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Chapter 1

Presentation of the field

In this section, we present notions related to our domains of interest. In particular, for tensors we give original definitions that are more appropriate for our study. In the neural network's section, we present the concepts necessary to understand the evolution of the state of the art research in this field. In the last section, we present graphs for their usage in deep learning.
Vector spaces considered in what follows are assumed to be finite-dimensional and over the field of real numbers $\mathbb{R}$.

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1.1 Tensors

Intuitively, tensors in the field of deep learning are defined as a generalization of vectors and matrices, as if vectors were tensors of rank 1 and matrices were tensors of rank 2. That is, they are objects in a vector space and their dimensions are indexed using as many indices as their rank, so that they can be represented by multidimensional arrays. In mathematics, a tensor can be defined as a special type of multilinear function (Bass, 1968; Marcus, 1975; Williamson, 2015), which image of a basis can be represented by a multidimensional array. Alternatively, Hackbush propose a mathematical construction of a tensor space as a quotient set of the span of an appropriately defined tensor product (Hackbusch, 2012), which coordinates in a basis can also be represented by a multidimensional array. In particular in the field of mathematics, tensors enjoy an intrinsic definition that neither depend on a representation nor would change the underlying object after a change of basis, whereas in our domain, tensors are confounded with their representation.

1.1.1 Definition

Our definition of tensors is such that they are a bit more than multidimensional arrays but not as much as mathematical tensors, for that they are embedded in a vector space so that deep learning objects can be later defined rigorously.
Given canonical bases, we first define a tensor space, then we relate it to the definition of the tensor product of vector spaces.

Definition 1.1.1. Tensor space
We define a *tensor space* $\mathbb{T}$ of rank r as a vector space such that its canonical basis is a cartesian product of the canonical bases of r other vector spaces. Its shape is denoted $n_1 \times n_2 \times \cdots \times n_r$, where the $\{n_k\}$ are the dimensions of the vector spaces.

Definition 1.1.2. Tensor product of vector spaces
Given r vector spaces $\mathbb{V}_1, \mathbb{V}_2, \ldots, \mathbb{V}_r$, their *tensor product* is the tensor space $\mathbb{T}$ spanned by the cartesian product of their canonical bases under coordinate-wise sum and outer product.
We use the notation $\mathbb{T} = \bigotimes_{k=1}^{r} \mathbb{V}_k$.

Remark 1.1.3. This simpler definition is indeed equivalent with the definition of the tensor product given in (Hackbusch, 2012, p. 51). The drawback of our definition is that it depends on the canonical bases, which at first can seem limiting as being canon implies that they are bounded to a certain system of coordinates. However this is not a concern in our domain as we need not distinguish tensors from their representation.

Remark 1.1.4. For naming convenience, from now on, we will distinguish between the terms *linear space* and *vector space i.e.* we will abusively use the term *vector space* only to refer to a linear space that is seen as a tensor space of rank 1. If we don't know its rank, we rather use the term *linear space*. We also make a clear distinction between the terms *dimension* (that is, for a tensor space it is equal to $\prod_{k=1}^{r} n_k$) and the term *rank* (equal to r). Note that some authors use the term *order* instead of *rank* (*e.g.* Hackbusch, 2012) as the latter is affected to another notion.

Definition 1.1.5. Tensor
A *tensor* t is an object of a tensor space. The *shape* of t, which is the same as the shape of the tensor space it belongs to, is denoted $n_1^{(t)} \times n_2^{(t)} \times \cdots \times n_r^{(t)}$.

1.1.2 Manipulation

In this subsection, we describe notations and operators used to manipulate data stored in tensors.

Definition 1.1.6. Indexing

An *entry* of a tensor $t \in \mathbb{T}$ is one of its scalar coordinates in the canonical basis, denoted $t[i_1, i_2, \ldots, i_r]$.

More precisely, if $\mathbb{T} = \bigotimes_{k=1}^{r} \mathbb{V}_k$, with bases $((e_k^i)_{i=1,\ldots,n_k})_{k=1,\ldots,r}$, then we have

$$t = \sum_{i_1=1}^{n_1} \cdots \sum_{i_r=1}^{n_r} t[i_1, i_2, \ldots, i_r](e_1^{i_1}, \ldots, e_r^{i_r})$$

The cartesian product $\mathbb{I} = \prod_{k=1}^{r} [\![1, n_k]\!]$ is called the *index space* of $\mathbb{T}$

Remark 1.1.7. When using an index i_k for an entry of a tensor t, we implicitly assume that $i_k \in [\![1, n_k^{(t)}]\!]$ if nothing is specified.

Definition 1.1.8. Subtensor

A *subtensor* t' is a tensor of same rank composed of entries of t that are contiguous in the indexing, with at least one entry per rank. We denote $t' = t[l_1{:}u_1, l_2{:}u_2, \ldots, l_r{:}u_r]$, where the $\{l_k\}$ and the $\{u_k\}$ are the lower and upper bounds of the indices used by the entries that compose t'.

Remark 1.1.9. We don't necessarily write the lower bound index if it is equal to 1, neither the upper bound index if it is equal to $n_k^{(t)}$.

Definition 1.1.10. Slicing

A *slice* operation, along the last ranks $\{r_1, r_2, \ldots, r_s\}$, and indexed by $(i_{r_1}, i_{r_2}, \ldots, i_{r_s})$, is a morphism $s : \mathbb{T} = \bigotimes_{k=1}^{r} \mathbb{V}_k \to \bigotimes_{k=1}^{r-s} \mathbb{V}_k$, such that:

$$s(t)[i'_1, i'_2, \ldots, i'_{r-s}] = t[i'_1, i'_2, \ldots, i'_{r-s}, i_{r_1}, i_{r_2}, \ldots, i_{r_s}]$$
$$i.e. \quad s(t) := t[:, :, \ldots, :, i_{r_1}, i_{r_2}, \ldots, i_{r_s}]$$

where := means that entries of the right operand are assigned to the left operand. We denote $t_{i_{r_1}, i_{r_2}, \ldots i_{r_s}}$ and call it the *slice* of t. Slicing along a

subset of ranks that are not the lasts is defined similarly. $s(\mathbb{T})$ is called a *slice subspace*.

Definition 1.1.11. Flattening
A *flatten* operation is an isomorphism $f : \mathbb{T} \to \mathbb{V}$, between a tensor space $\mathbb{T}$ of rank r and an n-dimensional vector space $\mathbb{V}$, where $n = \prod_{k=1}^{r} n_k$. It is characterized by a bijection in the index spaces $g : \prod_{k=1}^{r} [\![1, n_k]\!] \to [\![1, n]\!]$ such that

$$\forall t \in \mathbb{T}, f(t)[g(i_1, i_2, \ldots, i_r)] = f(t[i_1, i_2, \ldots, i_r])$$

We call an inverse operation a *de-flatten* operation.

Remark 1.1.12. **Row major ordering**
The choice of g determines in which order the indexing is made. g is reminiscent of how data of multidimensional arrays or tensors are stored internally by programming languages. In most tensor manipulation languages, incrementing the memory address (*i.e.* the output of g) will first increment the last index i_r if $i_r < n_r$ (and if else $i_r = n_r$, then $i_r := 1$ and ranks are ordered in reverse lexicographic order to decide what indices are incremented). This is called *row major ordering*, as opposed to *column major ordering*. That is, in row major, g is defined as

$$g(i_1, i_2, \ldots, i_r) = \sum_{p=1}^{r} \left(\prod_{k=p+1}^{r} n_k \right) i_p \tag{1.1}$$

Definition 1.1.13. Reshaping
A *reshape* operation is an isomorphism defined on a tensor space $\mathbb{T} = \bigotimes_{k=1}^{r} \mathbb{V}_k$ such that some of its basis vector spaces $\{\mathbb{V}_k\}$ are de-flattened and some of its slice subspaces are flattened.

1.1.3 Binary operations

We define binary operations on tensors that we'll later have use for. In particular, we define *tensor contraction* which is sometimes called *tensor multiplication*, *tensor product* or *tensor dotproduct* by other sources. We also define *convolution* and *pooling* which serve as the common building blocks of convolution neural network architectures (see Section 1.2.7).

Definition 1.1.14. Contraction
A *tensor contraction* between two tensors, along ranks of same dimensions, is defined by natural extension of the dot product operation to tensors.
More precisely, let $\mathbb{T}_1$ a tensor space of shape $n_1^{(1)} \times n_2^{(1)} \times \cdots \times n_{r_1}^{(1)}$, and $\mathbb{T}_2$ a tensor space of shape $n_1^{(2)} \times n_2^{(2)} \times \cdots \times n_{r_2}^{(2)}$, such that $\forall k \in [\![1, s]\!], n_{r_1-(s-k)}^{(1)} = n_k^{(2)}$, then the tensor contraction between $t_1 \in \mathbb{T}_1$ and $t_2 \in \mathbb{T}_2$ is defined as:

$$\begin{cases} t_1 \otimes t_2 = t_3 \in \mathbb{T}_3 \text{ of shape } n_1^{(1)} \times \cdots \times n_{r_1-s}^{(1)} \times n_{s+1}^{(2)} \times \cdots \times n_{r_2}^{(2)} \text{ where} \\ t_3[i_1^{(1)}, \ldots, i_{r_1-s}^{(1)}, i_{s+1}^{(2)}, \ldots, i_{r_2}^{(2)}] = \\ \displaystyle\sum_{k_1=1}^{n_1^{(2)}} \cdots \sum_{k_s=1}^{n_s^{(2)}} t_1[i_1^{(1)}, \ldots, i_{r_1-s}^{(1)}, k_1, \ldots, k_s]\, t_2[k_1, \ldots, k_s, i_{s+1}^{(2)}, \ldots, i_{r_2}^{(2)}] \end{cases}$$

For the sake of simplicity, we omit the case where the contracted ranks are not the last ones for t_1 and the first ones for t_2. But this definition still holds in the general case subject to a permutation of the indices.

Definition 1.1.15. Covariant and contravariant indices
Given a tensor contraction $t_1 \otimes t_2$, indices of the left hand operand t_1 that are not contracted are called *covariant* indices. Those that are contracted are called *contravariant* indices. For the right operand t_2, the naming convention is the opposite. The set of covariant and contravariant indices of both operands are called the *transformation laws* of the tensor contraction.

Remark 1.1.16. **Transformation law independency**
Contrary to most mathematical definitions, tensors in deep learning are inde-

pendent of any transformation law, so that they must be specified for tensor contractions.

Remark 1.1.17. **Einstein summation convention**
Using subscript notation for covariant indices and superscript notation for contravariant indices, the previous tensor contraction can be written using the Einstein summation convention as:

$$t_{1_{i_1^{(1)}\cdots i_{r_1-s}^{(1)}}}{}^{k_1\cdots k_s} t_{2_{k_1\cdots k_s}}{}^{i_{s+1}^{(2)}\cdots i_{r_2}^{(2)}} = t_{3_{i_1^{(1)}\cdots i_{r_1-s}^{(1)}}}{}^{i_{s+1}^{(2)}\cdots i_{r_2}^{(2)}} \tag{1.2}$$

Dot product $u_k v^k = \lambda$ and matrix product $A_i{}^k B_k{}^j = C_i{}^j$ are common examples of tensor contractions.

Proposition 1.1.18. A contraction can be rewritten as a matrix product.

Proof. Using notation of (1.2), with the reshapings $t_1 \mapsto T_1$, $t_2 \mapsto T_2$ and $t_3 \mapsto T_3$ defined by grouping all covariant indices into a single index and all contravariant indices into another single index, we can rewrite

$$T_{1_{g_i(i_1^{(1)},\ldots,i_{r_1-s}^{(1)})}}{}^{g_k(k_1,\ldots,k_s)} T_{2_{g_k(k_1,\ldots,k_s)}}{}^{g_j(i_{s+1}^{(2)},\ldots,i_{r_2}^{(2)})} = T_{3_{g_i(i_1^{(1)},\ldots,i_{r_1-s}^{(1)})}}{}^{g_j(i_{s+1}^{(2)},\ldots,i_{r_2}^{(2)})}$$

where g_i, g_k and g_j are bijections defined similarly as in (1.1). □

Definition 1.1.19. Convolution
The *n-dimensional convolution*, denoted $*^n$, between $t_1 \in \mathbb{T}_1$ and $t_2 \in \mathbb{T}_2$, where $\mathbb{T}_1$ and $\mathbb{T}_2$ are of the same rank n such that $\forall p \in [\![1, n]\!], n_p^{(1)} \geq n_p^{(2)}$, is defined as:

$$\begin{cases} t_1 *^n t_2 = t_3 \in \mathbb{T}_3 \text{ of shape } n_1^{(3)} \times \cdots \times n_n^{(3)} \text{ where} \\ \forall p \in [\![1, n]\!], n_p^{(3)} = n_p^{(1)} - n_p^{(2)} + 1 \\ t_3[i_1, \ldots, i_n] = \displaystyle\sum_{k_1=1}^{n_1^{(2)}} \cdots \sum_{k_n=1}^{n_n^{(2)}} t_1[i_1 + n_1^{(2)} - k_1, \ldots, i_n + n_n^{(2)} - k_n]\, t_2[k_1, \ldots, k_n] \end{cases}$$

Proposition 1.1.20. A convolution can be rewritten as a matrix product.

Proof. Let $t_1 *^n t_2 = t_3$ defined as previously with $\mathbb{T}_1 = \bigotimes_{k=1}^{r} \mathbb{V}_k^{(1)}$, $\mathbb{T}_2 = \bigotimes_{k=1}^{r} \mathbb{V}_k^{(2)}$. Let $t'_1 \in \bigotimes_{k=1}^{r} \mathbb{V}_k^{(1)} \otimes \bigotimes_{k=1}^{r} \mathbb{V}_k^{(2)}$ such that $t'_1[i_1, \ldots, i_n, k_1, \ldots, k_n] = t_1[i_1 + n_1^{(2)} - k_1, \ldots, i_n + n_n^{(2)} - k_n]$, then

$$t_3[i_1, \ldots, i_n] = \sum_{k_1=1}^{n_1^{(2)}} \cdots \sum_{k_n=1}^{n_n^{(2)}} t'_1[i_1, \ldots, i_n, k_1, \ldots, k_n]\, t_2[k_1, \ldots, k_n]$$

where we recognize a tensor contraction. Proposition 1.1.18 concludes. □

The two following operations are meant to further decrease the shape of the resulting output.

Definition 1.1.21. Strided convolution

The n-dimensional *strided* convolution, with strides $s = (s_1, s_2, \ldots, s_n)$, denoted $*_s^n$, between $t_1 \in \mathbb{T}_1$ and $t_2 \in \mathbb{T}_2$, where $\mathbb{T}_1$ and $\mathbb{T}_2$ are of the same rank n such that $\forall p \in [\![1, n]\!], n_p^{(1)} \geq n_p^{(2)}$, is defined as:

$$\begin{cases} t_1 *_s^n t_2 = t_4 \in \mathbb{T}_4 \text{ of shape } n_1^{(4)} \times \cdots \times n_n^{(4)} \text{ where} \\ \forall p \in [\![1, n]\!], n_p^{(4)} = \lfloor \frac{n_p^{(1)} - n_p^{(2)} + 1}{s_p} \rfloor \\ t_4[i_1, \ldots, i_n] = (t_1 *^n t_2)[(i_1 - 1)s_n + 1, \ldots, (i_n - 1)s_n + 1] \end{cases}$$

Remark 1.1.22. Informally, a strided convolution is defined as if it were a regular subsampling of a convolution. They match if $s = (1, 1, \ldots, 1)$.

Definition 1.1.23. Pooling

Let a real-valued function f defined on all tensor spaces of any shape, *e.g.* the *max* or *average* function. An f-pooling operation is a mapping $t \mapsto t'$ such that each entry of t' is an image by f of a subtensor of t.

Remark 1.1.24. Usually, the set of subtensors that are reduced by f into entries of t' are defined by a regular partition of the entries of t.

1.2 Neural Networks

A feed-forward neural network could originally be formalized as a composite function chaining linear and non-linear functions (Rumelhart et al., 1985; LeCun et al., 1989; LeCun et al., 1995), even up until the important breakthroughs that generated a surge of interest in the field (Hinton et al., 2012; Krizhevsky et al., 2012; Simonyan et al., 2014). However, in more recent advances, more complex architectures have emerged (Szegedy et al., 2015; He et al., 2016; Zoph et al., 2016; Huang et al., 2017), such that the former formalization does not suffice. We provide a definition for the first kind of neural networks (Definition 1.2.1) and use it to present its related concepts. Then we give a more generic definition (Definition 1.2.12).
Note that in this manuscript, we only consider neural networks that are *feed-forward* (Zell, 1994; Wikipedia, 2018).

1.2.1 Simple formalization

We denote by I_f the *domain of definition* of a function f ("I" stands for "input") and by $O_f = f(I_f)$ its *image* ("O" stands for "output"), and we represent it as $I_f \xrightarrow{f} O_f$.

Definition 1.2.1. Neural network (simply connected)
Let f be a function such that I_f and O_f are vector or tensor spaces.
f is a *(simply connected) neural network function* if there are a series of affine functions $(g_k)_{k=1,2,..,L}$ and a series of non-linear derivable univariate functions $(h_k)_{k=1,2,..,L}$ such that:

$$\begin{cases} \forall k \in [\![1, L]\!], f_k = h_k \circ g_k, \\ I_f = I_{f_1} \xrightarrow{f_1} O_{f_1} \cong I_{f_2} \xrightarrow{f_2} \dots \xrightarrow{f_L} O_{f_L} = O_f, \\ f = f_L \circ ... \circ f_2 \circ f_1 \end{cases}$$

The couple (g_k, h_k) is called the *k-th layer* of the neural network. L is its

depth. 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. We denote by $\mathcal{N}$ the set of neural network functions.

Definition 1.2.2. Activation function
An *activation function* h is a real-valued univariate function that is non-linear and derivable, that is also defined by extension on any linear space with the functional notation $h(v)[i] = h(v[i])$.

Definition 1.2.3. Layer
A couple (g, h), where g is an affine or linear function, and h is an activation function is called a *layer*. The set of layers is denoted $\mathcal{L}$.

Remark 1.2.4. **Adoption of ReLU activations**
Historically, sigmoidal and tanh activations were mostly used (Cybenko, 1989; LeCun et al., 1989). However in recent practice, the *rectified linear unit* (ReLU), which implements the *rectifier* function $h : x \mapsto max(0, x)$ with convention $h'(0) = 0$ (first introduced as the *positive part*, Jarrett et al., 2009), is the most used activation, as it was demonstrated to be faster and to obtain better results (Glorot et al., 2011). ReLU originated numerous variants *e.g. leaky rectified linear unit* (Maas et al., 2013), *parametric rectified linear unit* (PReLU, He et al., 2015), *exponential linear unit* (ELU, Clevert et al., 2015), *scaled exponential linear unit* (SELU, Klambauer et al., 2017).

Remark 1.2.5. **Universal approximation**
Early researches have shown that neural networks with one level of depth can approximate any real-valued function defined on a compact subset of $\mathbb{R}^n$. This result was first proved for sigmoidal activations (Cybenko, 1989), and then it was shown it did not depend on the sigmoidal activations (Hornik et al., 1989; Hornik, 1991).

For example, for the application of supervised learning when a neural network is trained from data (see Section 1.2.4), this result is quite important because it brings theoretical justification that the objective exists (even though it doesn't inform whether an algorithm to approach it exists or is efficient).

Remark 1.2.6. **Computational difficulty**
However, reaching such objective is a computationally difficult problem, which drove back interest from the field. Thanks to better hardware and to using better initialization schemes that speed up learning, researchers started to report more successes with deep neural networks (Hinton et al., 2006; Glorot et al., 2010) ; see (Bengio, 2009) for a review of this period. It ultimately came to a surge of interest in the field after a significant breakthrough on the imagenet dataset (Deng et al., 2009) with a deep convolutional architecture (Krizhevsky et al., 2012), see Section 1.2.7. The use of the fast ReLU activation function (Glorot et al., 2011) as well as leveraging graphical processing units with CUDA (Nickolls et al., 2008) were also key factors in overcoming this computational difficulty.

Remark 1.2.7. **Expressivity and expressive efficiency**
The study of the *expressivity* (also called *representational power*) of families of neural networks is the field that is interested in the range of functions that can be realized or approximated by this family (Håstad et al., 1991; Pascanu et al., 2013). In general, given a maximal error ϵ and an objective F, the more expressive is a family $N \subset \mathcal{N}$, the more likely it is to contain an approximation $f \in N$ such that $d(f, F) < \epsilon$. However, if we consider the approximation $f_{min} \in N$ that have the lowest number of neurons, it is possible that f_{min} is still too large and may be unpractical. For this reason, expressivity is often studied along the related notion of *expressive efficiency* (Delalleau et al., 2011; Cohen et al., 2018a).

Remark 1.2.8. **Rectifier neural netowrks**
Of particular interest for the intuition is a result stating that a simply connected neural networks with only ReLU activations (a rectifier neural network) is a piecewise linear function (Pascanu et al., 2013; Montufar et al., 2014), and that conversely any piecewise linear function is also a rectifier neural network such that an upper bound of its depth is logarithmically related to the input dimension (Arora et al., 2018, th. 2.1.). Their expressive

efficiency have also been demonstrated compared to neural networks using threshold or sigmoid activations (Pan et al., 2016).

Remark 1.2.9. **Benefits of depth**
Expressive efficiency analysis have demonstrated the benefits of depth, *i.e.* a shallow neural network would need an unfeasible large number of neurons to approximate the function of a deep neural network (*e.g.* Delalleau et al., 2011; Bianchini et al., 2014; Poggio et al., 2015; Eldan et al., 2016; Poole et al., 2016; Raghu et al., 2016; Cohen et al., 2016a; Mhaskar et al., 2016; Lin et al., 2017; Arora et al., 2018).

Remark 1.2.10. **Bias**
Note that affine functions $\widetilde{g}$ can be written as a sum between a linear function g and a constant vector b which is called the *bias*. It augments the expressivity of the neural network's family of functions. For notational convenience, we will often omit to write down the biases in the layer's equations.

1.2.2 Generic formalization

The former neural networks are said to be *simply connected* because each layer only takes as input the output of the previous one. We'll give a more general definition after first defining branching operations.

Definition 1.2.11. Branching
A *binary branching operation* between two tensors, $x_{k_1} \bowtie x_{k_2}$, outputs, subject to shape compatibility, either their addition, either their concatenation along a rank, or their concatenation as a list.
A *branching operation* between n tensors, $x_{k_1} \bowtie x_{k_2} \bowtie \cdots \bowtie x_{k_n}$, is a composition of binary branching operations, or is the identity function Id if $n = 1$. Branching operations are also naturally defined on tensor-valued functions through their realizations.

Definition 1.2.12. Neural network (generic definition)
The set of *neural network* functions $\mathcal{N}$ is defined inductively as follows

1. $Id \in \mathcal{N}$
2. $f \in \mathcal{N} \wedge (g, h) \in \mathcal{L} \wedge O_f \subset I_g \Rightarrow h \circ g \circ f \in \mathcal{N}$
3. for all shape compatible branching operations:
   $f_1, f_2, \ldots, f_n \in \mathcal{N} \Rightarrow f_1 \bowtie f_2 \bowtie \cdots \bowtie f_n \in \mathcal{N}$

Remark 1.2.13. **Examples**
The neural network proposed in (Szegedy et al., 2015), called *Inception*, use depth-wise concatenation of feature maps. Residual networks (ResNets, He et al., 2016) make use of *residual connections*, also called *skip connections*, *i.e.* an activation that is used as input in a lower level is added to another activation at an upper level. Densely connected networks (DenseNets, Huang et al., 2017) have their activations concatenated with all lower level activations. These neural networks had demonstrated state of the art performances on the imagenet classification challenge (Deng et al., 2009), outperforming simply connected neural networks.

Remark 1.2.14. **Benefits of branching operations**
Recent works have provided rationales supporting benefits of using branching operations, thus giving justifications for architectures obtained with the generic formalization. In particular, (Cohen et al., 2018a) have analyzed the impact of residual connections used in Wavenet-like architectures (Van Den Oord et al., 2016) in terms of expressive efficiency (see Remark 1.2.7) using tools from the field of tensor analysis ; (Orhan et al., 2018) have empirically demonstrated that skip connections can resolve some inefficiency problems inherent of fully-connected networks (dead activations, activations that are always equal, linearly dependent sets of activations).

For layer indexing convenience, we still use the simple formalization in the subsequent subsections, even though the presentation would be similar with the generic formalization.

1.2.3 Interpretation

Until now, we have formally introduced a neural network as a mathematical function. As its name suggests, such function can be interpreted from a connectivity viewpoint (LeCun, 1987).

Definition 1.2.15. Connectivity matrix
Let g a linear function. Without loss of generality subject to a flattening, let's suppose I_g and O_g are vector spaces. Then there exists a *connectivity matrix* W_g, such that:

$$\forall x \in I_g, g(x) = W_g x$$

We denote W_k the connectivity matrix of the k-th layer.

Remark 1.2.16. **Biological inspiration**
A *(computational) neuron* is a computational unit that is biologically inspired (McCulloch et al., 1943). Each neuron is capable of:

1. receiving modulated signals from other neurons and aggregate them,
2. applying to the result a derivable activation,
3. passing the signal to other neurons.

That is to say, each domain $\{I_{f_k}\}$ and O_f can be interpreted as a layer of neurons, with one neuron for each dimension. The connectivity matrices $\{W_k\}$ describe the connections between each successive layers. A neuron is illustrated on Figure 1.1.

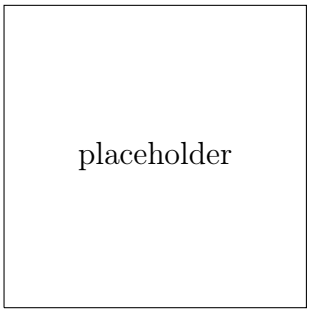

Figure 1.1: A neuron

1.2.4 Parameterization and training

Given an objective function F, training is the process of incrementally modifying a neural network f upon obtaining a better approximation of F. The most used training algorithms are based on gradient descent, as proposed in (Widrow et al., 1960). These algorithms became popular since (Rumelhart et al., 1985). Informally, f is parameterized with initial weights that characterize its linear parts. These weights are modified step by step in the opposite direction of their gradient with respect to a loss. All possible realizations of f through its weights draw a family N which expressivity is crucial for the success of the training. The common points between f and other objects of N define what is called a neural network *architecture*. That is
We present gradient based learning more formally in what follows.

Definition 1.2.17. Architecture Let $f \in \mathcal{N}$ with weights $(\theta_k)_k \in$.

Remark 1.2.18. **Gradient descent**
The most used training algorithms are based on gradient descent, as proposed in (Widrow et al., 1960). These algorithms became popular since (Rumelhart et al., 1985). In order to be trained, f is parameterized with initial weights that characterize its linear parts. These weights are modified step by step in the opposite direction of their gradient with respect to a loss.

Remark 1.2.19. **Architecture**
All possible realizations of f through its weights draw a family N which expressivity is crucial for the success of the training. The common points between f and other objects of N define what is called a neural network *architecture*.

Definition 1.2.20. Weights
Let consider the k-th layer of a neural network f. We define its weights as coordinates of a vector θ_k, called the *weight kernel*, such that:

$$\forall (i,j), \begin{cases} \exists p, W_k[i,j] := \theta_k[p] \\ \text{or } W_k[i,j] = 0 \end{cases}$$

A weight p that appears multiple times in W_k is said to be *shared*. Two parameters of W_k that share a same weight p are said to be *tied*. The number of weights of the k-th layer is $n_1^{(\theta_k)}$.

Remark 1.2.21. **Learning**
A *loss* function $\mathcal{L}$ penalizes the output $x_L = f(x)$ relatively to the approximation error $|f(x) - F(x)|$. Gradient w.r.t. θ_k, denoted $\vec{\nabla}_{\theta_k}$, is used to update the weights via an optimization algorithm based on gradient descent and a learning rate α, that is:

$$\theta_k^{(\text{new})} = \theta_k^{(\text{old})} - \alpha \cdot \vec{\nabla}_{\theta_k} \left(\mathcal{L}\left(x_L, \theta_k^{(\text{old})}\right) + R\left(\theta_k^{(\text{old})}\right) \right) \tag{1.3}$$

where α can be a scalar or a vector, $\cdot$ can denote outer or pointwise product, and R is a regularizer. They depend on the optimization algorithm.

TODO: examples of optimization

Remark 1.2.22. **Linear complexity**
The complexity of computing the gradients is linear with the number of weights.

Proof. Without loss of generality, we assume that the neural network is simply connected. Thanks to the chain rule, $\vec{\nabla}_{\theta_k}$ can be computed using gradients that are w.r.t. x_k, denoted $\vec{\nabla}_{x_k}$, which in turn can be computed using gradients w.r.t. outputs of the next layer $k+1$, up to the gradients given on the output layer.

That is:

$$\vec{\nabla}_{\theta_k} = J_{\theta_k}(x_k)\vec{\nabla}_{x_k} \tag{1.4}$$

$$\begin{aligned} \vec{\nabla}_{x_k} &= J_{x_k}(x_{k+1})\vec{\nabla}_{x_{k+1}} \\ \vec{\nabla}_{x_{k+1}} &= J_{x_{k+1}}(x_{k+2})\vec{\nabla}_{x_{k+2}} \\ &\dots \\ \vec{\nabla}_{x_{L-1}} &= J_{x_{L-1}}(x_L)\vec{\nabla}_{x_L} \end{aligned} \tag{1.5}$$

Obtaining,

$$\vec{\nabla}_{\theta_k} = J_{\theta_k}(x_k)(\prod_{p=k}^{L-1} J_{x_p}(x_{p+1}))\vec{\nabla}_{x_L} \tag{1.6}$$

where $J_{\text{wrt}}(.)$ are the respective jacobians which can be determined with the layer's expressions and the $\{x_k\}$; and $\vec{\nabla}_{x_L}$ can be determined using $\mathcal{L}$, R and x_L. □

This allows to compute the gradients with a complexity that is linear with the number of weights (only one computation of the activations), instead of being quadratic if it were done with the difference quotient expression of the derivatives (one more computation of the activations for each weight).

Remark 1.2.23. **Backpropagation**

We can remark that (1.5) rewrites as

$$\begin{aligned}\vec{\nabla}_{x_k} &= J_{x_k}(x_{k+1})\vec{\nabla}_{x_{k+1}} \\ &= J_{x'_k}(h(x'_k))J_{x_k}(W_k x_k)\vec{\nabla}_{x_{k+1}}\end{aligned} \tag{1.7}$$

where $x'_k = W_k x_k$, and these jacobians can be expressed as:

$$J_{x'_k}(h(x'_k))[i,j] = \delta_i^j h'(x'_k[i]) \tag{1.8}$$

$$J_{x'_k}(h(x'_k)) = I\, h'(x'_k)$$

$$J_{x_k}(W_k x_k) = W_k^T \tag{1.9}$$

That means that we can write $\vec{\nabla}_{x_k} = (\widetilde{h}_k \circ \widetilde{g}_k)(\vec{\nabla}_{x_{k+1}})$ such that the connectivity matrix $\widetilde{W}_k$ is obtained by transposition. This can be interpreted as gradient calculation being a *back-propagation* on the same neural network, in opposition of the *forward-propagation* done to compute the output.

TODO: Overfitting remark

1.2.5 Examples of layer

Definition 1.2.24. Connections

The set of *connections* of a layer (g,h), denoted C_g, is defined as:

$$C_g = \{(i,j), \exists p, W_g[i,j] := \theta_g[p]\}$$

We have $0 \leq |C_g| \leq n_1^{(W_g)} n_2^{(W_g)}$.

Definition 1.2.25. Dense layer

A *dense layer* (g,h) is a layer such that $|C_g| = n_1^{(W_g)} n_2^{(W_g)}$, *i.e.* all possible connections exist. The map $(i,j) \mapsto p$ is usually a bijection, meaning that there is no weight sharing.

Definition 1.2.26. Partially connected layer
A *partially connected layer* (g, h) is a layer such that $|C_g| < n_1^{(W_g)} n_2^{(W_g)}$.
A *sparsely connected layer* (g, h) is a layer such that $|C_g| \ll n_1^{(W_g)} n_2^{(W_g)}$.

Definition 1.2.27. Convolutional layer
A *n-dimensional convolutional layer* (g, h) is such that the weight kernel θ_g can be reshaped into a tensor w of rank $n + 2$, and such that

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

where p and q index slices along the last ranks.

Definition 1.2.28. Feature maps and input channels
The slices $g(x)_q$ are typically called *feature maps*, and the slices x_p are called *input channels*. Let's denote by $n_o = n_{n+1}^{(O_g)}$ and $n_i = n_{n+1}^{(I_g)}$ the number of feature maps and input channels. In other words, Definition 1.2.27 means that for each feature maps, a convolution layer computes n_i convolutions and sums them, computing a total if $n_i \times n_o$ convolutions.

Remark 1.2.29. Note that because they are simply summed, entries of two different input channels that have the same coordinates are assumed to share some sort of relationship. For instance on images, entries of each input channel (typically corresponding to Red, Green and Blue channels) that have the same coordinates share the same pixel location.

Remark 1.2.30. Given a tensor input x, the n-dimensional convolutions between the inputs channels x_p and slices of a weight tensor $w_{p,q}$ would result in outputs y_q of shape $n_1^{(x)} - n_1^{(w)} + 1 \times \ldots \times n_n^{(x)} - n_n^{(w)} + 1$. So, in order to preserve shapes, a padding operation must pad x with $n_1^{(w)} - 1 \times \ldots \times n_n^{(w)} - 1$ zeros beforehand. For example, the padding function of the library *tensorflow* (Abadi et al., 2015) pads each rank with a balanced number of zeros on the left and right indices (except if $n_t^{(w)} - 1$ is odd then there is one more zero on the left).

Definition 1.2.31. Padding
A convolutional layer with *padding* (g, h) is such that g can be decomposed as $g = g_{\text{pad}} \circ g'$, where g' is the linear part of a convolution layer as in Definition 1.2.27, and g_{pad} is an operation that pads zeros to its inputs such that g preserves tensor shapes.

Remark 1.2.32. One asset of padding operations is that they limit the possible loss of information on the borders of the subsequent convolutions, as well as preventing a decrease in size. Moreover, preserving shape is needed to build some neural network architectures, especially for ones with branching operations *e.g.* Remark 1.2.13. On the other hand, they increase memory and computational footprints.

Proposition 1.2.33. Connectivity matrix of a convolution with padding
A convolutional layer with padding (g, h) is equivalently defined as W_g being a $n_i \times n_o$ block matrix such that its blocks are Toeplitz matrices.

Proof. Let's consider the slices indexed by p and q, and to simplify the notations, let's drop the subscripts ${}_{p,q}$. We recall from Definition 1.1.19 that

$$
\begin{aligned}
y &= (x *^n w)[j_1, \dots, j_n] \\
&= \sum_{k_1=1}^{n_1^{(w)}} \cdots \sum_{k_n=1}^{n_n^{(w)}} x[j_1 + n_1^{(w)} - k_1, \dots, j_n + n_n^{(w)} - k_n]\, w[k_1, \dots, k_n] \\
&= \sum_{i_1=j_1}^{j_1+n_1^{(w)}-1} \cdots \sum_{i_n=j_n}^{j_n+n_n^{(w)}-1} x[i_1, \dots, i_n]\, w[j_1 + n_1^{(w)} - i_1, \dots, j_n + n_n^{(w)} - i_n] \\
&= \sum_{i_1=1}^{n_1^{(x)}} \cdots \sum_{i_n=1}^{n_n^{(x)}} x[i_1, \dots, i_n]\, \widetilde{w}[i_1, j_1, \dots, i_n, j_n] \\
&\text{where } \widetilde{w}[i_1, j_1, \dots, i_n, j_n] = \\
&\qquad \begin{cases} w[j_1 + n_1^{(w)} - i_1, \dots, j_n + n_n^{(w)} - i_n] & \text{if } \forall t, 0 \leq i_t - j_t \leq n_t^{(w)} - 1 \\ 0 & \text{otherwise} \end{cases}
\end{aligned}
$$

Using Einstein summation convention as in (1.2) and permuting indices, we recognize the following tensor contraction

$$y_{j_1\cdots j_n} = x_{i_1\cdots i_n}\widetilde{w}^{i_1\cdots i_n}{}_{j_1\cdots j_n} \tag{1.10}$$

Following Proposition 1.1.18, we reshape (1.10) as a matrix product. To reshape $y \mapsto Y$, we use the row major order bijections g_j as in (1.1) defined onto $\{(j_1, \ldots, j_n), \forall t, 1 \leq j_t \leq n_t^{(y)}\}$. To reshape $x \mapsto X$, we use the same row major order bijection g_j, however defined on the indices that support non zero-padded values, so that zero-padded values are lost after reshaping. That is, we use a bijection g_i such that $g_i(i_1, i_2, \ldots, i_n) = g_j(i_1 - o_1, i_2 - o_2, \ldots, i_n - o_n)$ defined if and only if $\forall t, 1 + o_t \leq i_t \leq n_t^{(y)}$, where the $\{o_t\}$ are the starting offsets of the non zero-padded values. $\widetilde{w} \mapsto W$ is reshaped by using g_j for its covariant indices, and g_i for its contravariant indices. The entries lost by using g_i do not matter because they would have been nullified by the resulting matrix product. We remark that W is exactly the block (p, q) of W_g (and not of $W_{g'}$). Now let's prove that it is a Toeplitz matrix.

Thanks to the linearity of the expression (1.1) of g_j, by denoting $i'_t = i_t - o_t$, we obtain

$$g_i(i_1, i_2, \ldots, i_n) - g_j(j_1, j_2, \ldots, j_n) = g_j(i'_1 - j_1, i'_2 - j_2, \ldots, i'_n - j_n) \tag{1.11}$$

To simplify the notations, let's drop the arguments of g_i and g_j. By bijectivity of g_j, (1.11) tells us that $g_i - g_j$ remains constant if and only if $i'_t - j_t$ remains constant for all t. Recall that

$$W[g_i, g_j] = \begin{cases} w[j_1 + n_1^{(w)} - i'_1, \ldots, j_n + n_n^{(w)} - i'_n] & \text{if } \forall t, 0 \leq i'_t - j_t \leq n_t^{(w)} - 1 \\ 0 & \text{otherwise} \end{cases} \tag{1.12}$$

Hence, on a diagonal of W, $g_i - g_j$ remaining constant means that $W[g_i, g_j]$

also remains constants. So W is a Toeplitz matrix.
The converse is also true as we used invertible functions in the index spaces through the proof. □

Remark 1.2.34. The former proof makes clear that the result doesn't hold in case there is no padding. This is due to border effects when the index of the n^{th} rank resets in the definition of the row-major ordering function g_j that would be used. Indeed, under appropriate definitions, the matrices could be seen as almost Toeplitz.

Remark 1.2.35. Comparatively with dense layers, convolution layers enjoy a significant decrease in the number of weights. For example, an input 2×2 convolution on images with 3-color input channels, would breed only 12 weights per feature maps, independently of the numbers of input neurons. On image datasets, their usage also breeds a significant boost in performance compared with dense layers (Krizhevsky et al., 2012), for they allow to take advantage of the topology of the inputs while dense layers don't (LeCun et al., 1995). A more thorough comparison and explanation of their assets will be discussed in Section **??**.

Definition 1.2.36. Stride
A convolutional layer with *stride* is a convolutional layer that computes strided convolutions (with stride > 1) instead of convolutions.

Definition 1.2.37. Pooling
A layer with *pooling* (g, h) is such that g can be decomposed as $g = g' \circ g_{\text{pool}}$, where g_{pool} is a pooling operation.

Remark 1.2.38. **Downscaling**
Layers with stride or pooling downscale the signals that passes through the layer. These types of layers allows to compute features at a coarser level, giving the intuition that the deeper a layer is in the network, the more abstract is the information captured by the weights of the layer.

TODO: below

1.2.6 Examples of regularization

Remark 1.2.39. **Overfitting** TODO:

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 (Srivastava et al., 2014). 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.

1.2.7 Examples of architecture

TODO: rephrase

A multilayer perceptron (MLP) (Hornik et al., 1989) is a neural network composed of only dense layers. A convolutional neural network (CNN) (LeCun et al., 1998) 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 (Hornik et al., 1989) via the chain rule and according to a chosen optimization algorithm (*e.g.* Bottou, 2010).

1.3 Graphs and signals

1.3.1 Basic definitions

1.3.1.1 Graphs

Definition 1.3.1. Graph
A *graph* G is defined as a couple of sets $\langle V, E \rangle$ where V is the set of *vertices*, also called *nodes*, and $E \subseteq \binom{V}{2}$ is the set of *edges*. For all $u, v \in V$ we define the relation $u \sim v \Leftrightarrow \{u, v\} \in E$. Unless stated otherwise, we will consider only *weighted* graphs *i.e.* each graph G is associated with a weight mapping $w : E \to \mathbb{R}^*$.

Figure 1.2 illustrates an example of a graph. Note that we employ interchangeably the terms *vertex* and *node*.

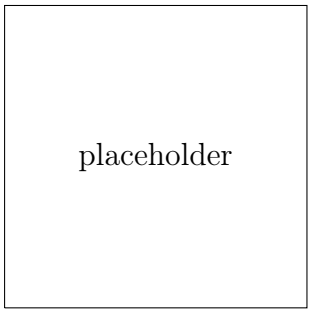

Figure 1.2: Example of a graph

Remark 1.3.2. According to this definition, we consider simple graphs *i.e.* no two edges share the same set of vertices and there is no self-loop.

Definition 1.3.3. Path
A *path* of length $n \in \mathbb{N}$ in a graph $G = \langle V, E \rangle$ is a sequence $(v_1 v_2 \cdots v_n)$ in V such that $\forall i, v_i \sim v_{i+1}$.

Remark 1.3.4. Our definition of graphs admit no self-loop so $\forall i, v_i \neq v_{i+1}$

Definition 1.3.5. Order
The order of a graph $G = \langle V, E \rangle$ is define as $\text{order}(G) = |V| \in \mathbb{N} \cup \{+\infty\}$

Definition 1.3.6. Adjacency matrix
The *adjacency matrix* of a finite graph $G = \langle V, E \rangle$ of order n, is a $n \times n$ real-valued matrix A associated to an indexing of $V = \{v_1, v_2, \dots v_n\}$, such that

$$A[i,j] = \begin{cases} w\left(\{v_i, v_j\}\right) & \text{if } v_i \sim v_j \\ 0 & \text{otherwise} \end{cases}$$

Definition 1.3.7. Degree
The *degree* of a vertex $v \in V$ of a graph $G = \langle V, E \rangle$ is defined as $\deg(v) = |\{u \in V, u \sim v\}| \in \mathbb{N} \cup \{+\infty\}$.
The *degree* of the graph G is defined as $\deg(G) = \max_{v \in V}\{\deg(v)\}$.
A graph is said to be *regular* if deg is constant on the vertices.

Definition 1.3.8. Degree matrix
The *degree matrix* of a finite graph $G = \langle V, E \rangle$ of order n, is the diagonal matrix D, associated to an indexing of $V = \{v_1, v_2, \dots v_n\}$, such that $D = \text{diag}(\deg(v_1), \deg(v_2), \dots, \deg(v_n))$.

Definition 1.3.9. Laplacian matrix
The *laplacian matrix* of a graph $G = \langle V, E \rangle$ of order n, associated to an indexing of $V = \{v_1, v_2, \dots v_n\}$, is defined as $L = D - A$, where D is the degree matrix and A is the adjacency matrix.

Definition 1.3.10. Digraph
A digraph is an oriented graph *i.e.* $E \subseteq V \times V - \{(v, v), v \in V\}$. Contrary to a graph, the weight mapping w, the relation $\sim$, the adjacency matrix A, and the laplacian matrix L are not symmetric. Notions defined on graphs naturally extends to digraphs where possible.

Definition 1.3.11. Bipartite graph
A *bipartite graph* is a triplet of sets $\langle V^{(1)}, V^{(2)}, E\rangle$, where $V^{(1)}$ and $V^{(2)}$ are sets of vertices, $V^{(1)} \cap V^{(2)} \neq \emptyset$, and $E \subseteq V^{(1)} \times V^{(2)}$. It is associated with a weight mapping $w : E \to \mathbb{R}^*$. Its adjacency matrix A is associated to indexings of $V^{(1)} = \{v_1^{(1)}, v_2^{(1)}, \dots v_n^{(1)}\}$ and $V^{(2)} = \{v_1^{(2)}, v_2^{(2)}, \dots v_n^{(2)}\}$, such that

$$A[i,j] = \begin{cases} w\left((v_i^{(1)}, v_j^{(2)})\right) & \text{if } (v_i^{(1)}, v_j^{(2)}) \in E \\ 0 & \text{otherwise} \end{cases}$$

Definition 1.3.12. Induced subgraph
The *subgraph* $\widetilde{G} = \langle \widetilde{V}, \widetilde{E}\rangle$ of a graph $G = \langle V, E\rangle$, *induced* by $\widetilde{V} \subseteq V$, is such that $\forall (u,v) \in \widetilde{V}^2, u \overset{\widetilde{G}}{\sim} v \Leftrightarrow u \overset{G}{\sim} v$.

Definition 1.3.13. Grid graph
A *grid graph* $G = \langle V, E\rangle$ is such that $V \cong \mathbb{Z}^2$, $v_1 \sim v_2 \Rightarrow \|v_2 - v_1\|_\infty \in \{0,1\}$ and either one of the following is true:

$$\begin{cases} (i_1,j_1) \sim (i_2,j_2) \Leftrightarrow |i_2 - i_1| \,\text{XOR}\, |j_2 - j_1| & \text{(4 neighbours)} \\ (i_1,j_1) \sim (i_2,j_2) \Leftrightarrow |i_2 - i_1| \,\text{AND}\, |j_2 - j_1| & \text{(4 neighbours)} \\ (i_1,j_1) \sim (i_2,j_2) \Leftrightarrow |i_2 - i_1| \,\text{OR}\, |j_2 - j_1| & \text{(8 neighbours)} \end{cases}$$

A *(rectangular) grid graph* of size $n \times m$ is the subgraph of a grid graph induced by $[\![1,n]\!] \times [\![1,m]\!]$.
A *square grid graph* is a rectangular grid graph of square size.

1.3.1.2 (Real-valued) Signals

Definition 1.3.14. Signal space
The *signal space* $\mathcal{S}(V)$, over the set V, is the linear space of real-valued functions defined on V.

We have $\dim(\mathcal{S}(V)) = |V| \in \mathbb{N} \cup \{+\infty\}$.

Remark 1.3.15. In particular, a vector space, and more generally a tensor space, are finite-dimensional signal spaces over any of their bases.

Definition 1.3.16. Signal
A *signal* over V, $s \in \mathcal{S}(V)$, is a function $s : V \to \mathbb{R}$.
An *entry* of a signal s is an image by s of some $v \in V$ and we denote $s[v]$.
If v is represented by a n-tuple, we can also write $s[v_1, v_2, \ldots, v_n]$.
The *support* of a signal $s \in \mathcal{S}(V)$ is $\text{supp}(s) = \{v \in V, s[v] \neq 0\}$.

Definition 1.3.17. Graph signal
A *graph signal* over G is a signal over its vertex set. We denote by $\mathcal{S}(G)$ the graph signal space.

We have $\dim(\mathcal{S}(G)) = \text{order}(G) \in \mathbb{N} \cup \{+\infty\}$.

Definition 1.3.18. Underlying structure
An *(underlying) structure* of a signal s over a set V, is a graph G with vertex set V.

Remark 1.3.19. **Example of images, time series and graph signals**
When their is a unique clear underlying structure, we say it is *the* underlying structure. For example, images are compactly supported signals over $\mathbb{Z}^2$ and their underlying structure is a rectangular grid graph. Time series are signals over $\mathbb{N}$ and their underlying structure is a line graph. The underlying structure of a graph signal is obviously the graph itself.

1.3.2 Graphs in deep learning

TODO: below

We come across 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, the *connectivity graph*. It encodes how

the information is propagated through a layer to another. See Section 1.3.2.1.

- Neural architectures can be represented by a graph. In particular, a computation graph is used by deep learning programming languages to keep track of the dependencies between layers of a deep learning model, in order to compute forward and back-propagation. See Section 1.3.2.2.
- A graph can represent the underlying structure of an object (often a vector or a signal). The nodes represent its features, and the edges represent some structural property. See Section 1.3.2.3.
- Datasets can also be graph-structured. The nodes represent the objects of the dataset, and its edge represent some sort of relation between them. See Section 1.3.2.4.

1.3.2.1 Connectivity graph

A Connectivity graph is the bipartite graph whose adjacency matrix is the connectivity matrix of 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 1.3.20. 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 1.3 depicts some examples.

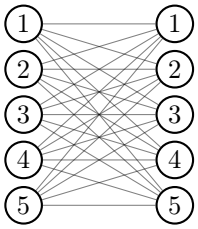

Figure 1.3: Examples

TODO: Figure 1.3. 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 1.4 depicts the connectivity graph of a 1-d convolution layer and its weight sharing scheme.

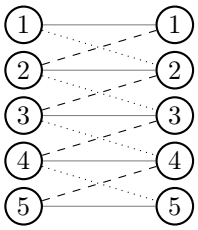

Figure 1.4: Depiction of a 1D-convolutional layer and its weight sharing scheme.

TODO: Add weight sharing scheme in Figure 1.4

1.3.2.2 Computation graph

1.3.2.3 Underlying graph structure and signals

1.3.2.4 Graph-structured dataset

Chapter 2

Currently Unnamed

2.1 Convolutions on graphs (draft that will be splitted in multiple sections) 40

2.1 Convolutions on graphs (draft that will be splitted in multiple sections)

Defining a convolution on graphs is a challenging problem. Obviously, the underlying structure determined by a graph is not necessarily isomorphic to a set onto which the convolution is already defined.
Related works: moura, spectral convolution with laplacian.
A convolution may comprise the following properties: bilinear, equivariant with respect to a certain class of isomorphism.
We shall first study classes of graphs onto which the convolution can be naturally defined before generalizing.
*Convolution without the edges
*Convolution on grids
*Convolution on lattice-regular graphs
*Convolution on product graphs
*Convolution on linear combination of circulant graphs
TODO: brief outline

2.1.1 Analysis of the classical convolution operator

In this subsection, we are exposing a few properties of the classical convolution that a generalization to graphs would likely try to preserve. For now let's consider a graph G agnostically of its edges *i.e.* $G \cong V$ is just the set of its vertices.
Let's recall what is a transformation, and how it acts on signals.

Definition 2.1.1. Transformation
A *transformation* $f : V \to V$ is a function with same domain and codomain. The set of transformations is denoted $\Phi(V)$. The set of bijective transformations is denoted $\Phi^*(V) \subset \Phi(V)$.

In case $f \in \Phi^*(V)$, it can act on $\mathcal{S}(V)$ through the linear operator $L_f \in \mathcal{L}(\mathcal{S}(V))$ defined as:

$$\forall s \in \mathcal{S}(V), \forall v \in V, f(s)[v] := L_f s[v] = s[f^{-1}(v)]$$

i.e. an entry of a transformed signal is obtained by doing a lookup of the entry of the original signal.
In case $f \notin \Phi^*(V)$, we can still define $L_f \in \mathcal{L}(\mathcal{S}(V))$, however we need to linearly aggregate the entries on the fibers:

$$\forall s \in \mathcal{S}(V), \forall v \in V, f(s)[v] := L_f s[v] = \text{AGGREGATE}\{s[u], u \in f^{-1}\{v\}\}$$

where AGGREGATE can be for example the sum, the average, or the max, and $\text{AGGREGATE}(\emptyset) = 0$.

2.1.1.1 Characterization on grid graphs

Consider an edge-less grid graph *i.e.* $G \cong \mathbb{Z}^2$. By restriction to compactly supported signals, this case encompass the case of images.

Definition 2.1.2. Translation on $\mathcal{S}(\mathbb{Z}^2)$
A translation on $\mathbb{Z}^2$ is defined as a transformation $t \in \Phi^*(\mathbb{Z}^2)$ such that

$$\exists (a, b) \in \mathbb{Z}^2, \forall (x, y) \in \mathbb{Z}^2, t(x, y) = (x + a, y + b)$$

It also acts on $\mathcal{S}(\mathbb{Z}^2)$ with the notation $t_{a,b}$ *i.e.*

$$\forall s \in \mathcal{S}(\mathbb{Z}^2), \forall (x, y) \in \mathbb{Z}^2, t_{a,b}(s)[x, y] = s[x - a, y - b]$$

For any set E, we denote by $\mathcal{T}(E)$ its translations if they are defined.

Definition 2.1.3. Convolution on $\mathcal{S}(\mathbb{Z}^2)$
Recall that the convolution between two signals s_1 and s_2 over $\mathbb{Z}^2$ is a binary

operator in $\mathcal{S}(\mathbb{Z}^2)$ defined as:

$$\forall (a,b) \in \mathbb{Z}^2, (s_1 * s_2)[a,b] = \sum_i \sum_j s_1[i,j]\, s_2[a-i, b-j]$$

The next proposition can be seen as a discretization of a classic result in distribution theory.

Proposition 2.1.4. Characterization of convolution operators on $\mathcal{S}(\mathbb{Z}^2)$ On real-valued signals over $\mathbb{Z}^2$, the class of linear transformations that are equivariant to translations is exactly the class of convolutive operations *i.e.*

$$\exists w \in \mathcal{S}(\mathbb{Z}^2), f = . * w \Leftrightarrow \begin{cases} f \in \mathcal{L}(\mathcal{S}(\mathbb{Z}^2)) \\ \forall t \in \mathcal{T}(\mathcal{S}(\mathbb{Z}^2)), f \circ t = t \circ f \end{cases}$$

Proof. The result from left to right is a direct consequence of the definitions:

$$\begin{aligned}
&\forall s \in \mathcal{S}(\mathbb{Z}^2), \forall s' \in \mathcal{S}(\mathbb{Z}^2), \forall (\alpha,\beta) \in \mathbb{R}^2, \forall (a,b) \in \mathbb{Z}^2, \\
&\qquad f_w(\alpha s + \beta s')[a,b] = \sum_i \sum_j (\alpha s + \beta s')[i,j]\, w[a-i, b-j] \\
&\qquad\qquad = \alpha f_w(s)[a,b] + \beta f_w(s')[a,b] \qquad \text{(linearity)} \\
&\forall s \in \mathcal{S}(\mathbb{Z}^2), \forall (\alpha,\beta) \in \mathbb{Z}^2, \forall (a,b) \in \mathbb{Z}^2, \\
&\qquad f_w \circ t_{\alpha,\beta}(s)[a,b] = \sum_i \sum_j t_{\alpha,\beta}(s)[i,j]\, w[a-i, b-j] \\
&\qquad\qquad = \sum_i \sum_j s[i-\alpha, j-\beta]\, w[a-i, b-j] \\
&\qquad\qquad = \sum_{i'} \sum_{j'} s[i', j']\, w[a-i'-\alpha, b-j'-\beta] \qquad (2.1) \\
&\qquad\qquad = f_w(s)[a-\alpha, b-\beta] \\
&\qquad\qquad = t_{\alpha,\beta} \circ f_w(s)[a,b] \qquad \text{(equivariance)}
\end{aligned}$$

Now let's prove the result from right to left .

Let $f \in \mathcal{L}(\mathcal{S}(\mathbb{Z}^2))$, $s \in \mathcal{S}(\mathbb{Z}^2)$. We suppose that f commutes with translations. Recall that s can be linearly decomposed on the infinite family of dirac signals:

$$s = \sum_i \sum_j s[i,j]\,\delta_{i,j}, \text{ where } \delta_{i,j}[x,y] = \begin{cases} 1 & \text{if } (x,y) = (i,j) \\ 0 & \text{otherwise} \end{cases}$$

By linearity of f and then equivariance to translations:

$$\begin{aligned} f(s) &= \sum_i \sum_j s[i,j]\, f(\delta_{i,j}) \\ &= \sum_i \sum_j s[i,j]\, f \circ t_{i,j}(\delta_{0,0}) \\ &= \sum_i \sum_j s[i,j]\, t_{i,j} \circ f(\delta_{0,0}) \end{aligned}$$

By denoting $w = f(\delta_{0,0}) \in \mathcal{S}(\mathbb{Z}^2)$, we obtain:

$$\begin{aligned} \forall (a,b) \in \mathbb{Z}^2, f(s)[a,b] &= \sum_i \sum_j s[i,j]\, t_{i,j}(w)[a,b] \\ &= \sum_i \sum_j s[i,j]\, w[a-i, b-j] \\ \textit{i.e. } f(s) &= s * w \end{aligned} \tag{2.2}$$

□

Remark 2.1.5. **Equivariance property of CNNs**
In deep learning, an important argument in favor of CNNs is that convolutional layers are equivariant to translations. Intuitively, that means that a detail of an object in an image should produce the same features independently of its position in the image.

Remark 2.1.6. **Lossless superiority of CNNs over MLPs**
The converse result, as a consequence of Proposition 2.1.24, is never men-

tioned in deep learning literature. However it is also a strong one: it means that layers of CNNs have every translational equivariant functions in their search space, so it implies that the reduction of parameters from an MLP to a CNN is done with strictly no loss of expressivity (provided the objective function is know to bear this property). Besides, it helps the training to search in a much more confined space.

2.1.1.2 Construction on groups

As Proposition 2.1.24 is a complete characterization of convolutions, it can be used to define them *i.e.* convolutive operations can be constructed as the set of linear transformations that are equivariant to translations. However, in the general case where G is not a grid graph, translations are not defined, so that construction needs to be generalized beyond translational equivariances.
TODO: reword sentence below (not exactly true)
A classic result from group theory is that one sense of this characterization (equivariance) hold for groups of (bijective) transformations, where the group of translations is a particular case. More generally, it also holds for groupoids (Weinstein, 1996). The converse sense will be discussed later.
Note that our approach is different than in (Cohen et al., 2016b), where the authors define group-equivariant convolutions from an already defined one. On graphs, convolutions aren't already defined. We are studying group convolutions in view of constructing one.

Definition 2.1.7. Group convolution I
Let a group $\mathcal{G}$, the group convolution between two signals s_1 and $s_2 \in \mathcal{S}(\mathcal{G})$ is defined as:

$$\forall h \in \mathcal{G}, (s_1 * s_2)[h] = \sum_{g \in \mathcal{G}} s_1[g]\, s_2[g^{-1}h]$$

provided one of the signals has finite support if $\mathcal{G}$ is not finite.

For a graph $G = \langle V, E \rangle$ and a subgroup $\Gamma \subset \Phi^*(V)$, this definition is applicable for $\mathcal{S}(\Gamma)$, but not for $\mathcal{S}(V)$ as V is not a group.
Nonetheless, let's assume we can provide V with a group structure by exhibiting an isomorphism φ from Γ to V. Then, the linear morphism $\widetilde{\varphi}$ from $\mathcal{S}(\Gamma)$ to $\mathcal{S}(V)$ defined by $\widetilde{\varphi}(\delta_g) = \delta_{\varphi(g)}$ is also an isomorphism. Hence, V and $\mathcal{S}(V)$ would inherit the same inherent structural properties as Γ and $\mathcal{S}(\Gamma)$, in addition of being related in the same way. For notational simplicity, we will use the same symbol φ for φ and $\widetilde{\varphi}$ (as done between f and L_f). A Commutative diagram between the sets is depicted on Figure 2.1.

$$\begin{array}{ccc} \Gamma & \xrightarrow{\varphi} & V \\ {\scriptstyle s}\downarrow & & \downarrow{\scriptstyle s} \\ \mathcal{S}(\Gamma) & \xrightarrow[\varphi]{} & \mathcal{S}(V) \end{array}$$

Figure 2.1: Commutative diagram

Hence, we can steer the definition of the group convolution from $\mathcal{S}(\Gamma)$ to $\mathcal{S}(V)$ as follows:

Definition 2.1.8. Group convolution II
Let $\Gamma \subset \Phi^*(V)$ such that $V \cong \Gamma$ through an isomorphism $g_v \overset{\varphi}{\mapsto} v$. The group convolution between two signals s_1 and $s_2 \in \mathcal{S}(V)$ is defined as:

$$\begin{aligned} \forall u \in V, (s_1 * s_2)[u] &= \sum_{v \in V} s_1[v]\, s_2[\varphi(g_v^{-1} g_u)] \\ &= \sum_{\substack{(a,b) \in V^2 \\ s.t.\ \ g_a g_b = g_u}} s_1[a]\, s_2[b] \end{aligned}$$

Proposition 2.1.9. Equivariance to $\varphi(\Gamma)$
With Definition 2.1.8, convolution operators on $\mathcal{S}(V)$ are equivariant to $\varphi(\Gamma)$

i.e.

$$\exists w \in \mathcal{S}(V), f = . * w \Rightarrow \forall v \in V, f \circ \varphi(g_v) = \varphi(g_v) \circ f$$

Proof.

$$\begin{aligned}
&\forall s \in \mathcal{S}(V), \forall u \in V, \forall v \in V, \\
&\quad f_w \circ \varphi(g_u)(s)[v] = \sum_{\substack{(a,b) \in V^2 \\ s.t.\ g_a g_b = g_v}} \varphi(g_u)(s)[a]\, w[b] \\
&\qquad\qquad = \sum_{\substack{(a,b) \in V^2 \\ s.t.\ g_a g_b = g_v}} s[\varphi(g_u)^{-1}(a)]\, w[b] \\
&\qquad\qquad = \sum_{\substack{(a,b) \in V^2 \\ s.t.\ g_{\varphi(g_u)(a)} g_b = g_v}} s[a]\, w[b]
\end{aligned}$$

Because φ is an isomorphism, its inverse $c \mapsto g_c$ is also an isomorphism and so $g_{\varphi(g_u)(a)} g_b = g_v \Leftrightarrow g_a g_b = g_{\varphi(g_u)^{-1}(v)}$. So we have:

$$\begin{aligned}
f_w \circ \varphi(g_u)(s)[v] &= \sum_{\substack{(a,b) \in V^2 \\ s.t.\ g_a g_b = g_{\varphi(g_u)^{-1}(v)}}} s[a]\, w[b] \\
&= s * w[\varphi(g_u)^{-1}(v)] \\
&= g_u \circ f_w(s)[v]
\end{aligned}$$

□

In fact, both group convolutions are the same as the latter one borrows the algebraic structure of the first one, regardless of the fact that the group Γ contains bijective transformations of V. We can exploit this fact to obtain equivariance to Γ for both (instead of only to $\varphi(\Gamma)$ for the latter). By noticing

that $g \in \Gamma$ can act on both $\mathcal{S}(\Gamma)$ through the linear transformation of the left multiplication and on $\mathcal{S}(V)$ as being an object of $\Phi^*(V)$, we define:

Definition 2.1.10. Group convolution III
Let $\Gamma \subset \Phi^*(V)$ such that $V \cong \Gamma$ through an isomorphism $g_v \overset{\varphi}{\mapsto} v$ which verifies the property:

$$\forall v \in V, \forall u \in V, g_v(u) = \varphi(g_v g_u) \tag{P}$$

The group convolution between two signals s_1 and $s_2 \in \mathcal{S}(V)$ is defined as:

$$\begin{aligned} \forall u \in V, (s_1 * s_2)[u] &= \sum_{v \in V} s_1[v]\, s_2[\varphi(g_v^{-1} g_u)] \\ &= \sum_{v \in V} s_1[v]\, s_2[g_v^{-1}(u)] \\ i.e.\ s_1 * s_2 &= \sum_{v \in V} s_1[v]\, g_v(s_2) \\ &= \sum_{g \in \Gamma} s_1[\varphi(g)]\, g(s_2) \end{aligned}$$

Remark 2.1.11. For example, this property holds for translations as $t_{i,j}(a,b) = \varphi(t_{i,j} \circ t_{a,b})$ (with $\varphi(t_{i,j}) = (i,j)$).

Proposition 2.1.12. Equivariance to Γ
With Definition 2.1.10, convolution operators on $\mathcal{S}(V)$ are equivariant to Γ *i.e.*

$$\exists w \in \mathcal{S}(V), f = . * w \Rightarrow \forall v \in V, f \circ g_v = g_v \circ f$$

Proof. In the following equations, (2.3) is obtained because left multiplication in a group is an isomorphism, and (2.4) is obtained from the property of

Definition 2.1.10.

$$\begin{aligned}
&\forall g \in \Gamma, \forall s \in \mathcal{S}(V), \\
&\qquad f_w \circ g(s) = \sum_{h\in\Gamma} g(s)[\varphi(h)]\, h(w) \\
&\qquad\qquad = \sum_{h\in\Gamma} g(s)[\varphi(gh)]\, gh(w) \qquad (2.3) \\
&\qquad\qquad = \sum_{h\in\Gamma} g(s)[g(\varphi(h))]\, gh(w) \qquad (2.4) \\
&\qquad\qquad = \sum_{h\in\Gamma} s[\varphi(h)]\, gh(w) \\
&\forall g \in \Gamma, \forall s \in \mathcal{S}(V), \forall u \in V, \\
&\qquad f_w \circ g(s)[u] = \sum_{h\in\Gamma} s[\varphi(h)]\, h(w)[g^{-1}(u)] \\
&\qquad\qquad = f_w(s)[g^{-1}(u)] \\
&\qquad\qquad = g \circ f_w(s)[u]
\end{aligned}$$

□

At this point, there are a two drawbacks: (D1) that $V \cong \Gamma$, (D2) the converse of of the characterization don't hold. Let's now consider the edge set in our construction and keep these drawbacks in mind.

2.1.1.3 Construction on Cayley graphs

The property (P) naturally holds for Cayley (di)graphs.

Definition 2.1.13. Cayley graph
$a \sim c \Leftrightarrow \exists b \in \mathcal{U} \subset \Gamma, g_a g_b = g_c$, and the corresponding digraph $\vec{G}$

The convolution from Definition 2.1.10 is defined on Cayley graphs. We can alleviate (D1) by summing onto the generating set $\mathcal{U}$ instead of onto Γ, which makes the convolution edge-constrained.

Definition 2.1.14. Cayley graph convolution

$$\forall u \in V, (s_1 * s_2)[u] = \sum_{g \in \mathcal{U}} s_1[g]\, g(s_2)$$

TODO: operator and characterization
TODO: which graph is a Cayley graph ?

2.1.1.4 Mixed convolution

Draft:
Hypothesis: $w \in \mathcal{S}(\Gamma), s \in \mathcal{S}(V), w * s \in \mathcal{S}(V), V \ncong \Gamma$

$$\forall v \in V, (w * s)[u] = \sum_{g \in \Gamma} w[g]\, s[g^{-1}(u)]$$

Bastnet in here.

2.1.1.5 Construction on graph groupoids

TODO: work in progress

On graphs, we notice that the property (P) can be realized by transformations acting on edges. However, unless the graph is complete, these actions can't be composed everywhere to form another edge constrained action. The algebraic structure that posesses the same kind of properties than a group except that its composition law is not defined everywhere is called a groupoid. The following definitions clarify our discussion.

Definition 2.1.15. Groupoid
A groupoid is a set equiped with a closed partial composition law, a unique identity element, and every unique inverses.

Remark 2.1.16. We use the convention than left and right inverses must be the same.

Definition 2.1.17. Graph groupoid
The *groupoid* $\mathcal{P}(G)$ of a graph $G = \langle V, E \rangle$ is the set of its paths equiped with:

1. two maps ψ and φ that respectively map a path to its first and last element,

2. a closed partial composition law gh defined if and only if $\psi(g) = \varphi(h)$, which concatenates g behind h and ~~removes adjacent duplicate vertices~~ to rewrite,

3. an inverse operator $^{-1}$ which maps a path to its reverse,

4. an identity element Id which is the path of length 0.

Remark 2.1.18. Recall from Definition 1.3.3 that a path can't contain adjacent duplicates.

Remark 2.1.19. Note that even though the composite path gh has elements of h before those of g we write gh instead of hg because we'll need the left operand to act on the right one through functional notation $g(h)$.

Definition 2.1.20. Graph k-groupoid
The *k-groupoid* $\mathcal{P}_k(G)$ of a graph $G = \langle V, E \rangle$, for $k \in \mathbb{N}^*$, is the groupoid obtained by restricting $\mathcal{P}(G)$ to paths of length at most k (the definition domain of its composition law is also further restricted by the length of the resulting paths in $\mathcal{P}(G)$).

Definition 2.1.21. k-Groupoid convolution
Let a graph $G = \langle V, E \rangle$. Let a subgroupoid $\Gamma \subseteq \mathcal{P}_k(G)$. The k-groupoid

convolution between two signals s_1 and $s_2 \in \mathcal{S}(\Gamma)$ is defined as:

$$\begin{aligned}\forall h \in \Gamma, (s_1 * s_2)[h] &= \sum_{\substack{(a,b)\in\Gamma^2 \\ s.t.\ ab=h}} s_1[a]\, s_2[b] \\ &= \sum_{\substack{g\in\Gamma \\ s.t.\ \varphi(g)=\varphi(h)}} s_1[g]\, s_2[g^{-1}h] \\ &= \sum_{\substack{g\in\Gamma \\ s.t.\ \psi(g)=\psi(h)}} s_1[hg^{-1}]\, s_2[g]\end{aligned}$$

Claim 2.1.22. Path transformation
Let a graph $G = \langle V, E\rangle$. By identifying vertices with paths of length 1, a path $g \in \mathcal{P}(G)$ can act as a transformation on $v \in V$ through the composition law of $\mathcal{P}(G)$. Also note that $g(v) = g(v^{-1})$.

We can nom define the k-Groupoid convolution operator on $\mathcal{S}(G)$ by restriction of the second operand from $\mathcal{S}(\Gamma)$ to paths of length 1:

Definition 2.1.23. k-Groupoid convolution operator
Let a graph $G = \langle V, E\rangle$. Let a subgroupoid $\Gamma \subseteq \mathcal{P}_k(G)$. The k-groupoid convolution operator f_w with parameter $w \in \mathcal{S}(\Gamma)$ is defined as:

$$\forall s \in \mathcal{S}(\Gamma), \forall h \in \Gamma, f_w(s)[h] = (s * w)[h]$$

And when restricted to $\mathcal{S}(G)$ it is defined as:

$$\forall s \in \mathcal{S}(G), \forall v \in V, f_w(s)[v] = \sum_{\substack{g\in\Gamma \\ s.t.\ \psi(g)=v}} s[g(v)]\, w[g]$$

$$\forall s \in \mathcal{S}(G), \forall v \in V, f_w(s)[v] = \sum_{\substack{g\in\Gamma \\ s.t.\ \varphi(g)=v}} s[g]\, w[g^{-1}(v)]$$

Proposition 2.1.24. Groupoid equivariance to Γ
k-Groupoid convolution operators on $\mathcal{S}(G)$ are groupoid equivariant to Γ *i.e.*

$$\exists w \in \mathcal{S}(\Gamma), f = w * . \Rightarrow \forall v \in V, \forall g \in \Gamma s.t.\ \psi(g^{-1}) = v, f \circ g[v] = g \circ f[v]$$

$$g(h(v)) maybe false \tag{2.5}$$

Mini patron of todo:

- Equivariance to Γ holds, proof
- Converse of characterization does not hold yet, except on orbits
- property for it to hold
- relaxing one-to-one correspondence constraint but keeping other properties
- other avenue instead of property: should make use of edges to build a group structure
- ideal graph (lattice-regular)
- if group is too much then just groupoid structure from edges is enough

TODO: finish this section

2.1.2 To rename

Definition 2.1.25. Graph automorphisms
A graph automorphism of a graph $G = \langle V, E \rangle$ is a bijection in the vertex

domain $\phi : V \to V$ such that $\{u, v\} \in E \Leftrightarrow \{\phi(u), \phi(v)\} \in E$. We denote $\mathcal{A}(G)$ the group of automorphism on G.
We denote by $\mathcal{E}(\phi)$ the set of input-output mapping of ϕ, defined as $\mathcal{E}(\phi) = \{(x, y) \in V^2, \phi(x) = y\}$.
A graph automorphism ϕ is said to be *edge-constrained* (EC) if $\mathcal{E}(\phi) \subseteq E$. We denote $\mathcal{A}_{\text{EC}}(G)$ the set of edge-constrained automorphism on G.

Definition 2.1.26. Orthogonality
Two graph automorphisms ϕ_1 and ϕ_2 are said to be orthogonal, if and only if $\mathcal{E}(\phi_1) \cap \mathcal{E}(\phi_2) = \emptyset$, denoted $\phi_1 \perp \phi_2$. They are said to be aligned otherwise. Similarly, we define orthogonality of r automophisms as $\phi_1 \perp \cdots \perp \phi_r \Leftrightarrow \mathcal{E}(\phi_1) \cap \cdots \cap \mathcal{E}(\phi_r) = \emptyset$

2.1.3 Lattice-regular graph

Definition 2.1.27. Lattice-regular graph
A lattice-regular graph is a regular graph that admits r orthogonal edge-constrained automorphisms, where r is its degree.

Chapter 0

Trash bin and more drafts

... that we may use in some section.

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TODO: Rework 1.1

0.1 Naming conventions

0.1.1 Basic notions

Let's recall the naming conventions of basic notions.
A *function* $f : E \to F$ maps objects $x \in E$ to objects $y \in F$, as $y = f(x)$.
Its *definition domain* $\mathcal{D}_f = E$ is the set of objects onto which it is defined.
We will often just use the term *domain*.
We also say that f is *taking values* in its *codomain* F.
The *image per* f of the subset $U \subset E$, denoted $f(U)$, is $\{y \in F, \exists x \in E, y = f(x)\}$.
The *image of* f is the image of its domain. We denote $\mathcal{I}_f$.
A vector space E, which we will always assume to be finite-dimensional in our context, is defined as $\mathbb{R}^n$, and is equipped with pointwise addition and scalar multiplication.
A *signal* s is a function taking values in a vector space. In other words, a signal can also be seen as a *vector* with an *underlying structure*, where the vector is composed from its image, and the underlying structure is defined by its *domain*.

For example, images are signals defined on a set of pixels. Typically, an image s in RGB representation is a mapping from pixels p to a 3d vector space, as $s_p = (r, g, b)$.
TODO?: figure

0.1.2 Graphs and graph signals

TODO: more defs on grid graphs and other graphs

A *graph* $G = (V, E)$ is defined as a set of nodes V, and a set of edges $E \subseteq \binom{V}{2}$. The words *node* and *vertex* will be used equivalently, but we will rather use the first.

A *graph signal*, or *graph-structured signal* is a signal defined on the nodes of a graph, for which the underlying structure is the graph itself. A *node signal* is a signal defined on a node, in which case it is a *node embedding* in a vector space.

Although this is rarely seen, a signal can also be defined on the edges of a graph, or on an edge. We then coin it respectively *dual graph signal*, or *edge signal / edge embedding*.

Graph-structured data can refer to any of these type of signals.

0.1.3 Data and datasets

A dataset of signals is said to be *static* if all its signals share the same underlying structure, it is said to be *non-static* otherwise.
For image datasets, being non-static would mean that the dataset contains images of different sizes or different scales. For graph signal datasets, it would mean thats the underlying graph structures of the signals are different.

The point in specifying that objects of a dataset of a machine learning task are signals is that we can hope to leverage their underlying structure.

TODO: figure

0.2 Disambiguation of the subject

This thesis is entitled *Deep learning models for data without a regular structure*. So either the data of interest in this manuscript do not have any structure, or either their structure is not regular.

0.2.1 Irregularly structured data

By structured data, we mean that there exists an underlying structure over which the data is defined. This kind of data are usually modelized as signals defined over a domain. These domains are then composed of objects that are related together by some sort of structural properties. For example, pixels of images can be seen as located on a grid with integer spatial coordinates (a 2d cartesian grid graph).
It then come in handy to define the notions of structure and regularity with the help of graph signals.

Definition 0.2.1. Structure
Let $s : D \to F$ be a signal defined over a finite domain.
An *underlying structure* of the signal s is a graph G that has the domain of s for nodes.
A dataset is said to be *structured*, if its objects can be modelized as signals with an underlying structure.
It is said to be *static* if all its objects share the same underlying structure, and *non-static* otherwise.

In other words, we chose to define "structured data" as "graph-structured data" by some graph. Hence we need to specify for which graphs this structure would be said to be regular, and for which it would not.

Definition 0.2.2. Regularity
An underlying structure is said to be *regular*, if it is a regular grid graph. It is said to be *irregular* otherwise.
A dataset is said to be *regularly structured*, if the underlying structures of its objects are regular. It is said to be *irregularly structured* otherwise.

TODO: examples

0.2.2 Unstructured data

Data can also be unstructured. If the data is not yet embedded into a finite dimensional vector space, then we will be interested in embedding techniques used in representation learning. In the other case, it is often possible to fall back to the case of irregularly structured data. For example, vectors can be seen as signals defined over the canonical basis of the vector space, and the vectors of this basis can be related together by their covariances through the dataset. It is typical to use the graph structure that has the canonical basis for nodes, with edges obtained by covariance thresholding.
TODO: examples
What follows is a draft

0.3 Datasets

0.4 Tasks

0.5 Goals

0.6 Invariance

In order to be observed, invariances must be defined relatively to an observation. Let's give a formal definition to support our discussion.
...

0.7 Methods

0.8 Expressivity analysis of dense versus sparse connectivity

Let consider a tensor input x of a neural network layer l. Without loss of generality, we consider that x is a matrix of shape $n \times p$. Its rows are supposed structured by a graph $G =< V, E >$, with $|V| = n$, its columns are its feature maps.

In what follows, we discuss the expressivity and efficiency of a dense layer with x as input versus a layer that would leverage G. We start with the regular case and continue onto non-regular structures.

0.8.1 Strong regular case

In the strong regular case, G is a lattice graph such that a convolution is defined naturally on it. For example, this is the case where rows of x defines ticks of a time series, or flattened pixels of an image.

Let consider a convolutional layer $c = (g_c, h_c)$ with padding, defined by q filters of width k. Define y_c its output of shape $n \times q$.

We are interested in knowing if there exists a dense layer that can efficiently replicate c.

Its connectivity matrix W_c is of shape $npxnq$. Obviously, the function g_c can be replicated by a dummy dense layer $d = (g_c, h_d)$ through W_c. However, whereas c has only kpq weights, d has n^2pq. If we consider the families of neural networks $\mathcal{C}$, $\mathcal{D}$ spaned by their weights θ_c, θ_d, then we realize the $\mathcal{C}$ is less expressive, but in the same time it is more efficient at representing its functions.

Let's define the notion of partial expressivity with respect to a family of functions.

Let $\mathcal{F}$ a family of functions, $\mathcal{L}$ a family of layer functions, and ϵ the approximation coefficient. For $f \in \mathcal{F}$, define $S_\epsilon(\mathcal{L}, f) = \{l \in \mathcal{L}, d(l, f) < \epsilon\}$ and

$S_\epsilon(\mathcal{L}, \mathcal{F}) = \bigcup_{f \in \mathcal{F}} S_\epsilon(\mathcal{L}, f)$.
TODO: reword above

By abusing and anticipating future correction of this manuscript, we consider that $\mathcal{C}$ and $\mathcal{D}$ are vector spaces. We are interesting in 1. proving that $S_\epsilon(\mathcal{C}, \mathcal{F})$ and $S_\epsilon(\mathcal{D}, \mathcal{F})$ are also vector spaces, and 2. analysing for which $\mathcal{F}$, $\frac{dim(S_\epsilon(\mathcal{C},\mathcal{F}))}{dim(S_\epsilon(\mathcal{D},\mathcal{F}))}$ is maximized.
Obviously 1. is false, so 2. is ill-posed (this draft is to be reworded afterward). Instead of using dim, we should rather use $card$. However they are potentially infinite families so we should rather use a notion of volume, except if we discretize. So let's discretize.
By the way, ''modified'' 2. is trivially maximized for $\mathcal{F} = \mathcal{C}$ (and then the ratio equals 1), so let's weaken $\mathcal{F}$ and say it's any family with translation equivariance. We are then interested in proving that if $\mathcal{F}$ is the family on translation equivariant function (on this domains that has to be specified when rewriting this section), then $\frac{card(S_\epsilon(\mathcal{C},\mathcal{F}))}{card(S_\epsilon(\mathcal{D},\mathcal{F}))}$ is close to 1. Equivariant in our context means commuting with translations (we should rather use the latter expression btw).
The result might be obtained without discretizing as convolutions with padding commutes with translations. Let's guess that they are close to other commuters. In fact that is even it. Proof with Fourier analysis.

0.8.2 Draft

The only dense layer that replicate g_c is obtained through the connectivity matrix W_c. $\mathcal{D}$ is more expressive, however less efficient as we are looking for equivariant functions. It happens that equivariant functions are exactly convolutions with padding.

0.9 Conv drafts

TODO: point

In particular, we have

$$\begin{aligned}
\forall s \in \mathcal{S}(\Gamma), \widetilde{\varphi}(s) &= \widetilde{\varphi}\left(\sum_{g\in\Gamma} s[g]\delta_g\right) \\
&= \sum_{g\in\Gamma} s[g]\widetilde{\varphi}\left(\delta_g\right) \\
&= \sum_{g\in\Gamma} s[g]\delta_{\varphi(g)} \\
&= \sum_{v\in V} s[\varphi^{-1}(v)]\delta_v \\
\widetilde{\varphi}(s) &= \sum_{v\in V} \widetilde{\varphi}(s)[v]\delta_v
\end{aligned}$$

So $\widetilde{\varphi}(s)[v] = s[\varphi^{-1}(v)]$ and $\widetilde{\varphi}(s)[\varphi(g)] = s[g]$. Let's simplify the notations with $\widetilde{\varphi}(s) = t$ and $\varphi(g) = v$, *i.e.* $t[v] = s[g]$ as expected. We then define the group convolution on $\mathcal{S}(V)$ as

$$\begin{aligned}
(t_1 * t_2)[v] &= (s_1 * s_2)[g] \\
&= \sum_{h\in\mathcal{G}} s_1[h]\, s_2[h^{-1}g] \\
&= \sum_{u\in V} s_1[\varphi^{-1}(u)]\, h_u(s_2)[\varphi^{-1}(v)] \\
&= \sum_{u\in V} t_1[u]\, \widetilde{\varphi}(h_u(s_2))[v]
\end{aligned}$$

$$(t_1 * t_2)[v] = \sum_{u \in V} t_1[u]\, h_u(t_2)[v] \tag{1}$$

$$\tag{2}$$

TODO: stop sign

Recall that

$$\begin{aligned}\delta_g[h] &= \begin{cases} 1 & \text{if } h = g \Leftrightarrow \varphi(h) = \varphi(g) \\ 0 & \text{otherwise} \end{cases} \\ &= \delta_{\varphi(g)}[\varphi(h)]\end{aligned}$$

$$s = \sum_{v \in V} s[v]\, \delta_v$$

TODO: lemme on existence of uncountable linearly independent irrational family ?

Proposition 0.9.1. The group convolution on $\mathcal{S}(\Gamma)$ has a unique neutral element which is the dirac signal on the identity tranformation.

Proof. Denote δ a neutral element for the group convolution. Note as because of the commutativity the group convolution, a left neutral element is also a right neutral element. We have

$$s[h] = (\delta * s)[h] = \sum_{g \in \Gamma} \delta[g]\, s[g^{-1}h]$$

which is true for any real valued signal. By chosing a signal π having linearly

independant irrational entries (and using the axiom of choice in case G is not finite), we obtain that

$$\delta[g] = \begin{cases} 1 \text{ if } g = \mathrm{Id} \\ 0 \text{ otherwise} \end{cases} \quad i.e. \quad \delta = \delta_{\mathrm{Id}}$$

Conversely, $(\delta_{\mathrm{Id}} * s)[h] = 1.s[\mathrm{Id}^{-1}h] = s[h]$. □

In other therms, if there is an isomorphism between Γ and V, the group structure pass to V as well as the definition of the group convolution.

To alleviate this issue, let's introduce the neutral elements δ of the convolution, and the neutral element $\mathrm{Id} \in \Phi^*(V)$.

With the help of δ, we follow the same process as in the proof of Proposition 2.1.24, see (2.2), to construct the class of group convolutional operators which defines exactly the class of linear transformations that are equivariant to a certain group.

On graphs, this could be used provided we defined meaningful translations beforehand (see Section **??**). Another possibilty would be to search for invariances with respect to graph equivariances and derive a convolution operator similarly than for translations. This approach, which uses group convolutions (Weinstein, 1996), has already been discussed on regular domain to extend CNNs to other invariances than translational ones (Cohen et al., 2016b; Hoogeboom et al., 2018), as well as on spherical domain with rotation equivariant CNNs (Cohen et al., 2018b). As stated from the previous remark, the big advantage of this approach is that there is no loss of expressivity. However on graphs, this would be more challenging as it's not likely there exists transformations with equivariances. However, let's suppose we found such a set of transformations on a graph, then for Proposition 2.1.24 to hold (instead as for regular translations), we see in the proof that they need to be bijective (2.1) and vertex dependent 2.2.

0.9.1

Definition 0.9.2. Grounded set of transformations
A set of transformations over a graph $G = \langle V, E \rangle$, *grounded* on a vertex $v_0 \in V$, denoted $\mathcal{P}_{v_0} \subset \Phi(V)$, is a set that is in one-to-one correspondence with V, such that $\forall v \in V, \exists! p_v \in \mathcal{P}_{v_0}, p_v(v_0) = v$.

We have $\mathcal{P}_{v_0} = \text{order}(G) \in \mathbb{N} \cup \{+\infty\}$. For notational convenience we drop the subscript $_{v_0}$ in what follows.

Definition 0.9.3. $\mathcal{P}$-equivariant convolution operator
Let $G = \langle V, E \rangle$ a graph, not necessarily a grid. Let $\mathcal{P}$ a grounded set of transformations. Then, the $\mathcal{P}$-equivariant convolution operator f_w is defined as

$$\forall s \in \mathcal{S}(V), f_w(s) = s *_{\mathcal{P}} w = \sum_v s[v]\, p_v(w)$$

Claim 0.9.4. Characterization of $\mathcal{P}$-eq. convolution operator
The class of linear graph signal transformations that are equivariant to a grounded set $\mathcal{P}$ is exactly the class of $\mathcal{P}$-equivariant convolutive operations.

Proof. By construction of $\mathcal{P}$-equivariant convolutions, the proof is similar to the one of Proposition 2.1.24. □

Index terms— Deep learning, representation learning, propagation learning, visualization, structured, unstructured regular, irregular, covariant, invariant, equivariant, tensor, scheme, weight sharing, graphs, manifold, euclidean, signal processing, graph signal processing, time series, time series database, distributed application, spatial-time series, geo time series, industrial applications, warp 10, warpscript, ...

Temptative titles

- Learning propagational representations of irregular and unstructured data
- Learning representations of unstructured or irregularly structured datasets
- Propagational learning of unstructured or irregularly structured datasets
- Learning tensorial representation of irregular and unstructured data
- Tensorial representation of propagation in deep learning for irregular and unstructured dataset
- Structural representation learning for irregular or unstructured data
- Word for both "irregularly structured" + "unstructured" = ? (maybe "unorthodox" ?)
- Unorthdox deep learning

- ...
- Deep learning of unstructured or irregularly structured datasets
- Deep learning models for data without a regular structure
- On structures in deep learning
- On deep learning for when data is lacking a regular structure
- Deep learning for non regularly structured data

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