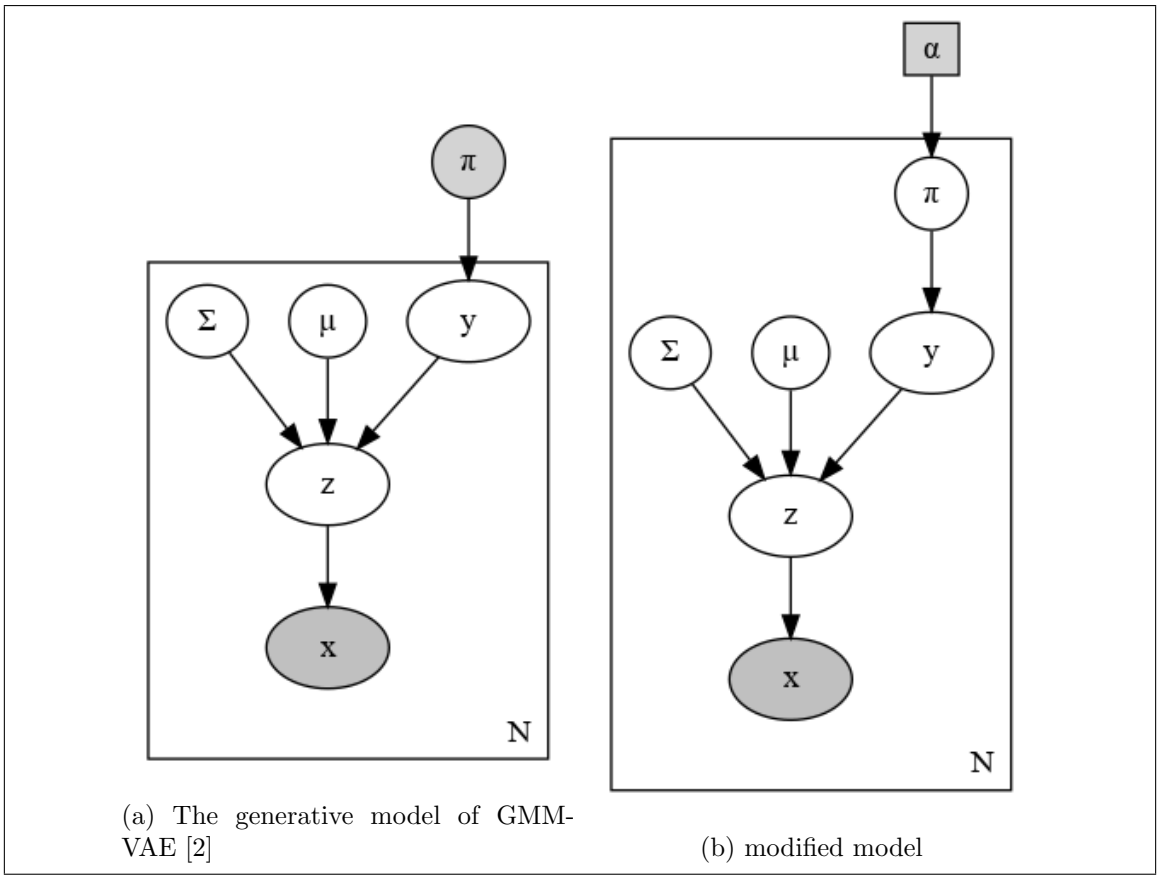
(a) "vanilla" Gauss mixture model with fixed centroids.

(b) a more complex mixture where the centroids are moved into the plate.

Figure 5.1

encoder) $q(\mathbf{y}|\mathbf{x})$ to be a good classifier so we don't want to impose it to be close to uniform. If we move π inside and give it a symmetric Dirichlet prior, we allow more flexibility on π, so it can be be heavily biased towards one category, making it a good predictor. α is a symmetric Dirichlet hyper-parameter and "tweaking" with it has influence on the number of non-empty categories that the model finds during training.

Figure 5.2a shows the generative model of the GMMVAE [2], where the mixtures components (μ, σ) are inside the plate but the selection distribution (π) is a fixed parameter which is outside the of the plate. The latent $\mathbf{z}$ space is a mixture distribution. As explained above, the $\mathbf{y}$-prior is "bad" because it will be uniform categorical, while we want to use the inference model $q(\mathbf{y}|\mathbf{z})$ to predict the category. In figure 5.2b π is moved inside the plate and becomes a variable. Its prior is a symmetric Dirichlet with hyper-parameter α. We call our modification the *DGMMVAE* model (D stands for the Dirichlet prior obviously).



(a) The generative model of GMM-VAE [2]

(b) modified model

Figure 5.2: On the left we see the generative model used by GMMVAE [2], where π is a fixed hyper parameter and resides outside of the plate. On the right: modification of the GMMVAE model, where π moves inside the plate and becomes a variable with a symmetric Dirichlet prior.

5.2 The DGMMVAE model

Our DGMMVAE model is based on figure 5.2b. In addition to the latent variables $\mathbf{z}$ (mixture), and $\mathbf{y}$ (categorical), there 2 more variables. The third latent variabel $\mathbf{w}$ has standard normal prior. With $\mathbf{w}$ the model generates the means and variances μ, σ for the mixture's components, by a of neural network. A fourth variable $\mathbf{d}$ is the Dirichlet prior. The full generative model factors as (figure 5.3):

$$\begin{aligned} p(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{w},\mathbf{d}) &= p(\mathbf{x}|\mathbf{z})p(\mathbf{z}|\mathbf{w},\mathbf{y})p(\mathbf{y}|\mathbf{d})p(\mathbf{d})p(\mathbf{w}) \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{0},\mathbf{1}) \\ p(\mathbf{d}) &= \mathrm{Dir}(\mathbf{d}|\alpha) \\ p(\mathbf{y}|\mathbf{d}) &= \mathrm{Cat}(\mathbf{y}|\mathbf{d}) \\ p(\mathbf{z}|\mathbf{w},\mathbf{y}) &= \mathcal{N}(\mathbf{z}|\mu(\mathbf{w})_{\mathbf{y}},\sigma(\mathbf{w})_{\mathbf{y}})) \\ p(\mathbf{x}|\mathbf{z}) &= \mathcal{N}(\mathbf{x}|\mu(\mathbf{z}),\sigma(\mathbf{z})) \end{aligned} \tag{5.1}$$

$\mu(\mathbf{w}), \sigma(\mathbf{w}), \mu(\mathbf{z}), \sigma(\mathbf{z})$ are neural networks of the decoder. $\mu(\mathbf{w})$, $(\sigma(\mathbf{w}))$ is not just one mean (variance) but a set of k (=number of categories) means (variances), and we are selecting the component $\mu(\mathbf{w})_{\mathbf{y}}, \sigma(\mathbf{w})_{\mathbf{y}}$ indicated by $\mathbf{y}$, the categorical random variable.

The generative process can be described as follows:

1. draw from the prior $\mathbf{w} \sim p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \mathbf{1})$
2. draw a categorical distribution from the Dirichlet prior $\mathbf{d} \sim p(\mathbf{d}) = \text{Dir}(\mathbf{d}|\alpha)$
3. draw a category $\mathbf{y} \sim p(\mathbf{y}|\mathbf{d}) = \text{Cat}(\mathbf{y}|\mathbf{d})$
4. generate the k centroids and diagonal variances by the decoder's NN: $\boldsymbol{\mu}(\mathbf{w}), \boldsymbol{\sigma}(\mathbf{w})$.
5. draw from the mixture $\mathbf{z} \sim p(\mathbf{z}|\mathbf{w}, \mathbf{y}) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}(\mathbf{w})_\mathbf{y}, \boldsymbol{\sigma}(\mathbf{w})_\mathbf{y})$
6. generate the means $\boldsymbol{\mu}(\mathbf{z})$ and diagonal variances $\boldsymbol{\sigma}(\mathbf{z})$ (or use fixed variance 1) by the decoder NN.
7. draw observation $\mathbf{x} \sim p(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}(\mathbf{z}))$

There are several ways to factor the inference model and it is not immediately clear which one is better. Here is the factorization depicted in figure 5.3:

$$\begin{aligned} q(\mathbf{y}, \mathbf{z}, \mathbf{w}, \mathbf{d}|\mathbf{x}) &= q(\mathbf{z}|\mathbf{x})q(\mathbf{w}|\mathbf{x})q(\mathbf{y}|\mathbf{z})q(\mathbf{d}|\mathbf{z}) \\ q(\mathbf{z}|\mathbf{x}) &= \mathcal{N}(\mathbf{z}|\mu_z(\mathbf{x}), \sigma_z(\mathbf{x})) \\ q(\mathbf{w}|\mathbf{x}) &= \mathcal{N}(\mathbf{w}|\mu_w(\mathbf{x}), \sigma_w(\mathbf{x})) \\ q(\mathbf{y}|\mathbf{z}) &= \text{Cat}(\mathbf{y}|f(\mathbf{z})) \\ q(\mathbf{d}|\mathbf{z}) &= \text{Dir}(\mathbf{d}|g(\mathbf{z})) \end{aligned} \tag{5.2}$$

And $f(\mathbf{z}), g(\mathbf{z}), \mu_w(\mathbf{x}), \sigma_w(\mathbf{x}), \mu_z(\mathbf{x}), \sigma_z(\mathbf{x})$ are the neural networks of the encoder.

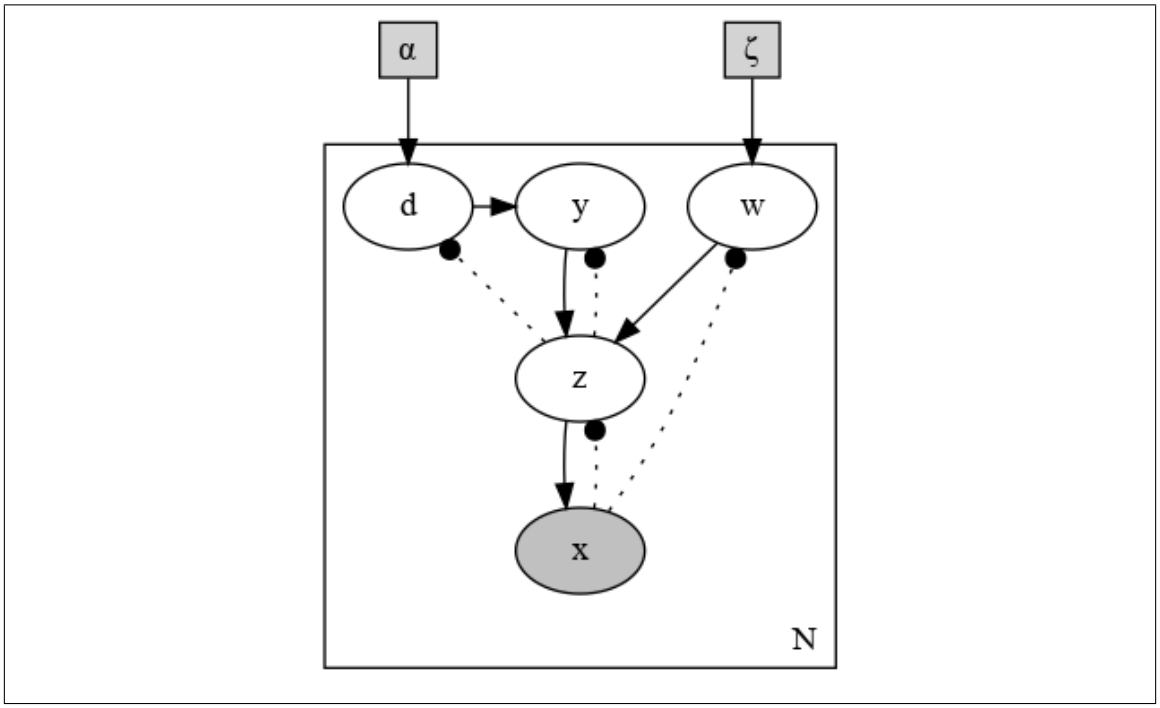


Figure 5.3: DGMMVAE: GMMVAE with Dirichlet prior

5.3 Computing the loss function of DGMMVAE model

The loss function remains the -ELBO and we can break it into different terms:

$$\mathcal{L}(p,q,\mathbf{x}) = \int -\log \frac{p(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{w},\mathbf{d})}{q(\mathbf{z},\mathbf{y},\mathbf{w},\mathbf{d}|\mathbf{x})} dq(\mathbf{z},\mathbf{y},\mathbf{w},\mathbf{d}|\mathbf{x}) \tag{5.3}$$

$$= \int -\log \frac{p(\mathbf{x}|\mathbf{z})p(\mathbf{z}|\mathbf{w},\mathbf{y})p(\mathbf{y}|\mathbf{d})p(\mathbf{w})p(\mathbf{d})}{q(\mathbf{z}|\mathbf{x})q(\mathbf{w}|\mathbf{x})q(\mathbf{y}|\mathbf{z})q(\mathbf{d}|\mathbf{z})} dq \tag{5.4}$$

$$= \int -\log p(\mathbf{x}|\mathbf{z}) dq \tag{5.5}$$

$$+ \int \log \frac{q(\mathbf{z}|\mathbf{x})}{p(\mathbf{z}|\mathbf{w},\mathbf{y})} dq \tag{5.6}$$

$$+ \int \log \frac{q(\mathbf{w}|\mathbf{x})}{p(\mathbf{w})} dq \tag{5.7}$$

$$+ \int \log \frac{q(\mathbf{y}|\mathbf{z})}{p(\mathbf{y}|\mathbf{d})} dq \tag{5.8}$$

$$+ \int \log \frac{q(\mathbf{d}|\mathbf{z})}{p(\mathbf{d})} dq \tag{5.9}$$

As we see there are five terms in the reconstruction loss function. 5.14 is called the reconstruction error. The rest of the terms get the repetitive, mundane names: 5.15 is called the z-error or z-kl-term, 5.16 is the w-error or w-kl-term, 5.18 is the y-error or y-kl-term, and 5.9 is called the d-error or d-kl-term.

To actually compute the loss function we will use Monte Carlo integration, with one sample for each observation. We will need to sample $\mathbf{z}$, $\mathbf{w}$ and $\mathbf{d}$. For $\mathbf{y}$ we will not sample but rather integrate over the categorical probabilities.

1. sample $\mathbf{z} \sim q(\mathbf{z}|\mathbf{x})$ using the reparameterization trick
2. sample $\mathbf{w} \sim q(\mathbf{w}|\mathbf{x})$ using the reparameterization trick
3. sample $\mathbf{d} \sim q(\mathbf{d}|\mathbf{z})$ using the reparameterization trick
4. Reconstruction error estimation:
$$-\log p(\mathbf{x}|\mathbf{z}) = -\log \mathcal{N}(\mathbf{x}|\mu(\mathbf{z}),\sigma(\mathbf{z}))$$
5. $\mathbf{z}$-error: calculate $KL(q(\mathbf{z}|\mathbf{x})\|p(\mathbf{z}|\mathbf{w},\mathbf{y}))$ analytically using equation 4.13 for every mixture component of $p(\mathbf{z}|\mathbf{w},\mathbf{y})$, and then take the weighted average with respect to $q(\mathbf{y}|\mathbf{z})$:
$$\sum_{j=1}^{k} [q(\mathbf{y}=j|\mathbf{z}) KL(q(\mathbf{z}|\mathbf{x})\|p(\mathbf{z}|\mathbf{w},\mathbf{y}=j))]$$
.
6. $\mathbf{w}$-error: calculate $KL(q(\mathbf{w}|\mathbf{x})\|p(\mathbf{w}))$ analytically the kl-divergence between two diagonal Gaussians (equation 4.13).
7. $\mathbf{y}$-error: calculate $KL(q(\mathbf{y}|\mathbf{z})\|p(\mathbf{y}|\mathbf{d}))$ analytically (kl-div of two categorical distributions,):
$$KL(q(\mathbf{y}|\mathbf{z})\|p(\mathbf{y}|\mathbf{d})) = \sum_{j=1}^{k} [q(\mathbf{y}=j|\mathbf{z}) \log \frac{q(\mathbf{y}=j|\mathbf{z})}{p(\mathbf{y}=j|\mathbf{d})}]$$
8. $\mathbf{d}$-error: calculate $KL(q(\mathbf{d}|\mathbf{z})\|p(\mathbf{d}))$ analytically (kl-divergence of two Dirichlet distributions also has a closed formed formula and it's builtin function in Pytorch).

5.4 The DGMMVAE model in the supervised case

The DGMMVAE model can also be used for supervised training. While the architecture of the neural network remains the same, the probabilistic interpretation and consequently the calculation of the loss function is different.

Figure 5.4 describes the generative and the inference model in the supervised case. Since in this case $\mathbf{y}$ is observed, we regard $\mathbf{z}$ in the generative model as only dependent on $\mathbf{w}$. Internally we keep the same architecture but during supervised training we always select just the given $\mathbf{y}$ component and so we can stop regarding $\mathbf{z}$ as depending on $\mathbf{y}$. $p(\mathbf{z}|\mathbf{w},\mathbf{y}) = p(\mathbf{z}|\mathbf{w}) = \mathcal{N}(\mathbf{z}|\mu(\mathbf{w})_y, \sigma(\mathbf{w})_y)$. In the figure we show the dashed arrow from $\mathbf{y}$ to $\mathbf{w}$ but if it were a real dependency we would get an "illegal" cycle in the p-graph. However the $\mathbf{y}$ which we used to select the $\mu(\mathbf{w}), \sigma(\mathbf{w})$ mixture components are not drawn from $p(\mathbf{y}|\mathbf{z})$, rather we use the observation $\mathbf{y}$ (=the category label) itself which is given to us in the supervised case. Thus there is no actual cycle in the dependency graph but the effect of $\mathbf{y}$ remains in the implementation of the network architecture.

Moreover in the supervised case the random variable $\mathbf{y}$ becomes dependent on both $\mathbf{d}$ and $\mathbf{z}$. We make an assumption that $\mathbf{y}|\mathbf{d}$ and $\mathbf{y}|\mathbf{z}$ are independent, so $p(\mathbf{y}|\mathbf{d},\mathbf{z}) = p(\mathbf{y}|\mathbf{d})p(\mathbf{y}|\mathbf{z})$, thus enabling us to retain the same network architecture. $p(\mathbf{y}|\mathbf{d})$ is determined by the same decoder component as in the unsupervised case but $p(\mathbf{y}|\mathbf{z})$ equals $q(\mathbf{y}|\mathbf{z})$ of the encoder in the unsupervised case. So while again we keep the same architecture we will compute the loss function differently. As for the inference model it becomes other than losing the $q(\mathbf{y}|\mathbf{z})$ component the rest remains the same. The full factorization in the supervised case becomes:

$$
\begin{aligned}
p(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{w},\mathbf{d}) &= p(\mathbf{x}|\mathbf{z})p(\mathbf{y}|\mathbf{d})p(\mathbf{y}|\mathbf{z})p(\mathbf{z}|\mathbf{w})p(\mathbf{d})p(\mathbf{w}) \\
q(\mathbf{z},\mathbf{w},\mathbf{d}|\mathbf{x},\mathbf{y}) &= q(\mathbf{z}|\mathbf{x})q(\mathbf{w}|\mathbf{x})q(\mathbf{d}|\mathbf{z}) \\
p(\mathbf{x}|\mathbf{z}) &= \mathcal{N}(\mathbf{x}|\mu(\mathbf{z}),\sigma(\mathbf{z})) \\
p(\mathbf{y}|\mathbf{z}) &= \mathrm{Cat}(\mathbf{y}|f(\mathbf{z})) \\
p(\mathbf{y}|\mathbf{d}) &= \mathrm{Cat}(\mathbf{y}|\mathbf{d}) \\
p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}|\mathbf{0},\mathbf{1}) \\
p(\mathbf{d}) &= \mathrm{Dir}(\mathbf{d}|\alpha) \\
p(\mathbf{z}|\mathbf{w}) &= \mathcal{N}(\mathbf{z}|\mu(\mathbf{w})_{\mathbf{y}},\sigma(\mathbf{w})_{\mathbf{y}})) \\
q(\mathbf{z}|\mathbf{x}) &= \mathcal{N}(\mathbf{z}|\mu_z(\mathbf{x}),\sigma_z(\mathbf{x})) \\
q(\mathbf{w}|\mathbf{x}) &= \mathcal{N}(\mathbf{w}|\mu_w(\mathbf{x}),\sigma_w(\mathbf{x})) \\
q(\mathbf{d}|\mathbf{z}) &= \mathrm{Dir}(\mathbf{d}|g(\mathbf{z}))
\end{aligned}
\tag{5.10}
$$

The loss function in the supervised case is:

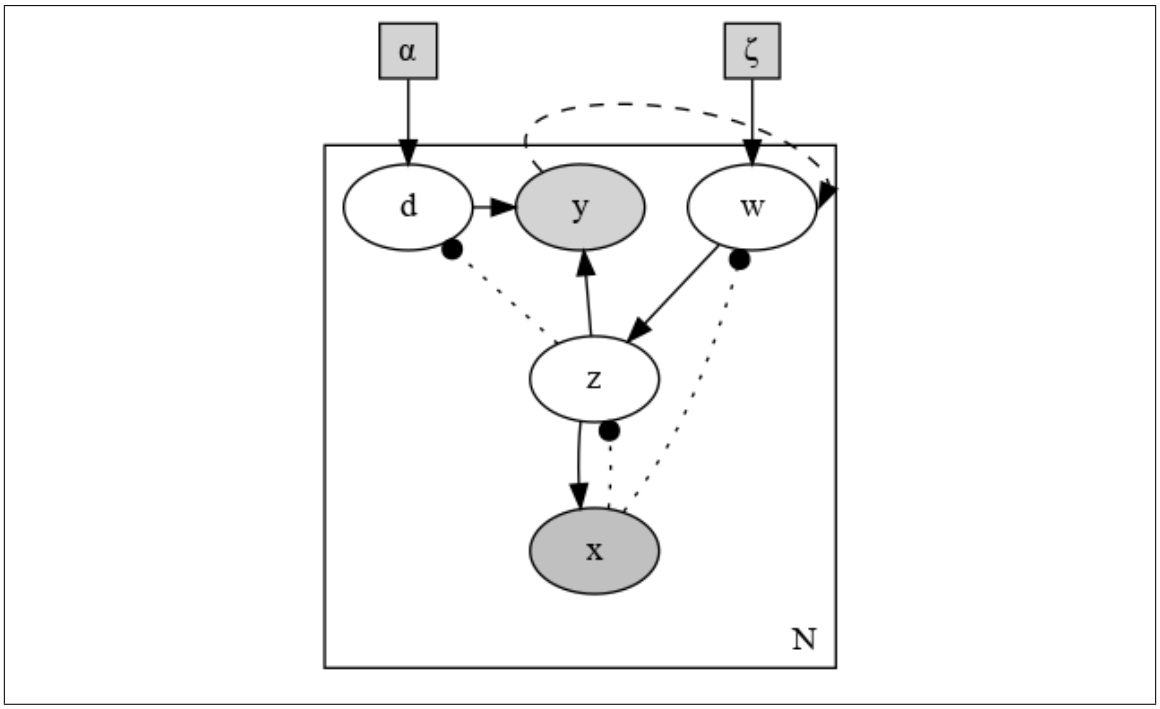


Figure 5.4: DGMMVAE: the supervised case, where $\mathbf{y}$ is an observed variable.

$$\mathcal{L}(p,q,\mathbf{x}) = \int -\log \frac{p(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{w},\mathbf{d})}{q(\mathbf{z},\mathbf{w},\mathbf{d}|\mathbf{x},\mathbf{y})} dq(\mathbf{z},\mathbf{y},\mathbf{w},\mathbf{d}|\mathbf{x}) \tag{5.11}$$

$$= \int -\log \frac{p(\mathbf{x}|\mathbf{z})p(\mathbf{z}|\mathbf{w})p(\mathbf{y}|\mathbf{d})p(\mathbf{y}|\mathbf{z})p(\mathbf{w})p(\mathbf{d})}{q(\mathbf{z}|\mathbf{x})q(\mathbf{w}|\mathbf{x})q(\mathbf{d}|\mathbf{z})} dq \tag{5.12}$$

$$= \int -\log p(\mathbf{x}|\mathbf{z}) dq \tag{5.13}$$

$$+ \int \log \frac{q(\mathbf{z}|\mathbf{x})}{p(\mathbf{z}|\mathbf{w})} dq \tag{5.14}$$

$$+ \int \log \frac{q(\mathbf{w}|\mathbf{x})}{p(\mathbf{w})} dq \tag{5.15}$$

$$+ \int \log p(\mathbf{y}|\mathbf{z}) dq \tag{5.16}$$

$$+ \int \log p(\mathbf{y}|\mathbf{d}) dq \tag{5.17}$$

$$+ \int \log \frac{q(\mathbf{d}|\mathbf{z})}{p(\mathbf{d})} dq \tag{5.18}$$

The reconstruction error, the w-error and the d-error are calculated exactly like in the unsupervised loss. The z-term is also calculated in exactly the same procedure as in unsupervised case except that we only need to take the component indicated by the obseved $\mathbf{y}$ in the weighted sum. The two y-terms are the log probability of the observed category given the sampled $\mathbf{z}$ and $\mathbf{d}$.

5.5 Combining GMMVAE with another clustering method

Because GMMVAE performs particularly well in (semi)supervised it can learn a given cluster/class assignment of a dataset by. But when might it be useful to train GMMVAE if we already have a different clustering algorithm or any other unsupervised classifier that works well? Suppose that we have a "nice" training set where a given clustering algorithm performs well on. We can supervised train GMMVAE on the nice dataset using the cluster assignment as labels. At this point the model should learn to represent the data clusters nearly perfect. It is often the case that the GMMVAE trained in this manner will out-perform a "naive" GMMVAE which was unsupervised trained.

We can than run unsupervised training on the dataset, if we are lucky the accuracy might improve. So that's one use case but a minor one.

The more important usage is that we can now classify with GMMVAE other datasets of the same kind. We should compare the performance of the trained model on the testing set with the performance of the clustering algorithm *on the testing set* which per assumption was not that good. If we are lucky the GMMVAE might outperform the clustering algorithm on the not–so–nice testing data.

We tested a combination of GMMVAE with Louvain [16] clustering on several datasets (results shown in subsequent chapters).

5.6 The conditional mixture model, cDGMMVAE

We have seen two types of models that deal with data that is both numerical and categorical, namely the conditional VAE (CVAE), and the GMMVAE. The cDGMMVAE is a combination of both, a conditional DGMMVAE. It is technically very easy to implement a conditional version from a given VAE model. Basically it just requires concatenating the condition c to whatever variable we want to condition. But why do we need it?

Suppose that we have again numerical/categorical type of data $(\mathbf{x}, \mathbf{y})$ which comes in two or more types of "flavors" c, so the full data type is $(\mathbf{x}, \mathbf{y}, c)$. For example $\mathbf{x}$ can be an image of on of k different faces, $\mathbf{y}$ is the identity of the person, c is an indicator of whether the person smiles or not. Also suppose that $\mathbf{y}$ might not be provided at all or just for a subset of the data but c is always provided for us.

The data we actually use for this model is scRNAseq data that comes from two types of conditions (control and stimulated), which are the conditions before and after exposure to some pathogen or some chemical. $\mathbf{x}$ is normalized gene expression levels, $\mathbf{y}$ is the cell type we want to infer but may not know the ground truth, and c indicates from which group the measurement was taken (control/stimulate) and this information is visible to use because we know for each sample from which group it was taken.

The factorization in the unsupervised case is:

$$\begin{aligned} p(\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{w}, \mathbf{d}, c) &= p(\mathbf{x}|\mathbf{z}, c)p(\mathbf{z}|\mathbf{w}, \mathbf{y})p(\mathbf{y}|\mathbf{d})p(\mathbf{d})p(\mathbf{w}|c) \\ q(\mathbf{z}, \mathbf{w}, \mathbf{d}|\mathbf{x}, \mathbf{y}, c) &= q(\mathbf{z}|\mathbf{x}, c)q(\mathbf{w}|\mathbf{x}, c)q(\mathbf{y}|\mathbf{z})q(\mathbf{d}|\mathbf{z}) \end{aligned} \tag{5.19}$$

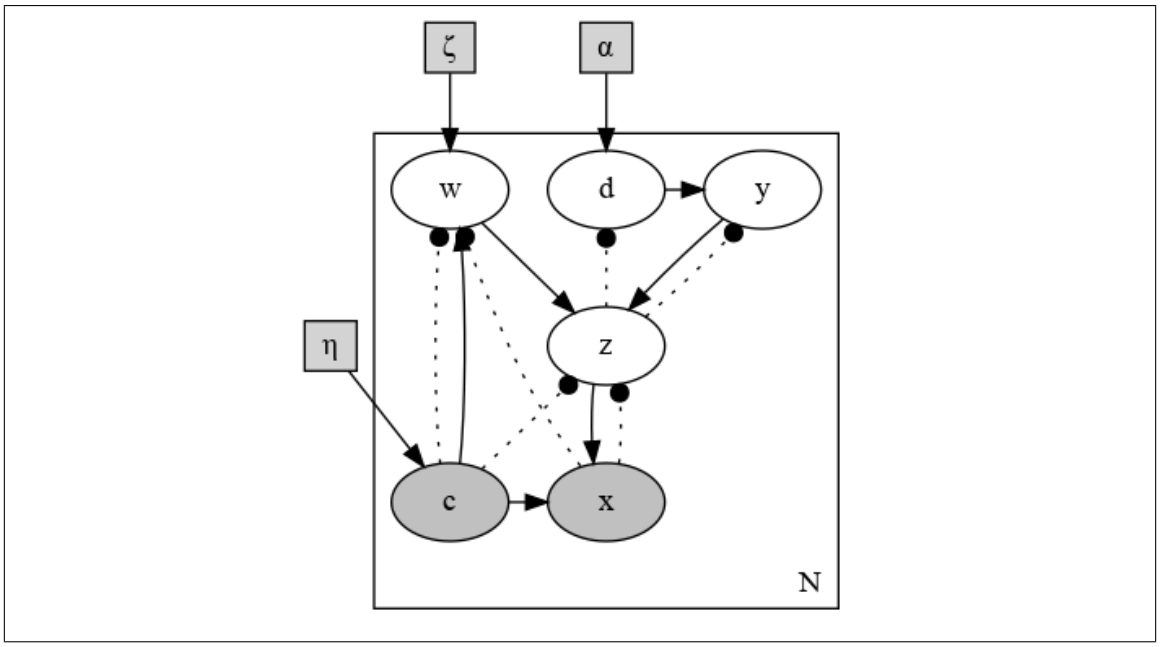


Figure 5.5: cDGMMVAE, unsupervised case

And in the supervised case:

$$\begin{aligned} p(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{w},\mathbf{d},c) &= p(\mathbf{x}|\mathbf{z},c)p(\mathbf{y}|\mathbf{d})p(\mathbf{y}|\mathbf{z})p(\mathbf{z}|\mathbf{w})p(\mathbf{d})p(\mathbf{w}|c) \\ q(\mathbf{z},\mathbf{w},\mathbf{d}|\mathbf{x},\mathbf{y}) &= q(\mathbf{z}|\mathbf{x},c)q(\mathbf{w}|\mathbf{x},c)q(\mathbf{d}|\mathbf{z}) \end{aligned} \tag{5.20}$$

In this model we want to keep the dependency of $\mathbf{x}$ on c, hence $p(\mathbf{x}|\mathbf{z},c)$. This allows us to "flip" condition of the reconstruction, which we can interpret as converting for example control cells to stimulated cells, as we'll see in a later chapter.

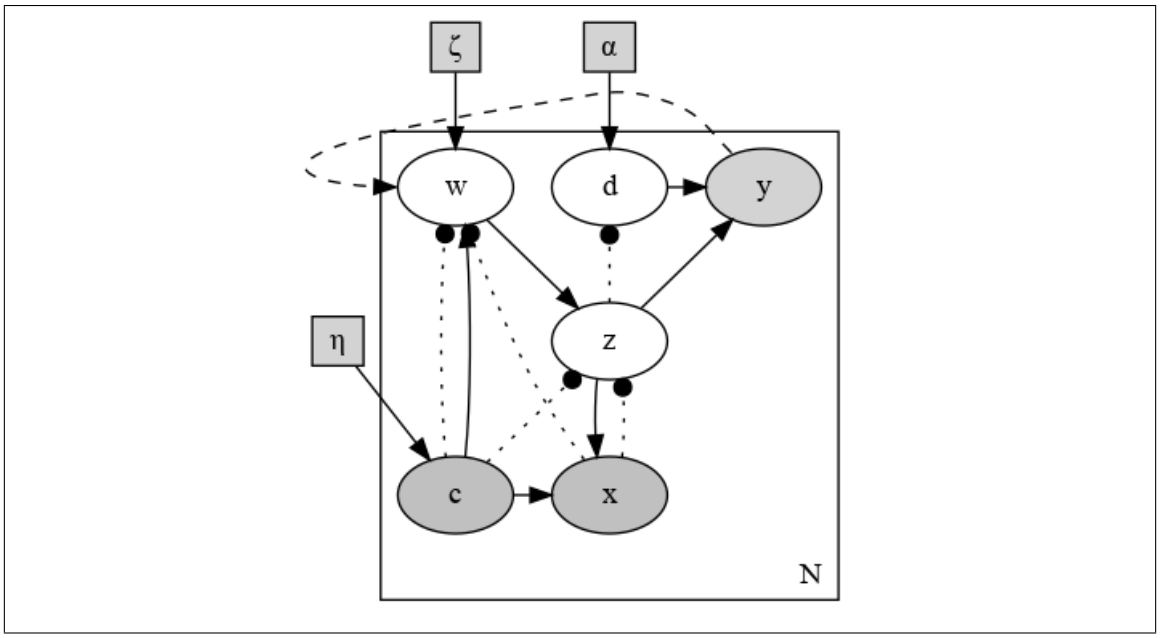


Figure 5.6: cDGMMVAE, supervised case

Chapter 6

Experiments and results MNIST

The first dataset we tested the model on was MNIST [19] which is easy to machine learn yet it is also the most tested and compared dataset. This is a collection of 28×28 pixel gray–scale images of hand written digits. The images are labeled with the ground truth so it is an $(\mathbf{X}, \mathbf{Y})$ kind of data, with $\mathbf{X}$ being numerical and $\mathbf{Y}$ categorical.

MNIST images are close to being binary black and wight (either close to 0 or close to 1), so it is better to model them with Bernoulli distribution than with Gaussian, with the intensity of each pixel is regarded as a Bernoulli probability. Unless otherwise stated, for MNIST we set $p(\mathbf{x}|\mathbf{z})$ to be Bernoulli distribution.

6.1 semi-supervised learning

In the first test we partition the training set into labeled (5% of the total) and unlabeled subset (the other 95%). As we have some labeled images, we set the number–of–categories hyperparameter on 10 and the goal here is to be able to predict the true categorical partitioning of the testing set.

There are several qualitative aspects that we are particularly interested in this experiment:

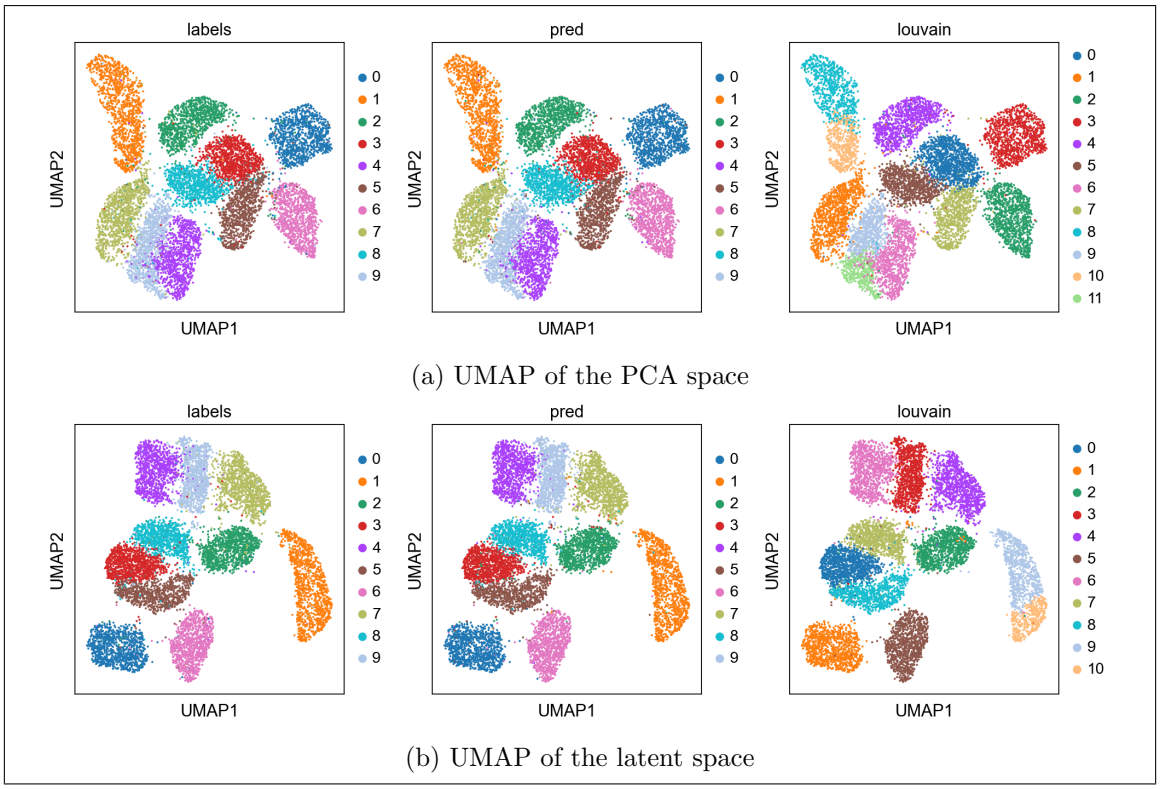
- The overall prediction accuracy of the model
- Comparing the models predicted clusters to Louvain clusters

  in the PCA space

  in the latent space

The overall accuracy of the model is 0.955 and as the figures 6.1 the prediction basically identifies the real classes. When performed on the PCA space, Louvain clustering with default settings identifies 12 clusters . The "0" and "9" classes each are split between two Louvain clusters. The Louvain clusters themselves appear to be homogeneous (each cluster contain practically only samples from one ground-truth class).

It is interesting to compare the PCA results to the same procedure done on the latent space. The umap appears a little bit better (the ground truth classes have more separation



(a) UMAP of the PCA space

(b) UMAP of the latent space

Figure 6.1: Comparison of the predictive quality of the model vs. Louvain clustering on the PCA space (top) and on the latent space (bottom).

from each other). This time there are 11 louvain clusters and only the "9" category is split between two louvain clusters. This is despite the latent z space being only 16-dimensional, while the PCA is done on the 50 most significant components.

Figure 6.2 shows the decoder's reconstruction of random samples from the mixture distribution which was imposed on the latent space. As we can see each component generates exactly one of the digit classes. Sampling from the latent mixture distribution (z-space) is done as follows: Firs we take random samples from the w-space, on which we imposed a standard normal diagonal distribution. Each sample corresponds to one row in the image. Then each w-sample is projected by the decoder into 10 (number of defined classes) mixture component. Each of these component if then further projected by the decoder network into the sample space (x).

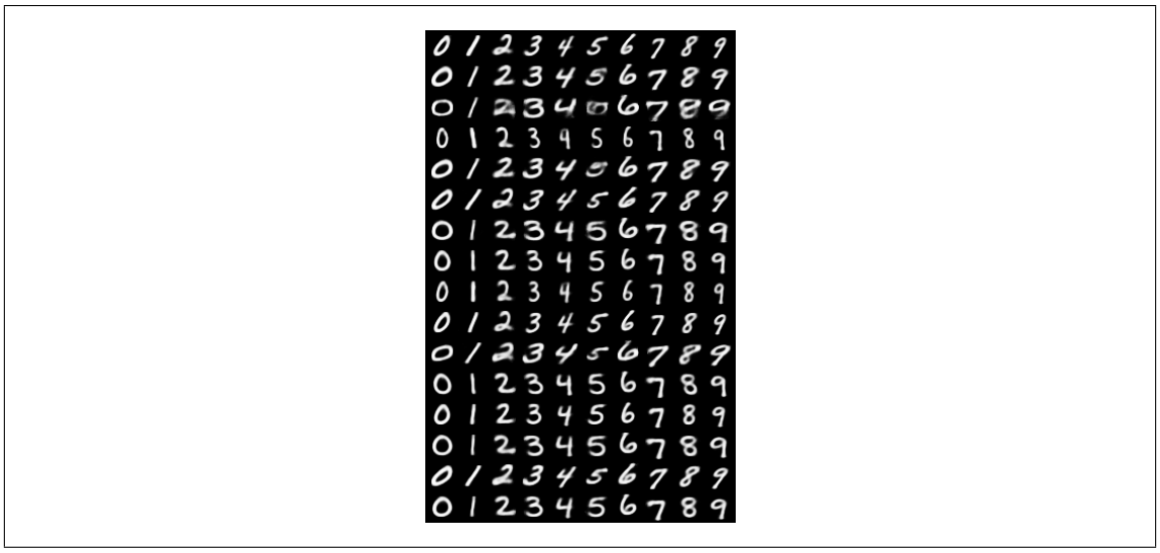


Figure 6.2: Images generated by random sampling from the latent mixture distribution. As we can see it fits perfectly with the right ground truth classes.

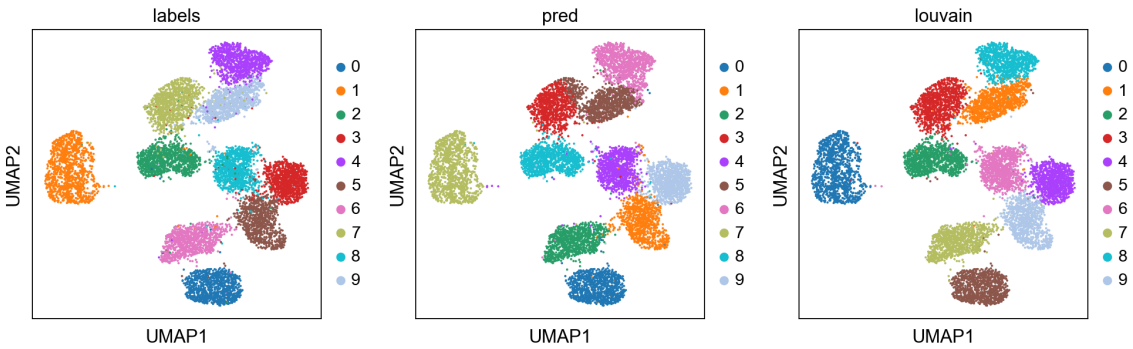
6.2 Unsupervised learning

6.2.1 10 Clusters (exact clustering)

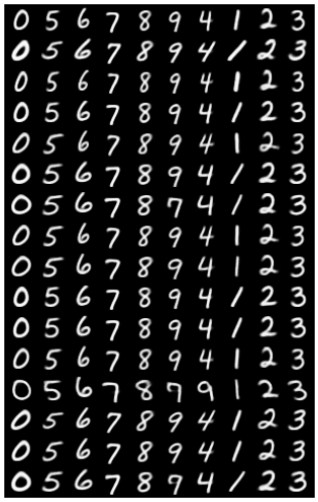
Getting the model to learn exactly the 10 ground truth classes is a daunting task. It requires a lot of tuning and micromanaging of the training procedure. In my experiments, the model first needs to be trained with standard learning rate ($1e-3$) to the point where it can adequately reconstruct digits and uses all 10 classes. Then the learning rate should be reduced to the range $5e-2$ — $5e-3$. This makes reconstruction less exact and allows the model to "jump" class predictions during training. If the learning rate is too big eventually the model might completely drift away and become inaccurate and unstable and if it is not sufficiently large the model remains stuck on a suboptimal classification. After this course training finds the correct classes, it needs to be further trained to improve accuracy and reconstruction with decreasing learning rates.

In my experiments, an accuracy of about 0.9—0.95 can be achieved however due the micromanagement involved it is hard to make the training fully automated. Moreover it may be completely unrealistic to expect the model to perform that well in unsupervised exact clustering tasks with harder datasets.

Figures 6.3 shows the results of unsupervised, exact clustering of MNIST by the GM-MVAE model with 8 dimensional latent z-space and w-space. As both the umap and the generated samples show, there is still a little bit inaccuracies left, mainly with "7","4", and "9" digits. Despite this, the actual latent space is very nicely clustered and louvain clustering over this space retrieves the true classification of the the data set, even to higher accuracy than the model prediction. Note that in unsupervised learning the predicted classes are naturally untagged with the ground truth class tag, the point is that it should find essentially the true partitioning of the data. The tag assignment can be done later. for example each predicted cluster is tagged with the class with which it has the most overlap.



(a) UMAP of the latent space



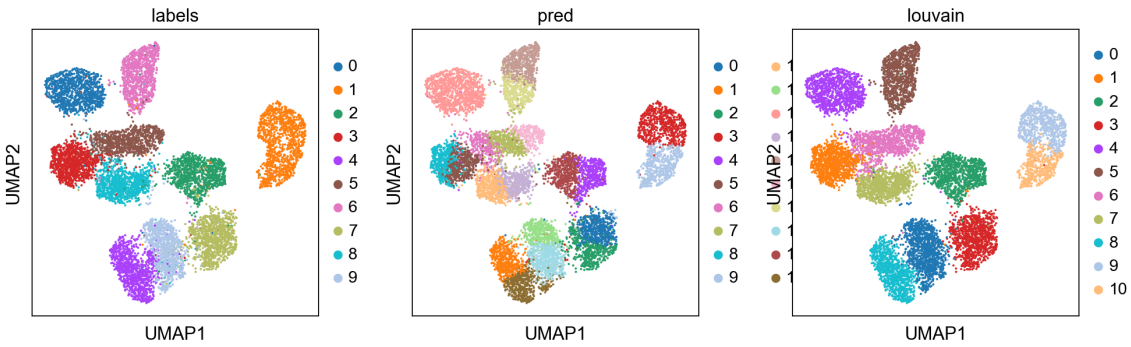
(b) Randomly generated samples

Figure 6.3: GMMVAE: unsupervised learning of MNIST. This particular model achieved 0.93 accyracy which probably could be a little bit further improved with fine-tune training. The Louvain clustering of the latent space is even better than the prediction.

6.2.2 With overclustering

Overclustering means defining a mixture distribution with more components then ground truth classes. This helps the model to create homogenous classes, where each component is nearly a subset of a single class. Moreover In the case of MNIST each digit has actually 2 or more basic appearance (e.g. strait vs. italic version, closed vs. open top "4" figure etc.). One can argue that there are more "natural" classes in this dataset than the 10 digits. We ran unsupervised training of a GMMVAE model with 20 components.

Figures 6.4 show the results of the 20–component GMMVAE model. "0" constitutes its own cluster, while "5" is split between 3 clusters. The rest of the classes are each split between two clusters. Each cluster has its own digit-style (e.g. a strait "7" in one cluster, and more cursive version in the other cluster). Unfortunately there is some misclassifications between "4" and "9". Overall accuracy is about 0.946, probably with some room for improvement with additional training rounds. Louvain clustering of the latent space is able to almost perfectly capture the true classes, with the "1" class split between two Louvain clusters and the other classes correspond each to a single Louvain cluster.



(a) UMAP (20 components, MNIST)

(b) 20 components: generated digits

Figure 6.4: GMMVAE with 20 components, unsupervised learning of MNIST.

Training an overclustering model provides much more consistent results without training micromanagement. It is probably advisable to set up a model with more mixture components than the ground truth classes when trying unsupervised classification of more complex datasets.

6.3 Combination with Louvain clustering

Louvain clustering achieves on its own an accuracy of 0.967 on the *training set* which is larger (60k images) and 0.925 on the smaller (10k) testing set.

We performed supervised training of GMMVAE model using Louvain clusters as the labels. After this step, the model was 0.966 accurate *on the testing set*. After further unsupervised training of the model the accuracy marginally improved to 0.968.

MNIST is an easy data set but still the improvement over Louvain from 0.92 to 0.968 is noticeable. There was also an improvement over the unsupervised model and it basically solved the misclassification issue between 9,7 and 4 which is the main problem we observes with unsupervised learning as we see in figure 6.5.

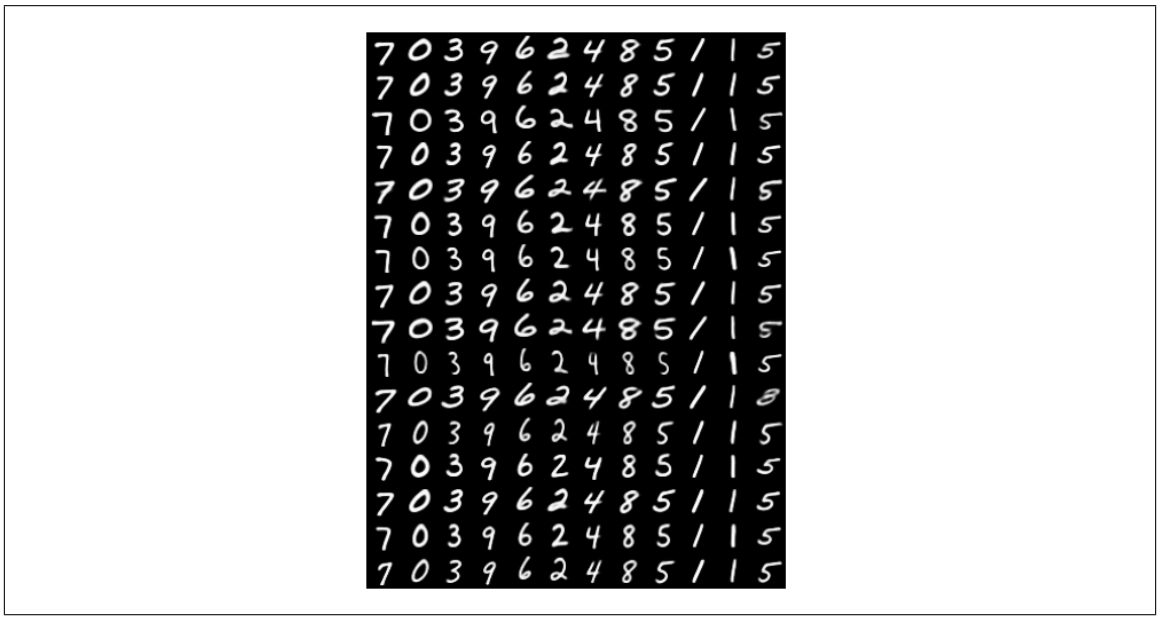


Figure 6.5: GMMVAE with 12 components guided by Louvain clustering: randomly generated digits

Chapter 7

Experiments and results fashion-MNIST

Fashion-MNIST (FMNIST) [3] is a drop-in replacement for MNIST which is a lot more challenging to machine–learn. Instead of digits we are dealing here with greyscale images of clothing and accessory items of 10 classes: *T-shirt, trouser, pullover, dress, coat, sandal, shirt, sneaker, bag, boot.* Although each image is tagged with a single category, it is not always obvious even for a human observer whether a certain image is actually a coat or a shirt, for example. There might be a little bit of this type of unclaritty in MNIST too, but it is much more pronounced in the fashion-MNIST dataset.

7.1 Unsupervised learning

GMMVAE achieved an overall 0.75 accuracy after *a lot* of training epochs. It is easier to achieve about 0.67 accuracy after a quick training (about 10 epochs). Choice of hyperparameters also have significant effect. For example choosing a high dimensional latent space or deepening the networks tend to make the model perform to not use all the components of the mixture.

Judging from the randomly generated images in figure 7.1, the model learns to generate what looks like a distinct classes in each of the mixture components. However as far as prediction accuracy, there is a major confusion between "shirt", "coat", and "pullover" classes, which is apparent from the UMAP in figure 7.2.

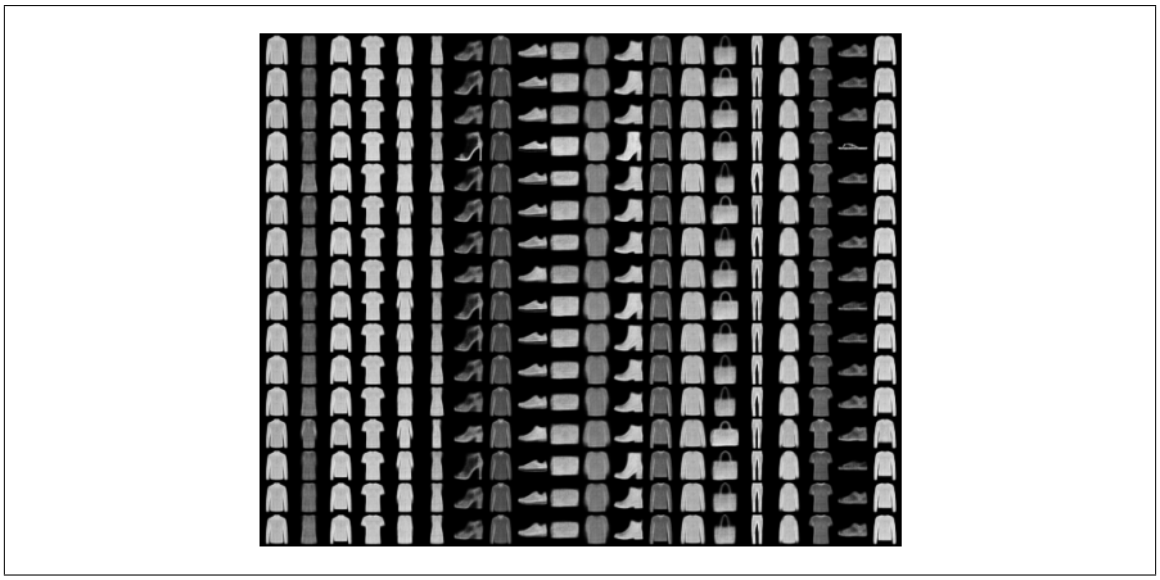


Figure 7.1: 20 components: generated digits

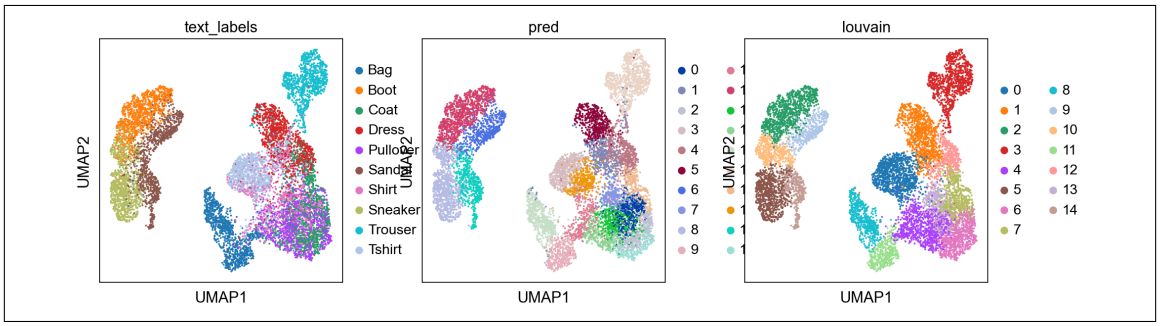


Figure 7.2: UMAP (20 components, MNIST)

7.2 Semisupervised learning

Our GMMVAE model achieved accuracy of 0.85 on semisupervised learning with 0.1 — 0.9 split between known and hidden labels. Considering that this accuracy was semisupervised and that the network layer architecture we used was just fully connected with 2 hidden layers we think this accuracy is not bad.

Figure 7.3 shows randomly generated samples by the model. The 10 components match the ground truth classes fairly well.

Figure 7.4 shows UMAP of the laten space. The top-wear (shirt, coat, pullover, T-shirt) are still pretty mixed and that's where most of the misclassifications occur.

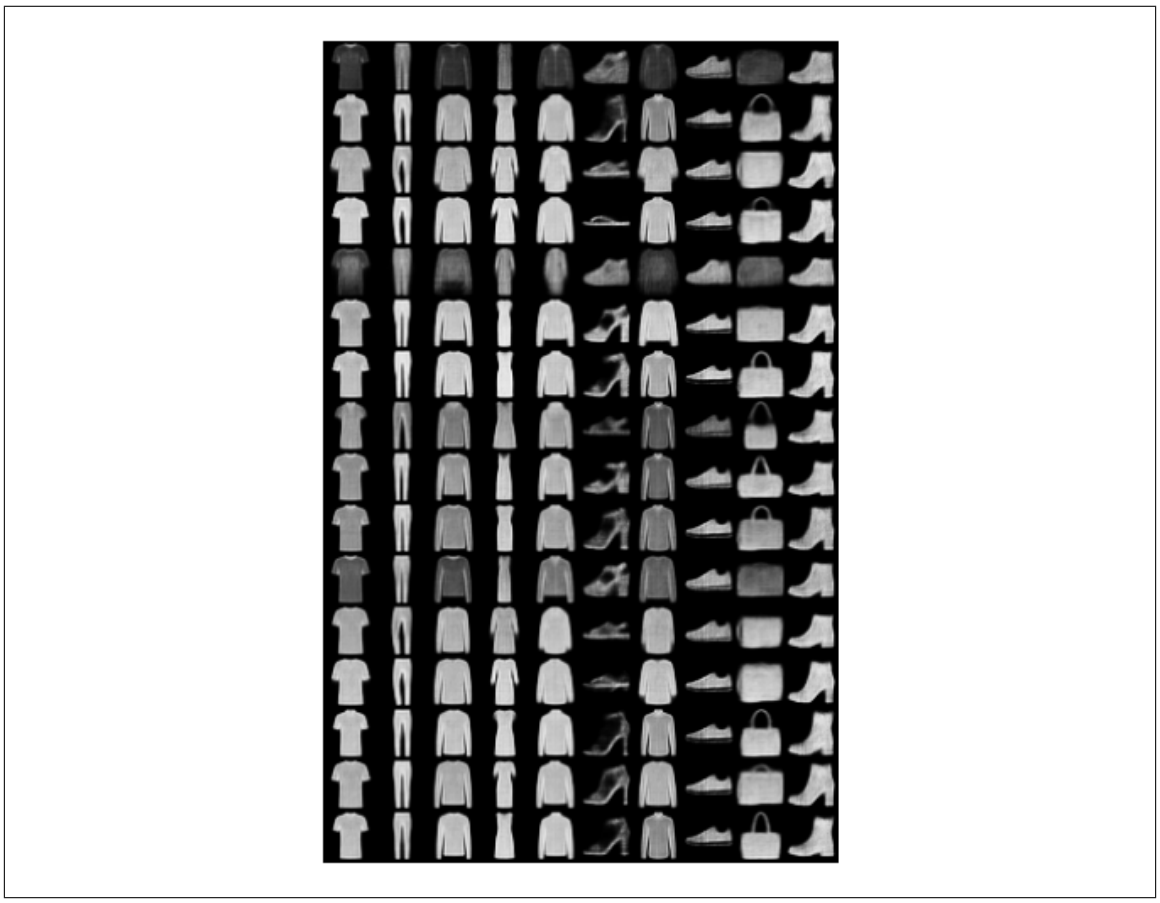


Figure 7.3: FMNIST, semisupervised. Randomly generated samples.

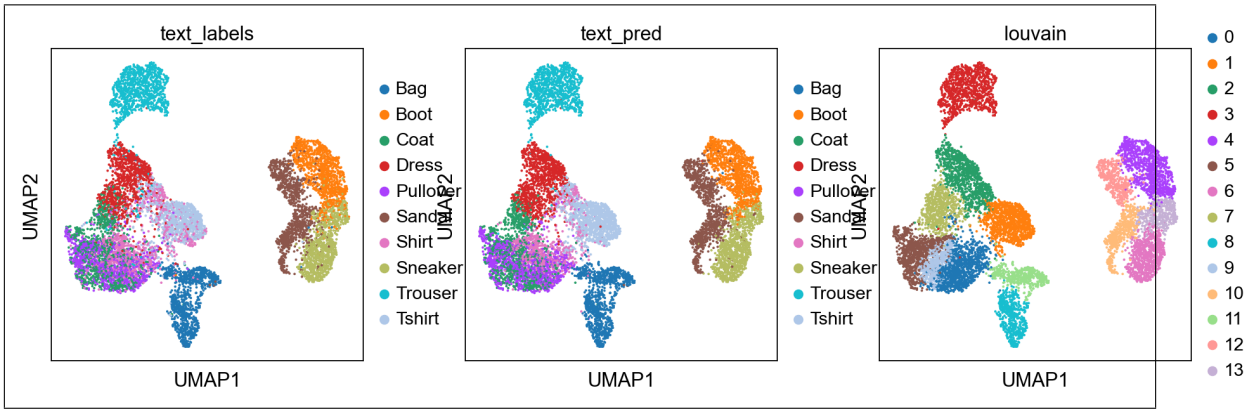


Figure 7.4: FMNIST, semisupervised. UMAP

7.3 Combination with Louvain clustering

Louvain clustering achieves accuracy of 0.71 on both the training and the testing sets. We supervised trained a GMMVAE and it achieved 0.714 accuracy, an insignificant difference from Louvain. With further unsupervised training rounds it reached 0.725 accuracy. Still below the 0.75 we achieved with the best model during unsupervised only training but but we were only able to achieve it with much trying and tuning. The combination with Louvain is much more consistent as a method.

Chapter 8

Tests with PBMCs scRNAseq Data – Zheng et al

We first selected a scRNAseq data set [20] which is easy because the cells are nicely clustered by cell type. The main challenge with this data is that it is imbalanced. It has 2623 samples of 7 cell types overall but in particularly one type (dendritic cells) only has 37 samples.

While Louvain clustering performs well: it achieved 0.93–0.94 accuracy and found 9 clusters, GMMVAE failed to cluster the smallest cell type (see figure 8.1). With the other types it did ok with accuracy of around 0.92.

In order to overcome this issue we generated a rebalanced data set by selecting 300 samples from each types with repetitions. In addition we added small Gaussian noise. We also scaled the log-count matrix of the original data set so each gene has near standard normal distribution across the samples.

We trained a GMMVAE model by taking turns, first on the rebalanced data, then on the original data, repeating several times. We were able to achieve 0.93 accuracy consistently and probably the method can be a little bit improved by tuning the model and the balancing preprocessing. In particular it appears that adding the small noise to the rebalanced data helped the model to learn all the cell types with fewer components. Figure 8.2 visualize with umaps the results of this rebalancing method.

Of course for this particular data it would be easier and faster to use Louvain clustering and train a GMMVAE model on the clustering if it were needed for some purpose. However this experiment gives some insight on the importance of data balancing.

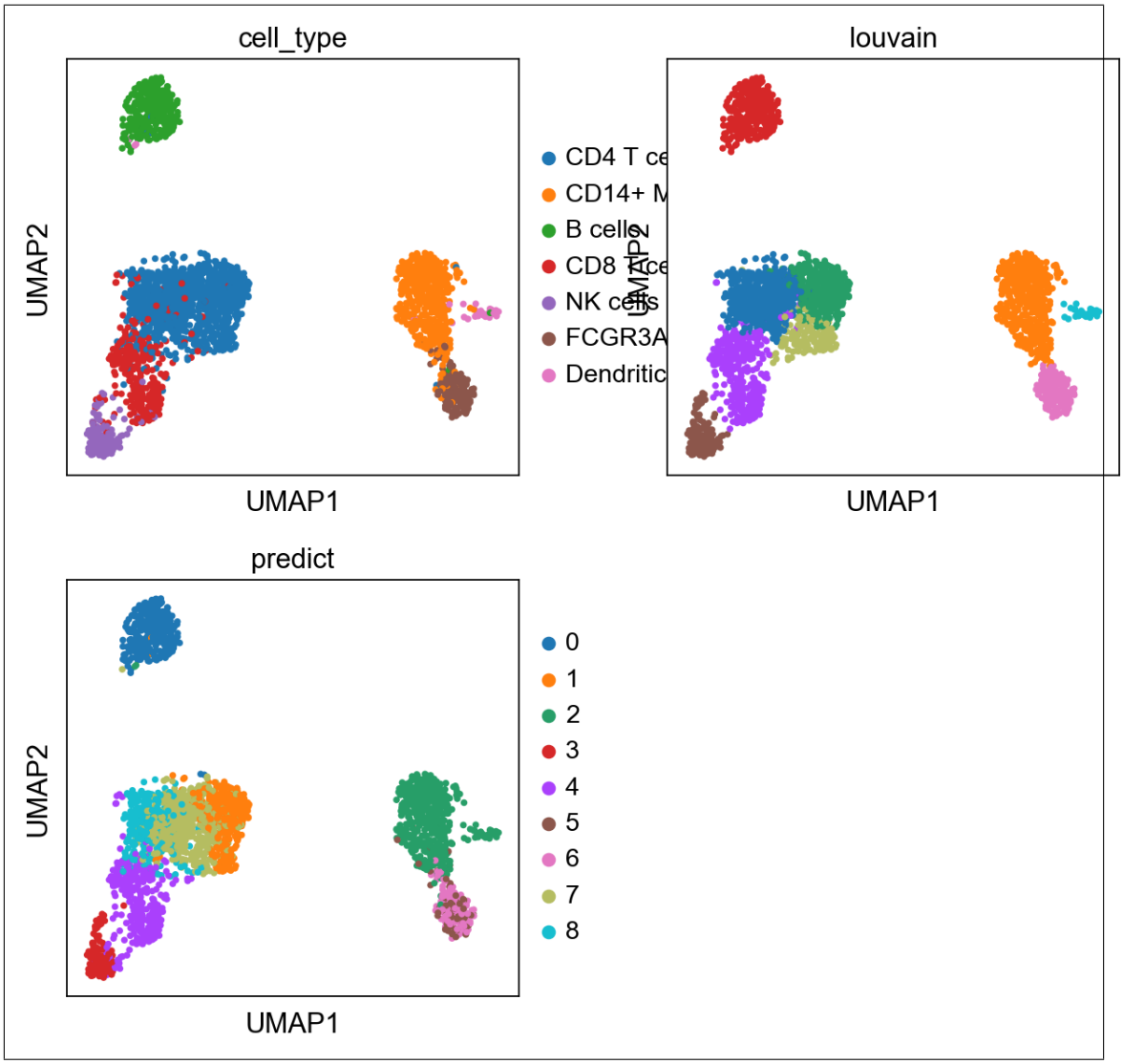


Figure 8.1: Zheng dataset, UMAPs. The main issue with GMMVAE is it fails to classify the smallest group (Dendritic) in its own cluster.

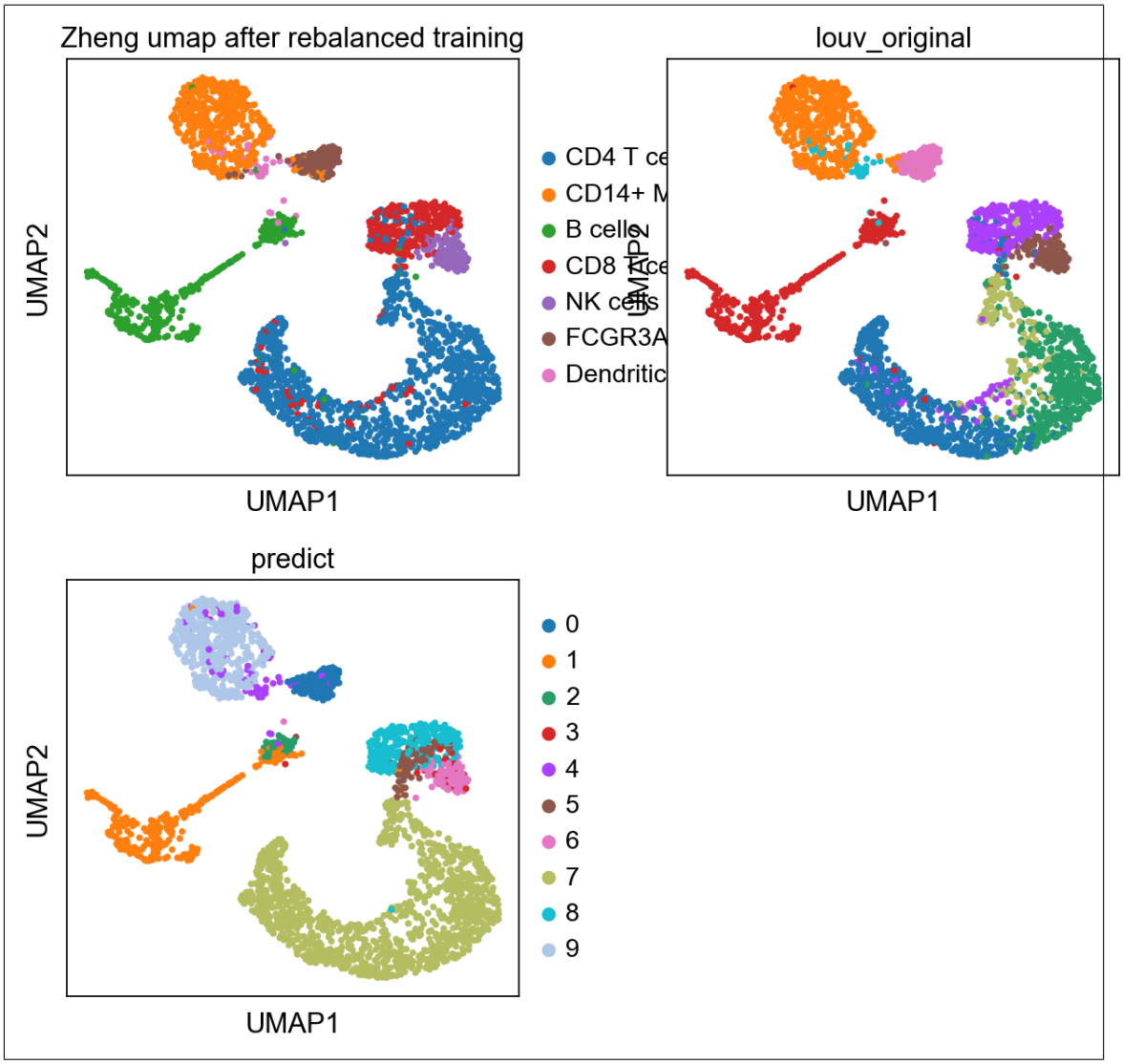


Figure 8.2: Zheng dataset, UMAPs of the latent space after training on the rebalanced and the original data set.

Chapter 9

Tests with PBMCs scRNAseq Data (Kang et al)

In these tests we used a scRNAseq dataset [6] of PBMCs (peripheral blood mononuclear cells) of 7 cell types which comes from two groups: control and treatment. The cells in the treatment group have been exposed to interferon beta (INF-β).

Because the data comes from different classes (=cell types) and from two different batches (control/treatment), the conditional version of our mixture model, cDGMMVAE, seems to be the most suitable for this type of data. The mixture components correspond to the cell types, and the condition corresponds to control/treatment.

9.0.1 Unsupervised learning

Chapter 10

Discussion, some remarks and conclusions

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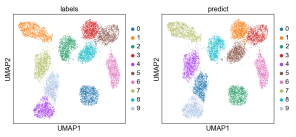
(a)



(b)

Figure 10.1: a figure

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