1 Definitions

1.1 Deep learning

1.2 Todo

TODO:

1.3 Formal description

We denote by I_f the *domain of definition* of a function f ("I" for "input") and by $O_f = f(I_f)$ its *image* ("O" for "output"), and we represent it as $I_f \xrightarrow{f} O_f$. An activation function is a function f such that $I_f = O_f$. Vector spaces considered in this thesis are always assumed to be finite-dimensional. A tensor space is a cartesian product of vector spaces, equipped with the canonical operators.

Definition 1.1. Neural network
Let F be a function such that I_f and O_f are vector spaces.
F is said to be a *functional formulation* of a *neural network* if there are a series of linear functions $(g_k)_{k=1,2,..,L}$ and a series of non-linear derivable activation functions $(h_k)_{k=1,2,..,L}$ such that:

$$\begin{cases} \forall k \in \{1, 2, .., L\}, f_k = h_k \circ g_k, \\ I_F = I_{f_1} \xrightarrow{f_1} O_{f_1} \cong I_{f_2} \xrightarrow{f_2} \dots \xrightarrow{f_L} O_{f_L} = O_F, \\ F = f_L \circ ... \circ f_2 \circ f_1 \end{cases}$$

The couple (g_k, h_k) is called the *k-th layer* of the neural network. For $x \in I_f$, we denote by $x_k = f_k \circ ... \circ f_2 \circ f_1(x)$ the *activations* of the k-th layer.

Any linear function g is characterized by a *set of parameters* θ_g. Without loss of generality, let's suppose I_g and O_g are vector spaces[1]. Then there exists a *connectivity matrix* W for which:

$$\begin{cases} \forall x \in I_g, g(x) = Wx \\ \forall (i, j), W_{ij} \in \theta_g \text{ or } W_{ij} = 0 \end{cases}$$

The *weights* of the k-th layer of a neural network, denoted θ_k, are defined as the set of parameters of its linear part.
Usually, a *loss* function $\mathcal{L}$ penalizes the output $F(x)$, and its gradient w.r.t. θ_k is used to update the weights via an optimization algorithm based on gradient descent and a learning rate α, that is:

$$\theta_k^{\text{new}} = \theta_k^{\text{old}} - \alpha \bigtriangledown (\mathcal{L})_{\theta_k}$$

Thanks to the chain rule, gradients w.r.t. weights of a layer k, denoted $\bigtriangledown_{\theta_k}$, can be computed using gradients that are w.r.t. the elementary basis of O_{f_k},

[1] for instance if they are tensor spaces, they can be reshaped to vector spaces

denoted $\bigtriangledown_k$, which in turn can be computed using gradients w.r.t. weights of the next layer $k+1$, up to the gradients given on the output layer. That is:

$$\begin{cases} \bigtriangledown_{\theta_k} = J(W_k)_{\theta_k} \bigtriangledown_{W_k} \\ \bigtriangledown_{W_k} = J(x_k)_{W_k} \bigtriangledown_k \\ \bigtriangledown_k = J(W_{k+1})_k \bigtriangledown_{W_{k+1}} \\ \bigtriangledown_{W_{k+1}} = \dots \\ \quad \dots \\ \bigtriangledown_L = \bigtriangledown(\mathcal{L}(x_L))_L \end{cases}$$

where $J(.)_{\text{wrt}}$ are the respective jacobians which can be determined with the layer's expressions.
This allows to compute the gradients with a complexity that is linear with the number of weights, instead of being quadratic if it were done with the difference quotient expression of the derivatives.

Remark 1. Neural interpretation
TODO:

Definition 1.2. Dense layer
A *dense layer* (g, h) is a layer such that there is a *weight matrix* W for which

$$\begin{cases} I_g \text{ and } O_g \text{ are vector spaces} \\ \forall x \in I_g, g(x) = Wx \end{cases}$$

Definition 1.3. Partially connected layer
A *partially connected layer* is a dense layer such that $\exists (i, j), W_{i,j} = 0$.

Definition 1.4. Convolutional layer
A *n-dimensional convolutional layer* (g, h) is a layer such that there is a *weight tensor* W of rank $n+2$ for which

$$\begin{cases} I_g \text{ and } O_g \text{ are tensor spaces of rank } n+1 \\ \forall x \in I_g, g(x) = (g(x)_q = \sum_p W_{pq} *_n x_p)_{\forall q} \end{cases}$$

where p and q index the last ranks and $*_n$ denotes the n-d convolution. The tensor slices indexed by p and q are typically called *feature maps*.

Note that a n-dimensional convolutional layer that has its domain and image reshaped to vector spaces is a partially connected layer for which the weight matrix W is a Toeplitz matrix.

Definition 1.5. Pooling A layer with *pooling* (g, h) is such that $g = g_1 \circ g_2$, where (g_1, h) is a layer and g_2 is a pooling operation.

A layer with *dropout* (g, h) is such that $h = h_1 \circ h_2$, where (g, h_2) is a layer and h_1 is a dropout operation [**?**]. When dropout is used, a certain number of neurons are randomly set to zero during the training phase, compensated at test time by scaling down the whole layer. This is done to prevent overfitting.

TODO: neuron interpretation
A multilayer perceptron (MLP) [**?**] is a neural network composed of only dense layers. A convolutional neural network (CNN) [**?**] is a neural network composed of convolutional layers.
Neural networks are commonly used for machine learning tasks. For example, to perform supervised classification, we usually add a dense output layer $s = (g_{L+1}, h_{L+1})$ with as many neurons as classes. We measure the error between an output and its expected output with a discriminative loss function $\mathcal{L}$. During the training phase, the weights of the network are adapted for the classification task based on the errors that are back-propagated [**?**] via the chain rule and according to a chosen optimization algorithm (e.g. [**?**]).

1.4 Graphs

A graph G is defined as a couple (V, E) where V represents the set of nodes and $E \subseteq \binom{V}{2}$ is the set of edges connecting these nodes.
TODO: Example of figure
We encounter the notion of graphs several times in deep learning:

- Connections between two layers of a deep learning model can be represented as a bipartite graph, coined *connectivity graph*. It encodes how the information is propagated through a layer to another. See section 1.4.1.
- A computation graph is used by deep learning frameworks to keep track of the dependencies between layers of a deep learning models, in order to compute forward and back-propagation. See section 1.4.2.
- A graph can represent the underlying structure of an object (often a vector), whose nodes represent its features. See section 1.4.3.
- Datasets can also be graph-structured, where the nodes represent the objects of the dataset. See section 1.4.4.

1.4.1 Connectivity graph

A Connectivity graph is a graphical representation of the linear part of the mathematical model implemented by a layer of neurons. Formally, given a linear part of a layer, let $\mathbf{x}$ and $\mathbf{y}$ be the input and output signals, n the size of the set of input neurons $N = \{u_1, u_2, \ldots, u_n\}$, and m the size of the set of output neurons $M = \{v_1, v_2, \ldots, v_m\}$. This layer implements the equation $y = \Theta x$ where Θ is a $n \times m$ matrix.

Definition 1.6. The *connectivity graph* $G = (V, E)$ is defined such that $V = N \cup M$ and $E = \{(u_i, v_j) \in N \times M, \Theta_{ij} \neq 0\}$.

I.e. the connectivity graph is obtained by drawing an edge between neurons for which $\Theta_{ij} \neq 0$. For instance, in the special case of a complete bipartite graph, we would obtain a dense layer. Connectivity graphs are especially useful

to represent partially connected layers, for which most of the Θ_{ij} are 0. For example, in the case of layers characterized by a small local receptive field, the connectivity graph would be sparse, and output neurons would be connected to a set of input neurons that corresponds to features that are close together in the input space. Figure 1 depicts some examples.

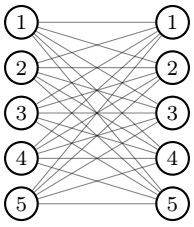

Figure 1: Examples

TODO: Figure 1. It's just a placeholder right now

Connectivity graphs also allow to graphically modelize how weights are tied in a neural layer. Let's suppose the $\Theta_i j$ are taking their values only into the finite set $K = \{w_1, w_2, \ldots, w_\kappa\}$ of size κ, which we will refer to as the *kernel* of *weights*. Then we can define a labelling of the edges $s : E \to K$. s is called the *weight sharing scheme* of the layer. This layer can then be formulated as $\forall v \in M, y_v = \sum_{u \in N, (u,v) \in E} w_{s(u,v)} x_u$. Figure 2 depicts the connectivity graph of a 1-d convolution layer and its weight sharing scheme.

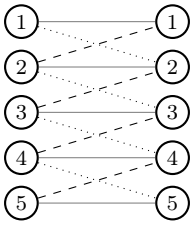

Figure 2: Depiction of a 1D-convolutional layer and its weight sharing scheme.

TODO: Add weight sharing scheme in Figure 2

1.4.2 Computation graph

1.4.3 Underlying graph structure

1.4.4 Graph-structured dataset

transductive vs inductive