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Chapter 2

Convolutions on graph domains

Introduction

Defining a convolution of signals over graph domains is a challenging problem. Obviously, if the graph is not a grid graph there exists no natural definition. We first analyze the reasons why the euclidean convolution operator is useful in deep learning, and give a characterization. Then we will search for domains onto which a convolution with these properties can be naturally obtained. This will lead us to put our interest on representation theory and convolutions defined on groups. As the euclidean convolution is just a particular case of the group convolution, it makes perfect sense to steer our construction in this direction. Hence, we will aim at transferring its representation on the vertex domain. First we will do this construction agnostically of the edge set. Then, we will introduce the role of the edge set and see how it should influence it. This will provide us with some particular classes of graphs for which we will obtain a natural construction with the wanted characteristics that we exposed in the first place. Finally, we can relax some aspect of the construction to adapt it to graphs that are not order-regular. The obtained construction is a set of general expressions that describes convolutions on graph domains, which preserve some key properties.

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2.1 Analysis of the classical convolution

In this section, 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.

2.1.1 Properties of the convolution

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 1. Convolution on $\mathcal{S}(\mathbb{Z}^2)$
Recall that the (discrete) convolution between two signals s_1 and s_2 over $\mathbb{Z}^2$ is a binary operation in $\mathcal{S}(\mathbb{Z}^2)$ defined as:

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

Definition 2. Convolution operator
A *convolution operator* is a function of the form $f_w : x \mapsto x * w$, where x and w are signals of domains for which the convolution $*$ is defined. When $*$ is not commutative, we differentiate the *right-action* operator $x \mapsto x * w$ from the *left-action* one $x \mapsto w * x$.

The following properties of the convolution on $\mathbb{Z}^2$ are of particular interest for our study.

Linearity

Operators produced by the convolution are linear. So they can be used as linear parts of layers of neural networks.

Locality and weight sharing

When w is compactly supported on K, an impulse response $f_w(x)[a,b]$ amounts to a w-weighted aggregation of entries of x in a neighbourhood of (a,b), called the *local receptive field*.

Commutativity

The convolution is commutative. However, it won't necessarily be the case on other domains.

Equivariance to translations

Convolution operators are equivariant to translations. Below, we show that the converse of this result also holds with Proposition 6.

2.1.2 Characterization on grid graphs

Let's recall first what is a transformation, and how it acts on signals.

Definition 3. 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 particular, $\Phi^*(V)$ forms the symmetric group of V and can move signals of $\mathcal{S}(V)$ by linear extension of its group action.

Lemma 4. Extension to $\mathcal{S}(V)$ by group action
A bijective transformation $f \in \Phi^*(V)$ can be extended linearly to the signal space $\mathcal{S}(V)$, and we have:

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

Proof. Let $s \in \mathcal{S}(V), f \in \Phi^*(V), L_f \in \mathcal{L}(\mathcal{S}(V))$ *s.t.* $\forall v \in V, L_f(\delta_v) = \delta_{f(v)}$. Then, we have:

$$\begin{aligned} L_f(s) &= \sum_{v \in V} s[v]\, L_f(\delta_v) \\ &= \sum_{v \in V} s[v]\, \delta_{f(v)} \\ \text{So, } \forall v \in V, L_f(s)[v] &= s[f^{-1}(v)] \end{aligned}$$

□

We also recall the formalism of translations.

Definition 5. 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.

The next proposition fully characterizes convolution operators with their translational equivariance property. This can be seen as a discretization of a classic result from the theory of distributions (Schwartz, 1957).

Proposition 6. 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:

$$
\begin{aligned}
&\forall s \in \mathcal{S}(\mathbb{Z}^2), \forall s' \in \mathcal{S}(\mathbb{Z}^2), \forall (\alpha, \beta) \in \mathbb{R}^2, \forall (a,b) \in \mathbb{Z}^2,\\
&\qquad f_w(\alpha s + \beta s')[a,b] = \sum_i \sum_j (\alpha s + \beta s')[i,j]\, w[a-i, b-j]\\
&\qquad\qquad = \alpha f_w(s)[a,b] + \beta f_w(s')[a,b] \qquad \text{(linearity)}\\
&\forall s \in \mathcal{S}(\mathbb{Z}^2), \forall (\alpha, \beta) \in \mathbb{Z}^2, \forall (a,b) \in \mathbb{Z}^2,\\
&\qquad f_w \circ t_{\alpha,\beta}(s)[a,b] = \sum_i \sum_j t_{\alpha,\beta}(s)[i,j]\, w[a-i, b-j]\\
&\qquad\qquad = \sum_i \sum_j s[i-\alpha, j-\beta]\, w[a-i, b-j]\\
&\qquad\qquad = \sum_{i'} \sum_{j'} s[i', j']\, w[a-i'-\alpha, b-j'-\beta] \qquad (1)\\
&\qquad\qquad = f_w(s)[a-\alpha, b-\beta]\\
&\qquad\qquad = t_{\alpha,\beta} \circ f_w(s)[a,b] \qquad \text{(equivariance)}
\end{aligned}
$$

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:

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

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

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

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

□

2.1.3 Usefulness of convolutions in deep learning

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.

Lossless superiority of CNNs over MLPs

The converse result, as a consequence of Proposition 6, is never mentioned in deep learning literature. However it is also a strong one. For example, let's consider a linear function that is equivariant to translations. Thanks to the converse result, we know that this function is a convolution operator parameterized by a weight vector w, $f_w : . * w$. If the domain is compactly supported, as in the case of images, we can break down the information of w in a finite number n_q of kernels w_q with small compact supports of same size (for instance of size 2×2), such that we have $f_w = \sum_{q \in \{1,2,\dots,n_q\}} f_{w_q}$. The convolution operators f_{w_q} are all in the search space of 2×2 convolutional layers. In other words, every translational equivariant linear function can have its information parameterized by these layers. So that means that the reduction of parameters from an MLP to a CNN is done with strictly no loss of expressivity (provided the objective function is known to bear this property). Besides, it also helps the training to search in a much more confined space.

Methodology for extending to general graphs

Hence, in our construction, we will try to preserve the characterization from Proposition 6 as it is mostly the reason why they are successful in deep learning. Note that the reduction of parameters compared to a dense layer is also a consequence of this characterization.

2.2 Construction from the vertex set

As Proposition 6 is a complete characterization of convolutions, it can be used to define them *i.e.* convolution operators 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. In mathematics, convolutions are more generally defined for signals defined over a group structure. The classical convolution that is used in deep learning is just a narrow case where the domain group is an euclidean space. Therefore, constructing a convolution on graphs should start from the more general definition of convolution on groups rather than convolution on euclidean domains.

Our construction is motivated by the following questions:

- Does the equivariance property holds ? Does the characterization from Proposition 6 still holds ?
- Is it possible to extend the construction on non-group domains, or at least on mixed domains ? (*i.e.* one signal is defined over a set, and the other is defined over a subgroup of the transformations of this set).
- Can a group domain draw an underlying graph structure ? Is the group convolution naturally defined on this class of graphs ?

We first recall the notion of group and group convolution.

Definition 7. Group
A group Γ is a set equipped with a closed, associative and invertible composition law that admits a unique left-right identity element.

The group convolution extends the notion of the classical discrete convolution.

Definition 8. Group convolution I
Let a group Γ, the group convolution I between two signals s_1 and $s_2 \in \mathcal{S}(\Gamma)$ is defined as:

$$\forall h \in \Gamma, (s_1 *_{\mathrm{I}} s_2)[h] = \sum_{g \in \Gamma} s_1[g]\, s_2[g^{-1}h]$$

provided at least one of the signals has finite support if Γ is not finite.

2.2.1 Steered construction from groups

For a graph $G = \langle V, E \rangle$ and a subgroup $\Gamma \subset \Phi^*(V)$ or its invertible transformations, Definition 8 is applicable for $\mathcal{S}(\Gamma)$, but not for $\mathcal{S}(V)$ as V is not a group. Nonetheless, our point here is that we will use the group convolution on $\mathcal{S}(\Gamma)$ to construct the convolutions on $\mathcal{S}(V)$.
For now, let's assume Γ is in one-to-one correspondence with V, and let's define a bijective map φ from Γ to V. We denote $\Gamma \overset{\varphi}{\cong} V$ and $g_v \overset{\varphi}{\mapsto} v$.
Then, the linear morphism $\widetilde{\varphi}$ from $\mathcal{S}(\Gamma)$ to $\mathcal{S}(V)$ defined on the Dirac bases by $\widetilde{\varphi}(\delta_g) = \delta_{\varphi(g)}$ is a linear isomorphism. Hence, $\mathcal{S}(V)$ would inherit the same inherent structural properties as $\mathcal{S}(\Gamma)$. For the sake of notational simplicity, we will use the same symbol φ for both φ and $\widetilde{\varphi}$ (as done between f and L_f). A commutative diagram between the sets is depicted on Figure 2.1.

$$\begin{tikzcd}
\Gamma \arrow[r, "\varphi"] \arrow[d, "\mathcal{S}"'] & V \arrow[d, "\mathcal{S}"] \\
\mathcal{S}(\Gamma) \arrow[r, "\varphi"'] & \mathcal{S}(V)
\end{tikzcd}$$

Figure 2.1: Commutative diagram between sets

We naturally obtain the following relation, which put in simpler words means that signals on $\mathcal{S}(\Gamma)$ are mapped to $\mathcal{S}(V)$ when φ is simultaneously applied on both the signal space and its domain.

Lemma 9. Relation between $\mathcal{S}(\Gamma)$ and $\mathcal{S}(V)$
$\forall s \in \mathcal{S}(\Gamma), \forall u \in V, \varphi(s)[u] = s[\varphi^{-1}(u)] = s[g_u]$

Proof.

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

So $\forall v \in V, \varphi(s)[u] = s[g_u]$

□

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

Definition 10. Group convolution II
Let a subgroup $\Gamma \subset \Phi^*(V)$ such that $\Gamma \overset{\varphi}{\cong} V$. The group convolution II between two signals s_1 and $s_2 \in \mathcal{S}(V)$ is defined as:

$$\forall u \in V, (s_1 *_{\text{II}} s_2)[u] = \sum_{v \in V} s_1[v]\, s_2[\varphi(g_v^{-1} g_u)]$$

Lemma 11. Relation between group convolution I and II
Let a subgroup $\Gamma \subset \Phi^*(V)$ such that $\Gamma \overset{\varphi}{\cong} V$,

$$\forall s_1, s_2 \in \mathcal{S}(\Gamma), \forall u \in V, (\varphi(s_1) *_{\text{II}} \varphi(s_2))[u] = (s_1 *_{\text{I}} s_2)[g_u]$$

Proof. Using Lemma 9,

$$\begin{aligned}(\varphi(s_1) *_{\text{II}} \varphi(s_2))[u] &= \sum_{v \in V} \varphi(s_1)[v]\, \varphi(s_2)[\varphi(g_v^{-1} g_u)] \\ &= \sum_{v \in V} s_1[g_v]\, s_2[g_v^{-1} g_u] \\ &= \sum_{g \in \Gamma} s_1[g]\, s_2[g^{-1} g_u] \\ &= (s_1 *_{\text{I}} s_2)[g_u]\end{aligned}$$

□

For convolution II, we only obtain a weak version of Proposition 6.

Proposition 12. Equivariance to $\varphi(\Gamma)$
If φ is a homomorphism, convolution operators acting on the right of $\mathcal{S}(V)$ are equivariant to $\varphi(\Gamma)$ *i.e.*

$$\begin{aligned}&\text{if } \varphi \in \text{ISO}(\Gamma, V), \\ &\exists w \in \mathcal{S}(V), f = .\, *_{\text{II}}\, w \Rightarrow \forall v \in V, f \circ \varphi(g_v) = \varphi(g_v) \circ f\end{aligned}$$

Proof.

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

$$= \sum_{\substack{(a,b)\in V^2 \\ s.t.\ g_{\varphi(g_u)(a)}g_b = g_v}} s[a]\, w[b]$$

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 both:

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

$\square$

Remark. Note that convolution operators of the form $f_w = . *_{\mathrm{I}} w$ are also equivariant to Γ, but the proposition and the proof are omitted as they are similar to the latter.

In fact, both group convolutions are the same as the latter one borrows the algebraic structure of the first one. Thus we only obtain equivariance to $\varphi(\Gamma)$ when φ also transfer the group structure from Γ to V, and the converse does not hold. To obtain equivariance to Γ (and its converse), we will drop the direct homomorphism condition, and instead we will take into account the fact that it contains invertible transformations of V.

2.2.2 Construction under group actions

Definition 13. Group action

An *action* of a group Γ on a set V is a function $L : \Gamma \times V \to V, (g, v) \mapsto L_g(v)$, such that the map $g \mapsto L_g$ is a homomorphism.

Given $g \in \Gamma$, the transformation L_g is called the action of g by L on V.

Remark. When there is no ambiguity, we use the same symbol for g and L_g. Hence, note that $g \in \Gamma$ can act on both Γ through the left multiplication and on V as being an object of $\Phi^*(V)$. This ambivalence can be seen on a commutative diagram, see Figure 2.2.

$$\begin{tikzcd}
g_u \arrow[r, "g_v"] \arrow[d, "\varphi"'] & g_v g_u \arrow[d, "\varphi"] \\
u \arrow[r, "(P)", "g_v"'] & \varphi(g_v g_u)
\end{tikzcd}$$

Figure 2.2: Commutative diagram. All arrows except for the one labeled with (P) are always True.

For (P) to be true means that φ is an equivariant map *i.e.* whether the mapping is done before or after the action of Γ has no impact on the result. When such φ exists, Γ and V are said to be equivalent and we denote $\Gamma \equiv V$.

Definition 14. Equivariant map

A map φ from a group Γ acting on the destination set V is said to be an *equivariant map* if

$$\forall g, h \in \Gamma, g(\varphi(h)) = \varphi(gh)$$

In our case we have $\Gamma \overset{\varphi}{\cong} V$. If we also have that $\Gamma \equiv V$, we are interested to know if then φ exhibits the equivalence.

Definition 15. φ-Equivalence
A subgroup $\Gamma \subset \Phi^*(V)$ such that $\Gamma \overset{\varphi}{\cong} V$, is said to be *$\varphi$-equivalent* if φ is a bijective equivariant map *i.e.* if it verifies the property:

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

In that case we denote $\Gamma \overset{\varphi}{\equiv} V$.

Remark. For example, translations on the grid graph, with $\varphi(t_{i,j}) = (i, j)$, are φ-equivalent as $t_{i,j}(a, b) = \varphi(t_{i,j} \circ t_{a,b})$. However, with $\varphi(t_{i,j}) = (-i, -j)$, they would not be φ-equivalent.

Definition 16. Group convolution III
Let a subgroup $\Gamma \subset \Phi^*(V)$ such that $\Gamma \overset{\varphi}{\cong} V$. The group convolution III between two signals s_1 and $s_2 \in \mathcal{S}(V)$ is defined as:

$$s_1 *_{\text{III}} s_2 = \sum_{v \in V} s_1[v]\, g_v(s_2) \tag{3}$$
$$= \sum_{g \in \Gamma} s_1[\varphi(g)]\, g(s_2) \tag{4}$$

The two expressions differ on the domain upon which the summation is done. The expression (3) put the emphasis on each vertex and its action, whereas the expression (4) emphasizes on each object of Γ.

Lemma 17. Relation with group convolution II
$\Gamma \overset{\varphi}{\equiv} V \Leftrightarrow *_{\text{II}} = *_{\text{III}}$

Proof.

$$\forall s_1, s_2 \in \mathcal{S}(V),$$
$$s_1 *_{\text{II}} s_2 = s_1 *_{\text{III}} s_2$$
$$\Leftrightarrow \forall u \in V, \sum_{v \in V} s_1[v]\, s_2[\varphi(g_v^{-1} g_u)] = \sum_{v \in V} s_1[v]\, s_2[g_v^{-1}(u)] \tag{5}$$

Hence, the direct sense is obtained by applying (P).

For the converse, given $u, v \in V$, we first realize (5) for $s_1 := \delta_v$, obtaining $s_2[\varphi(g_v^{-1} g_u)] = s_2[g_v^{-1}(u)]$, which we then realize for a real signal s_2 having no two equal entries, obtaining $\varphi(g_v^{-1} g_u) = g_v^{-1}(u)$. From the latter we finally obtain (P) with the one-to-one correspondence $g_{v'} := g_v^{-1}$. □

We can then coin the term φ-convolution.

Definition 18. φ-convolution

Let $\Gamma \overset{\varphi}{\equiv} V$, the *$\varphi$-convolution* between two signals s_1 and $s_2 \in \mathcal{S}(V)$ is defined as:

$$s_1 *_\varphi s_2 = s_1 *_{\text{II}} s_2 = s_1 *_{\text{III}} s_2$$

This time, we do obtain equivariance to Γ as expected, and the full characterization as well.

Proposition 19. Characterization by right-action equivariance to Γ

If Γ is φ-equivalent, the class of linear transformations of $\mathcal{S}(V)$ that are equivariant to Γ is exactly the class of φ-convolution operators acting on the right of $\mathcal{S}(V)$ *i.e.*

$$\begin{aligned} &\text{If } \Gamma \overset{\varphi}{\equiv} V, \\ &\exists w \in \mathcal{S}(V), f = \,.\, *_\varphi w \Leftrightarrow \begin{cases} f \in \mathcal{L}(\mathcal{S}(V)) \\ \forall g \in \Gamma, f \circ g = g \circ f \end{cases} \end{aligned}$$

Proof. 1. From left to right:

In the following equations, (6) is obtained by definition, (7) is obtained because left multiplication in a group is bijective, and (8) is obtained because of (P).

$$\begin{aligned}
&\forall g \in \Gamma, \forall s \in \mathcal{S}(V), \\
&\qquad f_w \circ g(s) = \sum_{h\in\Gamma} g(s)[\varphi(h)]\, h(w) && (6)\\
&\qquad = \sum_{h\in\Gamma} g(s)[\varphi(gh)]\, gh(w) && (7)\\
&\qquad = \sum_{h\in\Gamma} g(s)[g(\varphi(h))]\, gh(w) && (8)\\
&\qquad = \sum_{h\in\Gamma} s[\varphi(h)]\, gh(w)\\
&\qquad = \sum_{h\in\Gamma} s[\varphi(h)]\, h(w)[g^{-1}(.)]\\
&\qquad = f_w(s)[g^{-1}(.)]\\
&\qquad = g \circ f_w(s)
\end{aligned}$$

Of course, we also have that f_w is linear.

2. From right to left:
Let $f \in \mathcal{L}(\mathcal{S}(V)), s \in \mathcal{S}(V)$. By linearity of f, we distribute $f(s)$ on the family of dirac signals:

$$f(s) = \sum_{v\in V} s[v] f(\delta_v) \tag{9}$$

Thanks to (P), we have that:

$$\begin{aligned}
&g_v(\varphi(\mathrm{Id})) = \varphi(g_v\,\mathrm{Id}) = v\\
&\text{So, } v = u \Leftrightarrow \varphi(\mathrm{Id}) = g_v^{-1}(u)\\
&\text{So, } \delta_v = g_v(\delta_{\varphi(\mathrm{Id})})
\end{aligned}$$

By denoting $w = f(\delta_{\varphi(\mathrm{Id})})$, and using the hypothesis of equivariance, we obtain from (9) that:

$$\begin{aligned} f(s) &= \sum_{v\in V} s[v]\, f \circ g_v(\delta_{\varphi(\mathrm{Id})}) \\ &= \sum_{v\in V} s[v]\, g_v \circ f(\delta_{\varphi(\mathrm{Id})}) \\ &= \sum_{v\in V} s[v]\, g_v(w) \\ &= s *_\varphi w \end{aligned}$$

$\square$

Construction of φ-convolutions on vertex domains

Proposition 19 tells us that in order to define a convolution on the vertex domain of a graph $G = \langle V, E\rangle$, all we need is a subgroup Γ of invertible transformations of V, that is equivalent to V. The choice of Γ can be done with respect to E. This is discussed in more details in Section 2.3, where we will see that in fact, we only need a generating set of Γ.

Exposure of φ

This construction relies on exposing a bijective equivariant map φ between Γ and V. In the next subsection, we show that in cases where Γ is abelian, we even need not expose φ and the characterization still holds.

2.2.3 Mixed domain formulation

From (4), we can define a mixed domain convolution *i.e.* that is defined for $r \in \mathcal{S}(\Gamma)$ and $s \in \mathcal{S}(V)$, without the need of expliciting φ.

Definition 20. Mixed domain convolution
Let a subgroup $\Gamma \subset \Phi^*(V)$ such that $V \cong \Gamma$. The *mixed domain convolution* between two signals $r \in \mathcal{S}(\Gamma)$ and $s \in \mathcal{S}(V)$ results in a signal $r *_{\text{M}} s \in \mathcal{S}(V)$ and is defined as:

$$r *_{\text{M}} s = \sum_{g \in \Gamma} r[g]\, g(s)$$

We coin it M-convolution. From a practical point of view, this expression of the convolution is useful because it relegates φ as an underpinning object.

Lemma 21. Relation with group convolution III
$\forall \varphi \in \text{BIJ}(\Gamma, V), \forall (r, s) \in \mathcal{S}(\Gamma) \times \mathcal{S}(V)$,

$$r *_{\text{M}} s = \varphi(r) *_{\text{III}} s$$

Proof. Let $\varphi \in \text{BIJ}(\Gamma, V), (r, s) \in \mathcal{S}(\Gamma) \times \mathcal{S}(V)$,

$$\begin{aligned} r *_{\text{M}} s &= \sum_{g \in \Gamma} r[g]\, g(s) = \sum_{v \in V} r[g_v]\, g_v(s) \overset{(\diamond)}{=} \sum_{v \in V} \varphi(r)[v]\, g_v(s) \\ &= \varphi(r) *_{\text{III}} s \end{aligned}$$

Where $\overset{(\diamond)}{=}$ comes from Lemma 9. □

In other words, $*_{\text{M}}$ is a convenient reformulation of $*_{\text{III}}$ which does not depend on a particular φ.

Lemma 22. Relation with group convolution I, II and φ-convolution
Let $\varphi \in \text{BIJ}(\Gamma, V), (r, s) \in \mathcal{S}(\Gamma) \times \mathcal{S}(V)$, we have:

$$\begin{aligned} \Gamma \overset{\varphi}{\equiv} V &\Leftrightarrow \forall v \in V, (r *_{\text{M}} s)[v] = (r *_{\text{I}} \varphi^{-1}(s))[g_v] \\ &\Leftrightarrow r *_{\text{M}} s = \varphi(r) *_{\text{II}} s \\ &\Leftrightarrow r *_{\text{M}} s = \varphi(r) *_{\varphi} s \end{aligned}$$

Proof. On one hand, Lemma 21 gives $r *_{\text{M}} s = \varphi(r) *_{\text{III}} s$. On the other hand, Lemma 11 gives $\forall v \in V, (r *_{\text{I}} \varphi^{-1}(s))[g_v] = (\varphi(r) *_{\text{II}} s)[v]$. Then Lemma 17 concludes. □

Remark. The converse sense is meaningful because it justifies that when the M-convolution is employed, the property $\Gamma \equiv V$ underlies, without the need of expliciting φ.

From M-convolution, we can derive operators acting on the left of $\mathcal{S}(V)$, of the form $s \mapsto w *_{\text{M}} s$, parameterized by $w \in \mathcal{S}(\Gamma)$. In particular, these operators would be relevant as layers of neural networks. On the contrary, derived operators acting on the right such as $r \mapsto r *_{\text{M}} w$ wouldn't make sense with this formulation as they would make φ resurface. However, the equivariance to Γ incurring from Lemma 21 and Proposition 19 only holds for operators acting on the right. So we need to intertwine an abelian condition as follows. This is also a good excuse to see the influence of abelianity.

Proposition 23. Equivariance to Γ through left action
Let a subgroup $\Gamma \subset \Phi^*(V)$ such that $\Gamma \cong V$. Γ is abelian, if and only if, M-convolution operators acting on the left of $\mathcal{S}(V)$ are equivariant to it *i.e.*

$$\forall g, h \in \Gamma, gh = hg \Leftrightarrow \forall w, g \in \Gamma, w *_{\text{M}} g(.) = g \circ (w *_{\text{M}} .)$$

Proof. Let $w, g \in \Gamma$, and define $f_w : s \mapsto w *_{\text{M}} s$. In the following expressions, Γ is abelian if and only if (10) and (11) are equal (the converse is obtained by particularizing on well chosen signals):

$$\begin{aligned} f_w \circ g(s) &= \sum_{h \in \Gamma} w[h]\, hg(s) && (10) \\ &= \sum_{h \in \Gamma} w[h]\, gh(s) && (11) \\ &= \sum_{h \in \Gamma} w[h]\, h(s)[g^{-1}(.)] \\ &= (w *_{\text{M}} s)[g^{-1}(.)] \\ &= g \circ f_w(s) \end{aligned}$$

□

Remark. Similarly, $*_\varphi$ is also equivariant to Γ through left action if and only if Γ is abelian, as a consequence of being commutative if and only if Γ is abelian. On the contrary, note that commutativity of $*_{\text{M}}$ doesn't make sense.

Corrolary 24. Characterization by left-action equivariance to Γ
Let $\Gamma \cong V$. If Γ is abelian, the class of linear transformations of $\mathcal{S}(V)$ that are equivariant to Γ is exactly the class of M-convolution operators acting on the left of $\mathcal{S}(V)$ *i.e.*

$$\text{If } \Gamma \cong V \text{ and } \Gamma \text{ is abelian,}$$
$$\exists w \in \mathcal{S}(\Gamma), f = w *_{\text{M}} . \Leftrightarrow \begin{cases} f \in \mathcal{L}(\mathcal{S}(V)) \\ \forall g \in \Gamma, f \circ g = g \circ f \end{cases}$$

Proof. By picking φ such that $\Gamma \overset{\varphi}{\equiv} V$ with Lemma 22 and using the relation between $*_{\text{M}}$ and $*_\varphi$. □

Depending on the applications, we will build upon either $*_\varphi$ or $*_{\text{M}}$ when the abelian condition is satisfied.

2.3 Inclusion of the edge set in the construction

The constructions from the previous section involve the vertex set V and depend on Γ, a subgroup of the set of invertible transformations on V. Therefore, it looks natural to try to relate the edge set and Γ.

There are two approaches. Either Γ describes an underlying graph structure $G = \langle V, E\rangle$, either G can be used to define a relevant subgroup Γ to which the produced convolutive operators will be equivariant. Both approaches will help characterize classes of graphs that can support natural definitions of convolutions.

2.3.1 Edge-constrained convolutions

In this subsection, we are trying to answser the following question:

- What graphs admit a φ-convolution, or an M-convolution (in the sense that they can be defined with the characterization), under the condition that Γ is generated by a set of edge-constrained transformations ?

Definition 25. Edge-constrained transformation

An *edge-constrained* (EC) transformation on a graph $G = \langle V, E\rangle$ is a transformation $f : V \mapsto V$ such that

$$\forall u, v \in V, f(u) = v \Rightarrow u \overset{E}{\sim} v$$

We denote $\Phi_{\text{EC}}(G)$ and $\Phi^*_{\text{EC}}(G)$ the sets of (EC) and invertible (EC) transformations. When a convolution is defined as a sum over a set that is in one-to-one correspondence with a group that is generated from a set of (EC) transformations, we call it an (EC) convolution.

Remark. Note that $\Phi^*_{\text{EC}}(G)$ is not a group, thus why we are interested in groups and their generating sets.

This leads us to consider Cayley graphs (Cayley, 1878).

Definition 26. Cayley graph
Let a group Γ and one of its generating set $\mathcal{U}$. The *Cayley graph* generated by $\mathcal{U}$, is the digraph $\vec{G} = \langle V, E\rangle$ such that $V = \Gamma$ and E is such that:

$$u \to v \Leftrightarrow \exists g \in \mathcal{U}, ga = b$$

Also, if Γ is abelian, we call it an *abelian Cayley graph*. We call *Cayley subgraph*, a subgraph that is isomorph to a Cayley graph.

Remark. Note that for compatibility with the functional notation that we use, we define Cayley graphs with $ga = b$ instead of $ag = b$.

Convolution on Cayley graphs

In the case of Cayley graphs, it is clear that $\mathcal{U} \subseteq \Phi^*_{\text{EC}}$ and $\Phi^* \supseteq \langle \mathcal{U}\rangle \equiv V$. So that they admit (EC) φ-convolutions, and (EC) M-convolutions in the abelian case.
More precisely, we obtain the following characterization:

Proposition 27. Characterization by Cayley subgraph isomorphism
Let a graph $G = \langle V, E\rangle$, then:

(i) G admits an (EC) φ-convolution if and only if it contains a subgraph isomorph to a Cayley graph

(ii) G admits an (EC) M-convolution if and only if it contains a subgraph isomorph to an abelian Cayley graph

Proof. We show the result only in the general case as the proof for the abelian case is similar.

1. From left to right: as a direct application of the definitions.

2. From right to left:
   Let a graph $G = \langle V, E\rangle$. We suppose it contains a subgraph $\vec{G_s} = \langle V_s, E_s\rangle$ that is graph-isomorph to a Cayley graph $\vec{G_c} = \langle V_c, E_c\rangle$, generated by $\mathcal{U}$. Let ψ be a graph isomorphism from G_s to G_c. To obtain the proof, we need to find a group of invertible transformations Γ of V_s generated by a set of (EC) transformations, such that $\Gamma \equiv V_s$.

   Let's define the group action $L : V_c \times V_s \to V_s$ inductively as follows:

   (a) $\forall g \in \mathcal{U}, L_g(u) = v \Leftrightarrow g\psi(u) = \psi(v)$

   (b) Whenever L_g and L_h are defined, the action of gh is defined by homomorphism as $L_{gh} = L_g \circ L_h$

   (c) Whenever L_g is defined, the action of g^{-1} is defined by homomorphism as $L_{g^{-1}} = L_g^{-1}$ *i.e.* $L_{g^{-1}}(u) = v \Leftrightarrow \psi(u) = g\psi(v)$

   Note that the induction transfers the property (a) to all $g \in V_c$ in a transitive manner because

   $$L_{gh}(u) = L_g(L_h(u)) = w \Leftrightarrow \exists v \in V_s \begin{cases} L_h(u) = v \\ L_g(v) = w \end{cases}$$

   and

   $$\exists v \in V_s \begin{cases} h\psi(u) = \psi(v) \\ g\psi(v) = \psi(w) \end{cases} \quad \Leftrightarrow gh\psi(u) = \psi(w)$$

   We must also verify that this construction is well-defined, *i.e.* whenever we define an action with (b) or (c), if the action was already defined, then they must be equal. This is the case because the homomorphism

$g \mapsto L_g$ on V_c is in fact an isomorphism as

$$\begin{aligned} L_g = L_h &\Leftrightarrow \forall u \in V, L_g(u) = L_h(u) \\ &\Leftrightarrow \forall u \in V, g\psi(u) = h\psi(u) \\ &\Leftrightarrow g = h \end{aligned}$$

Also note that (c) is needed only in case that V_c is infinite.

Denote the set $L_{\mathcal{U}} = \{L_g, g \in \mathcal{U}\}$ and $\Gamma = \langle L_{\mathcal{U}} \rangle \cong V_c$. Let's define the map φ as:

$$\begin{aligned} \Gamma &\to V_s \\ \varphi : L_g &\mapsto L_g(\psi^{-1}(\mathrm{Id})) \end{aligned}$$

φ is bijective because $\forall g \in V_c, \varphi(L_g) = \psi^{-1}(g)$ thanks to (a).

Additionally, we have:

$$\begin{aligned} L_h(\varphi(L_g) &= L_h(L_g(\psi^{-1}(\mathrm{Id}))) \\ &= L_h \circ L_g(\psi^{-1}(\mathrm{Id})) \\ &= L_{hg}(\psi^{-1}(\mathrm{Id})) \\ &= \varphi(L_{hg}) \\ &= \varphi(L_h \circ L_g) \end{aligned}$$

That is, φ is a bijective equivariant map and $\langle L_{\mathcal{U}} \rangle = \Gamma \overset{\varphi}{\equiv} V_s$. Moreover, $L_{\mathcal{U}}$ is a set of (EC) transformations thanks to (a). Therefore, G admits an (EC) φ-convolution.

$\square$

Corrolary 28. Characterization by φ
Let a graph $G = \langle V, E \rangle$, and a set $\mathcal{U} \subset \Phi^*_{\text{EC}}(G)$ *s.t.*

$$\langle \mathcal{U} \rangle \cong \Gamma \equiv V' \subset V$$

G admits an (EC) φ-convolution, if and only if, φ is a graph isomorphism between the Cayley graph generated by $\mathcal{U}$ and the subgraph induced by V'.

The proof is omitted as it would be highly similar to the previous one.

2.3.2 Intrinsic properties

- Obviously the constructed convolutions are linear. But do they also preserve the locality and weight sharing properties ?

Let $\vec{G} = \langle V, E \rangle$ be a Cayley subgraph, generated by $\mathcal{U}$, of some graph G. Recall that its (EC) φ-convolution operator is a right operator, and can be expressed as

$$\begin{aligned} &\forall s \in \mathcal{S}(V), \forall u \in V, \\ f_w(s)[u] &= (s *_\varphi w)[u] \\ &= \sum_{v \in V} s[v]\, w[g_v^{-1}(u)] \end{aligned} \tag{12}$$

From this expression, it is not obvious that f_w is a local operator. To see this, we can show for example the following proposition.

Proposition 29. Locality
When the support of w is a compact (in the sense that its induced subgraph in G is connected), of diameter d, the same holds for the support of the sum Σ in (12). More precisely, the subgraph induced by the support of Σ is isomorphic to the transpose of the subgraph induced by the support of w.

Proof. Without loss of generality subject to growing $\mathcal{U}$, let's suppose that w has a support $\mathcal{M} = \varphi(\mathcal{N})$, such that $\mathcal{N} \subset \mathcal{U}$. $\mathcal{N}$ and $\mathcal{M}$ are obviously compacts of diameter 2. Thanks to (P), we have

$$\begin{aligned} g_v^{-1}(u) \in \mathcal{M} &\Leftrightarrow u \in g_v(\mathcal{M}) = g_v(\varphi(\mathcal{N})) = \varphi(g_v\mathcal{N}) \\ &\Leftrightarrow g_u \in g_v\mathcal{N} \\ &\Leftrightarrow g_v^{-1} \in \mathcal{N} g_u^{-1} \\ &\Leftrightarrow g_v \in g_u\mathcal{N}^{-1} \\ &\Leftrightarrow v \in g_u(\varphi(\mathcal{N}^{-1})) \end{aligned}$$

where $\mathcal{N}^{-1}$ reverses the edges of $\mathcal{N}$. Let's denote $\mathcal{K}_u = g_u(\varphi(\mathcal{N}^{-1})) \subset V$. By composing edge reversal and graph isomorphisms (as φ and its inverse are graph isomorphisms by Proposition 28), the compactness and diameter of $\mathcal{M}$ is preserved for $\mathcal{K}_u$. More precisely, the transposed subgraph structure is also preserved. □

Let's define $\mathcal{M}$, $\mathcal{N}$ and $\mathcal{K}_u$ as in the previous proof.

Definition 30. Supporting set
The *supporting set* of an (EC) convolution operator f_w, is a set $\mathcal{N} \subset \Phi^*_{\text{EC}}$, such that

(i) when $*$ is $*_\varphi$: $0 \notin w[\mathcal{M}]$, where $\mathcal{M} = \varphi(\mathcal{N})$

(ii) when $*$ is $*_{\text{M}}$: $0 \notin w[\mathcal{N}]$

Definition 31. Local patch for $*_\varphi$
The *local patch* at $u \in V$ of an (EC) φ-convolution operator f_w is defined as $\mathcal{K}_u = g_u(\varphi(\mathcal{N}^{-1}))$.

Remark. In other terms, $\mathcal{K}_{\text{Id}} = \varphi(\mathcal{N}^{-1})$ is the *initial local patch*, which is composed of all vertices that are connected in direction to $\varphi(\text{Id})$; and $\mathcal{K}_u$ is obtained by moving $\mathcal{K}_{\text{Id}}$ on the Cayley subgraph via the edges corresponding to the decomposition of g_u on the generating set $\mathcal{U}$.

To see that the weights are tied in the general case (i), we can show the following proposition.

Proposition 32. Weight sharing
$\forall a, \alpha \in V, \forall b \in \mathcal{K}_a : \exists \beta \in \mathcal{K}_\alpha \Leftrightarrow g_\beta^{-1}(\alpha) = g_b^{-1}(a)$

Proof. By using (P),

$$
\begin{aligned}
g_{\mathcal{K}_\alpha}^{-1}(\alpha) = g_{\mathcal{K}_a}^{-1}(a) &\Leftrightarrow g_\alpha^{-1} g_{\mathcal{K}_\alpha} = g_a^{-1} g_{\mathcal{K}_a} \\
&\Leftrightarrow \mathcal{K}_\alpha = g_\alpha g_a^{-1}(\mathcal{K}_a) = g_\alpha g_a^{-1} g_a(\varphi(\mathcal{N}^{-1})) \\
&\Leftrightarrow \mathcal{K}_\alpha = g_\alpha(\varphi(\mathcal{N}^{-1}))
\end{aligned}
$$

□

2.3.3 Stricly edge-constrained convolutions

We make the disctinction between general (EC) convolution operators and those for which the weight kernel w is smaller and is supported only on (EC) transformations of $\mathcal{U}$.

Definition 33. Strictly (EC) convolution operator
A *strictly* edge-constrained (EC*) convolution operator f_w, is an (EC) convolution operator such that its supporting set $\mathcal{N} \subset \mathcal{U}$.

Remark. (EC*) convolution operators are simpler to obtain as we can construct them just with $\mathcal{U} \subset \Phi^*_{\text{EC}}(G)$ without composing the transformations.

Let f_w be an (EC*) convolutional operator. In the general case (i), $w \in \mathcal{S}(V)$, so its support is $\mathcal{M} = \varphi(\mathcal{N})$ such that $\mathcal{N} \subseteq \mathcal{U}$. In the abelian case (ii), we use instead $w \in \mathcal{S}(\Gamma)$, and thus its support is directly $\mathcal{N}$. Therefore, we can rewrite the expressions of the convolution operator as:

(i) $\forall s \in \mathcal{S}(V), \forall u \in V, f_w(s)[u] \overset{(\varphi)}{=} \sum_{v \in \mathcal{K}_u} s[v]\, w[g_v^{-1}(u)]$

(ii) $\forall s \in \mathcal{S}(V), f_w(s) \overset{(\text{M})}{=} \sum_{g \in \mathcal{N}} w[g]\, g(s)$

Remark. Note that in the abelian case, we can see from (ii) that a definition of a local patch would coincide with the supporting set, so that locality and weight sharing is straightforward.

From these expressions, it is clear that Γ needs not to be fully determined to calculate $f_w(s)[u]$. The case (ii) is the simplest as the only requirement is a supporting set $\mathcal{N}$ of (EC) invertible transformations. In the case (i), we only need to determine $\mathcal{K}_u$.

2.4 From groups to groupoids

2.4.1 Motivation

One possible limitation coming from searching for Cayley subgraphs is that they are order-regular *i.e.* the in- and the out-degree $d = |\mathcal{U}|$ of each vertex is the same. That is, for a general graph G, the size of the weight kernel w of an (EC*) convolution operator f_w supported on $\mathcal{U}$ is bounded by d, which in turn is bounded by twice the mininimal degree of G (twice because G is undirected and $\mathcal{U}$ can contain every inverse).
There are a lot of possible strategies to overcome this limitation. For example:

1. connecting each vertex with its k-hop neighbors, with $k > 1$,
2. artificially creating new connections for less connected vertices,
3. allowing the supporting set $\mathcal{N}$ to exceed $\mathcal{U}$ *i.e.* dropping * in (EC*).

These strategies require to concede that the topological structure supported by G is not the best one to support an (EC*) convolution on it, which breeds the following question:

- What can we relax in the previous (EC*) contruction in order to unbound the supporting set, and still preserve the equivariance characterization?

The latter constraint is a consequence that every vertex of the Cayley subgraph $\vec{G}$ must be composable with every generator from $\mathcal{U}$. Therefore, an answer consists in considering groupoids (Brandt, 1927) instead of groups. Roughly speaking, a groupoid is almost a group except that its composition law needs not be defined everywhere. Weinstein, 1996, unveiled the benefits to base convolutions on groupoids instead of groups in order to exploit partial symmetries.

2.4.2 Definition of notions related to groupoids

Definition 34. Groupoid

A *groupoid* Υ is a set equipped with a partial composition law with domain $\mathcal{D} \subset \Upsilon \times \Upsilon$, called *composition rule*, that is

1. closed into Υ *i.e.* $\forall (g,h) \in \mathcal{D}, gh \in \Upsilon$
2. associative *i.e.* $\forall f,g,h \in \Upsilon, \begin{cases} (f,g),(g,h) \in \mathcal{D} \Leftrightarrow (fg,h),(f,gh) \in \mathcal{D} \\ (f,g),(fg,h) \in \mathcal{D} \Leftrightarrow (g,h),(f,gh) \in \mathcal{D} \\ \text{when defined, } (fg)h = f(gh) \end{cases}$
3. invertible *i.e.* $\forall g \in \Upsilon, \exists! g^{-1} \in \Upsilon \quad s.t. \begin{cases} (g,g^{-1}),(g^{-1},g) \in \mathcal{D} \\ (g,h) \in \mathcal{D} \Rightarrow g^{-1}gh = h \\ (h,g) \in \mathcal{D} \Rightarrow hgg^{-1} = h \end{cases}$

Optionally, it can be *domain-symmetric* *i.e.* $(g,h) \in \mathcal{D} \Leftrightarrow (h,g) \in \mathcal{D}$, and *abelian* *i.e.* domain-symmetric with $gh = hg$.

Remark. Note that left and right inverses are necessarily equal (because $(gg^{-1})g = g(g^{-1}g)$). Also note we can define a right identity element $e_g^r = g^{-1}g$, and a left one $e_g^l = gg^{-1}$, but they are not necessarily equal and depend on g.

Most definitions related to groups can be adapted to groupoids. In particular, let's adapt a few notions.

Definition 35. Groupoid partial action

A partial *action* of a groupoid Υ on a set V, is a function L, with domain $\mathcal{D}_L \subset \Upsilon \times V$ and valued in V, such that the map $g \mapsto L_g$ is a groupoid homomorphism.

Remark. As usual, we will confound L_g and g when there is no possible confusion, and we denote $\mathcal{D}_{L_g} = \mathcal{D}_g = \{v \in V, (g, v) \in \mathcal{D}_L\}$.

Definition 36. Partial equivariant map
A map φ from a groupoid Υ partially acting on the destination set V is said to be a *partial equivariant map* if

$$\forall g, h \in \Upsilon, \begin{cases} \varphi(h) \in \mathcal{D}_g \Leftrightarrow (g, h) \in \mathcal{D} \\ g(\varphi(h)) = \varphi(gh) \end{cases}$$

Also, φ-equivalence between a subgroupoid and a set is defined similarly with φ being a bijective *partial* equivariant map between them.

Definition 37. Partial transformations groupoid
The *partial transformations groupoid* $\Psi^*(V)$, is the set of invertible partial transformations, equipped with the functional composition law with domain $\mathcal{D}$ such that

$$\begin{cases} \mathcal{D}_{gh} = h(\mathcal{D}_h) \cap \mathcal{D}_g \\ (g, h) \in \mathcal{D} \Leftrightarrow \mathcal{D}_{gh} \neq \emptyset \end{cases}$$

Remark. Note that a subgroupoid $\Upsilon \subset \Psi^*(V)$ is domain-symmetric when $\exists v \in V, g(v) \in \mathcal{D}_h \Leftrightarrow \exists u \in V, h(u) \in \mathcal{D}_g$

2.4.3 Construction of partial convolutions

The expression of the convolution we constructed in the previous section cannot be applied as is. We first need to extend the algebraic objects we work with. Extending a partial transformation g on the signal space $\mathcal{S}(V)$ (and thus the convolutions) is a bit tricky, because only the signal entries corresponding to $\mathcal{D}_g$ are moved. A convenient way to do this is to consider the groupoid closure obtained with the addition of an absorbing element.

Definition 38. Zero-closure
The *zero-closure* of a groupoid Υ, denoted Υ^0, is the set $\Upsilon \cup 0$, such that the groupoid axioms 1, 2 and 3, and the domain $\mathcal{D}$ are left unchanged, and

4. the composition law is extended to $\Upsilon^0 \times \Upsilon^0$ with $\forall (g,h) \notin \mathcal{D}, gh = 0$

Remark. Note that this is coherent as the properties 2 and 3 are still partially defined on the original domain $\mathcal{D}$.

Now, we will also extend every other algebraic object used in the expression of the φ-convolution and the M-convolution, so that we can directly apply our previous constructions.

Lemma 39. Extension of φ on V^0
Let a partial equivariant map $\varphi : \Upsilon \to V$. It can be extended to a (total) equivariant map $\varphi : \Upsilon^0 \to V^0 = V \cup \varphi(0)$, such that $\varphi(0) \notin V$, that we denote $0_V = \varphi(0)$, and such that

$$\forall g \in \Upsilon^0, \forall v \in V^0, g(v) = \begin{cases} \varphi(gg_v) & \text{if } g_v \in \mathcal{D}_g \\ 0_V & \text{else} \end{cases}$$

Proof. We have $\varphi(0) \notin V$ because φ is bijective. Additionaly, we must have $\forall (g,h) \notin \mathcal{D}, g(\varphi(h)) = \varphi(gh) = \varphi(0) = 0_V$. □

Remark. Note that for notational conveniency, we may use the same symbol 0 for 0_Υ, 0_V and $0_\mathbb{R}$.

Similarly to $\Phi^*(V)$, $\Psi^*(V)$ can also move signals of $\mathcal{S}(V)$.

Lemma 40. Extension of injective partial transformations to $\mathcal{S}(V)$
Let $g \in \Psi^*(V)$. Its extension is done in two steps:

1. g is extended to $V^0 = V \cup \{0_V\}$ as $g(v) = 0_V \Leftrightarrow v \notin \mathcal{D}_g$.

2. Under the convention $\forall s \in \mathcal{S}(V), s[0_V] = 0_{\mathbb{R}}$, g is extended via linear extension to $\mathcal{S}(V)$, and we have

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

Proof. Straightforward. □

With these extensions, we can obtain the partial φ- and M-convolutions related to Υ almost by substituting Υ^0 to Γ in Definition 18 and Definition 20.

Definition 41. Partial convolution
Let a subgroupoid $\Upsilon \subset \Psi^*(V)$, such that $\Upsilon \overset{\varphi}{\equiv} V$. The partial φ- and M-convolutions, based on Υ, are defined on its zero-closure, with the same expression as if Υ^0 were a subgroup, and by extension of φ and of the groupoid partial actions *i.e.*

(i) $\forall s, w \in \mathcal{S}(V), s *_\varphi w = \sum_{v \in V} s[v]\, g_v(w) = \sum_{g \in \Upsilon} s[\varphi(g)]\, g(w)$

(ii) $\forall (w, s) \in \mathcal{S}(\Upsilon) \times \mathcal{S}(V), w *_{\mathrm{M}} s = \sum_{g \in \Upsilon} w[g]\, g(s)$

Symmetrical expressions
Note that, as $\forall r, r[0] = 0$, the partial convolutions can also be expressed on the domain $\mathcal{D}$ with a convenient symmetrical expression:

(i) $\forall u \in V, (s *_\varphi w)[u] = \sum_{\substack{(g_a, g_b) \in \mathcal{D} \\ s.t.\ g_a g_b = g_u}} s[a]\, w[b]$

(ii) $\forall u \in V, (w *_{\mathrm{M}} s)[u] = \sum_{\substack{v \in \mathcal{D}_g \\ s.t.\ g(v) = u}} w[g]\, s[v]$

We obtain an equivariance characterization similar to Proposition 19 and Corrolary 24.

Proposition 42. Characterization by equivariance to Υ
Let a subgroupoid $\Upsilon \subset \Psi^*(V)$, such that $\Upsilon \overset{\varphi}{\equiv} V$, with $*$ based on Υ.

1. Then,

   (i) partial φ-convolution right-operators are equivariant to Υ,

   (ii) if Υ is abelian, partial M-convolution left-operators are equiv to Υ.

2. Conversely,

   (i) if Υ is domain-symmetric, linear transformations of $\mathcal{S}(V)$ that are equivariant to Υ are partial φ-convolution right-operators,

   (ii) if Υ is abelian, they are also partial M-convolution left-operators.

Proof. (i) (a) Direct sense:
Using the symmetrical expressions, and the fact that $\forall r, r[0] = 0$, we have

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

(b) Converse:

Let $v \in V$. Denote $e^r_{g_v} = g_v^{-1} g_v$ the right identity element of g_v, and $e^r_v = \varphi(e^r_{g_v})$. We have that

$$g_v(e^r_v) = v$$
$$\text{So, } \delta_v = g_v(\delta_{e^r_v})$$

Let $f \in \mathcal{L}(\mathcal{S}(V))$ that is equivariant to Υ, and $s \in \mathcal{S}(V)$. Thanks to the previous remark we obtain that

$$\begin{aligned} f(s) &= \sum_{v \in V} s[v]\, f(\delta_v) \\ &= \sum_{v \in V} s[v]\, f(g_v(\delta_{e^r_v})) \\ &= \sum_{v \in V} s[v]\, g_v(f(\delta_{e^r_v})) \\ &= \sum_{v \in V} s[v]\, g_v(w_v) \end{aligned} \tag{13}$$

where $w_v = f(\delta_{e^r_v})$. In order to finish the proof, we need to find w such that $\forall v \in V, g_v(w) = g_v(w_v)$.

Let's consider the equivalence relation $\mathcal{R}$ defined on $V \times V$ such that:

$$\begin{aligned} a\mathcal{R}b &\Leftrightarrow w_a = w_b \\ &\Leftrightarrow e^r_a = e^r_b \\ &\Leftrightarrow g_a^{-1} g_a = g_b^{-1} g_b \\ &\Leftrightarrow (g_b, g_a^{-1}) \in \mathcal{D} \\ &\Leftrightarrow (g_a^{-1}, g_b) \in \mathcal{D} \end{aligned} \tag{14}$$

with (14) owing to the fact that Υ is domain-symmetric.

Given $x \in V$, denote its equivalence class $\mathcal{R}(x)$. Under the hypothesis of the axiom of choice (Zermelo, 1904) (if V is infinite), define the set $\aleph$ that contains exactly one representative per equivalence class. Let $w = \sum_{n \in \aleph} w_n$. Then V is the disjoint union $V = \cup_{n \in \aleph} \mathcal{R}(n)$ and (13) rewrites:

$$\begin{aligned}
\forall u \in V, f(s)[u] &= \sum_{n \in \aleph} \sum_{v \in \mathcal{R}(n)} s[v]\, g_v(w_n)[u] \\
&= \sum_{n \in \aleph} \sum_{v \in \mathcal{R}(n)} s[v]\, w_n[g_v^{-1}(u)] \\
&= \sum_{n \in \aleph} \sum_{v \in \mathcal{R}(n)} s[v]\, w[g_v^{-1}(u)] \qquad (15) \\
&= (s *_\varphi w)[u]
\end{aligned}$$

where (15) is obtained thanks to (14).

(ii) With symmetrical expressions, it is clear that the convolution is abelian, if and only if, Υ is abelian. Then (i) concludes.

$\square$

Inclusion of (EC)

Similarly to the construction in Section 2.3, partial convolutions can define (EC) and (EC*) counterparts with a characterization of admissibility by groupoid Cayley subgraph isomorphism, and similar intrinsic properties.

Limitation of partial convolutions

However, because of the groupoid associativity, if $g \in \Psi^*_{\text{EC}}(G)$, then, any $v \in V$ *s.t.* $g(u) = v$ would be constrained to allow to be acted by every h *s.t.* $(h, g) \in \mathcal{D}$, which fails at unbounding the supporting set of a partial (EC*) convolutions.

2.4.4 Construction of path convolutions

To answer the limitation of partial convolutions, given $g \in \langle \mathcal{U} \rangle$ where $\mathcal{U} \subset \Psi^*_{\mathrm{EC}}(G)$, the idea is to proceed with a foliation of g into pieces, each corresponding to an edge $e \in E$, and together generating another groupoid with a different associativity law, as follows.

Definition 43. Path groupoid
Let $\mathcal{U} \subset \Psi^*_{\mathrm{EC}}(G)$. The *path groupoid* generated from $\mathcal{U}$, denoted $\mathcal{U} \ltimes G$, with composition rule $\mathcal{D}_\ltimes$, is the groupoid obtained inductively with:

1. $\mathcal{U} \ltimes_1 G = \{(g, v) \in \mathcal{U} \times V, v \in \mathcal{D}_g\} \subset \mathcal{U} \ltimes G$
2. $((g_n, v_n) \cdots (g_1, v_1), (h_m, u_m) \cdots (h_1, u_1)) \in \mathcal{D}_\ltimes \Leftrightarrow h_m(u_m) = v_1$
3. $((g_n, v_n) \cdots (g_1, v_1))^{-1} = (g_1^{-1}, g_1(v_1)) \cdots (g_n^{-1}, g_n(v_n))$

Call path its objects. Given a length $l \in \mathbb{N}$, denote $\mathcal{U} \ltimes_l G$ the subset composed of the paths that are the composition of exactly l paths of $\mathcal{U} \ltimes_1 G$.

Remark. This groupoid construction is inspired from the field of operator algebra where partial action groupoids have been extensively studied, *e.g.* Nica, 1994; Exel, 1998; Li, 2016.

Such groupoids usually come equipped with source and target maps. We also define the path map.

Definition 44. Source, target and path maps
Let a path groupoid $\mathcal{U} \ltimes G$. We define on it the *source map* α the *target map* β and the *path map* γ as:

$$\begin{cases} \alpha : (g_n, v_n) \cdots (g_1, v_1) \mapsto v_1 \in V \\ \beta : (g_n, v_n) \cdots (g_1, v_1) \mapsto g_n(v_n) \in V \\ \gamma : (g_n, v_n) \cdots (g_1, v_1) \mapsto g_n g_{n-1} \ldots g_1 \in \Psi^*(V^0) \end{cases}$$

Remark. Note that the path groupoid can also be obtained by derivation of the partial transformation groupoid (*i.e.* $p \in \mathcal{U} \ltimes G$ can be seen as a derivative of $\gamma(p)$ *w.r.t.* $\alpha(p)$), and can thus be seen as the local structure of it.

Lemma 45.

Note the following properties:

1. $(p,q) \in \mathcal{D}_\ltimes \Leftrightarrow \alpha(p) = \beta(q)$
2. $\alpha(p) = \beta(p^{-1})$
3. $e^l_p = pp^{-1} = (\mathrm{Id}, \beta(p))$ and $e^r_p = p^{-1}p = (\mathrm{Id}, \alpha(p))$
4. γ is a groupoid partial action. We will denote γ_p instead of $\gamma(p)$.

Remark. Note that this time we won't use the notation $p(v)$ for $\gamma_p(v)$ in order to better differentiate between the composition laws in $\langle \mathcal{U} \rangle$ and $\mathcal{U} \ltimes G$.

One of the key object of our contruction is the use of φ-equivalence in order to transform a sum over a group(oid) of (partial) transformations, into a sum over the vertex set. With the current notion of path groupoid, searching for something similar amounts to searching for a graph traversal.

Definition 46. Traversal set

Let a graph $G = \langle V, E \rangle$ that is connected. A *traversal set* is a pair $(\mathcal{U}, \mathcal{T})$ of (EC) partial transformations subsets $\subset \Psi^*_{\mathrm{EC}}(G)$, such that

1. An edge can only correspond to a unique $g \in \mathcal{U}$,
   i.e. $\forall g, h \in \mathcal{U} : \exists v \in V, g(v) = h(v) \Rightarrow g = h$
2. The (EC) partial transformations of $\mathcal{T}$ are restrictions of those of $\mathcal{U}$,
   i.e. $\forall g \in \mathcal{U}, \exists! h \in \mathcal{T}, \begin{cases} \mathcal{D}_h \subset \mathcal{D}_g \\ \forall v \in \mathcal{D}_h, h(v) = g(v) \end{cases}$
   (equivalently, $\mathcal{T} \ltimes G$ is a path subgroupoid of $\mathcal{U} \ltimes G$ *s.t.* $|\mathcal{T}| = |\mathcal{U}|$)
3. The subgraph $G_\mathcal{T} = \langle V, \mathcal{T} \ltimes_1 G \rangle$ is a spanning tree of G.

We denote $(\mathcal{U}, \mathcal{T}) \in \mathrm{trav}(G)$, and denote by r the root of $G_\mathcal{T}$.

Remark. The assumption that the graph G is connected doesn't lose generality as the construction can be replicated to each connected component in the general case.

A traversal set $(\mathcal{U}, \mathcal{T})$ defines a φ-equivalence between the α-fiber of the root r and the vertex set V as follows.

Lemma 47. Path φ-Equivalence
Let $(\mathcal{U}, \mathcal{T}) \in \mathrm{trav}(G)$. Given $v \in V$, there exists a unique $p_v \in \mathcal{T} \ltimes G$ such that $\alpha(p_v) = r$ and $\beta(p_v) = v$. Define $\varphi : p_v \mapsto v$. Then $\varphi : \alpha^{-1}_{\mathcal{T} \ltimes G}\{r\} \to V$ is a bijective partial equivariant map.

Proof. Bijectivity is a consequence of the spanning tree structure of $\mathcal{T}$. Equivariance because $\gamma_{p_v}(u) = \gamma_{p_v}\gamma_{p_u}(r) = \gamma_{p_v p_u}(r) = \varphi(p_v p_u)$. □

We can now define the convolution that is based on a path groupoid.

Definition 48. Path convolution
Let $(\mathcal{U}, \mathcal{T}) \in \mathrm{trav}(G)$. The *path convolution* is the partial convolution based on the path subgroupoid $\mathcal{T} \ltimes G$, which uses the groupoid partial action $\gamma := \gamma^{\mathcal{U} \ltimes G}$ of the embedding groupoid $\mathcal{U} \ltimes G$.

(i) In what follows are the three expressions of the path φ-convolution for signals $s_1, s_2 \in \mathcal{S}(V)$, and $u \in V$:

$$
\begin{aligned}
(s *_\varphi w) &= \sum_{v \in V} s[v]\, \gamma_{p_v}(w) \\
&= \sum_{\substack{p \in \mathcal{T} \ltimes G \\ s.t.\ \alpha(p) = r}} s[\varphi(p)]\, \gamma_p(w) \\
(s *_\varphi w)[u] &= \sum_{\substack{(a,b) \in V \\ s.t.\ \gamma_{p_a}(b) = u}} s[a]\, w[b]
\end{aligned}
$$

(ii) The mixed formulations with $w \in \mathcal{S}(\mathcal{T} \ltimes G)$ are:

$$(w *_{\mathrm{M}} s) = \sum_{\substack{p \in \mathcal{T} \ltimes G \\ s.t.\ \alpha(p)=r}} w[p]\, \gamma_p(s)$$

$$(w *_{\mathrm{M}} s)[u] = \sum_{\substack{(p,v) \in \mathcal{T} \ltimes G \times V \\ s.t.\ \alpha(p)=r \\ s.t.\ \gamma_p(v)=u}} w[p]\, s[v]$$

Remark. The role of $\mathcal{T}$ is to provide a φ-equivalence. The role of $\mathcal{U}$ is to extend every partial transformation $\gamma_g^{\mathcal{T} \ltimes G}$ to the domain of its unrestricted counterpart $\gamma_g^{\mathcal{U} \ltimes G}$.

Proposition 42 also holds for path groupoids, except that the domain-symmetric condition of 2.(i) is not needed.

Proposition 49. Characterization by equivariance to $\mathcal{U} \ltimes G$'s action Let $(\mathcal{U}, \mathcal{T}) \in \mathrm{trav}(G)$.

(i) The class of linear transformations of $\mathcal{S}(V)$ that are equivariant to the path actions of $\mathcal{U} \ltimes G$ is exactly the path φ-convolution right-operators;

(ii) in the abelian case, they are also exactly the M-convolution left-operators.

Proof. Instead of the domain-symmetric condition that was used in the proof of the converse of Proposition 42 (2.(i)), we use the fact that any vertex can be reached with an action from the root of the spanning tree of the traversal set. Indeed, given $v \in V$, as we have $\gamma_{p_v}(r) = v$, then $\gamma_{p_v}(\delta_r) = \delta_v$. Therefore, by developping a linear transformation $f(s)$ on the dirac family, and commuting f with γ_{p_v}, we obtain that $f(s) = s *_{\varphi} w$, where $w = f(\delta_r)$. The rest of the proof is similar to that of Proposition 42. □

Remark. Note that $\mathcal{U} \ltimes V$'s action is almost the same as the groupoid partial action of $\Upsilon = \langle \mathcal{U} \rangle$ (only "almost" because not all combinations of partial transformations might exist in the paths). However $\mathcal{U} \ltimes V$ associativy law doesn't have the limitation of Υ's.

(EC*) Path convolution operators

The counterparts of strictly edge-constrained (EC*) convolution operators for path convolutions, are indeed path convolution operators obtained with supporting set $\mathcal{N} \subset \mathcal{T} \ltimes_1 G$ which any graph can admit. As shown by this section, to construct one, all we need is a traversal set of partial transformations $(\mathcal{U}, \mathcal{T})$.

2.5 Conclusion

In this chapter, we constructed the convolution on graph domains.

1. We first saw that classical convolutions are in fact the class of linear transformations of the signal space that are equivariant to translations. For signals defined on graph domains, there is no natural definition of translations.

2. Therefore, we adopted a more abstract standpoint and considered in the first place any kind of transformation of the vertex set V. Hence, given a subgroup of transformation Γ, we constructed the class of linear transformations of the signal space that are equivariant to it. This provided us with an expression of a convolution based on this subgroup, and a bijective equivariant map between Γ and V, in order to transport a sum over Γ into a sum over V. We also proposed a simpler expression in the abelian case.

3. Then, we introduced the role of the edge set E, and we constrained Γ by it. This allows us to obtain a characterization of admissibility of convolutions by Cayley subgraph isomorphism, and to analyze intrinsic properties of the constructed convolution operator, namely locality and weight sharing. We also discussed operators with a smaller kernel, in particular those that are strictly edge-constrained (EC*), as they are simpler to construct.

4. Finally, we overcame the limitation that some graphs only have trivials or low order Cayley subgraphs. In this case, we rebased our construction on groupoids of partial transformations Υ as a first iteration, but this one didn't overcome fully the above-mentioned limitation. As a last iteration, we broke down the previous construction into elementary partial actions onto the edges, recomposed into path groupoids $\mathcal{U} \ltimes G$.

Similarly, equivariance characterization and intrinsic properties hold, and the simpler (EC*) construction is also possible.

Summary of practical (EC*) convolution operators

3. For graphs that are quite regular, in the sense that they contain an above-low-order Cayley subgraph (order $k \geq 4$), we saw in Section 2.3.3 that all we need to construct an (EC*) convolution operator is a generating set $\mathcal{U}$ of transformations, without the need of composing its elements, and optionally (in the non-abelian case) to move a local patch $\mathcal{K}_{\mathrm{Id}}$ over the graph domain.

4. For a general graph, we saw in Section 2.4.4 that all we need to construct an (EC*) path convolution operator is a traversal set $(\mathcal{U}, \mathcal{T})$ of partial transformations, without the need to compose the paths.

In the next chapter, we will encounter examples of (EC) and (EC*) convolution operators defined on graphs, that can be expressed under group representations or under path groupoid representations.

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