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Chapter 3
Application to neural networks on graph domains

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Introduction

TODO:

3.0.1 Graph structures of neural layers

Recall our notations. Let $\mathcal{L} = (g, h)$ a neural network layer, where $g : I \to O$ is its linear part, $h : O \to O$ is its activation function, I and O are its input and output spaces, which are tensor spaces. Recall from Definition **??**, that a tensor space has been defined such that its canonical basis is a cartesian product of canonical bases of vector spaces. Let $I = \bigotimes_{k=1}^{p} \mathbb{V}_k$ and $O = \bigotimes_{l=1}^{q} \mathbb{U}_l$. Their canonical bases are denoted $\mathbb{v}_k = (\mathbb{v}_k^1, \dots, \mathbb{v}_k^{n_k})$ and $\mathbb{u}_l = (\mathbb{u}_l^1, \dots, \mathbb{u}_l^{n_l})$.

Definition 1. Topoloical space and layer
We call *topological space* a set of points with their corresponding neighborhoods (which are sets belonging to a class of sets that is closed under intersection), and we call *topological layer*, a layer $\mathcal{L}$ such that some $\mathbb{v}_k$ and some $\mathbb{u}_l$ are topological spaces.

Hence, any layer is in fact a topological layer, which is characterized by a propagation graph, as depicted on Figure 3.1.

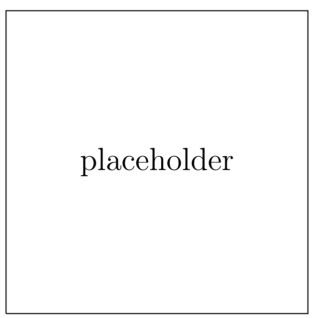

Figure 3.1: A propagation graph

Lemma 2. Propagation graph
Let a layer (g, h) with connectivity matrix W of shape $n \times m$. The connectivity matrix W defines a topological layer such that

1. $\mathcal{T}_O = (\mathcal{B}_O, \mathcal{N}_O)$, where $\mathcal{N}_O = \{\mathcal{N}_j = \{e_i^I, W[i,j] \neq 0\}, j \in \{1, 2, \dots, n\}\}$

2. $\mathcal{T}_I = (\mathcal{B}_I, \mathcal{N}_I)$, where $\mathcal{N}_I = \{\mathcal{N}_i = \{e^O_j, W[i,j] \neq 0\}, i \in \{1, 2, \dots, m\}\}$

We define the *propagation graph* $P = \langle \mathcal{B}^I, \mathcal{B}^O, E \rangle$ as the weighted bipartite graph characterized by W as its adjacency matrix. Then P also characterizes the topological spaces $\mathcal{T}_0$ and $\mathcal{T}_I$.

In the general case of partially connected layer, the latent canonical bases $\mathcal{B}_I$ and $\mathcal{B}_O$ are not the same. However, forthe example of convolutional layers, we can adopt an isomorphic point of view $O \cong I$, as we can obtain $\mathcal{T}_O \cong \mathcal{T}_I$ (if necessary with padding, and by setting the neighborhoods of the pads to $\emptyset$). Therefore, we can define the underlying graph structure as follows.

Definition 3. Underlying graph structure
Let a topological layer (g, h) such that $I = \mathcal{S}(\mathcal{B}_I) \cong O = \mathcal{S}(\mathcal{B}_O))$. By identifying their signal domains $V := \mathcal{B}_I \cong \mathcal{B}_O$, we define the *underlying graph structure* $G = \langle V, E \rangle$, such that $i \sim j \Leftrightarrow e^I_i \in \mathcal{N}_j$.

That is, when a convolution is defined over a graph like in the previous chapter (todo:insert ref here), its underlying graph structure is obviously a subgraph of the graph itself. Nonetheless, this definition also implies that every topological layer where $I \cong O$ is underpinned by a convolution on an underlying graph structure.
For instance:

- The underlying graph structure of classical 2d convolutions is a lattice graph. They can be redefined equivalently as a Cayley convolution on this lattice graph.

- The underlying graph structure of a dense layer is a complete graph. The matrix multiplication can be redefined equivalently as a partial convolution without φ-equivalence (*i.e.* with no equivariance characterization).

Figure **??** depicts a underlying graph strucuture basing a convolution, and the corresponding propagation graph.

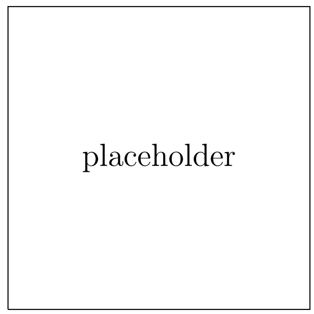

Figure 3.2: Underlying graph Vs Prop graph