Group invariant machine learning by fundamental domain projections

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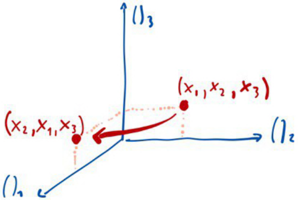
Abstract: In many applications one wants to learn a function that is invariant under a group action. For example, classifying images of digits, no matter how they are rotated. There exist many approaches in the literature to do this. I will mention two approaches that are very useful in many applications, but struggle if the group is big or acts in a complicated way. I will then explain our approach which does not have these two problems. The approach works by finding some "canonical representative" of each input element. In the example of images of digits, one may rotate the digit so that the brightest quarter is in the top-left, which would define a "canonical representative". In the general case, one has to define what that means. Our approach is useful if the group is big, and useless if the group is small, and I will present experiments for both cases. This is joint work with Benjamin Aslan and David Sheard.

Group actions

- Example: S_3 =permutation group of 3 elements
  $S_3 \curvearrowright \mathbb{R}^3$, e.g. $(1,2) \cdot (x_1, x_2, x_3) = (x_2, x_1, x_3)$



- $f : \mathbb{R}^3 \to \mathbb{R}$ group invariant $:\Leftrightarrow f(g \cdot x) = f(x)$ for all $g \in S_3$ and $x \in \mathbb{R}^3$
- Example:

$$\max : \mathbb{R}^3 \to \mathbb{R}$$
$$(x_1, x_2, x_3) \mapsto \max\{x_1, x_2, x_3\}$$

- Given many pairs $((x_1, x_2, x_3), \max\{x_1, x_2, x_3\})$ can train neural network NN
- Approximate max, but need not be group invariant
- Q1: how can find one group invariant NNs?
- Q2: does this improve performance of NNs?

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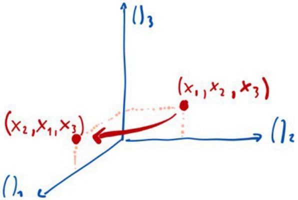

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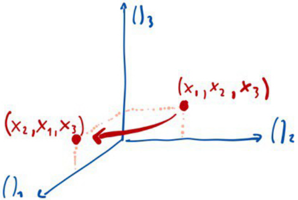

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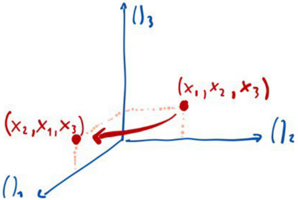

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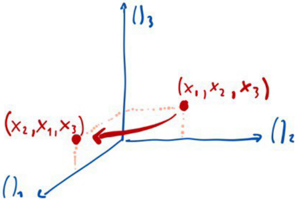

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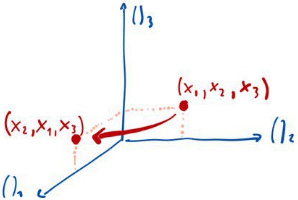

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2. Restricting weights of neural networks [Zaheer et al., 2017] ("Deep Sets"):

$$L : \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \mapsto \lambda_1 \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + \lambda_2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \text{ for } \lambda_1, \lambda_2 \in \mathbb{R}$$

   has $L(g \cdot x) = g \cdot L(x)$ (equivariant). Define $NN = \text{pool} \circ L \circ \sigma \circ L \circ \sigma \circ L$, where:
   - pool =some fixed group-invariant function $\mathbb{R}^3 \to \mathbb{R}$, e.g. $(x_1, x_2, x_3) \mapsto x_1 + x_2 + x_3$
   - σ =some non-linearity, e.g. ReLU

   Theorem: If $L : \mathbb{R}^3 \to \mathbb{R}^3$ is S_3-equivariant, then L is of this form.
3. Averaging techniques:
   Let $NN : \mathbb{R}^3 \to \mathbb{R}$ be a neural network architecture, not necessarily invariant

$$\widetilde{NN} : \mathbb{R}^3 \to \mathbb{R}$$

$$(x_1, x_2, x_3) \mapsto \sum_{g \in S_3} NN(g \cdot (x_1, x_2, x_3))$$

   $\Rightarrow \widetilde{NN}$ is group invariant $\rightsquigarrow$ train $\widetilde{NN}$ instead of NN

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New approach: group invariant pre-processing [Aslan et al., 2023]

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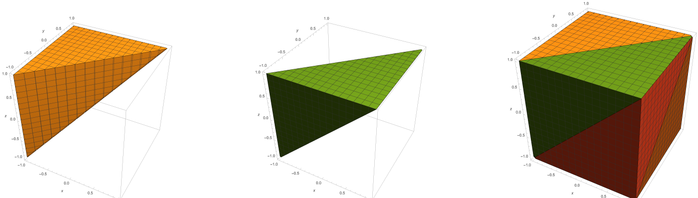
  Train $\widetilde{NN}$ instead of NN
  (Equivalent: train on data $(F(x), y)$ rather than (x, y))

How to get good F?

- $U \subset \mathbb{R}^N$ fundamental domain for $G \curvearrowright \mathbb{R}^N :\Leftrightarrow$
  1. U open and connected
  2. for all $x \in X$ the orbit $G \cdot x := \{g \cdot x : g \in G\}$ intersects $\overline{U}$
  3. if $G \cdot x$ intersects U, then the intersection is unique
- $F : \mathbb{R}^N \to \mathbb{R}^N$ def by $x \mapsto$ intersection of $G \cdot x$ and $\overline{U}$

Example: $G = S_3 \curvearrowright \mathbb{R}^3$, $U := \{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_1 > x_2 > x_3\}$



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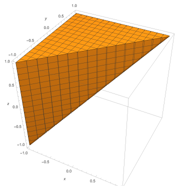

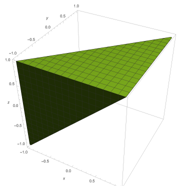

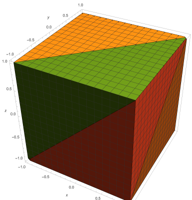

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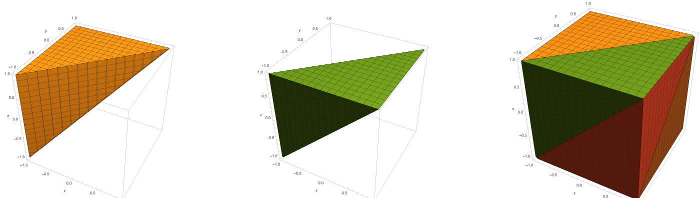

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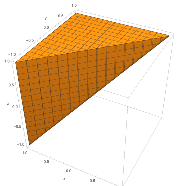
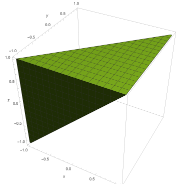
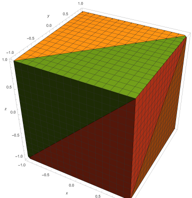

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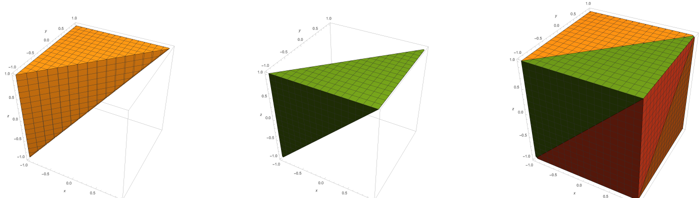

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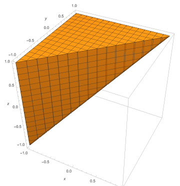
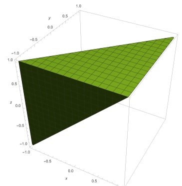
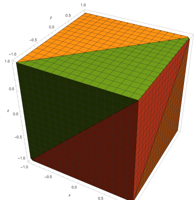

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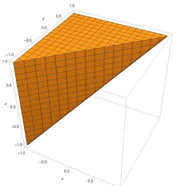

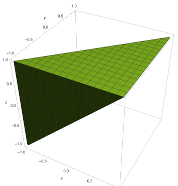

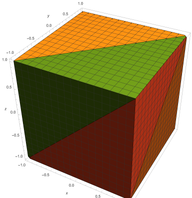

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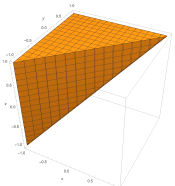

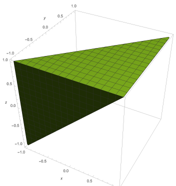

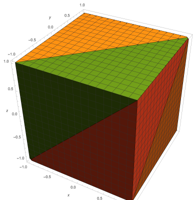

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For more general groups

- Groups can be large, e.g. $S_{15} \curvearrowright \mathbb{R}^{15}$ has $|S_{15}| = 15! \approx 10^{12}$
  $\Rightarrow$ data augmentation and averaging techniques impossible
  (NN with restricted weights still possible)
- Ours can be generalised to $G \curvearrowright M$ for M a complete Riemannian manifold

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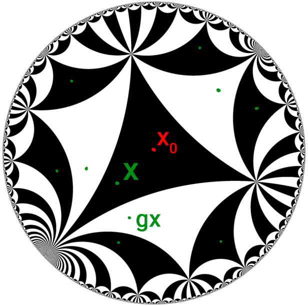
e.g. $SL(2, \mathbb{Z}) \curvearrowright \mathbb{H}^2$



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For more general groups

- Groups can be large, e.g. $S_{15} \curvearrowright \mathbb{R}^{15}$ has $|S_{15}| = 15! \approx 10^{12}$
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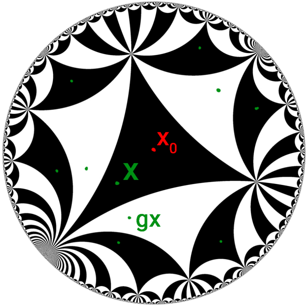

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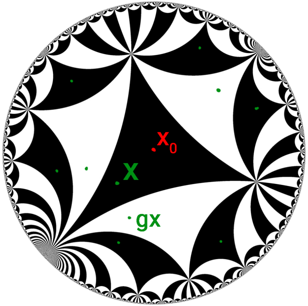

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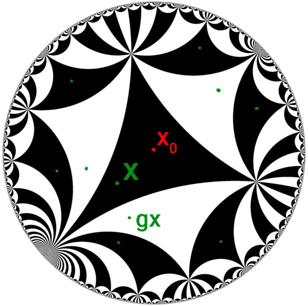

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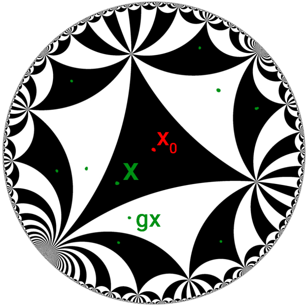

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Example 1: Rotated MNIST

- 28×28 pixel images showing a digit, possibly rotated by $90°, 180°, 270°$

- Learn

$$h : \mathbb{R}^{28\times 28} \to \{0, 1, 2, \ldots, 9\}$$
$$x \mapsto \text{the digit shown in } x$$

- Have $\mathbb{Z}_4 \curvearrowright \mathbb{R}^{28\times 28}$ by rotation and h is $\mathbb{Z}_4$-invariant (note $\mathbb{Z}_4 \subset S_{28\cdot 28} = S_{784}$)
- Define U (fundamental domain) and F (projection): (small lie, x_0 not generic)

$$x_0 = \left(\begin{array}{ccc|ccc} 4 & 4 & \ldots & 3 & 3 & \ldots \\ 4 & 4 & \ldots & 3 & 3 & \ldots \\ \vdots & \vdots & & \vdots & \vdots & \\ \hline 2 & 2 & \ldots & 1 & 1 & \ldots \\ 2 & 2 & \ldots & 1 & 1 & \ldots \\ \vdots & \vdots & & \vdots & \vdots & \end{array}\right), \quad \overline{U} := \left\{ x \in \mathbb{R}^{28\times 28} : \langle x, x_0\rangle = \max_{g\in S_4} \langle g\cdot x, x_0\rangle \right\}$$

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	No pre-processing	F
Linear	0.677 ± 0.001	0.784 ± 0.001
MLP	0.939 ± 0.001	0.953 ± 0.003
SimpNet (19)	0.979	0.979

(pre-processing useful for very small models)

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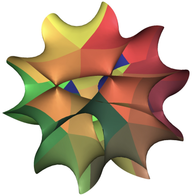
Example 2: Complete Intersection Calabi-Yau (CICY) matrices

- have procedure $M \in \mathbb{R}^{12\times 15} \rightsquigarrow f_1, \ldots, f_{15}$ polynomials such that

$$\mathrm{CY}(M) := \{x \in \mathbb{CP}^{k_1} \times \cdots \times \mathbb{CP}^{k_{12}} : f_1(x) = 0, \ldots, f_{15}(x) = 0\}$$



is Calabi-Yau manifold

$$\begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 & \ldots \\ 0 & 0 & 1 & 0 & 0 & 1 & \ldots \\ 0 & 0 & 0 & 0 & 1 & 1 & \ldots \\ 1 & 0 & 0 & 1 & 0 & 0 & \ldots \\ 1 & 0 & 0 & 0 & 0 & 1 & \ldots \\ 0 & 0 & 1 & 2 & 0 & 0 & \ldots \\ 0 & 1 & 0 & 0 & 2 & 0 & \ldots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \end{pmatrix}$$

- geometric invariant "second Hodge number" $h^2 : \{\text{Calabi-Yau mf}\} \to \mathbb{Z}$
- Learn

$$h : \mathbb{R}^{12\times 15} \to \mathbb{Z}$$
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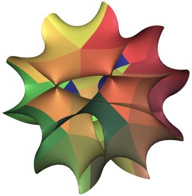

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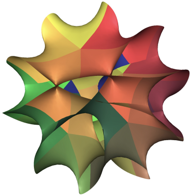

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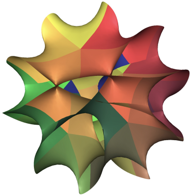

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- Let $x_0 = \begin{pmatrix} 10^{179} & 10^{178} & 10^{177} & \dots & 10^{165} \\ \vdots & \vdots & \vdots & & \vdots \\ 10^{29} & 10^{28} & 10^{27} & \dots & 10^{15} \\ 10^{14} & 10^{13} & 10^{12} & \dots & 10^{0} \end{pmatrix} \in \mathbb{R}^{12\times 15}$

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  E.g. $F\begin{pmatrix} 2 & 0 \\ 1 & 3 \end{pmatrix} = \begin{pmatrix} 0 & 2 \\ 3 & 1 \end{pmatrix}$
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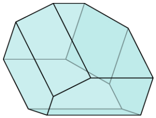
	Original dataset	Randomly permuted
MLP	0.554 ± 0.015	0.395 ± 0.029
MLP+pre-processing	0.858 ± 0.009	0.417 ± 0.086
Inception	0.970 ± 0.009	0.844 ± 0.117
G-inv MLP	0.895 ± 0.029	0.914 ± 0.023
F +Inception	$\mathbf{0.975 \pm 0.007}$	$\mathbf{0.963 \pm 0.016}$

Inception [Erbin and Finotello, 2021]

Example 3: Kreuzer-Skarke toric variety list

- $M \in \mathbb{R}^{4\times 26} \leftrightarrow$ polytope in $\mathbb{R}^4$ with 26 vertices



$\rightsquigarrow$ Calabi-Yau manifold $\mathrm{CY}(M)$

- Learn

$$h : \mathbb{R}^{4\times 26} \to \mathbb{Z}$$
$$M \mapsto h^2(\mathrm{CY}(M))$$

- x_0, U, F as before $\rightsquigarrow$

Model	Acc (orig)
MLP with reduced input	46.89%
MLP	82.96%
MLP+ **F**	85.56%
Invariant MLP	67.16%

First line from [Berglund et al., 2021]

Thank you for the attention!

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Image credit

- Polytope image: https://en.wikipedia.org/wiki/Simple_polytope#/media/File:Associahedron_K5.svg
- Tesselation of hyperbolic plane: https://www.pngwing.com/en/free-png-cmyrj