GEOMETRIC DEEP LEARNING

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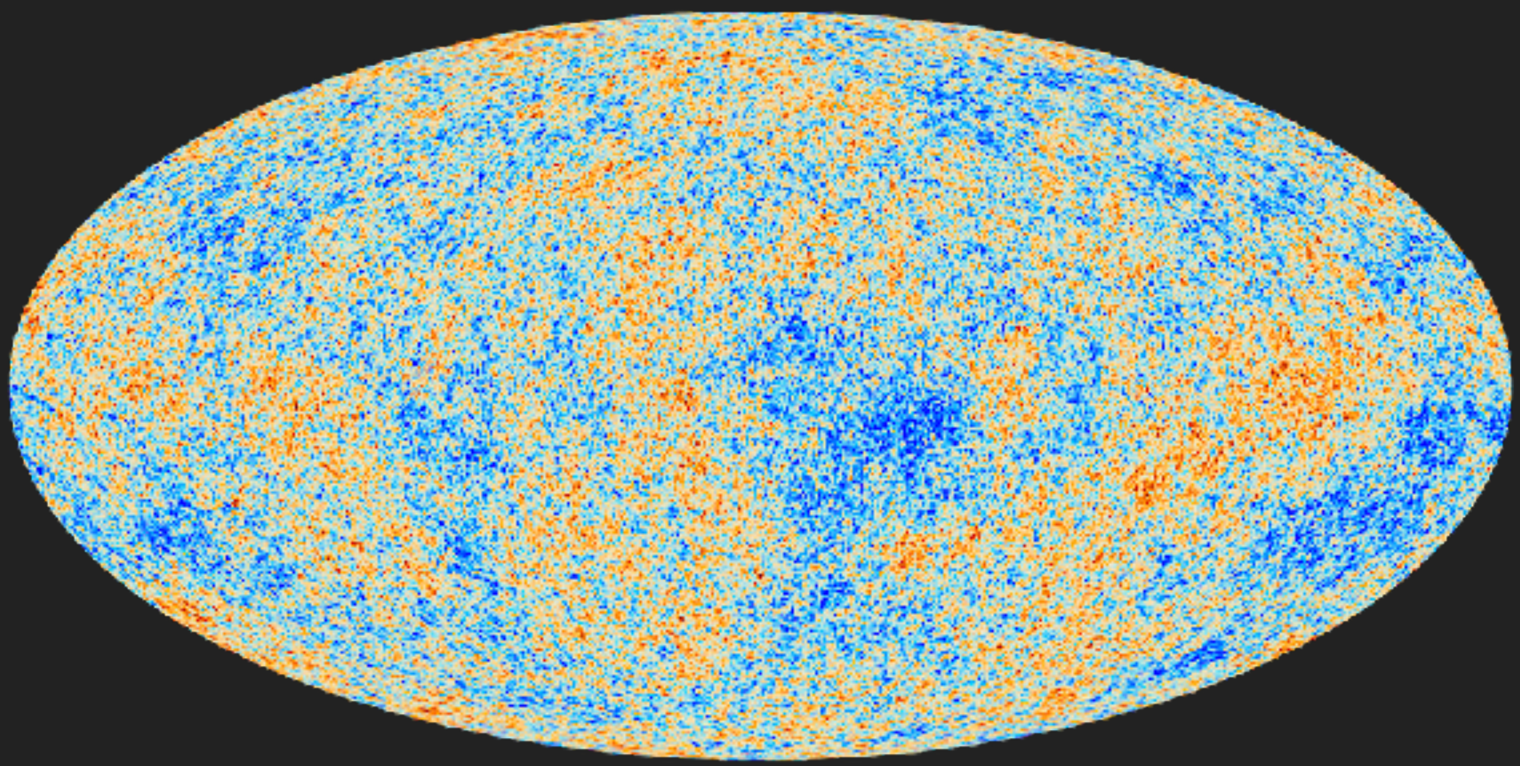
Symmetries are ubiquitous in physics

- The Universe is homogeneous & isotropic
- Gauge theory in particle physics
- Crystal structures in solid state physics

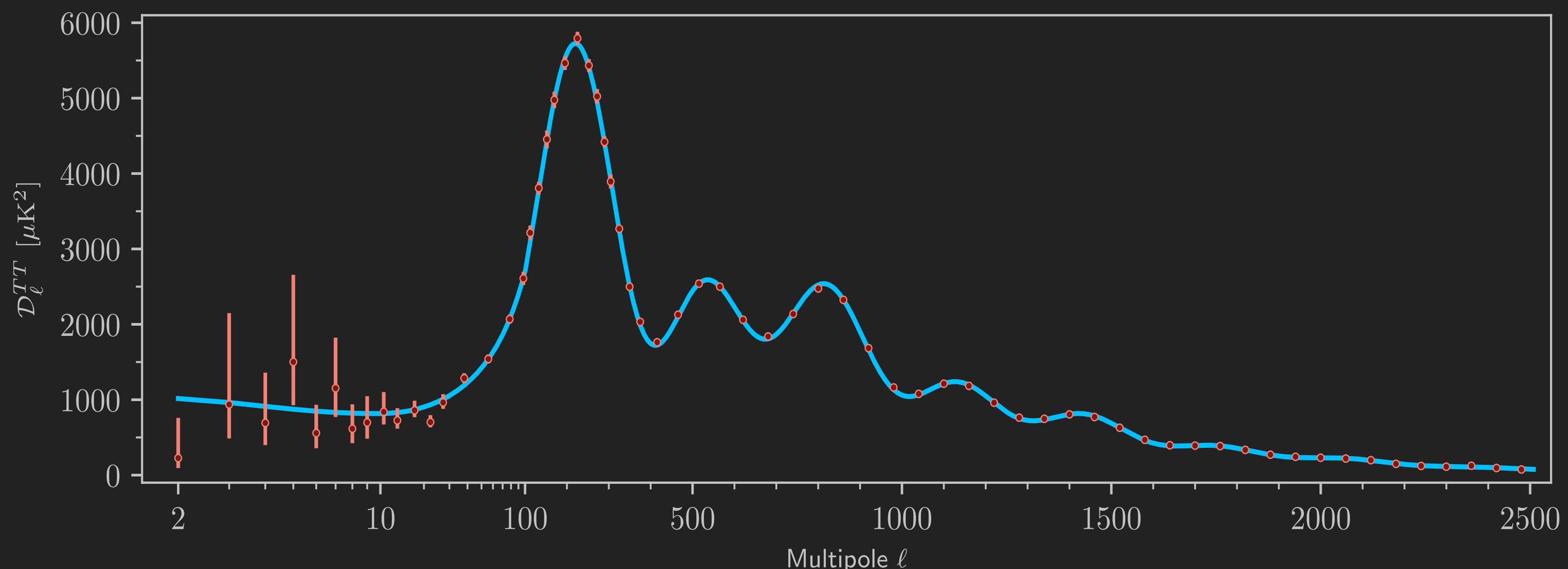
We should care about symmetries when using ML in physics

"Classical" data analysis respects symmetries

- The Universe is isotropic



- Summary statistics in cosmology are invariant to rotations



Planck Collaboration 2018

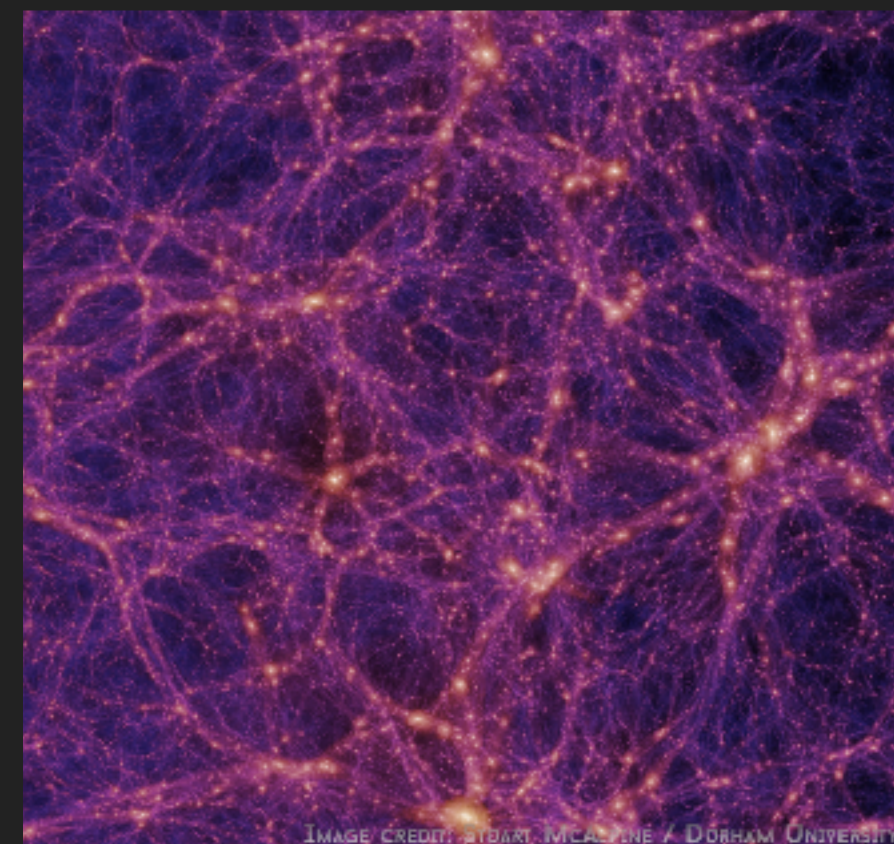
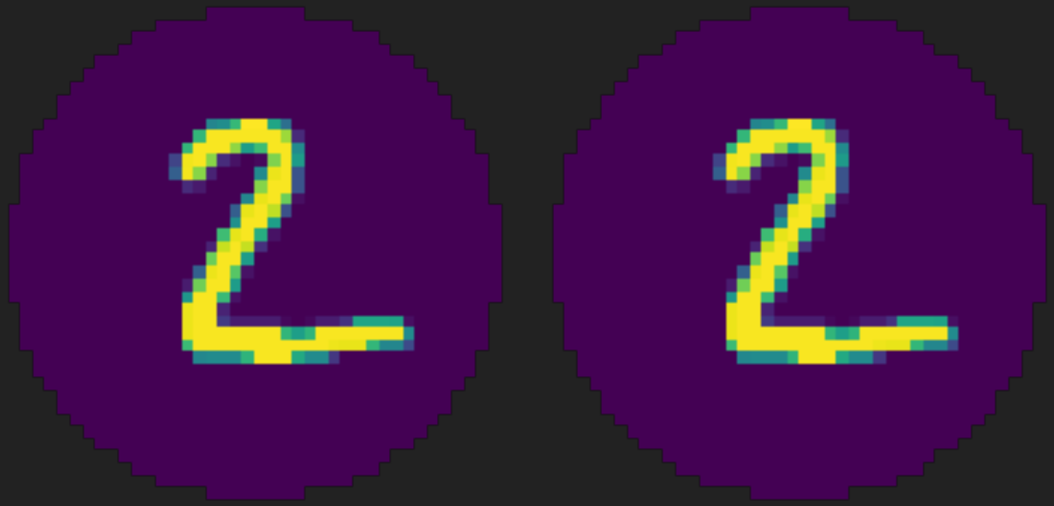


Image credit: Stuart McAlpine / Durham University

ML data analysis should respect symmetries too

- Ignore symmetries



Predicted label: 2

ML data analysis should respect symmetries too

- Data augmentation
  - No inductive bias
  - Need to learn symmetries
    - Redundant parameters
  - For 3D data, need many data augmentations
  - Inefficient, no guarantees

ML data analysis should respect symmetries too

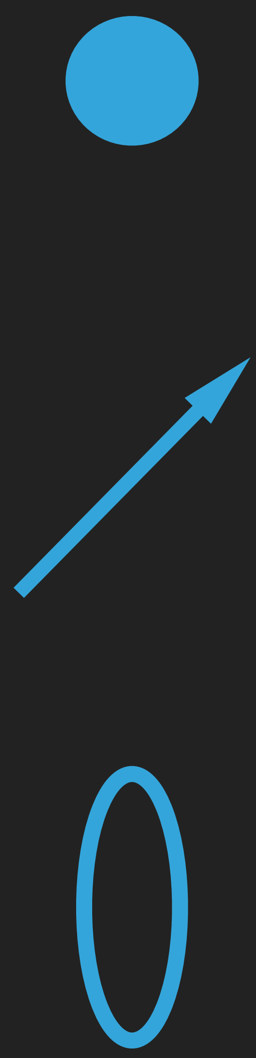
- Invariance
  - Output is invariant to transformations of the input
  - Example: Characterise a point cloud by distances and angles
  - Less model flexibility

ML data analysis should respect symmetries too

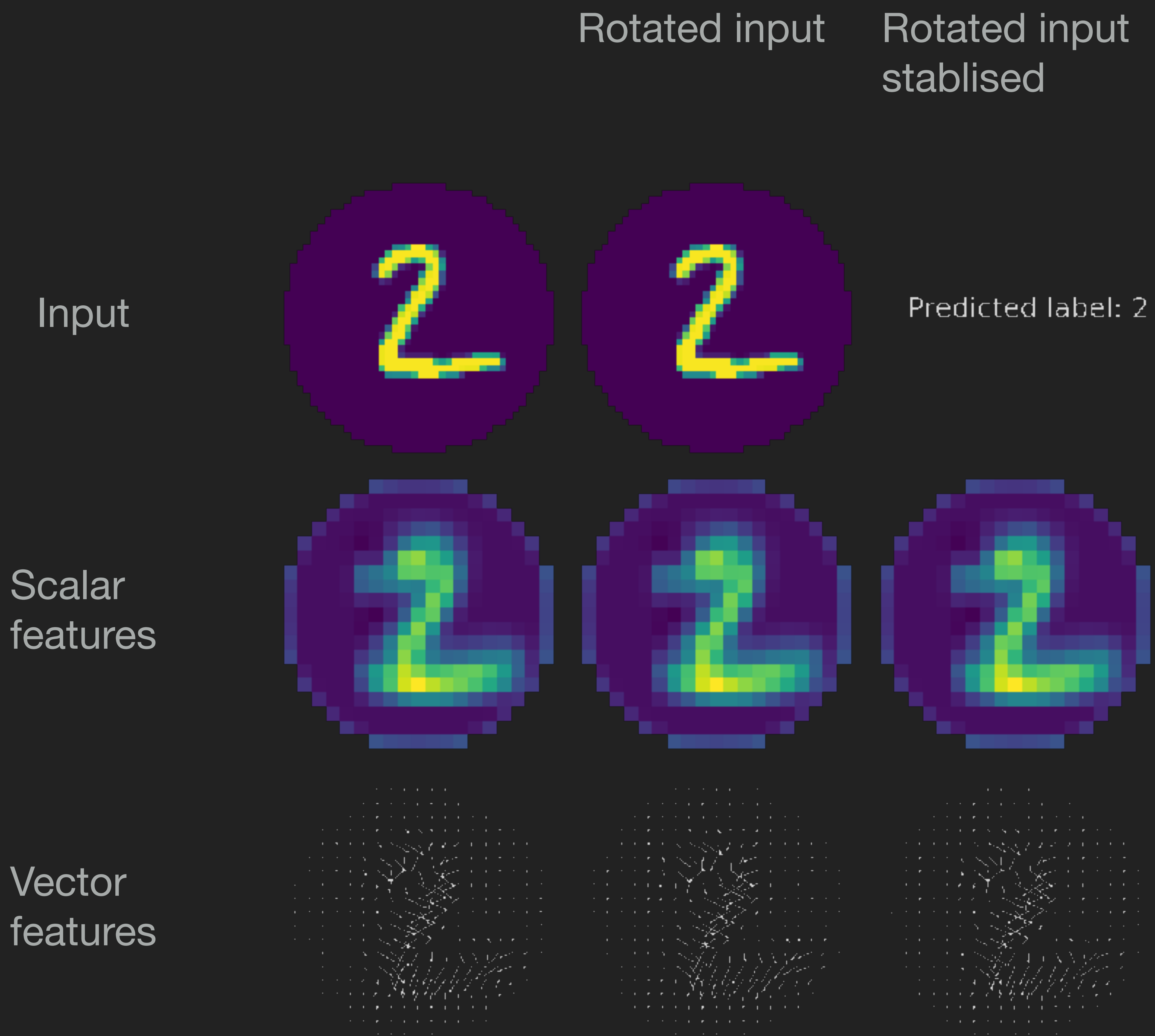
- Equivariance
  - Output transforms consistently with transformed input
  - Best of both worlds
    - No need for data augmentation
    - More flexible models than invariance

- Deep learning is about finding intermediate representations
  - These representations should respect the geometry of the data
- Output and intermediate representations should transform consistently or be invariant

Geometric features



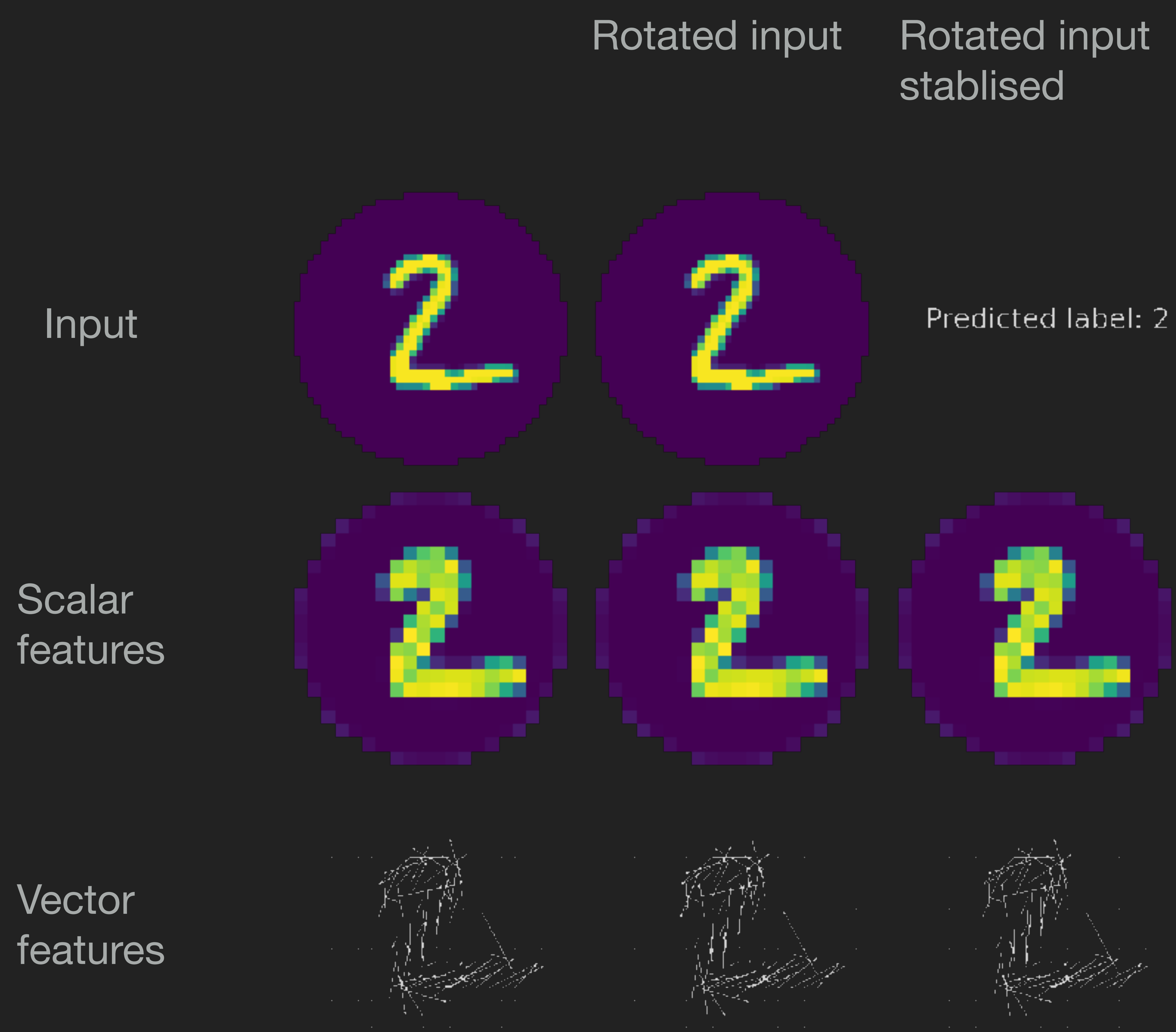
- Scalars
  - Images
- Vectors
  - Velocities
- Tensors
  - Polarisation



Rotated input
Rotated input stablised
Input
Predicted label: 2
Scalar features
Vector features

Invariance & Equivariance

- $f : X \to Y$
  - Example: n features on a 2d grid: $X = \mathbb{R}^2$, $Y = \mathbb{R}^n$
- Group element $g \in G$
  - Example: $G = SO(2)$
- Representations on X and Y: $\rho_X(g)$, $\rho_Y(g)$
  - Example: $X = \mathbb{R}^2$, $\rho_X(\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$
- Invariance: $f\left(\rho_X(g)x\right) = f(x)$
- Equivariance: $f\left(\rho_X(g)x\right) = \rho_Y(g)f(x)$


Rotated input
Rotated input stablised
Input
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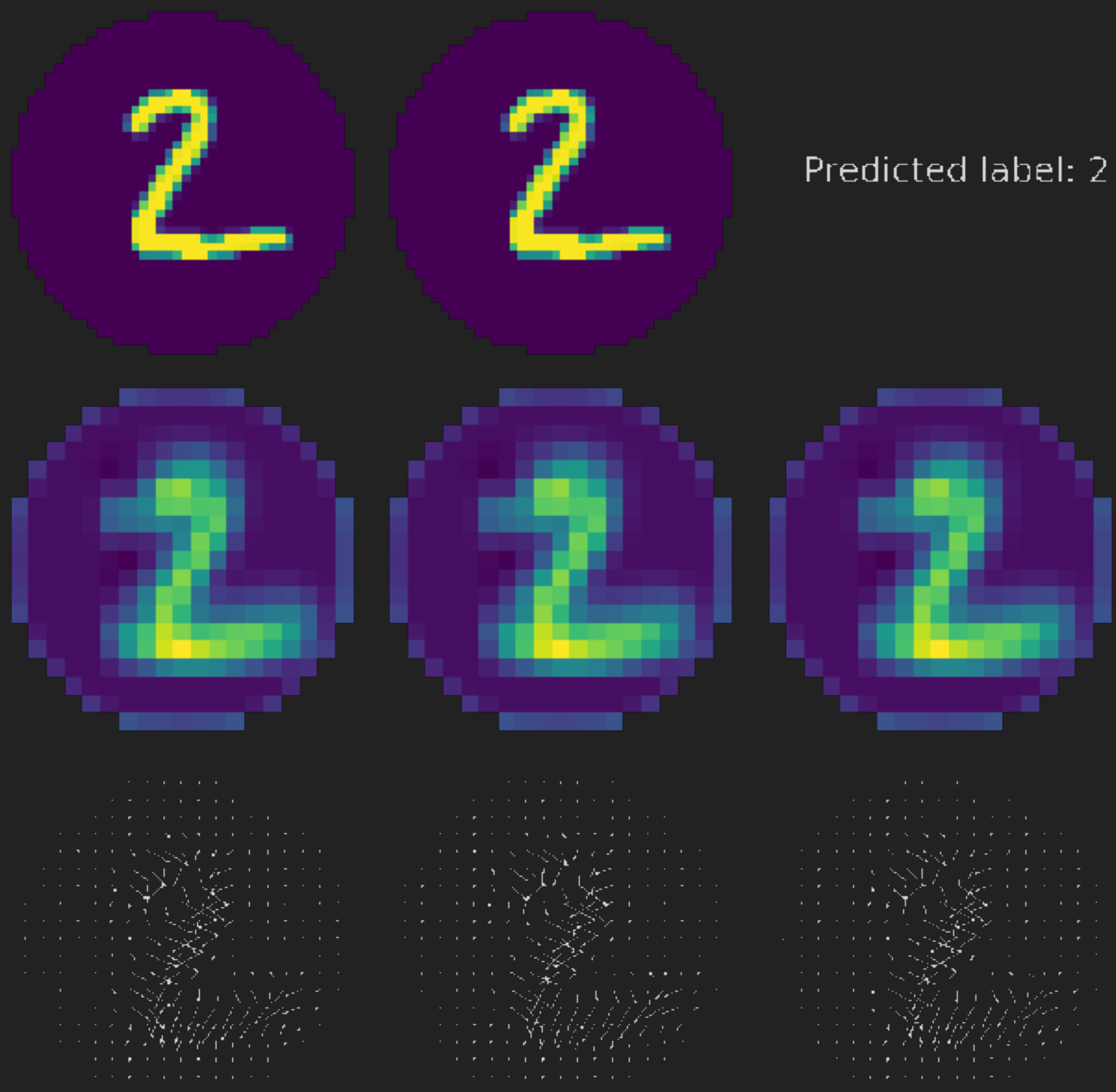
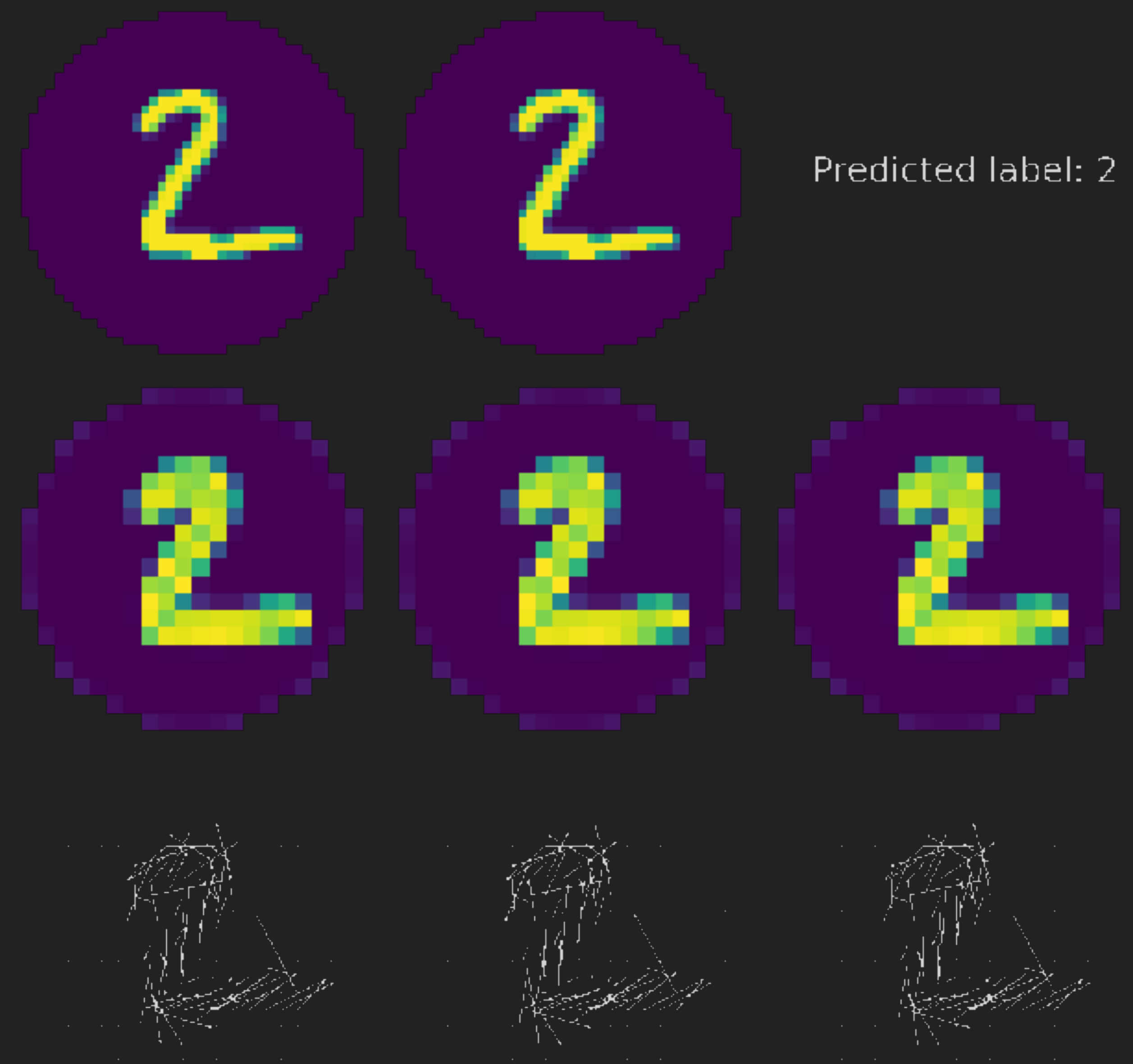
CNN



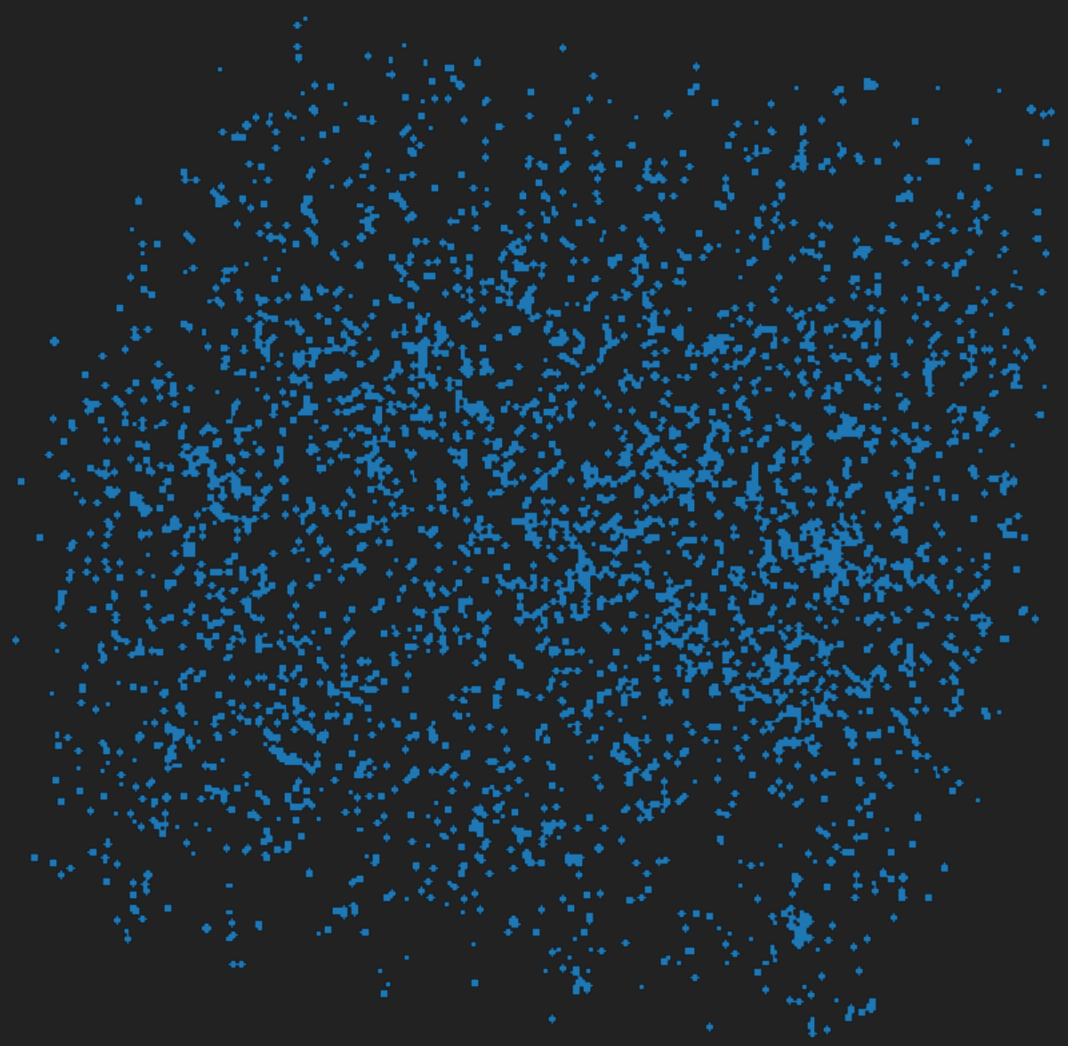
Equivariant CNN

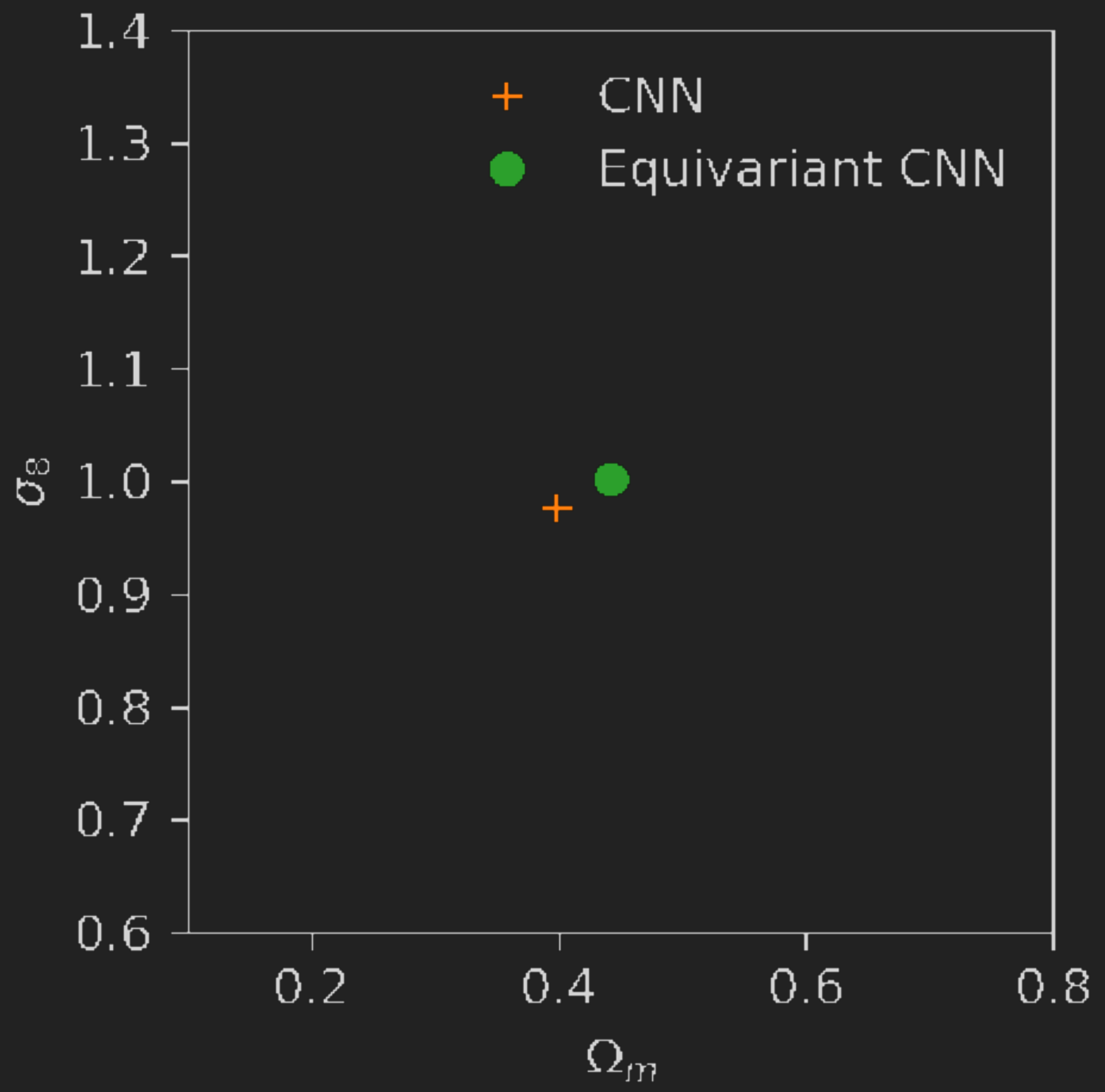


Ingredients for equivariant models

- Define geometric meaning of features:  …
    - Specify the irreducible representation of the features
- Use equivariant operations
    - E.g. steerable convolutions for SO(3)
        - Kernel constraint: $k(rx) = \rho_{\text{out}}(r)k(x)\rho_{\text{in}}(r)^{-1}$
        - $k(x) = F(|x|)\overline{Y^{\ell_{\text{out}}}(x/|x|)}Y^{\ell_{\text{in}}}(x/|x|)^T$
    - Tensor products of irreps
        - Decompose into irreps using Clebsch-Gordan coefficients

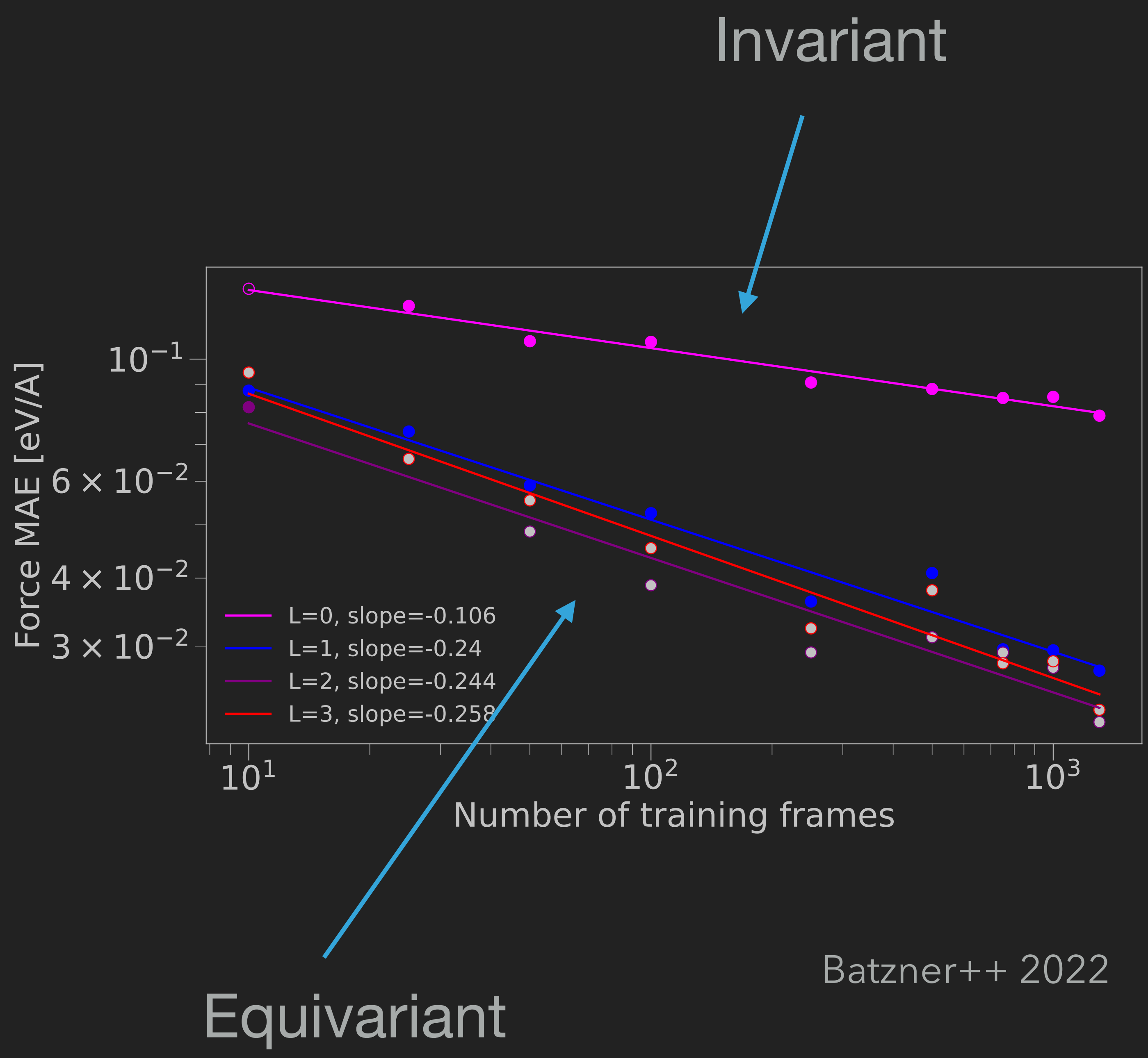
Preliminary application to galaxy point clouds





Why should you care?

- Guaranteed respect for symmetries in the data
- Sample efficiency
  - Preliminary: Equivariant point cloud model achieves same accuracy with order of magnitude less parameters
  - Equivariant models seem to scale better with number of training samples than invariant models



Batzner++ 2022

Geometric deep learning

- Deep learning on structured and geometric data
  - Graphs
  - Point clouds
  - Manifolds (e.g. S^2)
  - Meshes
  - …
- Consistent treatment of transformations
  - (Global) group equivariance
  - Gauge equivariance
  - …

Some (very incomplete) literature

- Early works
  - Group Equivariant Convolutional Networks: Cohen++ 2016 (1602.07576)
  - Tensorfield Networks: Thomas++ 2018 (1802.08219)
  - 3D Steerable CNN: Weiler++ 2018 (1807.02547)
- Reviews & background
  - A General Theory of Equivariant CNNs on Homogeneous Spaces: Cohen++ 2018 (1811.02017)
  - Theoretical Aspects of Group Equivariant Neural Networks: Esteves 2020 (2004.05154)
  - Geometric Deep Learning: Grids, Groups, Graphs, Geodesics, and Gauges: Bronstein++ 2021 (2104.13478)

Summary

- Geometric deep learning provides a framework to include inductive biases about symmetries of the data in our models
- Equivariant model preserve geometric meaning of inputs, intermediate representations, and outputs
- Greater interpretability, robust, and sample efficient