An introduction to groups, actions, and equivariance

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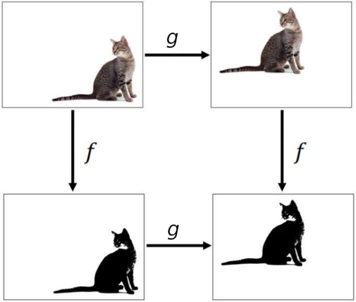
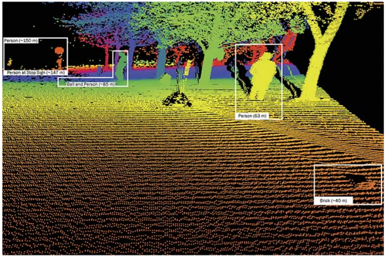
Motivation: “symmetry”



https://www.doc.ic.ac.uk/~bkainz/teaching/DL/notes/equivariance.pdf

Many other examples



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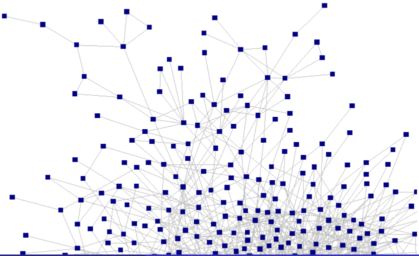

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- Group actions describe things like "translate the cat"

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Intuitively, in terms of our example:

- Group actions describe things like "translate the cat"
- Equivariance says that the network "respects this translation"

Groups: intuition

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Rough answer: a "symmetry" is an information-preserving transformation

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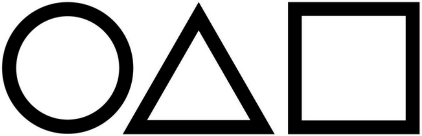
But what *are* "symmetries"?

Rough answer: a "symmetry" is an information-preserving transformation

Warning: many people use "symmetry" more specifically to mean a transformation that leaves an object unchanged



Towards a theory of symmetry

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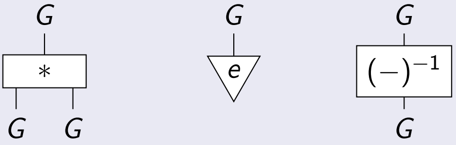
Basic idea: groups model collections of things that behave like this

Groups: formal definition

Definition

A group is a set G equipped with operations



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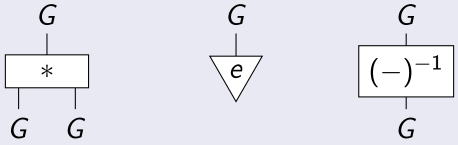

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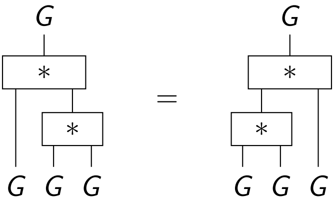
Refer to these as multiplication, unit, and inversion

Associativity

Group multiplication must be associative



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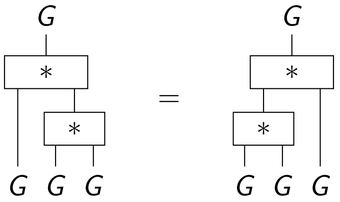
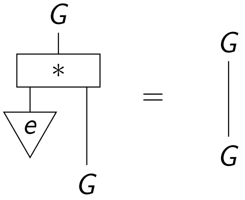


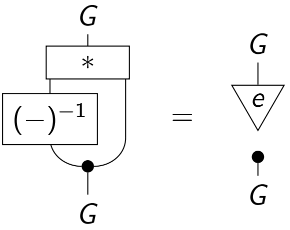
In classical notation, this just says:

$$g(hn) = (gh)n \qquad \text{for all } g, h, n \in G$$

Other group axioms

Group multiplication must also be unital and admit inverses





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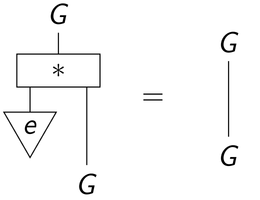

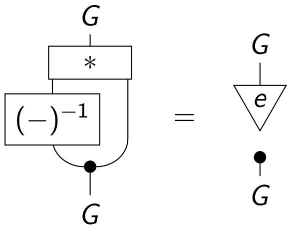

In classical notation, this says

$$eg = g \qquad \text{and} \qquad g^{-1}g = e \qquad\qquad \text{for all } g \in G$$

Examples of groups

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Representation theory gives descriptions of these in terms of matrices, e.g.:

$$\mathrm{O}(d) \cong \{Q \in \mathbb{R}^{d \times d} \mid QQ^T = I\}$$

Actions

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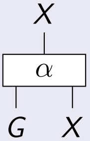
Definition

An action of a group G on a set X is a function of the form



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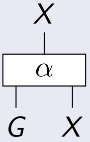


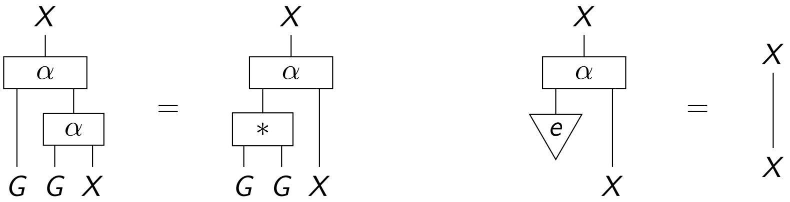
that satisfies some axioms (to come next)

In classical notation, actions are often written as

$$\alpha(g, x) = g \cdot x \qquad \text{where } g \in G \text{ and } x \in X$$

Action axioms

To be an action, α must satisfy the following:



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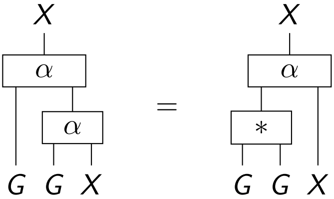
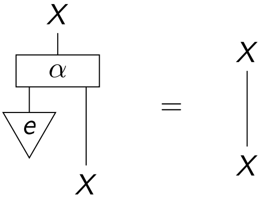


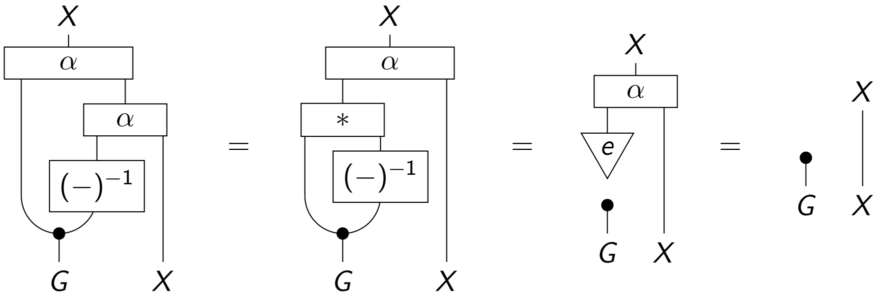


In classical notation, this says

$g \cdot (h \cdot x) = (gh) \cdot x$ and $e \cdot x = x$ for all $g, h \in G$ and $x \in X$

Invertibility

One consequence of this definition is the following:



This says that group actions are always invertible

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- $\mathrm{SE}(3)$ acts on 3D point cloud by rotation followed by a translation:

$$(t, R) \cdot x = Rx + t$$

- And many others

Equivariance

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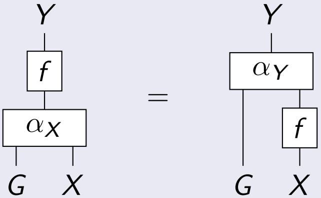
Definition

Given actions α_X and α_Y of a group G on some sets X and Y, a function $f : X \to Y$ is equivariant with respect to α_X and α_Y if



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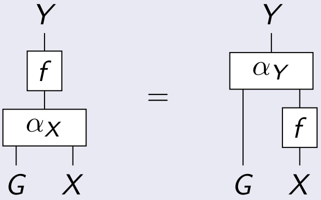

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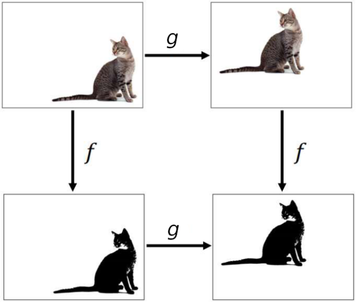
Examples of equivariance

We can now formalise the original example:



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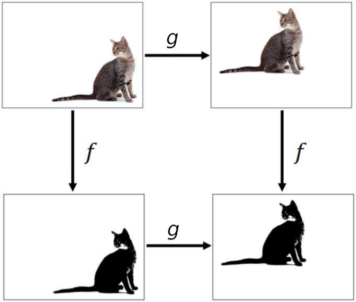


Here:

- G is $\mathbb{T}_2$, the group of 2D translations
- X is the set of colour images
- Y is the set of black-and-white images
- $\alpha_X(g, x)$ is the translation of x by g (with α_Y similar)

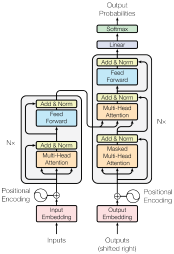


Figure 1: The Transformer - model architecture.

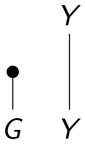
Attention is equivariant to the symmetric group: for $\sigma \in S_n$ we have

$$\begin{array}{ccc} (x_1, \ldots, x_n) & \stackrel{\sigma}{\longmapsto} & (x_{\sigma(1)}, \ldots, x_{\sigma(n)}) \\ \downarrow \text{Attn.} & & \downarrow \text{Attn.} \\ (e_1, \ldots, e_n) & \stackrel{\sigma}{\longmapsto} & (e_{\sigma(1)}, \ldots, e_{\sigma(n)}) \end{array}$$

This constitutes a very elegant solution to catastrophic forgetting

Invariance

For every set Y, we can define the trivial action ε as



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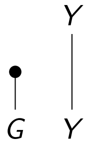

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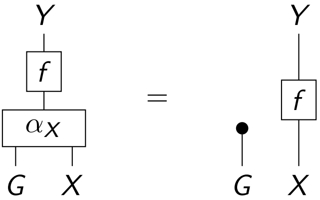
Equivariance with respect to α_X and ε is called invariance:



Example of invariance

For processing sequences, with $X = \mathbb{R}^n$, often want:

$$f(x_1, \ldots, x_n) = f(x_{\sigma(1)}, \ldots, x_{\sigma(n)}) \qquad \text{for all permutations } \sigma$$

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DeepSets [Zaheer et al., 2017] is a well-known example of such an f

Enforcing equivariance

Fundamental problem of GDL

Suppose G is a group acting on X and Y. How can we parameterise a function $f : X \to Y$ that is equivariant with respect to these actions?

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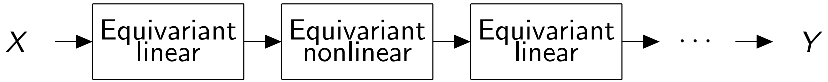
Two key approaches: intrinsic equivariance and symmetrisation

Intrinsic equivariance

Overall model $f : X \to Y$ has form



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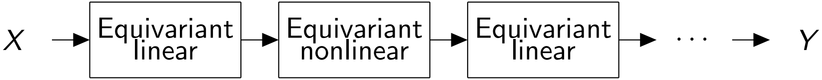

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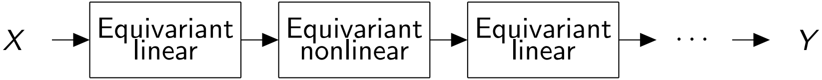

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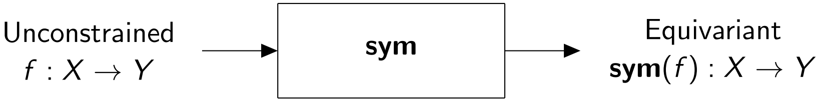
Many examples throughout GDL (CNNs, GNNs, etc.)

Works very well, but some caveats:

- Requires hand engineering for each case
- Can be somewhat brittle at scale (e.g. AlphaFold 2 vs. 3)

Symmetrisation

Recent interest instead in symmetrisation:



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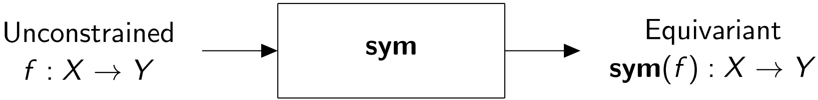

Here f is completely general and opaque

Symmetrisation: example

Early example is Janossy pooling [Murphy et al., 2019]: given

$$f : X^n \to \mathbb{R}^d,$$

the following function $X^n \to \mathbb{R}^n$ is always permutation invariant:

$$\frac{1}{n!} \sum_{\sigma \in S_n} f\big(x_{\sigma(1)}, \dots, x_{\sigma(n)}\big)$$

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In turn, this generalises deep sets [Zaheer et al., 2017]

Symmetrisation: other examples

Other recent examples, given $f : X \to \mathbb{R}^d$ and a group G

$\frac{1}{\lvert\mathcal{F}(x)\rvert} \sum_{g \in \mathcal{F}(x)} g \cdot f(g^{-1} \cdot x)$	[Puny et al., 2022]
$h(x) \cdot f(h(x)^{-1} \cdot x)$	[Kaba et al., 2023]
$\mathbb{E}_{\boldsymbol{G} \sim p(g \mid x)}[\boldsymbol{G} \cdot f(\boldsymbol{G}^{-1} \cdot x)]$	[Kim et al., 2023]

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Under some conditions, each is equivariant in $x \in X$, even if f is arbitrarily complex

Stochastic equivariance: illustration

Equivariance can also be generalised to stochastic models

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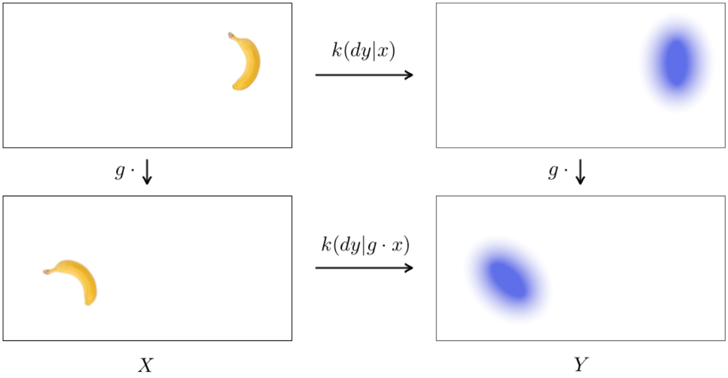
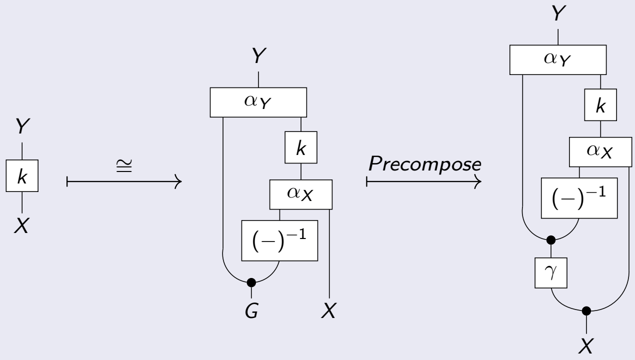


A general theory of symmetrisation

Theorem ([Cornish, 2024])

Given suitable $\gamma : X \to G$, can always symmetrise a general $k : X \to Y$ via:



Moreover, every (natural) symmetrisation procedure has this form.

Thank you!

References I

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