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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 analyse 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 S(V) by group action

An transformation  $f \in \Phi^*(V)$  can be extended linearly to the signal space S(V), and we have:

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

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:

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

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:

$$\forall s \in \mathcal{S}(\mathbb{Z}^{2}), \forall s' \in \mathcal{S}(\mathbb{Z}^{2}), \forall (\alpha, \beta) \in \mathbb{R}^{2}, \forall (a, b) \in \mathbb{Z}^{2},$$

$$f_{w}(\alpha s + \beta s')[a, b] = \sum_{i} \sum_{j} (\alpha s + \beta s')[i, j] w[a - i, b - j]$$

$$= \alpha f_{w}(s)[a, b] + \beta f_{w}(s')[a, b] \qquad \text{(linearity)}$$

$$\forall s \in \mathcal{S}(\mathbb{Z}^{2}), \forall (\alpha, \beta) \in \mathbb{Z}^{2}, \forall (a, b) \in \mathbb{Z}^{2},$$

$$f_{w} \circ t_{\alpha,\beta}(s)[a, b] = \sum_{i} \sum_{j} t_{\alpha,\beta}(s)[i, j] w[a - i, b - j]$$

$$= \sum_{i} \sum_{j} s[i - \alpha, j - \beta] w[a - i, b - j]$$

$$= \sum_{i'} \sum_{j'} s[i', j'] w[a - i' - \alpha, b - j' - \beta] \qquad \text{(1)}$$

$$= f_{w}(s)[a - \alpha, b - \beta]$$

$$= t_{\alpha,\beta} \circ f_{w}(s)[a, b] \qquad \text{(equivariance)}$$

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:

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

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

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

$$\forall (a,b) \in \mathbb{Z}^2, f(s)[a,b] = \sum_{i} \sum_{j} s[i,j] t_{i,j}(w)[a,b]$$

$$= \sum_{i} \sum_{j} s[i,j] w[a-i,b-j]$$
*i.e.*  $f(s) = s * w$  (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  $2 \times 2$ ), such that we have  $f_w = \sum_{q \in \{1,2,\ldots,n_q\}} f_{w_q}$ . The convolution operators  $f_{w_q}$  are all in the search space of  $2 \times 2$  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  $\Gamma$  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  $\Gamma$ , the group convolution I between two signals  $s_1$  and  $s_2 \in \mathcal{S}(\Gamma)$  is defined as:

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

provided at least one of the signals has finite support if  $\Gamma$  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  $\Gamma$  is in one-to-one correspondence with V, and let's define a bijective map  $\varphi$  from  $\Gamma$  to V. We denote  $\Gamma \stackrel{\varphi}{\cong} V$  and  $g_v \stackrel{\varphi}{\mapsto} v$ .

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  $\varphi$  for both  $\varphi$  and  $\widetilde{\varphi}$  (as done between f and  $L_f$ ). A commutative diagram between the sets is depicted on Figure 2.1.

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

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  $\varphi$  is simultaneously applied on both the signal space and its domain.

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Lemma 9. Relation between  $S(\Gamma)$  and S(V)

$$\forall s \in \mathcal{S}(\Gamma), \forall u \in V, \varphi(s)[u] = s[\varphi^{-1}(u)] = s[g_u]$$

Proof.

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

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  $\Gamma \stackrel{\varphi}{\cong} V$ . The group convolution II between two signals  $s_1$  and  $s_2 \in \mathcal{S}(V)$  is defined as:

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

# Lemma 11. Relation between group convolution I and II

Let a subgroup  $\Gamma \subset \Phi^*(V)$  such that  $\Gamma \stackrel{\varphi}{\cong} V$ ,

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

*Proof.* Using Lemma 9,

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

$$= \sum_{v \in V} s_1[g_v] s_2[g_v^{-1}g_u]$$

$$= \sum_{g \in \Gamma} s_1[g] s_2[g^{-1}g_u]$$

$$= (s_1 *_{\Pi} s_2)[g_u]$$

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

#### Proposition 12. Equivariance to $\varphi(\Gamma)$

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

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

Proof.

$$\forall s \in \mathcal{S}(V), \forall u \in V, \forall v \in V,$$

$$(f_w \circ \varphi(g_u))(s)[v] = \sum_{v \in V} \varphi(g_u)(s)[v] w[\varphi(g_v^{-1}g_u)]$$

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

$$= \sum_{\substack{(a,b) \in V^2 \\ s.t. \ g_a g_b = g_v}} s[\varphi(g_u)^{-1}(a)] w[b]$$

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

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

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

Remark. Note that convolution operators of the form  $f_w = . *_{\scriptscriptstyle \text{I}} w$  are also equivariant to  $\Gamma$ , 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  $\varphi$  also transfer the group structure from  $\Gamma$  to V, and the converse don't hold. To obtain equivariance to  $\Gamma$  (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  $\Gamma$  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  $\Gamma$  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.

$$g_{u} \xrightarrow{g_{v}} g_{v}g_{u}$$

$$\downarrow^{\varphi} \qquad \qquad \downarrow^{\varphi}$$

$$u \xrightarrow{(P)} \varphi(g_{v}g_{u})$$

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

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

#### Definition 14. Equivariant map

A map  $\varphi$  from a group  $\Gamma$  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  $\Gamma \stackrel{\varphi}{\cong} V$ . If we also have that  $\Gamma \equiv V$ , we are interested to know if then  $\varphi$  exhibits the equivalence.

## Definition 15. $\varphi$ -Equivalence

A subgroup  $\Gamma \subset \Phi^*(V)$  such that  $\Gamma \stackrel{\varphi}{\cong} V$ , is said to be  $\varphi$ -equivalent if  $\varphi$  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  $\Gamma \stackrel{\varphi}{\equiv} V$ .

Remark. For example, translations on the grid graph, with  $\varphi(t_{i,j}) = (i,j)$ , are  $\varphi$ -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  $\varphi$ -equivalent.

### Definition 16. Group convolution III

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

$$s_1 *_{\text{III}} s_2 = \sum_{v \in V} s_1[v] g_v(s_2)$$
 (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  $\Gamma$ .

#### Lemma 17. Relation with group convolution II

$$\Gamma \stackrel{\varphi}{\equiv} V \Leftrightarrow *_{\text{II}} = *_{\text{III}}$$

Proof.

$$\forall s_{1}, s_{2} \in \mathcal{S}(V),$$

$$s_{1} *_{II} s_{2} = s_{1} *_{III} s_{2}$$

$$\Leftrightarrow \forall u \in V, \sum_{v \in V} s_{1}[v] s_{2}[\varphi(g_{v}^{-1}g_{u})] = \sum_{v \in V} s_{1}[v] s_{2}[g_{v}^{-1}(u)]$$
(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  $\varphi$ -convolution.

#### Definition 18. $\varphi$ -convolution

Let  $\Gamma \stackrel{\varphi}{=} V$ , 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  $\Gamma$  as expected, and the full characterization as well.

Proposition 19. Characterization by right-action equivariance to  $\Gamma$  If  $\Gamma$  is  $\varphi$ -equivalent, the class of linear transformations of  $\mathcal{S}(V)$  that are equivariant to  $\Gamma$  is exactly the class of  $\varphi$ -convolution operators acting on the right of  $\mathcal{S}(V)$  *i.e.* 

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

## *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).

$$\forall g \in \Gamma, \forall s \in \mathcal{S}(V),$$

$$f_w \circ g(s) = \sum_{h \in \Gamma} g(s)[\varphi(h)] h(w) \qquad (6)$$

$$= \sum_{h \in \Gamma} g(s)[\varphi(gh)] gh(w) \qquad (7)$$

$$= \sum_{h \in \Gamma} g(s)[g(\varphi(h))] gh(w) \qquad (8)$$

$$= \sum_{h \in \Gamma} s[\varphi(h)] gh(w)$$

$$= \sum_{h \in \Gamma} s[\varphi(h)] h(w)[g^{-1}(.)]$$

$$= f_w(s)[g^{-1}(.)]$$

$$= g \circ f_w(s)$$

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:

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

By denoting  $w = f(\delta_{\varphi(\mathrm{Id})})$ , and using the hypothesis of equivariance,

we obtain from (9) that:

$$f(s) = \sum_{v \in V} s[v] f \circ g_v(\delta_{\varphi(\mathrm{Id})})$$

$$= \sum_{v \in V} s[v] g_v \circ f(\delta_{\varphi(\mathrm{Id})})$$

$$= \sum_{v \in V} s[v] g_v(w)$$

$$= s *_{\varphi} w$$

#### Construction of $\varphi$ -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  $\Gamma$  of invertible transformations of V, that is equivalent to V. The choice of  $\Gamma$  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  $\Gamma$ .

#### Exposure of $\varphi$

This construction relies on exposing a bijective equivariant map  $\varphi$  between  $\Gamma$  and V. In the next subsection, we show that in cases where  $\Gamma$  is abelian, we even need not expose  $\varphi$  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  $\varphi$ .

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#### 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  $r *_{\mathsf{M}} s \in \mathcal{S}(V)$  and is defined as:

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

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

#### Lemma 21. Relation with group convolution III

$$\forall \varphi \in \text{BIJ}(\Gamma, V), \forall (r, s) \in \mathcal{S}(\Gamma) \times \mathcal{S}(V),$$
$$r *_{\text{M}} s = \varphi(r) *_{\text{HI}} s$$

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

$$r *_{\mathsf{M}} s = \sum_{g \in \Gamma} r[g] g(s) = \sum_{v \in V} r[g_v] g_v(s) \stackrel{(\diamond)}{=} \sum_{v \in V} \varphi(r)[v] g_v(s)$$
$$= \varphi(r) *_{\mathsf{III}} s$$

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

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

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

$$\Gamma \stackrel{\varphi}{\equiv} V \Leftrightarrow \forall v \in V, (r *_{\mathsf{M}} s)[v] = (r *_{\mathsf{I}} \varphi^{-1}(s))[g_v]$$
$$\Leftrightarrow r *_{\mathsf{M}} s = \varphi(r) *_{\mathsf{II}} s$$
$$\Leftrightarrow r *_{\mathsf{M}} s = \varphi(r) *_{\mathsf{G}} s$$

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

From M-convolution, we can derive operators acting on the left of S(V), of the form  $s \mapsto w *_{\mathsf{M}} s$ , parameterized by  $w \in S(\Gamma)$ . In particular, these operators would be relevant as layers of neural networks. On the contrary, derived operators acting on the right such as  $r \mapsto r *_{\mathsf{M}} w$  wouldn't make sense with this formulation as they would make  $\varphi$  resurface. However, the equivariance to  $\Gamma$  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 $\Gamma$ through left action

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

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

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

by particularizing on well chosen signals):

$$f_{w} \circ g(s) = \sum_{h \in \Gamma} w[h] hg(s)$$

$$= \sum_{h \in \Gamma} w[h] gh(s)$$

$$= \sum_{h \in \Gamma} w[h] h(s)[g^{-1}(.)]$$

$$= (w *_{M} s)[g^{-1}(.)]$$

$$= g \circ f_{w}(s)$$
(10)

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

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

If 
$$\Gamma \cong V$$
 and  $\Gamma$  is abelian,

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

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

Depending on the applications, we will build upon either  $*_{\varphi}$  or  $*_{\mathsf{M}}$  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  $\Gamma$ , a subgroup of the set of invertible transformations on V. Therefore, it looks natural to try to relate the edge set and  $\Gamma$ .

There are two approaches. Either  $\Gamma$  describes an underlying graph structure  $G = \langle V, E \rangle$ , either G can be used to define a relevant subgroup  $\Gamma$  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 answer the following question:

• What graphs admit a  $\varphi$ -convolution, or an M-convolution (in the sense that they can be defined with the characterization), under the condition that  $\Gamma$  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

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

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; Wikipedia, 2018).

#### Definition 26. Cayley graph

Let a group  $\Gamma$  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:

$$u \to v \Leftrightarrow \exists q \in \mathcal{U}, qa = b$$

Also, if  $\Gamma$  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)  $\varphi$ -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)  $\varphi$ -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  $\psi$  be a graph isomorphism from  $G_s$  to  $G_c$ . To obtain the proof, we need to find a group of invertible transformations  $\Gamma$  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)  $\forall g \in \mathcal{U}, L_q(u) = v \Leftrightarrow g\psi(u) = \psi(v)$
- (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

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

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

$$L_g = L_h \Leftrightarrow \forall u \in V, L_g(u) = L_h(u)$$
  
 $\Leftrightarrow \forall u \in V, g\psi(u) = h\psi(u)$   
 $\Leftrightarrow g = h$ 

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  $\varphi$  as:

$$\Gamma \to V_s$$

$$\varphi: L_g \mapsto L_g(\psi^{-1}(\mathrm{Id}))$$

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

Additionally, we have:

$$L_h(\varphi(L_g) = L_h(L_g(\psi^{-1}(\mathrm{Id})))$$

$$= L_h \circ L_g(\psi^{-1}(\mathrm{Id}))$$

$$= L_{hg}(\psi^{-1}(\mathrm{Id}))$$

$$= \varphi(L_{hg})$$

$$= \varphi(L_h \circ L_g)$$

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

## Corrolary 28. Characterization by $\varphi$

Let a graph  $G = \langle V, E \rangle$ , and a set  $\mathcal{U} \subset \Phi_{\text{\tiny EC}}^*(G)$  s.t.

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

G admits an (EC)  $\varphi$ -convolution, if and only if,  $\varphi$  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 contructed 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)  $\varphi$ -convolution operator is a right operator, and can be expressed as

$$\forall s \in \mathcal{S}(V), \forall u \in V,$$

$$f_w(s)[u] = (s *_{\varphi} w)[u]$$

$$= \sum_{v \in V} s[v] w[g_v^{-1}(u)]$$
(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  $\Sigma$  in (12). More precisely, the subgraph induced by the support of  $\Sigma$  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

$$g_v^{-1}(u) \in \mathcal{M} \Leftrightarrow u \in g_v(\mathcal{M}) = g_v(\varphi(\mathcal{N})) = \varphi(g_v\mathcal{N})$$

$$\Leftrightarrow g_u \in g_v\mathcal{N}$$

$$\Leftrightarrow g_v^{-1} \in \mathcal{N}g_u^{-1}$$

$$\Leftrightarrow g_v \in g_u\mathcal{N}^{-1}$$

$$\Leftrightarrow v \in g_u(\varphi(\mathcal{N}^{-1}))$$

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  $\varphi$  and its inverse are graph isomorphisms by Proposition 28), the compactness and diameter of  $\mathcal{M}$  is preserved for  $\mathcal{K}_u$ . More preceisely, 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 \*<sub>M</sub>:  $0 \notin w[\mathcal{N}]$

## Definition 31. Local patch for $*_{\varphi}$

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

Remark. In other terms,  $\mathcal{K}_{\mathrm{Id}} = \varphi(\mathcal{N}^{-1})$  is the *initial local patch*, which is composed of all vertices that are connected in direction to  $\varphi(\mathrm{Id})$ ; and  $\mathcal{K}_u$  is obtained by moving  $\mathcal{K}_{\mathrm{Id}}$  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),

$$g_{\mathcal{K}_{\alpha}}^{-1}(\alpha) = g_{\mathcal{K}_{a}}^{-1}(a) \Leftrightarrow g_{\alpha}^{-1}g_{\mathcal{K}_{\alpha}} = g_{a}^{-1}g_{\mathcal{K}_{a}}$$
$$\Leftrightarrow \mathcal{K}_{\alpha} = g_{\alpha}g_{a}^{-1}(\mathcal{K}_{a}) = g_{\alpha}g_{a}^{-1}g_{a}(\varphi(\mathcal{N}^{-1}))$$
$$\Leftrightarrow \mathcal{K}_{\alpha} = g_{\alpha}(\varphi(\mathcal{N}^{-1}))$$

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  $\mathcal{N} \subset \mathcal{U}$ .

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

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

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  $\Gamma$  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 minimial 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 Definitions of some groupoid related notions

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#### Definition 34. Groupoid

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

- 1. closed into  $\Upsilon$  *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.  $\forall g \in \Upsilon, \exists ! g^{-1} \in \Upsilon$  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  $\Upsilon$  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  $\varphi$  from a groupoid  $\Upsilon$  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,  $\varphi$ -equivalence between a subgroupoid and a set is defined similarly with  $\varphi$  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

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

# 2.4.3 Construction of the groupoid convolution

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

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#### Definition 38. Zero-closure

The zero-closure of a groupoid  $\Upsilon$ , denoted  $\Upsilon^0$ , 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  $\varphi$ -convolution and the M-convolution, so that we can directly apply our previous constructions.

## Lemma 39. Extension of $\varphi$ 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  $\varphi$  is bijective. Additionally, 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  $0_{\Upsilon}$ ,  $0_{V}$  and  $0_{\mathbb{R}}$ .

# Lemma 40. Extension of the subgroupoid actions on $\mathcal{S}(V)$

Let a subgroupoid  $\Upsilon \subset \Psi^*(V)$  such that  $\Upsilon \stackrel{\varphi}{=} V$ . Under the convention that  $s[0_V] = 0_{\mathbb{R}}$ , a transformation  $g \in \Upsilon^0$  can be extended to the signal space S(V) as usual:

$$\forall s \in \mathcal{S}(V), \forall v \in V, g(s)[v] = \begin{cases} s[g^{-1}(v)] & \text{if } g \neq 0_{\Upsilon} \text{ and } v \in \mathcal{D}_{g^{-1}} \\ 0_{\mathbb{R}} & \text{else} \end{cases}$$

*Proof.* Straightforward.

With these extensions, we can obtain the  $\varphi$ - and M-convolutions related to  $\Upsilon$  almost by substituting  $\Upsilon^0$  to  $\Gamma$  in Definition 18 and Definition 20.

#### Definition 41. Groupoid convolution

Let a subgroupoid  $\Upsilon \subset \Psi^*(V)$ , such that  $\Upsilon \stackrel{\varphi}{\equiv} V$ . The  $\varphi$ - and M-convolutions, based on  $\Upsilon$ , are defined on its zero-closure, with the same expression as if  $\Upsilon^0$  were a subgroup, and by extension of  $\varphi$  and of the groupoid 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) 
$$\forall (w, s) \in \mathcal{S}(\Upsilon) \times \mathcal{S}(V), w *_{\mathsf{M}} s = \sum_{g \in \Upsilon} w[g] g(s)$$

where (ii) applies in the abelian case.

#### Symmetrical expressions

Note that, as  $\forall r, r[0] = 0$ , the groupoid 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) 
$$\forall u \in V, (w *_{\mathbf{M}} s)[u] = \sum_{\substack{v \in \mathcal{D}_g \\ s.t. \ g(v) = u}} w[g] \, s[v]$$

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

# Proposition 42. Characterization by equivariance to $\Upsilon$

Let a subgroupoid  $\Upsilon \subset \Psi^*(V)$ , such that  $\Upsilon \stackrel{\varphi}{\equiv} V$ . Then,

- (i) right  $\varphi$ -convolution operators are equivariant to  $\Upsilon$ ,
- (ii) if  $\Upsilon$  is abelian, left M-convolution operators are equivariant to  $\Upsilon$ .

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## Conversely,

- (i) if  $\Upsilon$  is domain-symmetric, linear transformations of  $\mathcal{S}(V)$  that are equivariant to  $\Upsilon$  are right  $\varphi$ -convolution operators,
- (ii) if  $\Upsilon$  is abelian, linear transformations of  $\mathcal{S}(V)$  that are equivariant to  $\Upsilon$  are also left M-convolution operators.

# *Proof.* (i) (a) Direct sense:

Using the symmetrical expressions, and the fact that  $\forall r, r[0] = 0$ , we have

$$(f_{w} \circ g(s))[u] = \sum_{\substack{(g_{a},g_{b}) \in \mathcal{D} \\ s.t. \ g_{a}g_{b} = g_{u}}} g(s)[a] w[b]$$

$$= \sum_{\substack{(g_{a},g_{b}) \in \mathcal{D} \\ s.t. \ g_{a}g_{b} = g_{u}}} s[g^{-1}(a)] w[b]$$

$$= \sum_{\substack{(g_{a},g_{b}) \in \mathcal{D} \\ s.t. \ (g,g_{a}) \in \mathcal{D} \\ s.t. \ (g,g_{a}) \in \mathcal{D}}} s[a] w[b]$$

$$= \sum_{\substack{(g_{a},g_{b}) \in \mathcal{D} \\ s.t. \ (g,g_{a}) \in \mathcal{D} \\ s.t. \ (g,g_{a}) \in \mathcal{D} \\ s.t. \ (g,g_{a}) \in \mathcal{D}}} s[a] w[b]$$

$$= f_{w}(s)[g^{-1}(u)]$$

$$= (q \circ f_{w}(s))[u]$$

# (b) Converse:

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

$$g_v(e_v^r) = v$$
  
So,  $\delta_v = g_v(\delta_{e_v^r})$ 

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

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

$$= \sum_{v \in V} s[v] f(g_v(\delta_{e_v^r}))$$

$$= \sum_{v \in V} s[v] g_v(f(\delta_{e_v^r}))$$

$$= \sum_{v \in V} s[v] g_v(w_v)$$
(13)

where  $w_v = f(\delta_{e_v^r})$ . 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:

$$a\mathcal{R}b \Leftrightarrow w_a = w_b$$

$$\Leftrightarrow e_a^r = e_b^r$$

$$\Leftrightarrow g_a^{-1}g_a = g_b^{-1}g_b$$

$$\Leftrightarrow (g_b, g_a^{-1}) \in \mathcal{D}$$

$$\Leftrightarrow (g_a^{-1}, g_b) \in \mathcal{D}$$
(14)

with (14) owing to the fact that  $\Upsilon$  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  $V = \bigcup_{n \in \aleph} \mathcal{R}(n)$  and (13) rewrites:

$$\forall u \in V, f(s)[u] = \sum_{n \in \mathbb{N}} \sum_{v \in \mathcal{R}(n)} s[v] g_v(w_n)[u]$$

$$= \sum_{n \in \mathbb{N}} \sum_{v \in \mathcal{R}(n)} s[v] w_n[g_v^{-1}(u)]$$

$$= \sum_{n \in \mathbb{N}} \sum_{v \in \mathcal{R}(n)} s[v] w[g_v^{-1}(u)]$$

$$= (s *_{\omega} w)[u]$$
(15)

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

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

# 2.4.4 Edge-constrained groupoid convolutions

TODO: Irrelevant because associativity and equivariant map property clash and we still have the same constraints as before

TODO: Erase and rewrite this subsection

Similarly to the construction with Cayley graphs of 2.3.1, we start by adapting the related notions.

## Definition 43. Groupoid generating set

A set  $\mathcal{U}$ , equipped with a partial composition law of domain  $\mathcal{D}_0$ , is a generating set of a groupoid  $\Upsilon$ , if every object of  $\Upsilon$  can be expressed as a composition of objects of  $\mathcal{U}$  and their inverses. In this case, the domain  $\mathcal{D}$  of the partial composition law of  $\Upsilon$  can be deducted inductively from  $\mathcal{D}_0$  with the associativity and invertibility axioms of  $\Upsilon$  (and eventually also with the domain-symmetric axiom if  $\Upsilon$  is domain-symmetric).

A partial Cayley graph is defined similarly as the (total) Cayley graph.

## Definition 44. Partial Cayley graph

Let a groupoid  $\Upsilon = \langle \mathcal{U}, \mathcal{D}_0 \rangle$ . The partial Cayley graph generated by  $\mathcal{U}$  and  $\mathcal{D}_0$ , is the digraph  $\vec{G} = \langle V, E \rangle$  such that  $V = \Upsilon$  and E is such that:

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

We call *partial Cayley subgraph*, a subgraph that is isomorph to a partial Cayley graph.

Remark. The characterization by a partial Cayley subgraph, of graphs admitting an (EC) convolution based on a groupoid, similar to Proposition 27 also holds for the groupoid representation.

In the case of the groupoid representation, what is more interesting is that an (EC) groupoid convolution can be characterized by a generating set of the groupoid it is based on.

## Proposition 45. Characterization by generating set

Let a graph  $G = \langle V, E \rangle$  such that it admits an (EC) convolution based on a groupoid  $\Upsilon$ . Then, G contains a sugraph  $\vec{G}$  that is isomorph to a partial Cayley subgraph  $\vec{G}_c$ , of generating set  $\mathcal{U} \subset \Psi_{\text{EC}}^*(G)$ , such that the underlying equivariant map  $\varphi$  of the (EC) convolution is also a graph isomorphism between  $\vec{G}_c$  and  $\vec{G}$ .

The proof is omitted because it would be highly similar with the one of Corrolary 28.

## Strictly edge-constrained groupoid convolution

Thanks to the previous construction, in order to define a meaningful convolution operator on a general graph  $G = \langle V, E \rangle$ , all we need is a set  $\mathcal{U}$  of (EC) partial transformations that need not to be defined on every vertex, and a composition rule  $\mathcal{D}_0$ . From the set  $\mathcal{U}$ , we can choose a supporting set  $\mathcal{N} \subset \mathcal{U}$  (from which we eventually need to derive the local patches  $\mathcal{K}_u$ ), and

obtain the (EC\*) convolution operator  $f_w$ , without the need of fully determining  $\Upsilon = \langle \mathcal{U} \rangle$ . We can choose between three levels of constraints, which are inherited from  $\mathcal{U}$  and  $\mathcal{D}_0$ :

- 1.  $\Upsilon$  is unconstrained, then  $f_w$  is an (EC\*)  $\varphi$ -convolution right-operator that is equivariant to  $\Upsilon$ , but the converse doesn't hold,
- 2.  $\Upsilon$  is domain-symmetric, then  $f_w$  is an (EC\*)  $\varphi$ -convolution right operator and the equivariance characterization holds,
- 3.  $\Upsilon$  is abelian, then  $f_w$  is an (EC\*) M-convolution operator, the equivariance characterization holds, and we don't need to compute the local patches  $\mathcal{K}_u$ .

In the next chapter, we will encounter examples of convolutions defined on graphs, that can be expressed under group representations or under groupoid representations.

TODO: Limitation: border effect because g goes in implies g goes out

#### TODO:

#### TODO

Use groupoids and  $\Psi^*$ . Show it is useless. But (ER) from  $\Psi^*$ , not  $\Phi^*$ 

# 2.5 Paths

TODO: work in progress

## 2.5.1 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 minimal 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?

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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.

# 2.5.2 Groupoids

## Definition 46. Groupoid

A groupoid  $\Upsilon$  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  $\Upsilon$  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. 
$$\forall g \in \Upsilon, \exists ! g^{-1} \in \Upsilon$$
 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.

The groupoid convolution may be expressed as the restriction of the group convolution to the composition rule  $\mathcal{D}$ , *i.e.*:

## Definition 47. Groupoid convolution

Let a groupoid  $\Upsilon$ , the groupoid convolution between two signals  $s_1, s_2 \in \mathcal{S}(\Upsilon)$  is defined as:

$$\forall h \in \Upsilon, (s_1 * s_2)[h] = \sum_{\substack{f \in \Upsilon \ s.t. \\ (f^{-1},h) \in \mathcal{D}}} s_1[f] \, s_2[f^{-1}h]$$

#### Symmetrical expression

Note that a convenient change of index gives the following symmetrical expression:

$$\forall h \in \Upsilon, (s_1 * s_2)[h] = \sum_{\substack{(f,g) \in \mathcal{D} \\ s.t. \ gf = h}} s_1[f] \, s_2[g]$$

Let a graph  $G = \langle V, E \rangle$ . As V is not a groupoid, we cannot apply the groupoid convolution on  $\mathcal{S}(V)$ . So we need to find a meaningful groupoid.

# 2.5.3 Edge-restricted convolutions

In what follows, our aim is to restrict the construction of the convolution we made on groups to a composition rule  $\mathcal{D}$  dicted by the edge set E.

# Definition 48. Edge-restricted transformation

Let a graph  $G = \langle V, E \rangle$ . An edge-restricted (ER) transformation  $g_{\text{ER}}$  is the restriction of a transformation  $g \in \Phi^*(V)$  to the domain

$$\mathcal{D}_g = \{ v \in V, v \sim g(v) \}$$

(or  $v \to g(v)$  in the case of a digraph  $\vec{G} = \langle V, E \rangle$ ).

The set of (ER) transformations, and injective (ER) transformations are denoted  $\Phi_{\text{er}}(G)$ , and  $\Phi_{\text{er}}^*(G)$  respectively.

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## Extension to S(V) by (ER) group action

As a restriction of the symmetric group of V,  $\Phi_{\text{ER}}^*(G)$  can also move signals of  $\mathcal{S}(V)$ . Let  $g \in \Phi_{\text{ER}}^*(G)$ . Its extension is done in two steps:

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

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

similarly to Lemma 2.1.2.

Note that even though  $\Phi_{\text{ER}}^*(G)$  can generate a groupoid, we won't use it to define the convolution of the graph G as its composition rule would be too narrow. Instead, we form another groupoid from the actions of a semigroup of (ER) transformations.

## Definition 49. Edge-restricted (EC) Groupoid

Let  $\mathcal{U} \subset \Phi^*(V)$ . The *(ER) groupoid* generated from  $\mathcal{U}_{ER}$ , denoted  $\mathcal{U}_{ER} \ltimes V$ , with composition rule  $\mathcal{D}$ , is the groupoid obtained inductively as:

1. 
$$\mathcal{U}_{\text{ER}} \ltimes_0 V = \{(g, v) \in \mathcal{U}_{\text{ER}} \times V, v \in \mathcal{D}_g\} \subset \mathcal{U} \ltimes V$$

2. 
$$((g_1, v_1) \cdots (g_n, v_n), (h_1, u_1) \cdots (h_m, u_m)) \in \mathcal{D} \Leftrightarrow g_n(v_n) = u_1$$

3. 
$$(g_1, v_1) \cdots (g_n, v_n) \in \mathcal{U}_{ER} \ltimes V \Rightarrow (g_n^{-1}, g_n(v_n)) \cdots (g_1^{-1}, g_1(v_1)) \in \mathcal{U}_{ER} \ltimes V$$

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

## Definition 50. Source, target, and path

Let an (ER) groupoid  $\mathcal{U}_{ER} \ltimes V$ . We define on it the *path map*  $\alpha$ , the *source map*  $\beta$ , and the *target map*  $\gamma$ , such that:

$$\begin{cases} \alpha : (g_1, v_1) \cdots (g_n, v_n) \mapsto g_1 g_2 \dots g_n \in \Phi^*(V) \\ \beta : (g_1, v_1) \cdots (g_n, v_n) \mapsto v_1 \in V \\ \gamma : (g_1, v_1) \cdots (g_n, v_n) \mapsto v_n \in V \end{cases}$$

Remark. Note that  $k \in \mathcal{U}_{ER} \ltimes V$  doesn't imply  $(\alpha(k), \beta(k)) \in \mathcal{U}_{ER} \ltimes V$ . We can now define the (ER) convolution based on an (ER) groupoid.

## Definition 51. Edge-restricted (EC) Convolution

(i) 
$$\forall u \in V, (s_1 *_{\varphi} s_2)[u] = \sum_{\substack{k \in \mathcal{U} \ltimes V \\ s.t. \ \gamma(k) = u}} s_1[\varphi(\alpha(k))] s_2[\beta(k)]$$

(ii) 
$$\forall u \in V, (s_1 *_{\mathbf{M}} s_2)[u] = \sum_{\substack{k \in \mathcal{U} \times V \\ s.t. \ \gamma(k) = u}} s_1[\alpha(k)] s_2[\beta(k)]$$

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