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22 Chapter 2

23 Convolutions on graph domains

24 Introduction

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

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65 2.1 Analysis of the classical convolution

66 In this section, we are exposing a few properties of the classical convolution
 67 that a generalization to graphs would likely try to preserve. For now let's
 68 consider a graph G agnostically of its edges *i.e.* $G \cong V$ is just the set of its
 69 vertices.

70 2.1.1 Properties of the convolution

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

73 **Definition 1. Convolution on $\mathcal{S}(\mathbb{Z}^2)$**

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

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

76 **Definition 2. Convolution operator**

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

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

83 **Linearity**

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

86 Locality and weight sharing

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

90 Commutativity

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

93 Equivariance to translations

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

96 2.1.2 Characterization on grid graphs

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

98 Definition 3. Transformation

99 A *transformation* $f : V \rightarrow V$ is a function with same domain and codomain.
 100 The set of transformations is denoted $\Phi(V)$. The set of bijective transforma-
 101 tions is denoted $\Phi^*(V) \subset \Phi(V)$.

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

104 Lemma 4. Extension to $\mathcal{S}(V)$ by group action

105 An transformation $f \in \Phi^*(V)$ can be extended linearly to the signal space
 106 $\mathcal{S}(V)$, and we have:

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

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

108 Then, we have:

$$\begin{aligned} L_f(s) &= \sum_{v \in V} s[v] L_f(\delta_v) \\ &= \sum_{v \in V} s[v] \delta_{f(v)} \end{aligned}$$

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

109

□

110 We also recall the formalism of translations.

111 **Definition 5. Translation on $\mathcal{S}(\mathbb{Z}^2)$**

112 A translation on \mathbb{Z}^2 is defined as a transformation $t \in \Phi^*(\mathbb{Z}^2)$ such that

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

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

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

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

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

118 **Proposition 6. Characterization of convolution operators on $\mathcal{S}(\mathbb{Z}^2)$**

119 On real-valued signals over \mathbb{Z}^2 , the class of linear transformations that are
120 equivariant to translations is exactly the class of convolutive operations i.e.

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

121

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

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

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

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

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

127 By linearity of f and then equivariance to translations:

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

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

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

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

129

□

130 2.1.3 Usefulness of convolutions in deep learning

131 Equivariance property of CNNs

132 In deep learning, an important argument in favor of CNNs is that convolu-
133 tional layers are equivariant to translations. Intuitively, that means that a
134 detail of an object in an image should produce the same features indepen-
135 dently of its position in the image.

136 Lossless superiority of CNNs over MLPs

137 The converse result, as a consequence of Proposition 6, is never mentioned
138 in deep learning literature. However it is also a strong one. For example,
139 let's consider a linear function that is equivariant to translations. Thanks
140 to the converse result, we know that this function is a convolution operator
141 parameterized by a weight vector w , $f_w : \cdot * w$. If the domain is compactly
142 supported, as in the case of images, we can break down the information of w
143 in a finite number n_q of kernels w_q with small compact supports of same size
144 (for instance of size 2×2), such that we have $f_w = \sum_{q \in \{1, 2, \dots, n_q\}} f_{w_q}$. The
145 convolution operators f_{w_q} are all in the search space of 2×2 convolutional
146 layers. In other words, every translational equivariant linear function can

147 have its information parameterized by these layers. So that means that the
148 reduction of parameters from an MLP to a CNN is done with strictly no loss of
149 expressivity (provided the objective function is known to bear this property).
150 Besides, it also helps the training to search in a much more confined space.

151 **Methodology for extending to general graphs**

152 Hence, in our construction, we will try to preserve the characterization from
153 Proposition 6 as it is mostly the reason why they are successful in deep
154 learning. Note that the reduction of parameters compared to a dense layer
155 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.

182 **Definition 8. Group convolution I**

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

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

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

186 **2.2.1 Steered construction from groups**

187 For a graph $G = \langle V, E \rangle$ and a subgroup $\Gamma \subset \Phi^*(V)$ or its invertible transfor-
 188 mations, Definition 8 is applicable for $\mathcal{S}(\Gamma)$, but not for $\mathcal{S}(V)$ as V is not a
 189 group. Nonetheless, our point here is that we will use the group convolution
 190 on $\mathcal{S}(\Gamma)$ to construct the convolutions on $\mathcal{S}(V)$.

191 For now, let's assume Γ is in one-to-one correspondence with V , and let's
 192 define a bijective map φ from Γ to V . We denote $\Gamma \xrightarrow{\varphi} V$ and $g_v \xrightarrow{\varphi} v$.

193 Then, the linear morphism $\tilde{\varphi}$ from $\mathcal{S}(\Gamma)$ to $\mathcal{S}(V)$ defined on the Dirac bases
 194 by $\tilde{\varphi}(\delta_g) = \delta_{\varphi(g)}$ is a linear isomorphism. Hence, $\mathcal{S}(V)$ would inherit the same
 195 inherent structural properties as $\mathcal{S}(\Gamma)$. For the sake of notational simplicity,
 196 we will use the same symbol φ for both φ and $\tilde{\varphi}$ (as done between f and
 197 L_f). A commutative diagram between the sets is depicted on Figure 2.1.

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

Figure 2.1: Commutative diagram between sets

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

201 **Lemma 9. Relation between $\mathcal{S}(\Gamma)$ and $\mathcal{S}(V)$**

202 $\forall s \in \mathcal{S}(\Gamma), \forall u \in V, \varphi(s)[u] = s[\varphi^{-1}(u)] = s[g_u]$

Proof.

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

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

203

□

204 Hence, we can steer the definition of the group convolution from $\mathcal{S}(\Gamma)$ to
205 $\mathcal{S}(V)$ as follows:

206 **Definition 10. Group convolution II**

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

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

209

210 **Lemma 11. Relation between group convolution I and II**

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

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

212

213 *Proof.* Using Lemma 9,

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

214

□

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

216 **Proposition 12. Equivariance to $\varphi(\Gamma)$**

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

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

219

Proof.

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

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

220 Because φ is an isomorphism, its inverse $c \mapsto g_c$ is also an isomorphism and

221 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:

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

222

□

223 *Remark.* Note that convolution operators of the form $f_w = . *_\Pi w$ are also
 224 equivariant to Γ , but the proposition and the proof are omitted as they are
 225 similar to the latter.

226 In fact, both group convolutions are the same as the latter one borrows the
 227 algebraic structure of the first one. Thus we only obtain equivariance to $\varphi(\Gamma)$
 228 when φ also transfer the group structure from Γ to V , and the converse don't
 229 hold. To obtain equivariance to Γ (and its converse), we will drop the direct
 230 homomorphism condition, and instead we will take into account the fact that
 231 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 $L : \Gamma \times V \rightarrow V, (g, v) \mapsto L_g(v)$, 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.

$$\begin{array}{ccc} g_u & \xrightarrow{g_v} & g_v g_u \\ \varphi \downarrow & & \downarrow \varphi \\ u & \xrightarrow[g_v]{(P)} & \varphi(g_v g_u) \end{array}$$

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

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

247

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 φ exhibits the equivalence.

249

250 **Definition 15. φ -Equivalence**

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

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

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

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

257 **Definition 16. Group convolution III**

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

$$s_1 *_{\text{III}} s_2 = \sum_{v \in V} s_1[v] g_v(s_2) \quad (3)$$

$$= \sum_{g \in \Gamma} s_1[\varphi(g)] g(s_2) \quad (4)$$

260

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

264 **Lemma 17. Relation with group convolution II**

265 $\Gamma \stackrel{\varphi}{\equiv} V \Leftrightarrow *_{\text{II}} = *_{\text{III}}$

Proof.

$$\forall s_1, s_2 \in \mathcal{S}(V),$$

$$\begin{aligned} s_1 *_{\text{II}} s_2 &= s_1 *_{\text{III}} s_2 \\ \Leftrightarrow \forall u \in V, \sum_{v \in V} s_1[v] s_2[\varphi(g_v^{-1} g_u)] &= \sum_{v \in V} s_1[v] s_2[g_v^{-1}(u)] \end{aligned} \quad (5)$$

266 Hence, the direct sense is obtained by applying (P).
 267 For the converse, given $u, v \in V$, we first realize (5) for $s_1 := \delta_v$, obtaining
 268 $s_2[\varphi(g_v^{-1}g_u)] = s_2[g_v^{-1}(u)]$, which we then realize for a real signal s_2 having no
 269 two equal entries, obtaining $\varphi(g_v^{-1}g_u) = g_v^{-1}(u)$. From the latter we finally
 270 obtain (P) with the one-to-one correspondence $g_{v'} := g_v^{-1}$. \square

271 We can then coin the term φ -convolution.

272 **Definition 18. φ -convolution**

273 Let $\Gamma \stackrel{\varphi}{\cong} V$, the φ -convolution between two signals s_1 and $s_2 \in \mathcal{S}(V)$ is
 274 defined as:

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

275

276 This time, we do obtain equivariance to Γ as expected, and the full charac-
 277 terization as well.

278 **Proposition 19. Characterization by right-action equivariance to Γ**

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

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

282

283 *Proof.* 1. From left to right:

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

286 because of (P).

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

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

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

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

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

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

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

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

287 Of course, we also have that f_w is linear.

288 2. From right to left:

289 Let $f \in \mathcal{L}(\mathcal{S}(V))$, $s \in \mathcal{S}(V)$. By linearity of f , we distribute $f(s)$ on
290 the family of dirac signals:

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

291 Thanks to (P), we have that:

$$g_v(\varphi(\text{Id})) = \varphi(g_v \text{Id}) = v$$

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

$$\text{So, } \delta_v = g_v(\delta_{\varphi(\text{Id})})$$

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

we obtain from (9) that:

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

□

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

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

Where $\stackrel{(\diamond)}{=}$ 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:

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

325

326 *Proof.* On one hand, Lemma 21 gives $r *_M s = \varphi(r) *_{III} s$. On the other hand,
 327 Lemma 11 gives $\forall v \in V, (r *_I \varphi^{-1}(s))[g_v] = (\varphi(r) *_{II} s)[v]$. Then Lemma 17
 328 concludes. \square

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

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

340 **Proposition 23. Equivariance to Γ through left action**

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

$$\forall g, h \in \Gamma, gh = hg \Leftrightarrow \forall w, g \in \Gamma, w *_M g(.) = g \circ (w *_M .)$$

343 *Proof.* Let $w, g \in \Gamma$, and define $f_w : s \mapsto w *_M s$. In the following expressions,
 344 Γ is abelian if and only if (10) and (11) are equal (the converse is obtained

345 by particularizing on well chosen signals):

$$f_w \circ g(s) = \sum_{h \in \Gamma} w[h] hg(s) \quad (10)$$

$$= \sum_{h \in \Gamma} w[h] gh(s) \quad (11)$$

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

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

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

346

□

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

350 **Corrolary 24. Characterization by left-action equivariance to Γ**

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

If $\Gamma \cong V$ and Γ is abelian,

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

354

355 *Proof.* By picking φ such that $\Gamma \stackrel{\varphi}{\cong} V$ with Lemma 22 and using the relation
 356 between $*_{\mathbf{M}}$ and $*_{\varphi}$. □

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

359 2.3 Inclusion of the edge set in the construction

360 The constructions from the previous section involve the vertex set V and de-
 361 pend on Γ , a subgroup of the set of invertible transformations on V . There-
 362 fore, it looks natural to try to relate the edge set and Γ .

363 There are two approaches. Either Γ describes an underlying graph structure
 364 $G = \langle V, E \rangle$, either G can be used to define a relevant subgroup Γ to which
 365 the produced convolutive operators will be equivariant. Both approaches
 366 will help characterize classes of graphs that can support natural definitions
 367 of convolutions.

368 2.3.1 Edge-constrained convolutions

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

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

373 Definition 25. Edge-constrained transformation

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

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

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

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

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

383 **Definition 26. Cayley graph**

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

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

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

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

390 **Convolution on Cayley graphs**

391 In the case of Cayley graphs, it is clear that $\mathcal{U} \subseteq \Phi_{\text{EC}}^*$ and $\Phi^* \supseteq \langle \mathcal{U} \rangle \equiv V$.
392 So that they admit (EC) φ -convolutions, and (EC) M-convolutions in the
393 abelian case.

394 More precisely, we obtain the following characterization:

395 **Proposition 27. Characterization by Cayley subgraph isomorphism**

396 Let a graph $G = \langle V, E \rangle$, then:

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

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

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

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

404 2. From right to left:

405 Let a graph $G = \langle V, E \rangle$. We suppose it contains a subgraph $\vec{G}_s =$
 406 $\langle V_s, E_s \rangle$ that is graph-isomorph to a Cayley graph $\vec{G}_c = \langle V_c, E_c \rangle$, gen-
 407 erated by \mathcal{U} . Let ψ be a graph isomorphism from G_s to G_c . To obtain
 408 the proof, we need to find a group of invertible transformations Γ of V_s
 409 generated by a set of (EC) transformations, such that $\Gamma \equiv V_s$.

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

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

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

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

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

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

418 and

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

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

422 $g \mapsto L_g$ on V_c is in fact an isomorphism as

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

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

424 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
425 map φ as:

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

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

427 Additionally, we have:

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

428 That is, φ is a bijective equivariant map and $\langle L_{\mathcal{U}} \rangle = \Gamma \stackrel{\varphi}{\cong} V_s$. Moreover,
429 $L_{\mathcal{U}}$ is a set of (EC) transformations thanks to (a). Therefore, G admits
430 an (EC) φ -convolution.

431 □

432 **Corrolary 28. Characterization by φ**

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

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

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

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

437 2.3.2 Intrinsic properties

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

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

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

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

445 Proposition 29. Locality

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

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

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

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

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

459 **Definition 30. Supporting set**

460 The *supporting set* of an (EC) convolution operator f_w , is a set $\mathcal{N} \subset \Phi_{\text{EC}}^*$,
 461 such that

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

464 **Definition 31. Local patch for $*_\varphi$**

465 The *local patch* at $u \in V$ of an (EC) φ -convolution operator f_w is defined as
 466 $\mathcal{K}_u = g_u(\varphi(\mathcal{N}^{-1}))$.

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

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

473 **Proposition 32. Weight sharing**

474 $\forall a, \alpha \in V, \forall b \in \mathcal{K}_a : \exists \beta \in \mathcal{K}_\alpha \Leftrightarrow g_\beta^{-1}(\alpha) = g_b^{-1}(a)$

475 *Proof.* By using (P),

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

476

□

477 2.3.3 Stricly edge-constrained convolutions

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

481 **Definition 33. Strictly (EC) convolution operator**

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

484 *Remark.* (EC*) convolution operators are simpler to obtain as we can con-
 485 struct them just with $\mathcal{U} \subset \Phi_{\text{EC}}^*(G)$ without composing the transformations.

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

$$490 \quad \text{(i)} \quad \forall s \in \mathcal{S}(V), \forall u \in V, f_w(s)[u] \stackrel{(\varphi)}{=} \sum_{v \in \mathcal{K}_u} s[v] w[g_v^{-1}(u)]$$

$$491 \quad \text{(ii)} \quad \forall s \in \mathcal{S}(V), f_w(s) \stackrel{(\text{M})}{=} \sum_{g \in \mathcal{N}} w[g] g(s)$$

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

495 From these expressions, it is clear that Γ needs not to be fully determined
 496 to calculate $f_w(s)[u]$. The case (ii) is the simplest as the only requirement
 497 is a supporting set \mathcal{N} of (EC) invertible transformations. In the case (i), we
 498 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 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*) construction 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. $\forall g \in \Upsilon, \exists ! g^{-1} \in \Upsilon$ 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.

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

546 **Definition 36. Partial equivariant map**

547 A map φ from a groupoid Υ partially acting on the destination set V is said
 548 to be a *partial equivariant map* if

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

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

551 **Definition 37. Partial transformations groupoid**

552 The *partial transformations groupoid* $\Psi^*(V)$, is the set of invertible par-
 553 tial transformations, equipped with the functional composition law with do-
 554 main \mathcal{D} such that

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

555 *Remark.* Note that a subgroupoid $\Upsilon \subset \Psi^*(V)$ is domain-symmetric when
 556 $\exists v \in V, g(v) \in \mathcal{D}_h \Leftrightarrow \exists u \in V, h(u) \in \mathcal{D}_g$

557 **2.4.3 Construction of partial convolutions**

558 The expression of the convolution we constructed in the previous section
 559 cannot be applied as is. We first need to extend the algebraic objects we
 560 work with. Extending a partial transformation g on the signal space $\mathcal{S}(V)$
 561 (and thus the convolutions) is a bit tricky, because only the signal entries
 562 corresponding to \mathcal{D}_g are moved. A convenient way to do this is to consider
 563 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 $\varphi : \Upsilon \rightarrow V$. It can be extended to a (total) equivariant map $\varphi : \Upsilon^0 \rightarrow V^0 = V \cup \varphi(0)$, 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. Additionally, we must have $\forall (g, h) \notin \mathcal{D}, g(\varphi(h)) = \varphi(gh) = \varphi(0) = 0_V$. \square

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 $g(v) = 0_V \Leftrightarrow v \notin \mathcal{D}_g$.

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

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

587 *Proof.* Straightforward. □

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

590 **Definition 41. Partial convolution**

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

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

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

597 **Symmetrical expressions**

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

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

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

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

Proposition 42. Characterization by equivariance to Υ

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

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

616 (b) Converse:

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

$$g_v(e_v^r) = v$$

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

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

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

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

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

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

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

626 Given $x \in V$, denote its equivalence class $\mathcal{R}(x)$. Under the hy-
 627 pothesis of the axiom of choice (Zermelo, 1904) (if V is infinite),
 628 define the set \aleph that contains exactly one representative per equiv-
 629 alence class. Let $w = \sum_{n \in \aleph} w_n$. Then V is the disjoint union
 630 $V = \cup_{n \in \aleph} \mathcal{R}(n)$ and (13) rewrites:

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

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

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

634 □

635 Inclusion of (EC)

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

639 Limitation of partial convolutions

640 However, because of the groupoid associativity, if $g \in \Psi_{\text{EC}}^*(G)$, then, any
 641 $v \in V$ s.t. $g(u) = v$ would be constrained to allow to be acted by every
 642 h s.t. $(h, g) \in \mathcal{D}$, which fails at unbounding the supporting set of a partial
 643 (EC*) convolutions.

2.4.4 Construction of path convolutions

To answer the limitation of partial convolutions, given $g \in \langle \mathcal{U} \rangle$ where $\mathcal{U} \subset \Psi_{\text{EC}}^*(G)$, 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 $\mathcal{U} \subset \Psi_{\text{EC}}^*(G)$. 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:

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

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

668 **Lemma 45.**

669 Note the following properties:

- 670 1. $(p, q) \in \mathcal{D}_\ltimes \Leftrightarrow \alpha(p) = \beta(q)$
- 671 2. $\alpha(p) = \beta(p^{-1})$
- 672 3. $e_p^l = pp^{-1} = (\text{Id}, \beta(p))$ and $e_p^r = p^{-1}p = (\text{Id}, \alpha(p))$
- 673 4. γ is a groupoid partial action. We will denote γ_p instead of $\gamma(p)$.

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

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

680 **Definition 46. Traversal set**

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

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

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

690 *Remark.* The assumption that the graph G is connected doesn't lose gener-
 691 ality as the construction can be replicated to each connected component in
 692 the general case.

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

695 **Lemma 47. Path φ -Equivalence**

696 Let $(\mathcal{U}, \mathcal{T}) \in \text{trav}(G)$. Given $v \in V$, there exists a unique $p_v \in \mathcal{T} \ltimes G$ such
 697 that $\alpha(p_v) = r$ and $\beta(p_v) = v$. Define $\varphi : p_v \mapsto v$. Then $\varphi : \alpha_{\mathcal{T} \ltimes G}^{-1}\{r\} \rightarrow V$ is
 698 a bijective partial equivariant map.

699 *Proof.* Bijectivity is a consequence of the spanning tree structure of \mathcal{T} . Equiv-
 700 ariance because $\gamma_{p_v}(u) = \gamma_{p_v} \gamma_{p_u}(r) = \gamma_{p_v p_u}(r) = \varphi(p_v p_u)$. \square

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

702 **Definition 48. Path convolution**

703 Let $(\mathcal{U}, \mathcal{T}) \in \text{trav}(G)$. The *path convolution* is the partial convolution based
 704 on the path subgroupoid $\mathcal{T} \ltimes G$, which uses the groupoid partial action
 705 $\gamma := \gamma^{\mathcal{U} \ltimes G}$ of the embedding groupoid $\mathcal{U} \ltimes G$.

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

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

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

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

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

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

714 **Proposition 49. Characterization by equivariance to $\mathcal{U} \ltimes G$'s action**

715 Let $(\mathcal{U}, \mathcal{T}) \in \text{trav}(G)$.

- 716 (i) The class of linear transformations of $\mathcal{S}(V)$ that are equivariant to the
 717 path actions of $\mathcal{U} \ltimes G$ is exactly the path φ -convolution right-operators;
 718 (ii) in the abelian case, they are also exactly the M-convolution left-operators.

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

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

730 **(EC*) Path convolution operators**

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

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

765 **Summary of practical (EC*) convolution operators**

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

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

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

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