Stochastic neural network symmetrisation in Markov categories

Rob Cornish

Department of Statistics, University of Oxford

June 19, 2024

Motivation

Top-down, formal constraints for machine learning models

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Top-down, formal constraints for machine learning models

Want new methodology as well as a better framework

Paper

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[Submitted on 17 Jun 2024]

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Subjects: **Machine Learning (stat.ML)**; Machine Learning (cs.LG); Category Theory (math.CT)

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Builds heavily on work in Markov categories, and CT more generally

Background: group equivariance

Often want a function $f : X \to Y$ to be equivariant with respect to the action of a group G, so that

$$f(g \cdot x) = g \cdot f(x) \qquad \text{for all } x \in X \text{ and } g \in G$$

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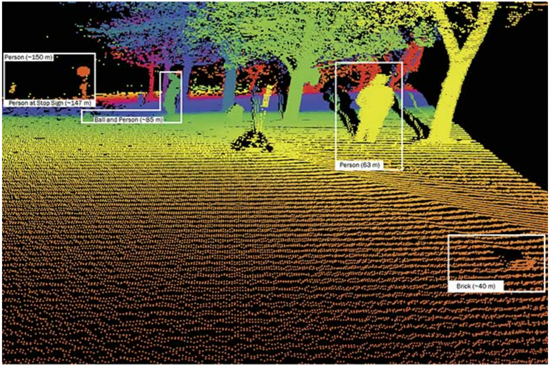
Invariance is a special case: $f(g \cdot x) = f(x)$

Examples

Very important for geometric data, such as point clouds:



Taken from www.photonics.com

Other examples: 2D images, sets, graphs, and more

Parametrising equivariance

How can we parameterise an equivariant neural network f?

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Instance of a more general problem: how to ensure a neural network satisfies some "top down" algebraic constraint?

Intrinsic equivariance

Major strategy is intrinsic equivariance:

- Constrain individual layers to obtain equivariance, then compose

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- Constrain individual layers to obtain equivariance, then compose

Some problems with this approach:

- Often quite specific to particular groups and actions
- Hand engineering (e.g. nonlinear layers are often ad hoc)
- Can be brittle and hard to scale

Symmetrisation

Recent interest in symmetrisation approaches: modify an arbitrary neural network to obtain equivariance

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Example: when it makes sense, the following is invariant:

$$x \mapsto \frac{1}{|G|} \sum_{g \in G} f(g^{-1} \cdot x)$$

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$$x \mapsto \frac{1}{|G|} \sum_{g \in G} f(g^{-1} \cdot x)$$

Various examples in the literature, including very recently, e.g. [Murphy et al., 2019, Puny et al., 2022, Kaba et al., 2023, Kim et al., 2023]

Stochastic equivariance

More general model: f depends on some additional randomness

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A natural equivariance condition is then:

$$f(g \cdot x, \boldsymbol{U}) \stackrel{\mathrm{d}}{=} g \cdot f(x, \boldsymbol{U})$$

Idea: equivariance across repeated executions

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Of interest in e.g. generative modelling and reinforcement learning, and for uncertainty quantification

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Stochastic symmetrisation does not appear to have been studied in the literature

Markov kernels

Convenient to model $(f, \boldsymbol{U})$ as a single entity, a Markov kernel $k : X \to Y$

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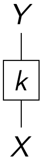
Leads to Markov categories as a natural framework:



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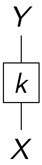

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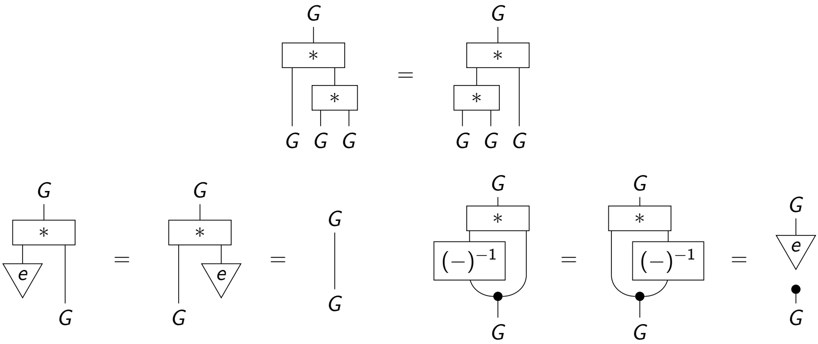
Covers deterministic case also

Group theory in Markov categories

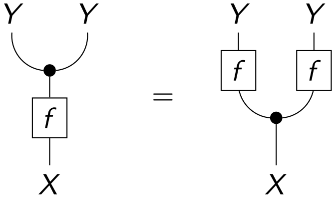
Basic axioms

A group is a Markov category C is an object G together with deterministic morphisms such that



Determinism

Recall: a morphism $f : X \to Y$ in C is deterministic if



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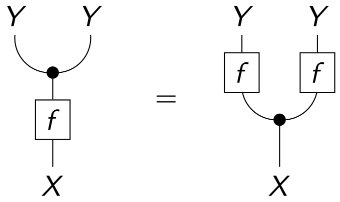

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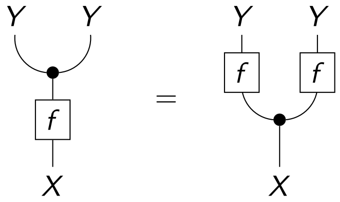
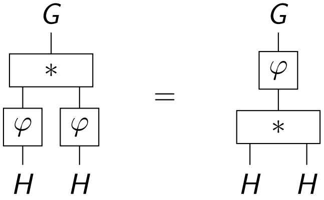


The deterministic morphisms in C form a cartesian monoidal subcategory called $\mathsf{C}_{\mathrm{det}}$

This lets us lift set-theoretic results (e.g. $(g^{-1})^{-1} = g$) to C via the Yoneda Embedding

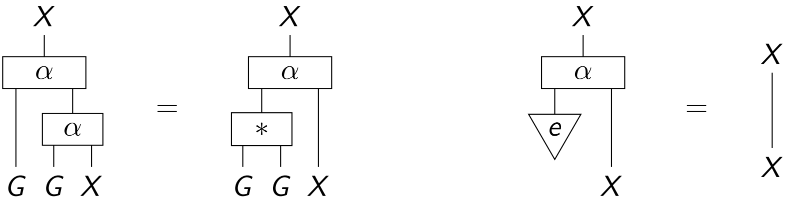
Homomorphisms

Also obtain natural definitions of homomorphism $\varphi : H \to G$ in $\mathsf{C}_{\mathrm{det}}$:



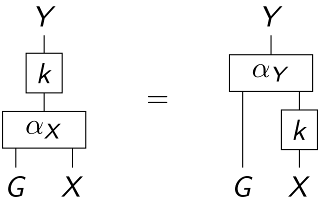
Actions

Similarly, action $\alpha : G \otimes X \to X$ in $\mathsf{C}_{\mathrm{det}}$:



Equivariance

This gives rise to a natural notion of equivariance (now in C): a morphism $k : X \to Y$ is equivariant with respect to α_X and α_Y if



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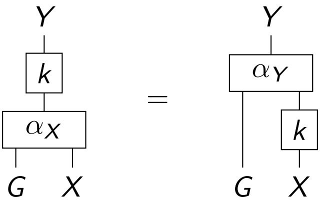

Becomes invariance when α_Y is trivial.

Recovers the desired definitions:

- For C = Set, $k(g \cdot x) = g \cdot k(x)$
- For C = Stoch, $k(dy|g \cdot x) = (g \cdot k)(dy|x)$ as desired

Orbits

Given an action $\alpha : G \otimes X \to X$, a orbit map is a deterministic coequaliser in C as follows:

$$G \otimes X \underset{\varepsilon}{\overset{\alpha}{\rightrightarrows}} X \xrightarrow{q} X/G$$

that is moreover preserved by every functor $(-) \otimes Y$

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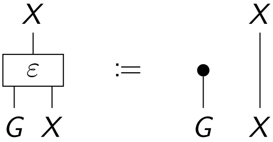
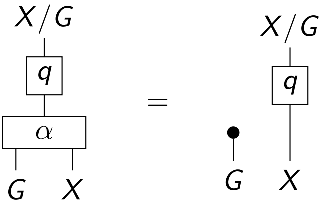
Here ε is the trivial action



Orbits: intuition

Key idea is that q is initial among invariant maps



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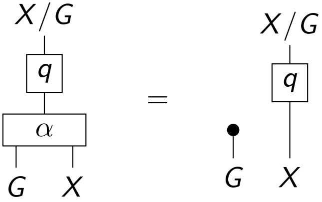

Preservation condition ensures: if q is an orbit map, then $q \otimes \mathrm{id}_Y$ is, where G acts trivially on Y

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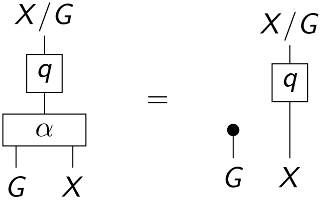

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Existence of orbits

Theorem

The Markov category TopStoch *of topological spaces and continuous Markov kernels admits all orbit maps.*

Not sure about the general case (although they seem forthcoming in practice)

Cosets

Recall from classical theory that a subgroup $H \subseteq G$ induces a space of cosets:

$$G/H := \{gH \mid g \in G\}$$

Corresponds to orbits under action $h \cdot g = gh^{-1}$

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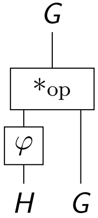
$$G/H := \{gH \mid g \in G\}$$

Corresponds to orbits under action $h \cdot g = gh^{-1}$

Given a homomorphism $\varphi : H \to G$, can define a φ-coset map as an orbit map of the following action:



where $*_{\mathrm{op}}$ does right-multiplication (by inverse)

Recap

In a general Markov category theory, we can talk about:

- Groups
- Homomorphisms
- Actions
- Orbits
- Cosets
- Also semidirect and direct products

Symmetrisation

Markov category of equivariant maps

Given a group G in C, always obtain a Markov category C^G as follows:

- Objects are pairs (X, α_X), where α_X is an action on X in C

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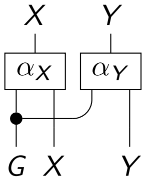

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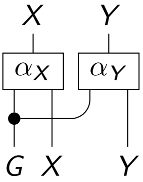

- Other components inherited from C

(*Almost* Eilenberg-Moore category of action monad)

Restriction

Given a homomorphism $\varphi : H \to G$, obtain a functor $R_\varphi : \mathsf{C}^G \to \mathsf{C}^H$ by restriction

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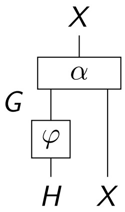
Idea: $R_\varphi(X, \alpha)$ is X equipped with the H-action



Symmetrisation procedures

In this context, can define a symmetrisation procedure as a function

$$\mathsf{C}^H(R_\varphi X, R_\varphi Y) \to \mathsf{C}^G(X, Y)$$

(where actions are denoted implicitly)

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Key idea: sends "less equivariant" morphisms to "more equivariant" ones

- E.g. consider $H = I$ the trivial group

Compositionality

Can compose procedures sequentially: given homomorphisms

$$K \xrightarrow{\phi} H \xrightarrow{\varphi} G$$

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can symmetrise as follows:

$$\mathsf{C}^K(R_\phi R_\varphi X, R_\phi R_\varphi Y) \xrightarrow{\mathsf{sym}_\phi} \mathsf{C}^H(R_\varphi X, R_\varphi Y) \xrightarrow{\mathsf{sym}_\varphi} \mathsf{C}^G(X, Y).$$

where here also $R_\phi R_\varphi = R_{\varphi \circ \phi}$

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where here also $R_\phi R_\varphi = R_{\varphi \circ \phi}$

Can therefore "build up" complex equivariance constraints in a structured way

Methodology

Motivating idea

Suppose R_φ has a left adjoint E (often true classically [May et al., 1997])

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$$\mathsf{C}^H(R_\varphi X, R_\varphi Y) \cong \mathsf{C}^G(ER_\varphi X, Y)$$

This recharacterises the problem of symmetrisation:

- Before, H-equivariance $\mapsto$ G-equivariance
- Now, G-equivariance $\mapsto$ G-equivariance (of another kind)

General approach

When a left adjoint $E \dashv R_\varphi$ exists, obtain the following methodology:

$$\mathsf{C}^H(R_\varphi X, R_\varphi Y) \xrightarrow{\quad\cong\quad} \mathsf{C}^G(ER_\varphi X, Y) \xrightarrow{\text{Precompose}} \mathsf{C}^G(X, Y)$$

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In the second step, require a morphism $X \to ER_\varphi X$ in C^G

This must be already G-equivariant, as for other symmetrisation approaches

- But now this can be very trivial compared with overall model

More general idea

A full left adjoint is quite onerous to obtain, and more than we need

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Classically in Set, have the following natural isomorphism:

$$ER_{\varphi} \cong G/H \otimes (-)$$

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Classically in Set, have the following natural isomorphism:

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Our idea: show directly that previous isomorphism of hom sets hold when ER_φ is replaced like this

- Now G/H is the codomain of a φ-coset map

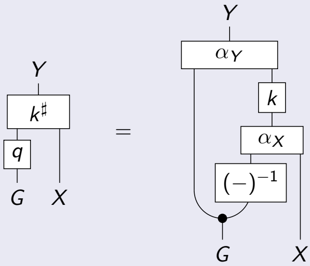
Main result

Theorem

Suppose a φ-coset map $q : G \to G/H$ exists. Then for all X and Y in C^G there is a bijection

$$\mathsf{C}^H(R_\varphi X, R_\varphi Y) \xrightarrow{\cong} \mathsf{C}^G(G/H \otimes X, Y)$$

that sends $k : R_\varphi X \to R_\varphi Y$ in C^H to the unique $k^\sharp$ such that



Some comments

Theoretically, corresponds to an equivalence of categories between:

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Practically, can compute bijection finding a section of φ-coset map

Resulting procedure

Overall procedure becomes as follows:

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Recovers all existing deterministic symmetrisation techniques I am aware of (in a sense inevitably) when combined with further averging step

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Directly gives rise to a novel procedure for stochastic symmetrisation also

Implementation

Application

The method of Kim et al. [2023] requires a stochastically equivariant subcomponent

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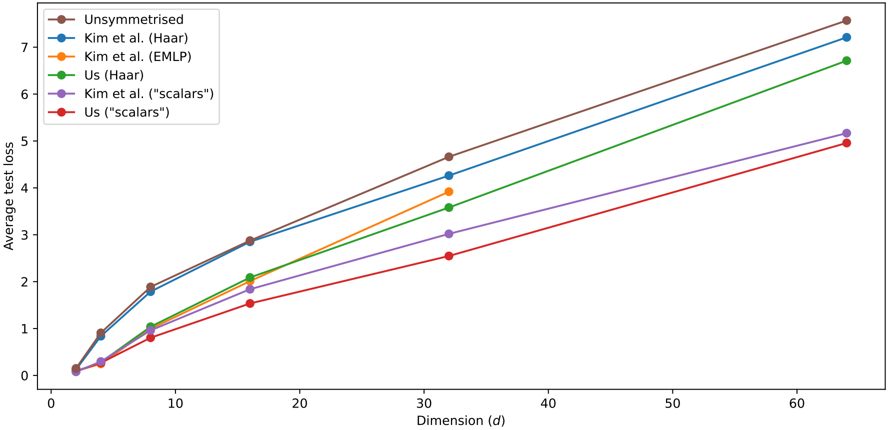
Consider learning the matrix inversion function $A \mapsto A^{-1}$, which is equivariant with respect to orthogonal group:

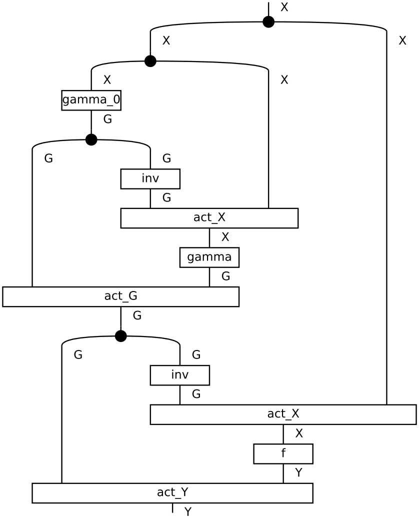
$$(QA)^{-1} = A^{-1}Q^{-1} = A^{-1}Q^T$$

More examples needed!

Results


Unsymmetrised
Kim et al. (Haar)
Kim et al. (EMLP)
Us (Haar)
Kim et al. ("scalars")
Us ("scalars")
Average test loss
Dimension (d)
0
1
2
3
4
5
6
7
0
10
20
30
40
50
60

Implementation - DisCoPy



Thank you!

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