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AMLAB Amsterdam Machine Learning Lab

Group Equivariant Deep Learning

Lecture 1 - Regular group convolutions

Lecture 1.1 - Introduction

Desirable properties of neural networks, invariance, equivariance, weight-sharing

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This mini-course serves as a module with the UvA Master AI course Deep Learning 2 https://uvadl2c.github.io/

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Group Equivariant Deep Learning

Lecture 1 - Regular group convolutions

Lecture 1.1 - Introduction

Desirable properties of neural networks, invariance, equivariance, weight-sharing

Lecture 1.2 - Group Theory | The basics

Groups, group product, inverse, action, representation, affine groups $G = \mathbb{R}^d \rtimes H$

Lecture 1.3 - Regular group convolutions | Template matching viewpoint

General group convolutional NN design with example for roto-translation equivariance (SE(2))

Lecture 1.4 - SE(2) Equivariant NN Example | With histopathology images

Visual example for roto-translation equivariance (SE(2))

Lecture 1.5 - A brief history of G-CNNs

Lecture 1.6 - Group Theory | Homogeneous/quotient spaces

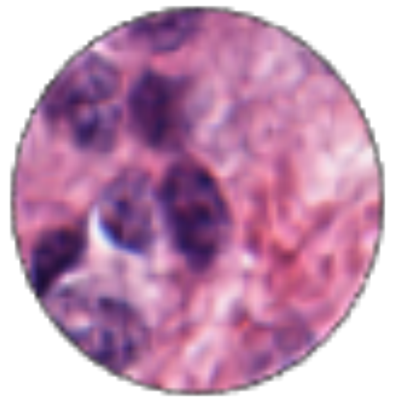
Transitive action, homogeneous space, quotient space, examples

Lecture 1.7 - Group convolutions are all you need!

Equivariant linear layers between feature maps are group convolutions

Geometric guarantees (invariance)

Example: Detection of pathological cells



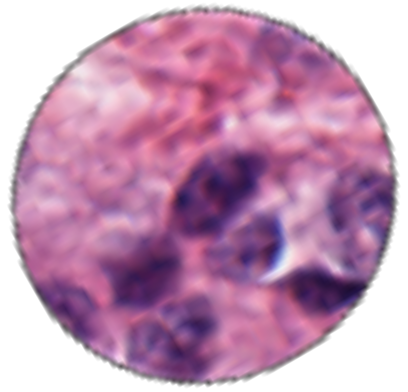
Geometric guarantees (invariance)

Example: Detection of pathological cells

Healthy

Geometric guarantees (invariance)

Example: Detection of pathological cells



Healthy

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Healthy

?

Geometric guarantees (invariance)

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Pathological

Geometric guarantees (invariance)

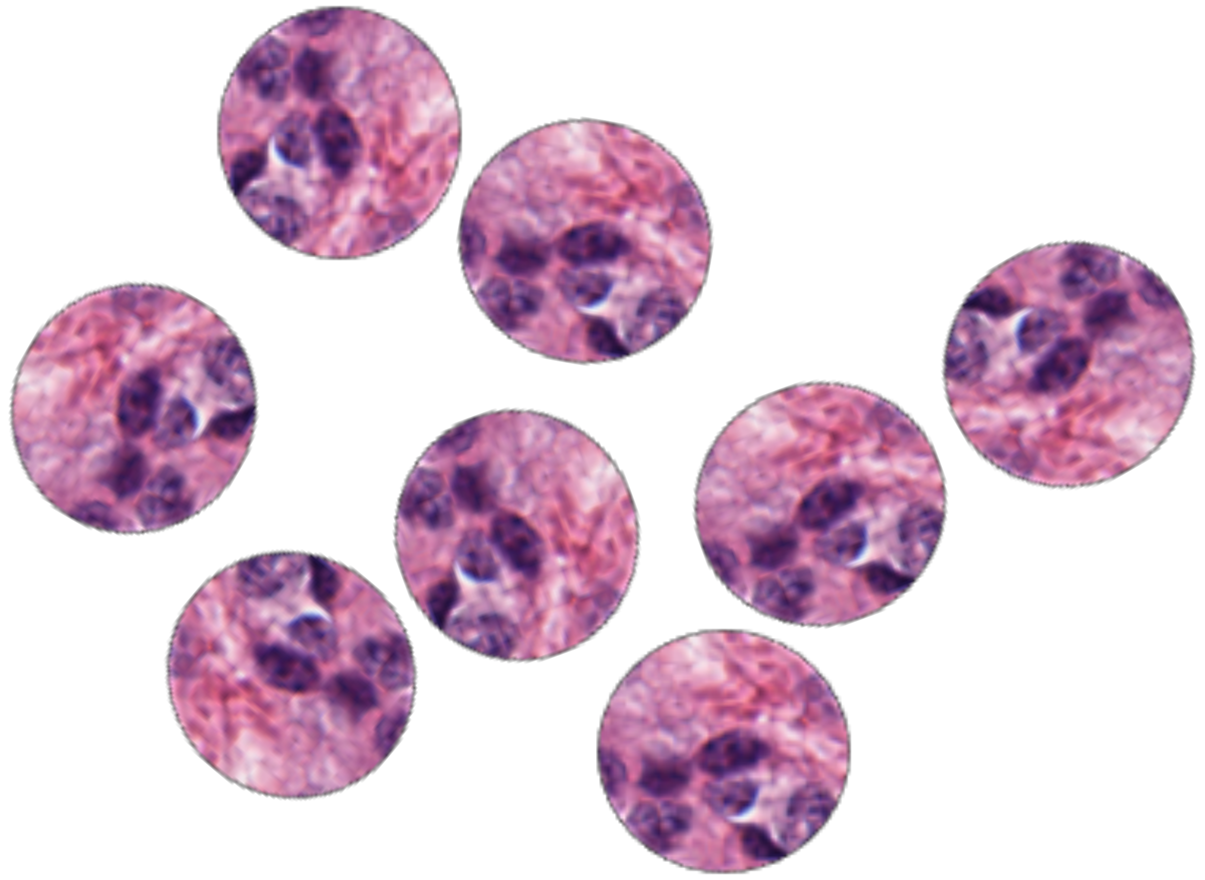
Example: Detection of pathological cells

Healthy

?

Pathological

Common approach: data-augmentation



Geometric guarantees (invariance)

Example: Detection of pathological cells

Healthy

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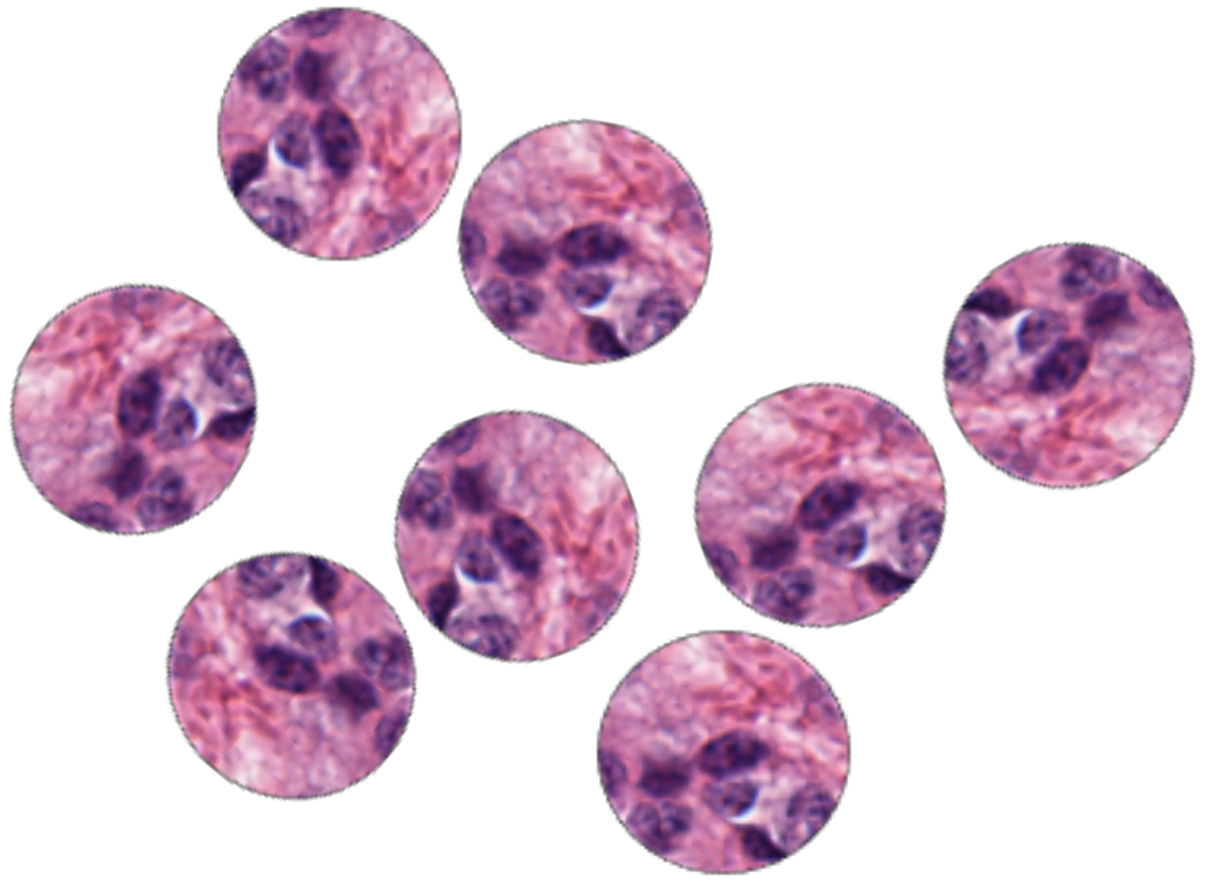
Pathological

Common approach: data-augmentation

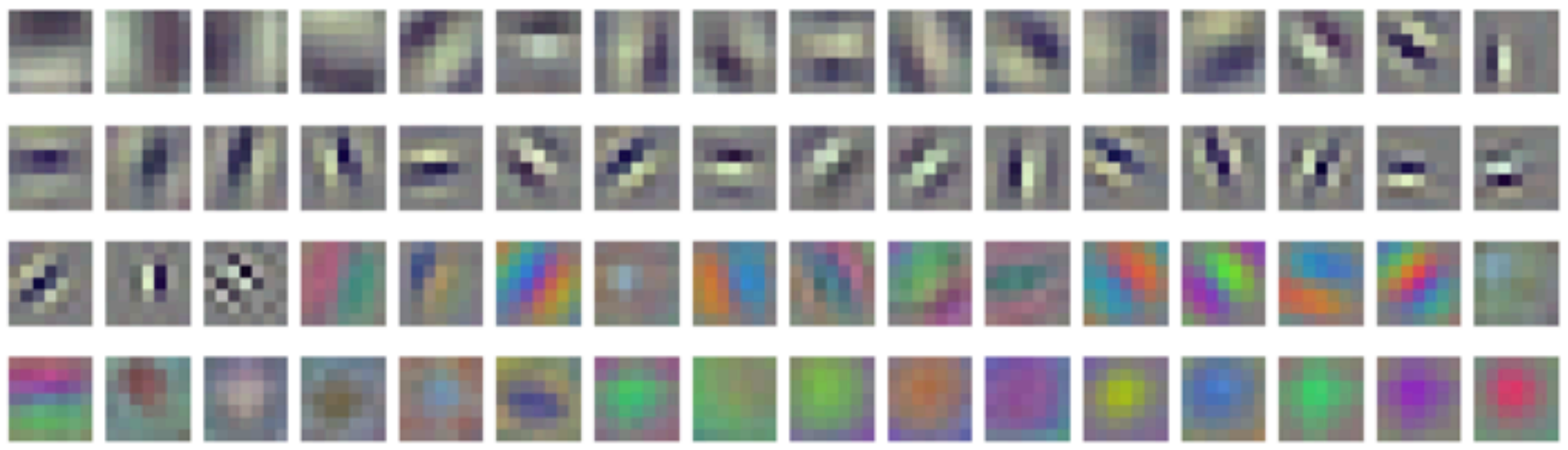


Issues:
- Still no guarantee of invariance
- Valuable net capacity is spend on learning invariance
- Redundancy in feature repr.

https://distill.pub/2020/circuits/equivariance/

Naturally Occurring Equivariance in Neural Networks

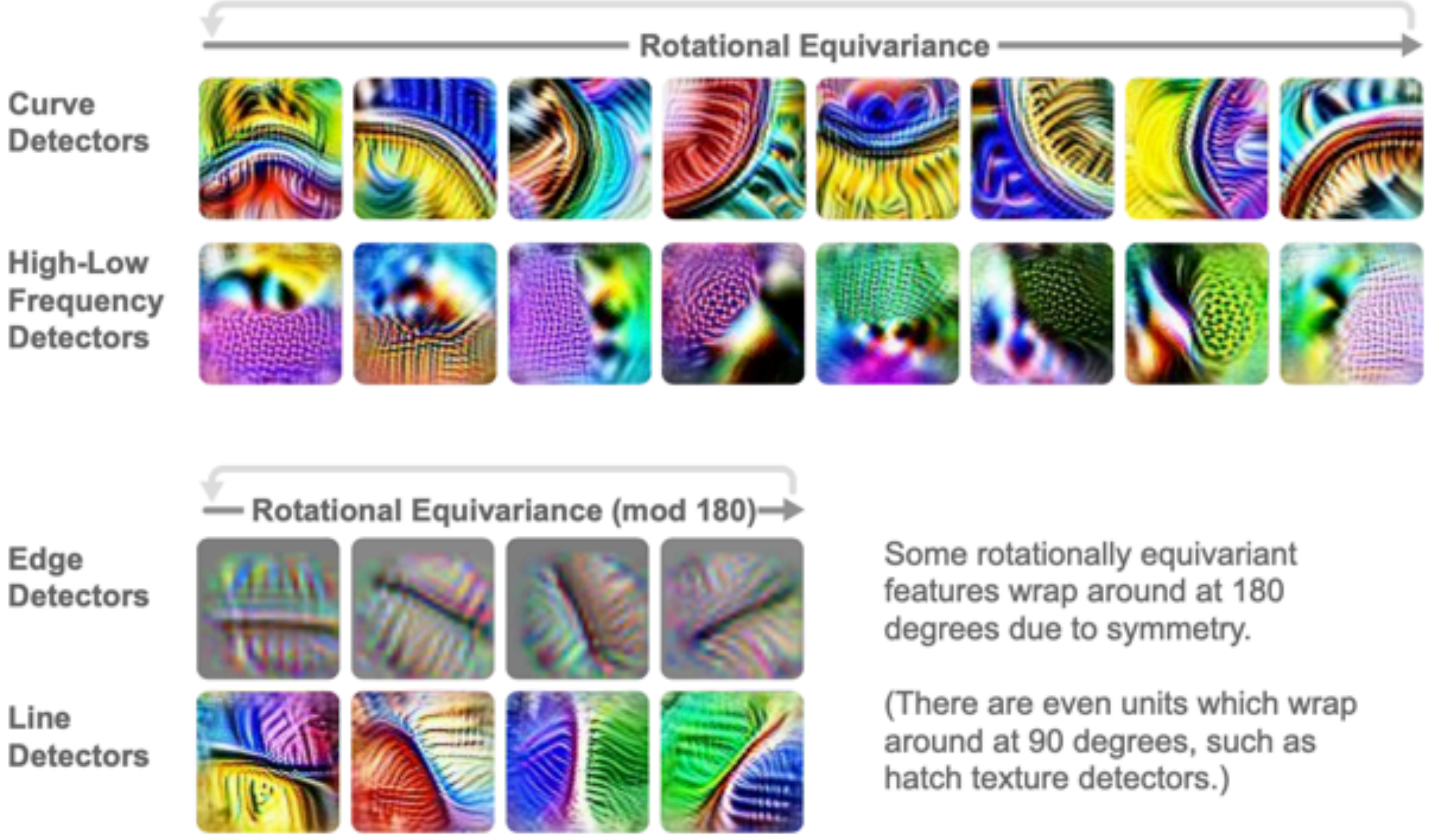
AUTHORS	AFFILIATIONS	PUBLISHED	DOI
Chris Olah	OpenAI	Dec. 8, 2020	10.23915/distill.00024.004
Nick Cammarata	OpenAI		
Chelsea Voss	OpenAI		
Ludwig Schubert			
Gabriel Goh	OpenAI		



The weights for the units in the first layer of the TF-Slim [11] version of InceptionV1 [8]. [5] Units are sorted by the first principal component of the adjacency matrix between the first and second layers. Note how many features are similar except for rotation, scale, and hue.

Equivariant Features

Rotational Equivariance: One example of equivariance is rotated versions of the same feature. These are especially common in early vision, for example curve detectors, high-low frequency detectors, and line detectors.



Some rotationally equivariant features wrap around at 180 degrees due to symmetry.

(There are even units which wrap around at 90 degrees, such as hatch texture detectors.)

Geometric guarantees (equivariance)

CNNs are translation equivariant

Via convolutions →

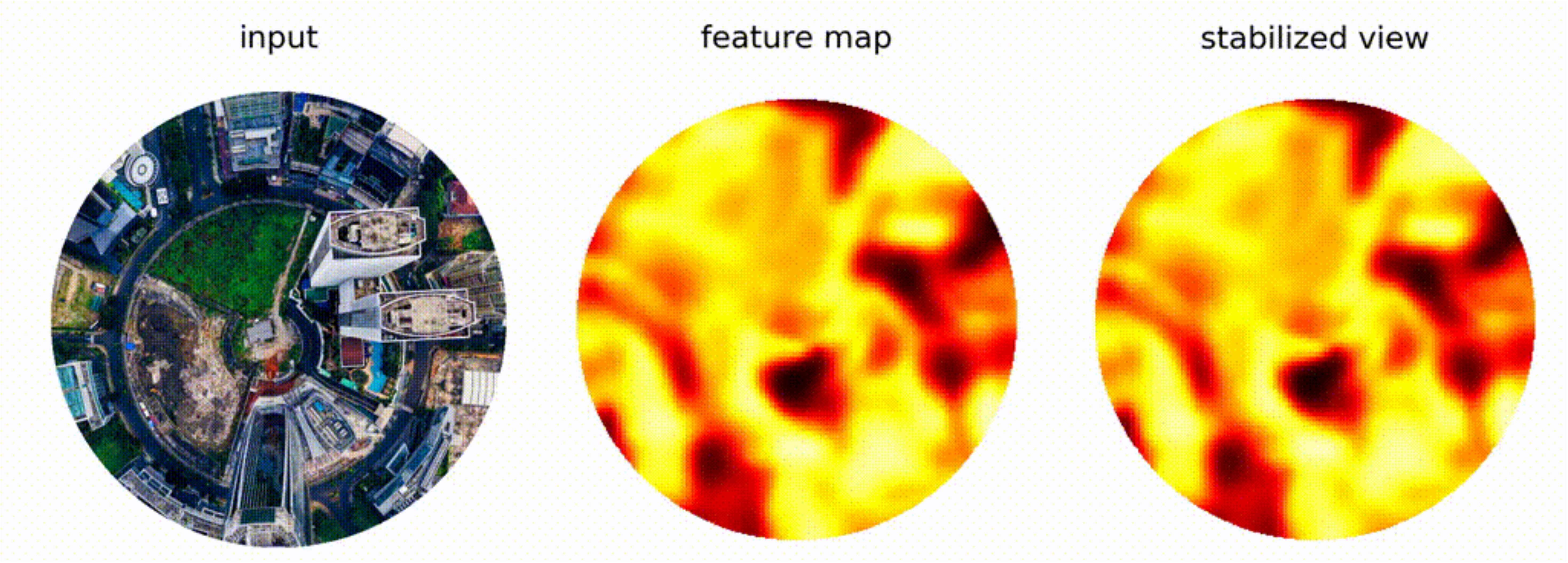
Geometric guarantees (equivariance)

CNNs are translation equivariant

Via convolutions

Geometric guarantees (equivariance)

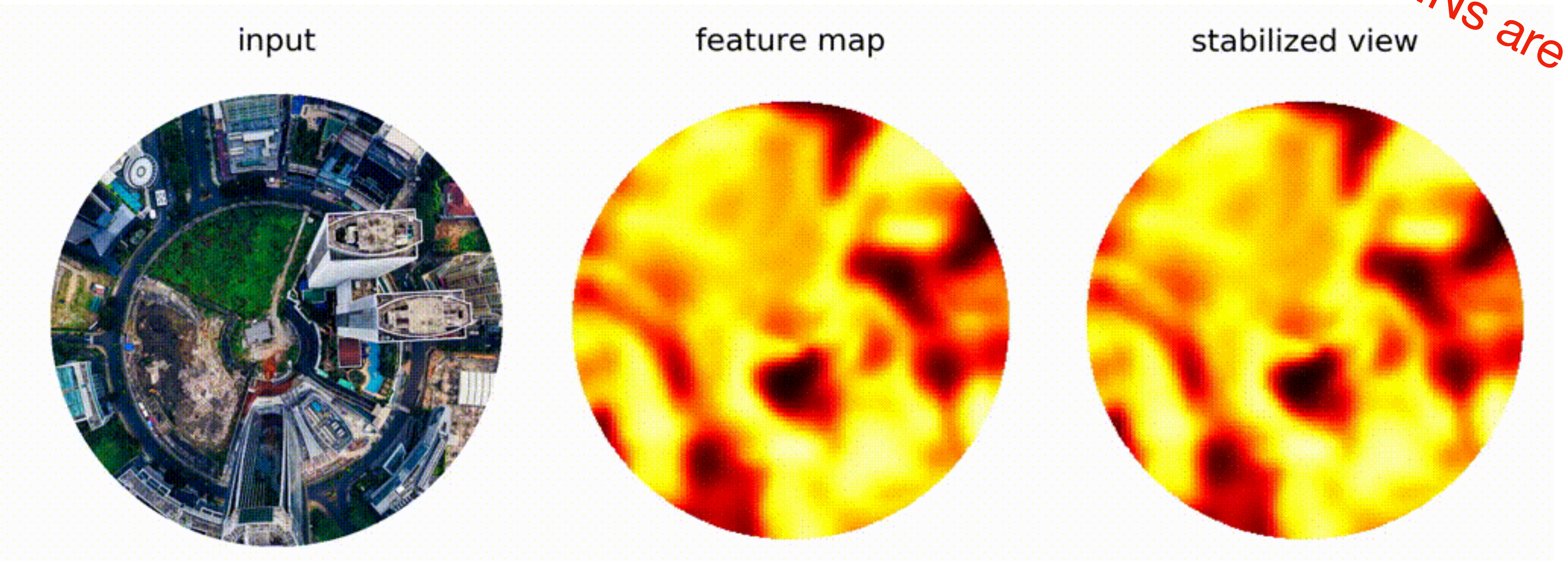
Normal CNN



Figures source:
https://github.com/QUVA-Lab/e2cnn

Geometric guarantees (equivariance)

Normal CNN



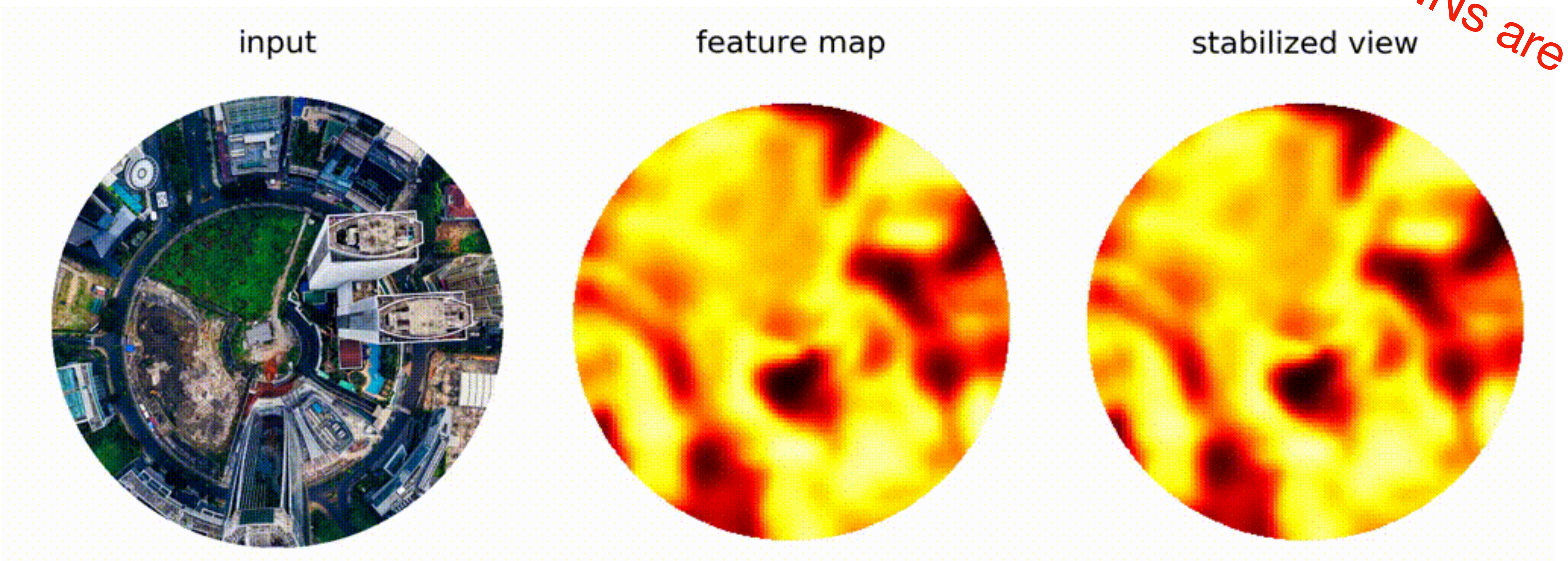
CNNs are not rotation equivariant

☹

Figures source:
https://github.com/QUVA-Lab/e2cnn

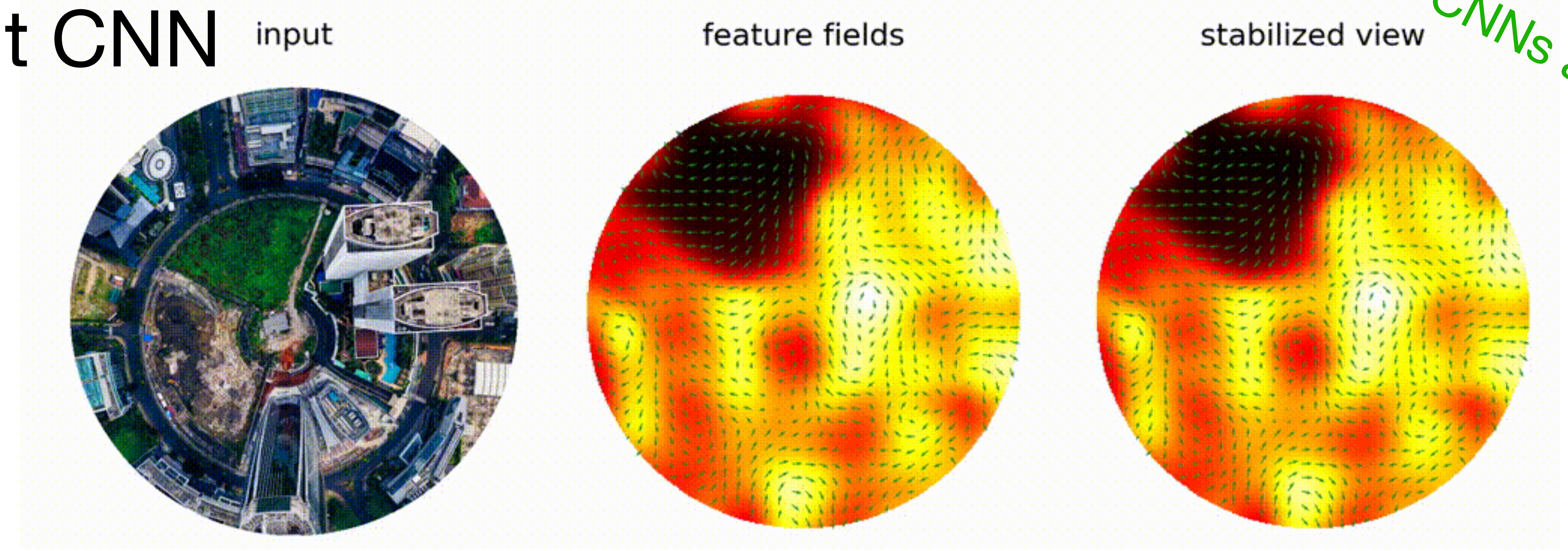
Geometric guarantees (equivariance)

Normal CNN



CNNs are not rotation equivariant

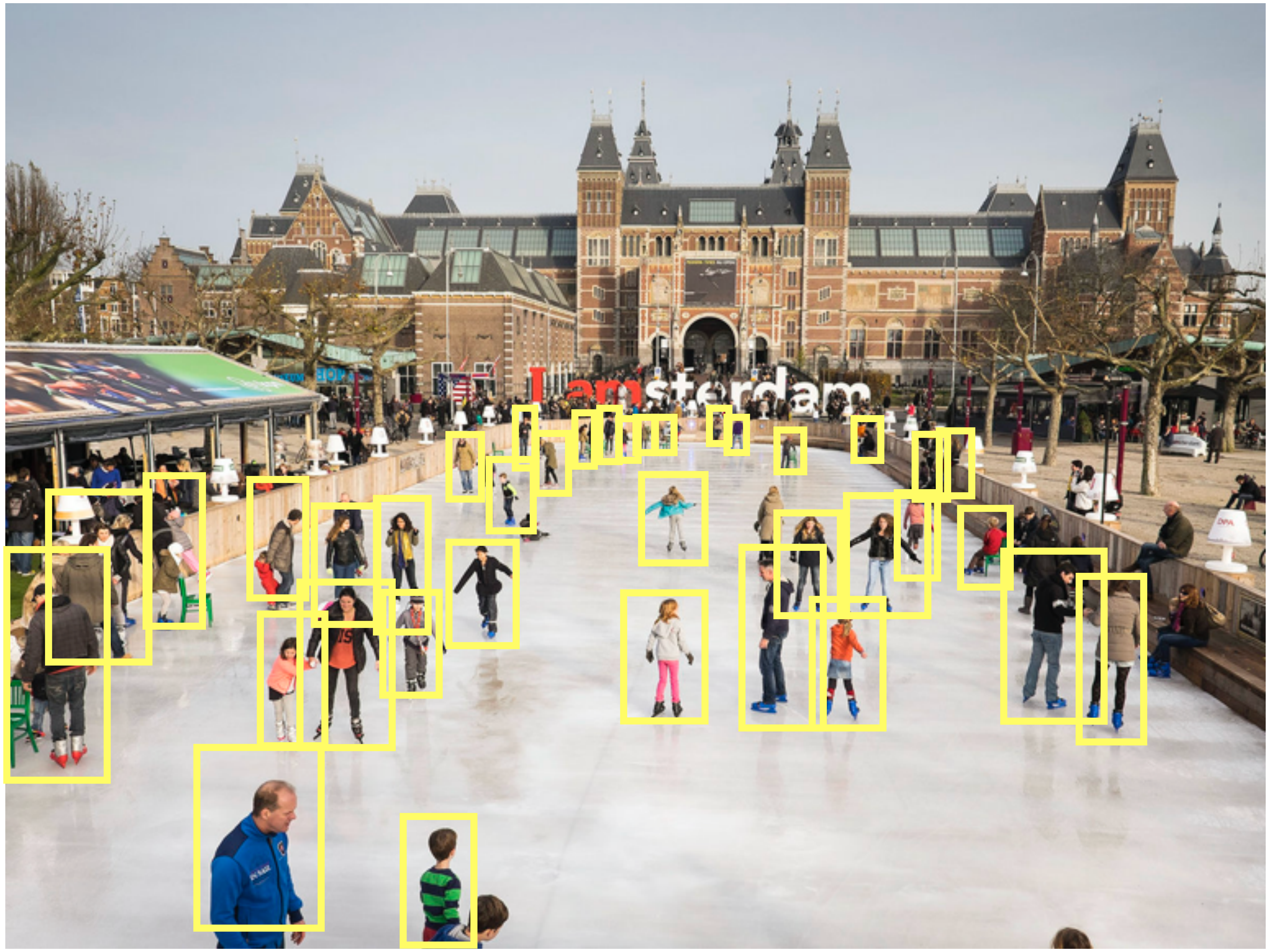
Group equivariant CNN



G-CNNs are rotation equivariant!

Figures source:
https://github.com/QUVA-Lab/e2cnn

Geometric guarantees (equivariance)



Importance of equivariance:

- No information is lost when the input is transformed
- Guaranteed stability to (local + global) transformations

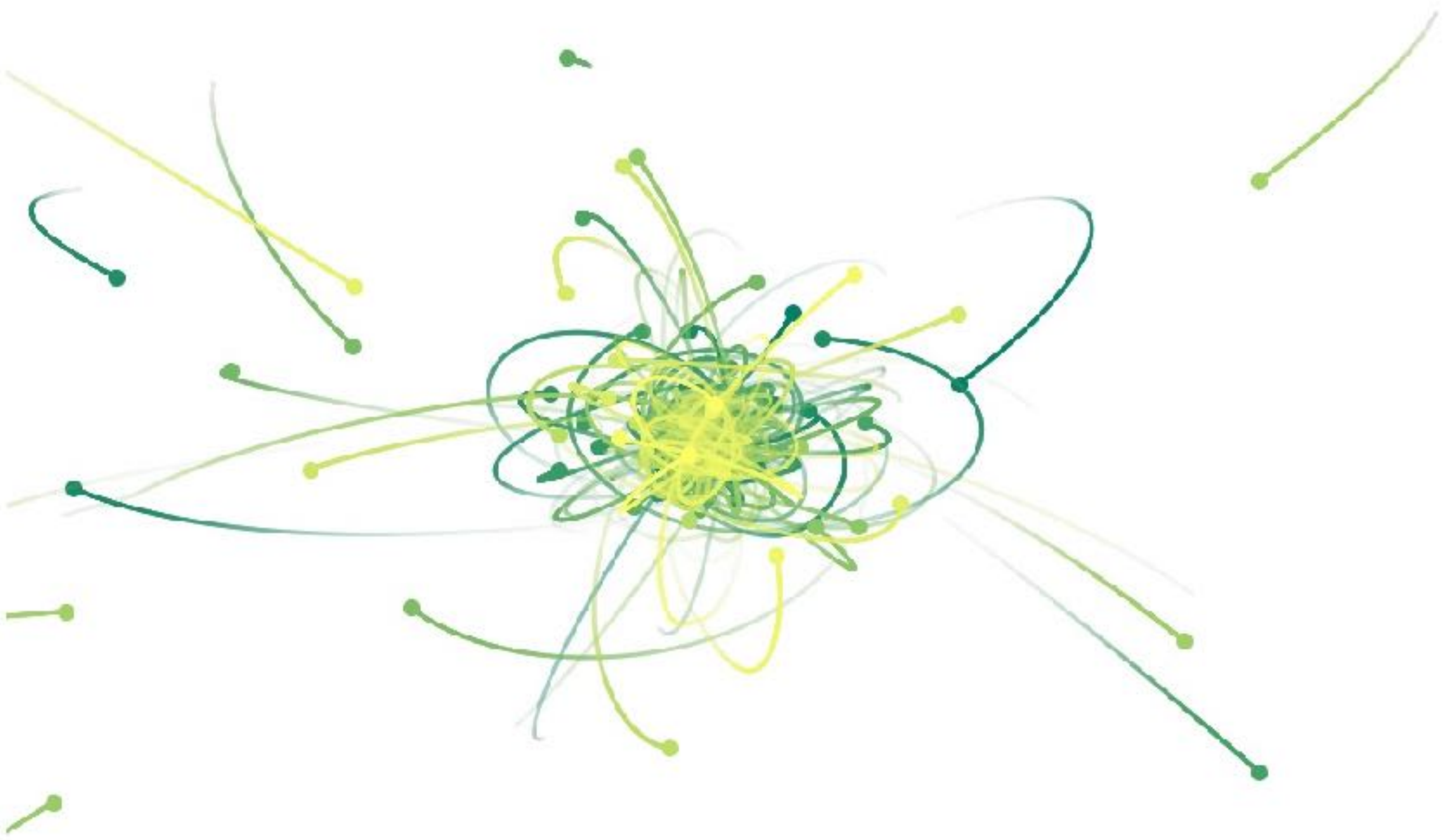
Group convolutions:

- Equivariance beyond translations
- Geometric guarantees
- Increased weight sharing

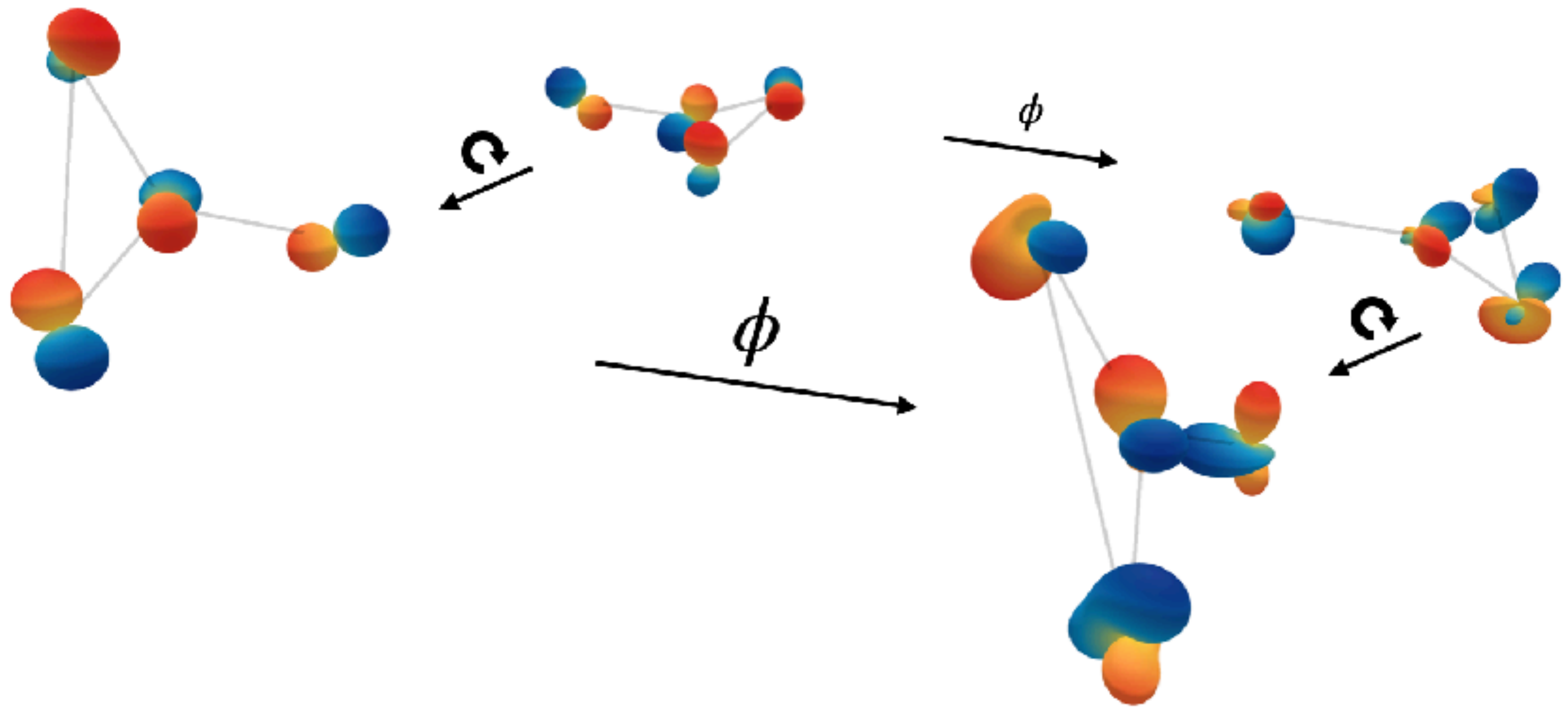
G-CNNs are not only relevant for invariant problems but for any type of structured data!

Geometric guarantees (equivariance)

Equivariant problem:
N-body problem (force/velocity prediction)

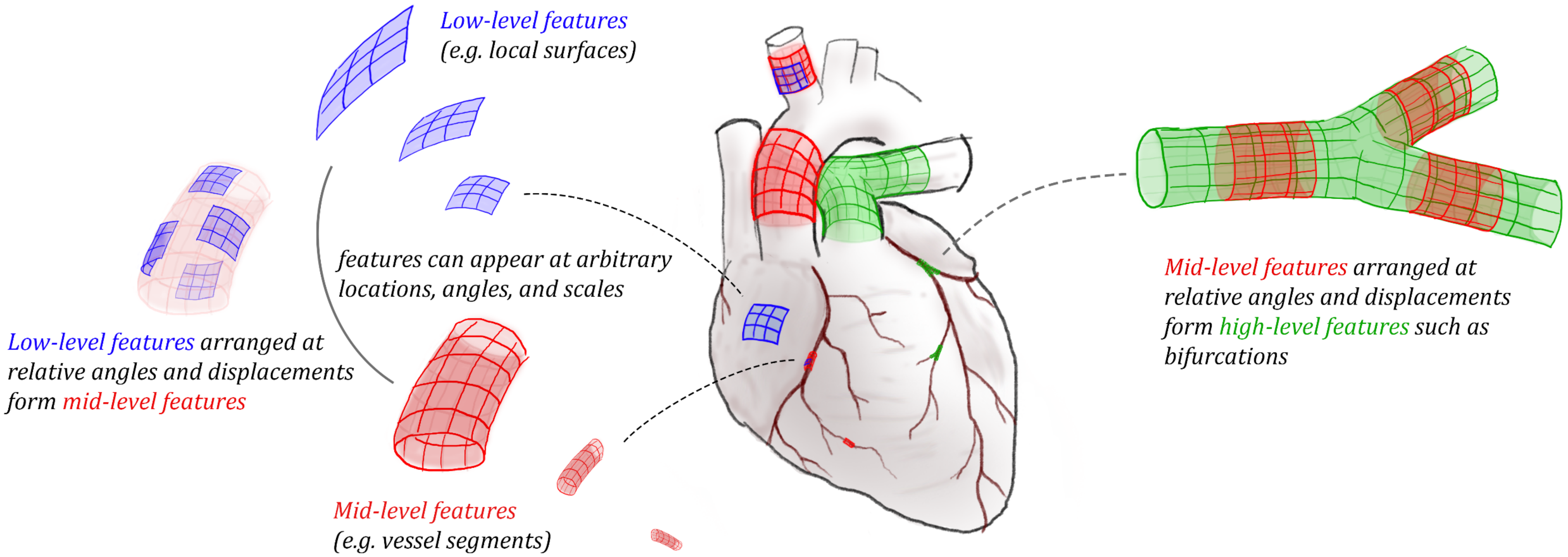


Equivariant problem:
Molecule conformer generation

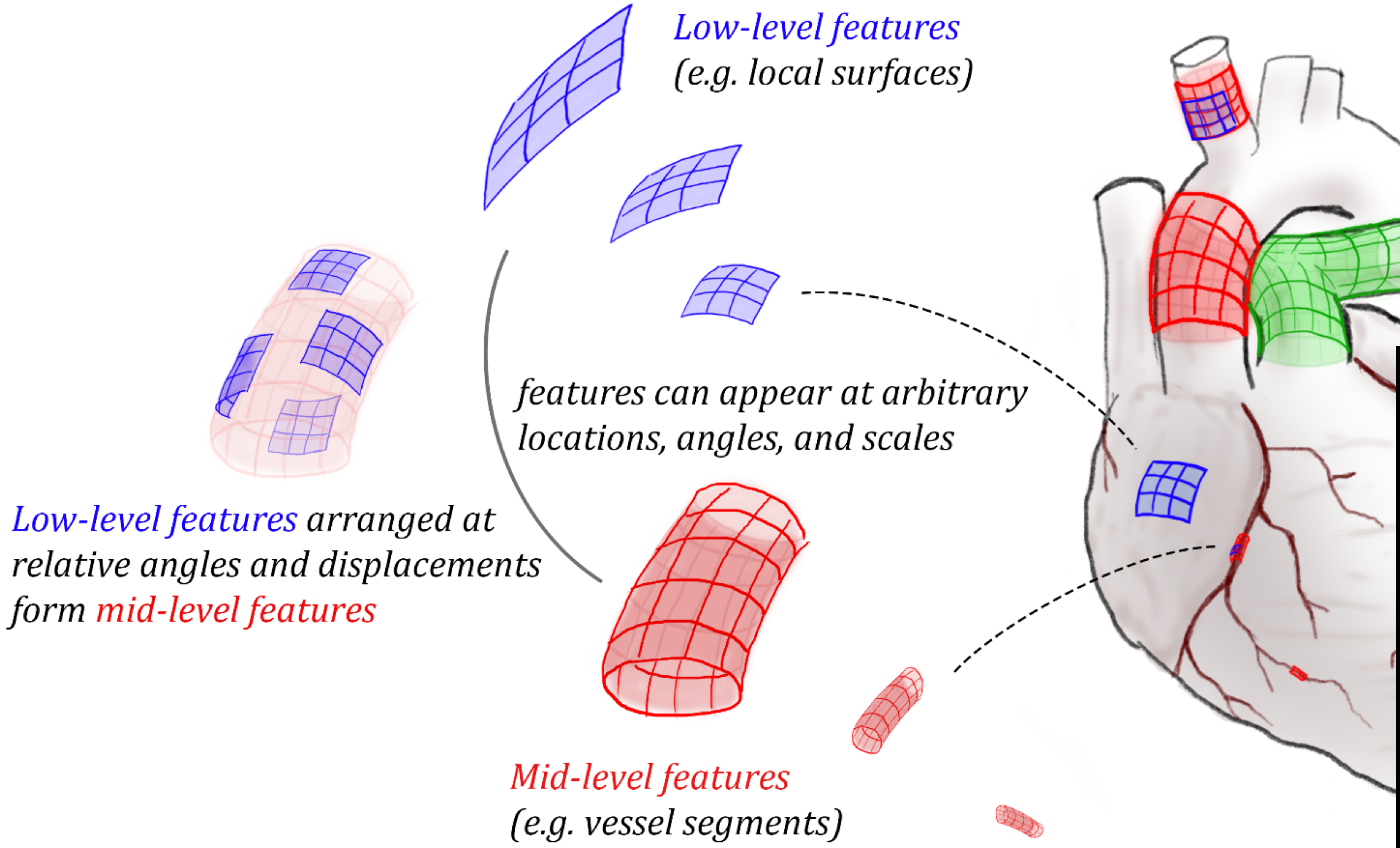


Invariant problem:
Molecule property prediction

Psychology of vision: recognition by components



Psychology of vision: recognition by components



Rationale behind capsule networks

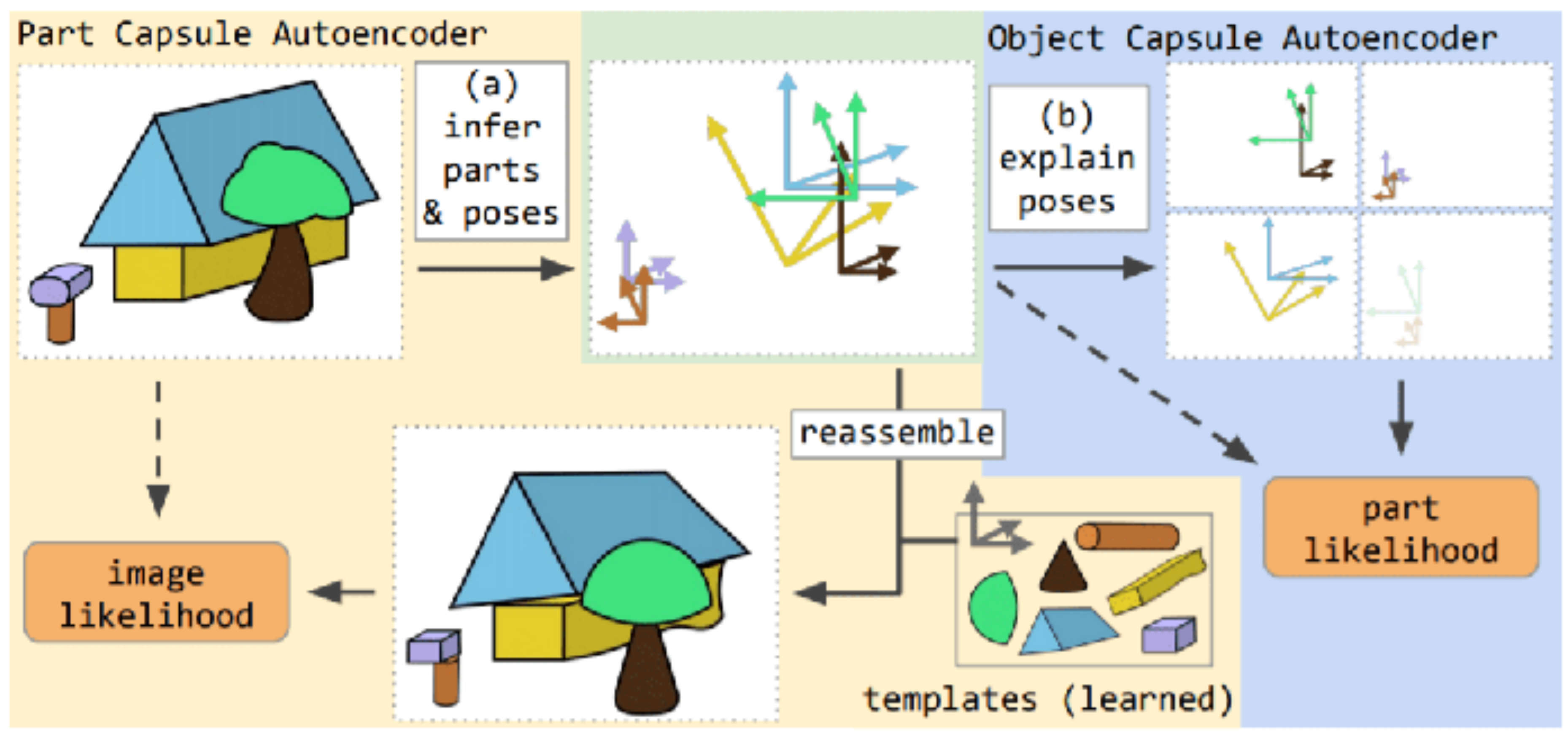


Fig from Kosiorek et al. 2019

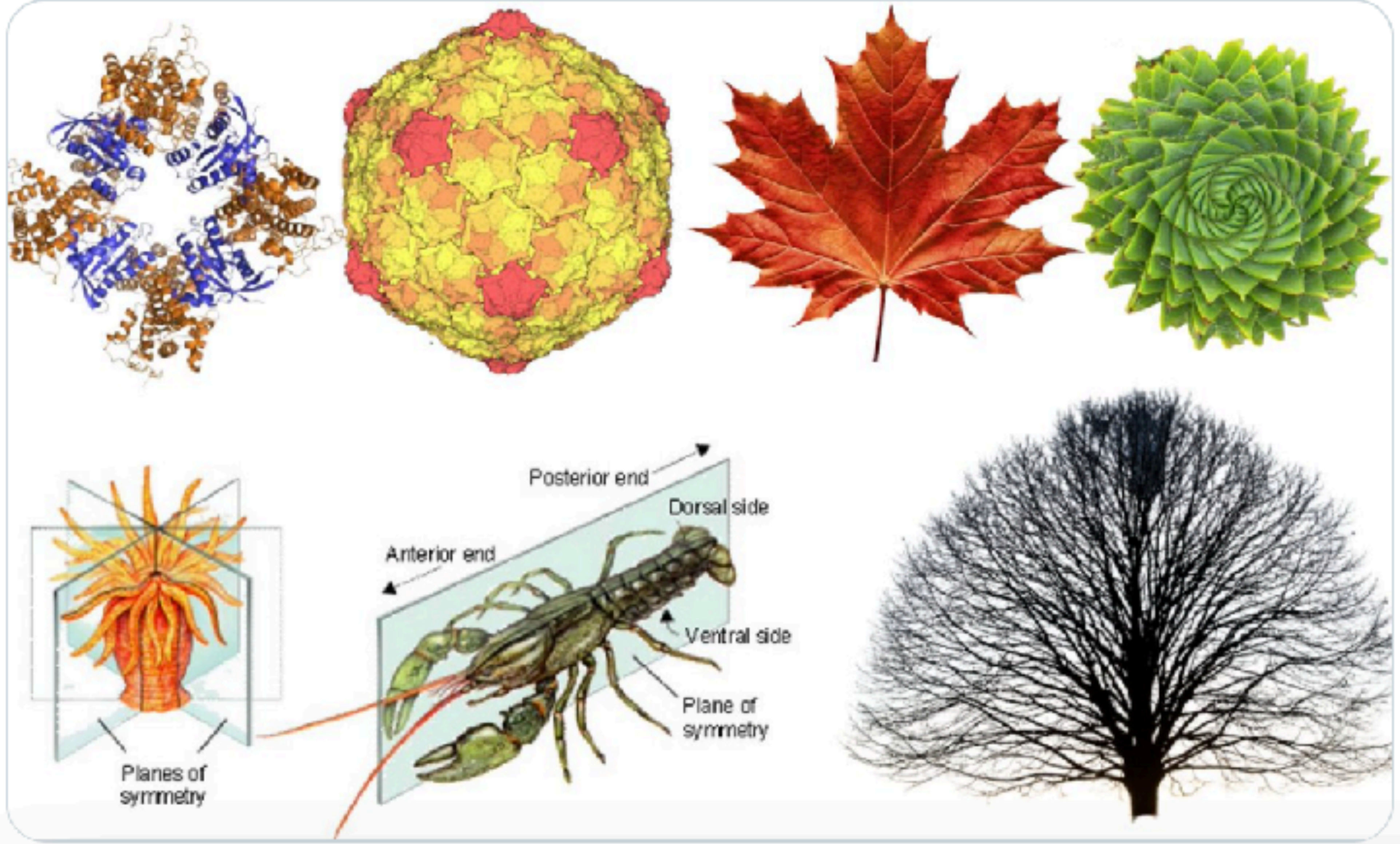
Symmetries in nature

Chico Camargo
@evoluchico

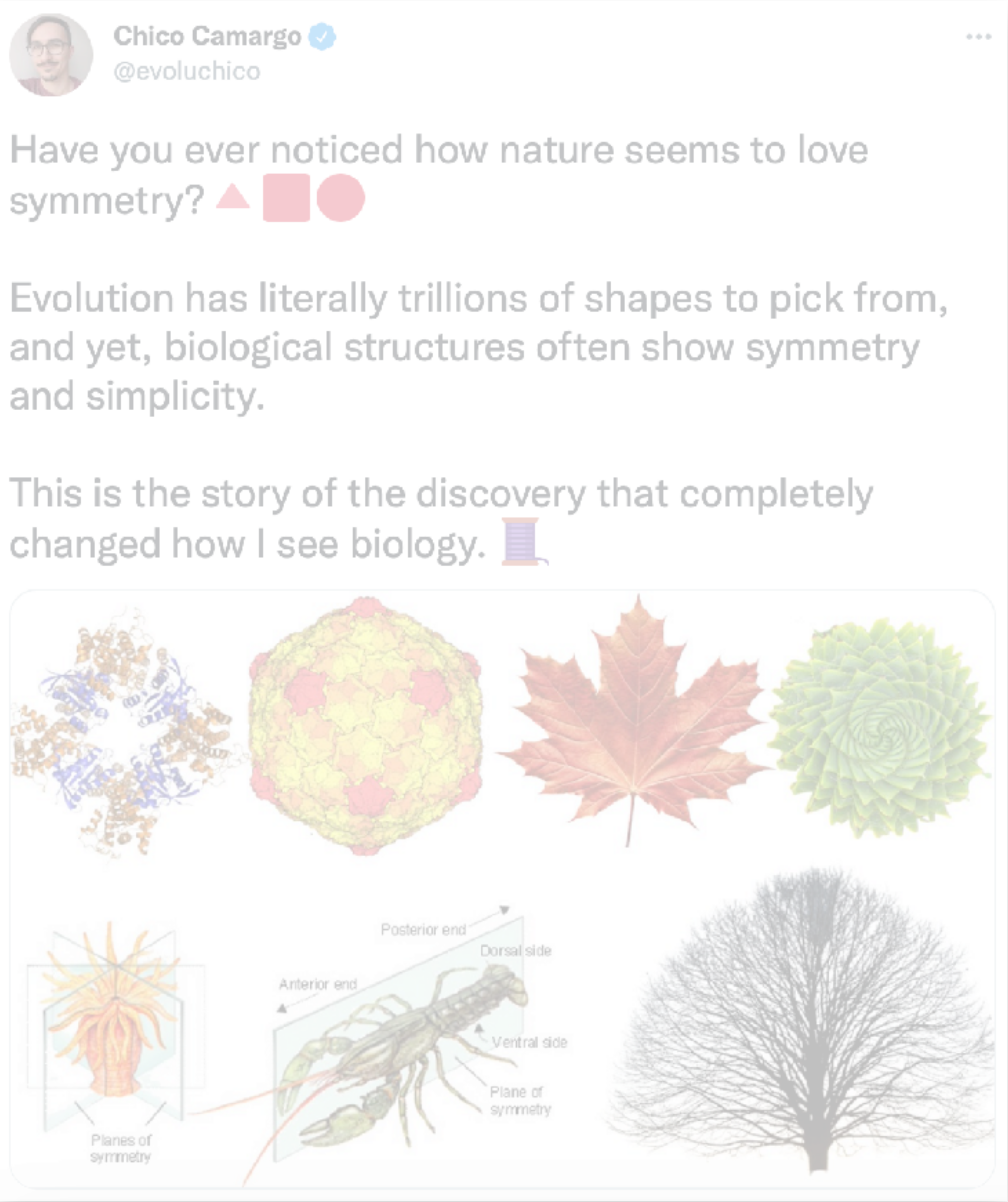
Have you ever noticed how nature seems to love symmetry? 🔺🟥🔴

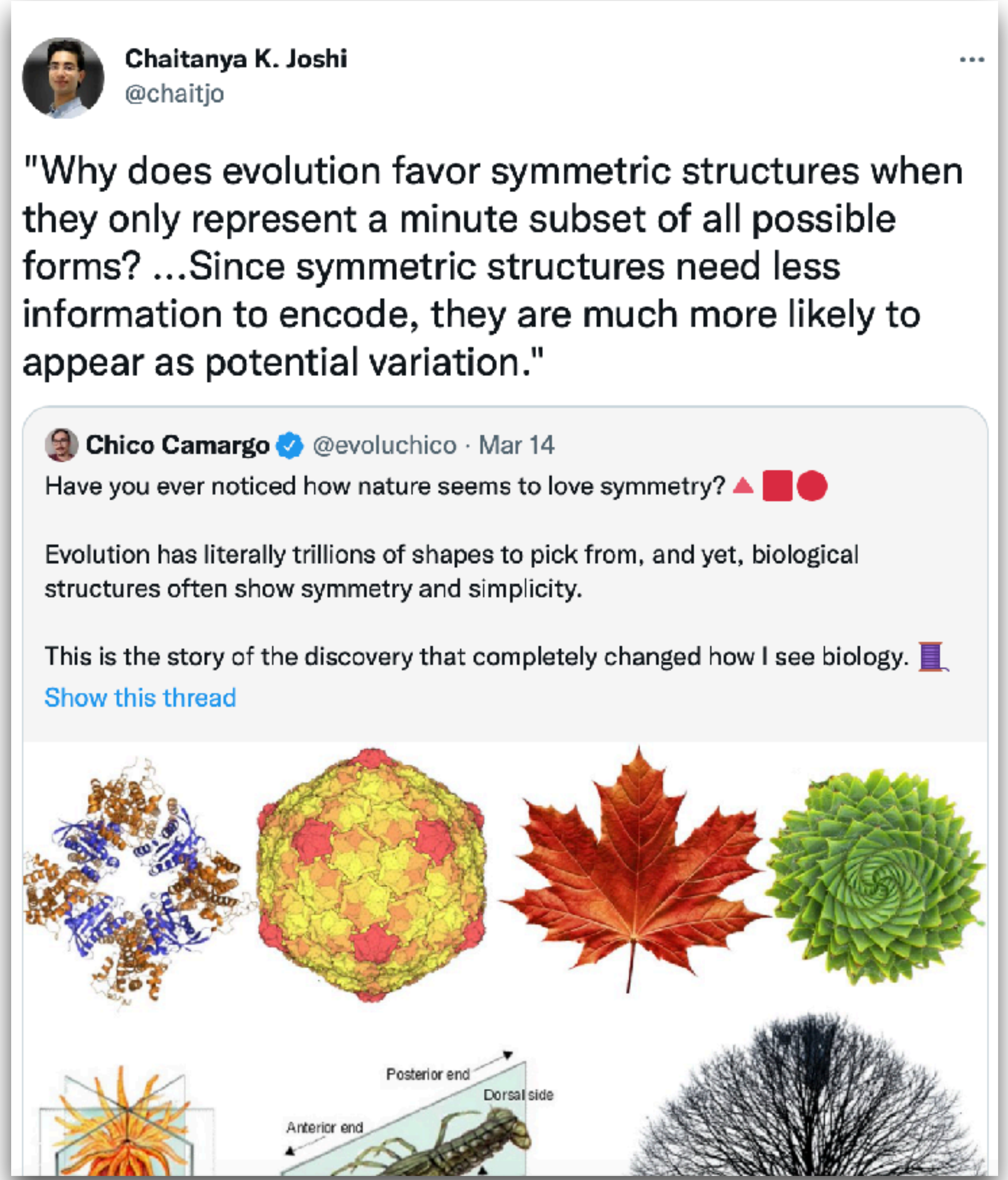
Evolution has literally trillions of shapes to pick from, and yet, biological structures often show symmetry and simplicity.

This is the story of the discovery that completely changed how I see biology. 🧵

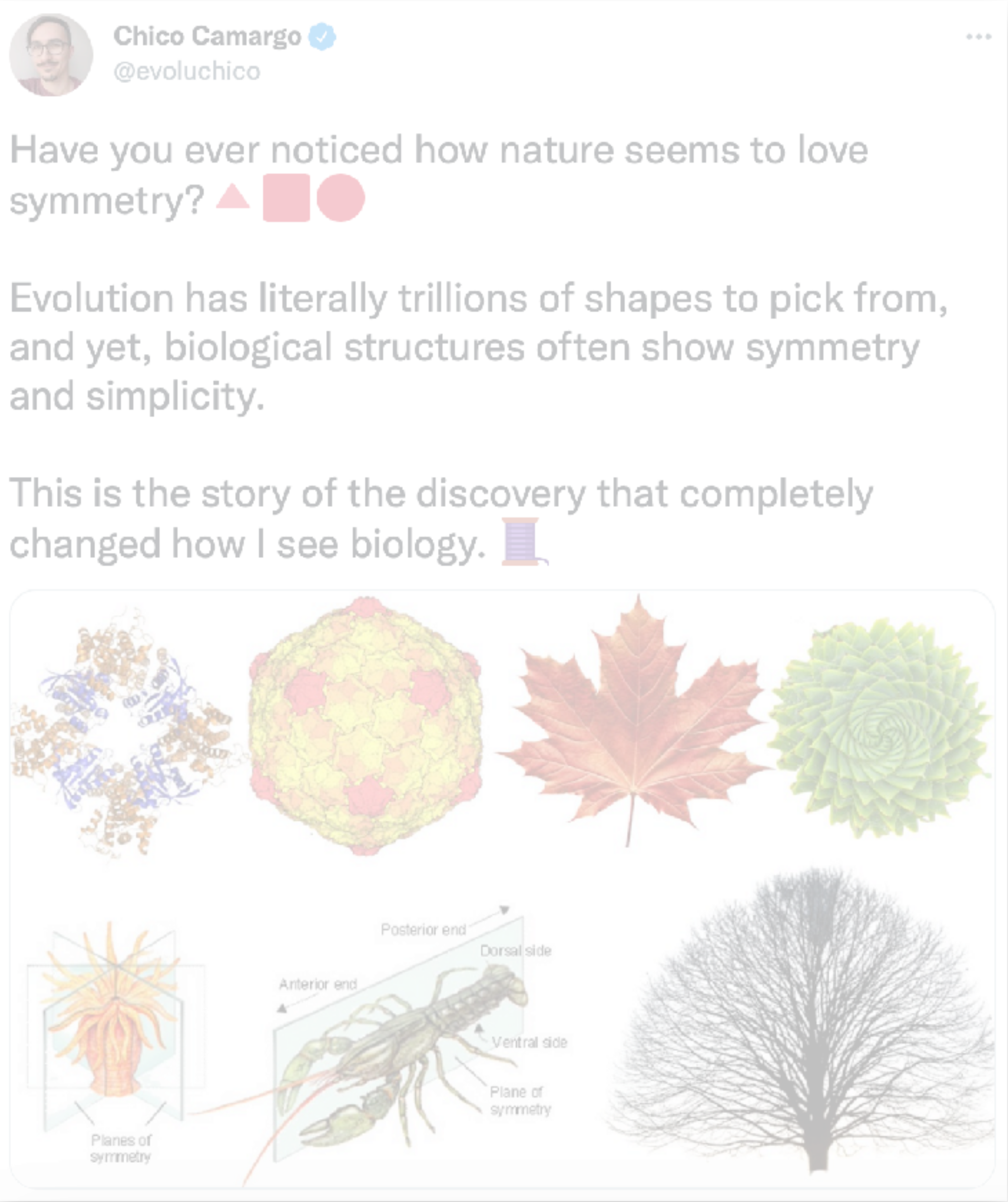


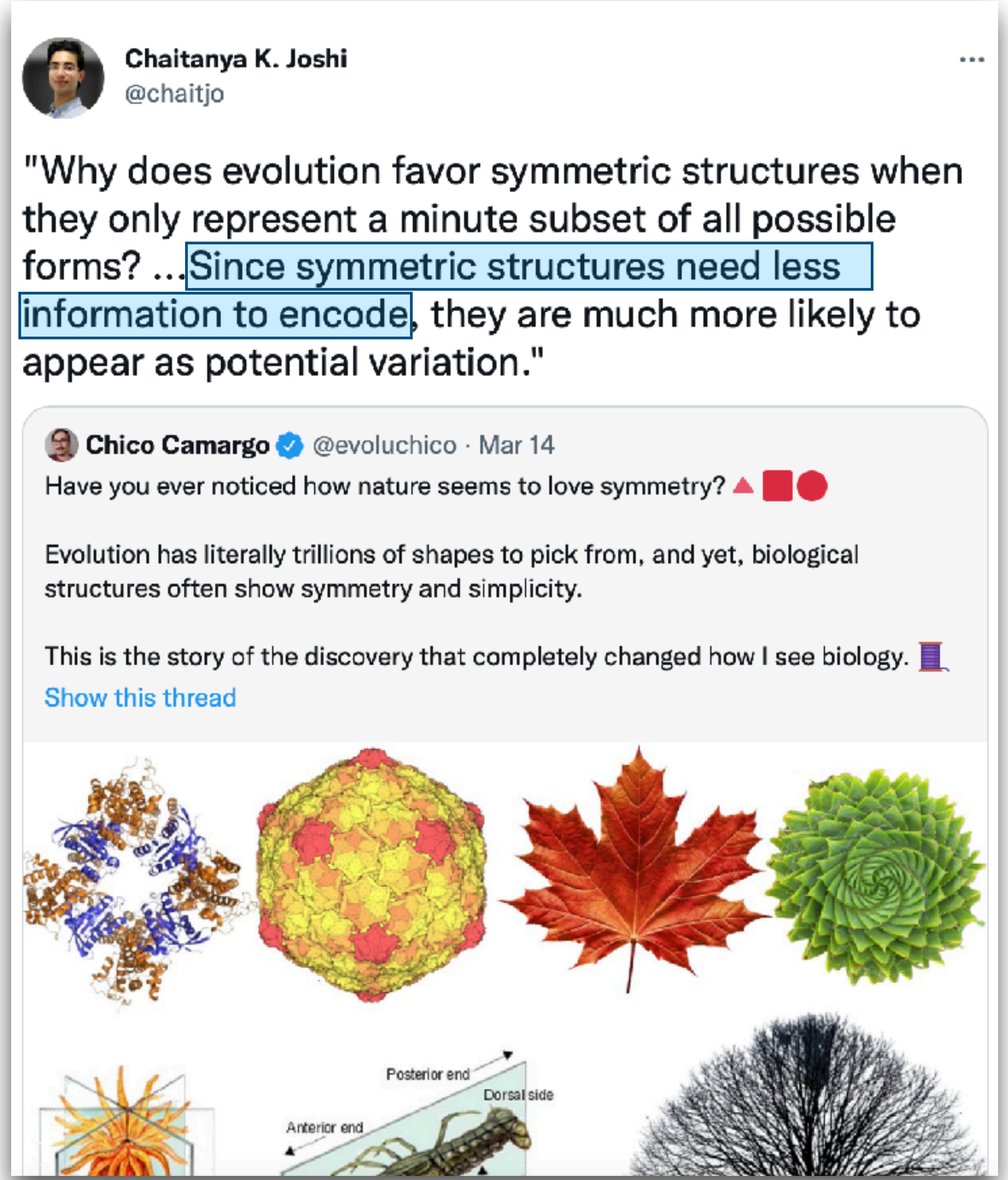
Symmetries in nature





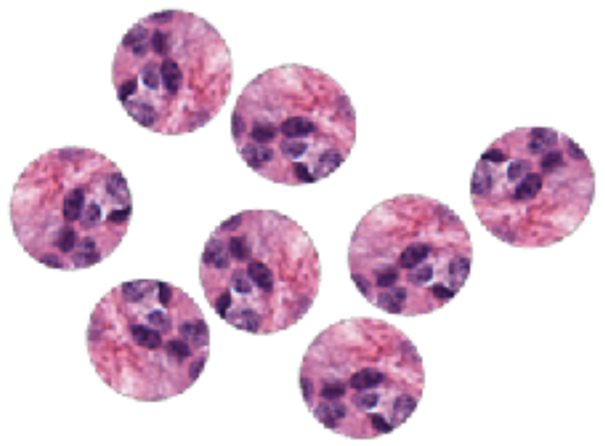
Symmetries in nature

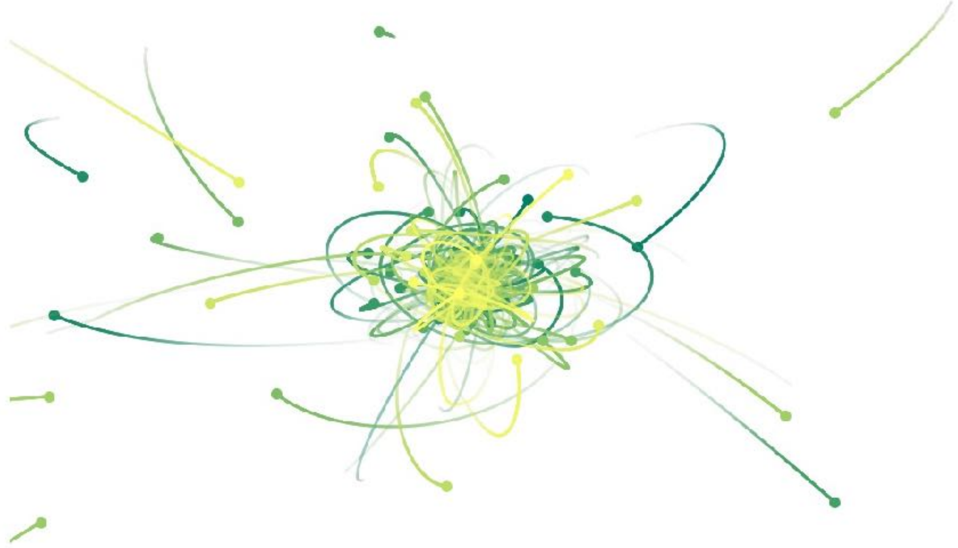


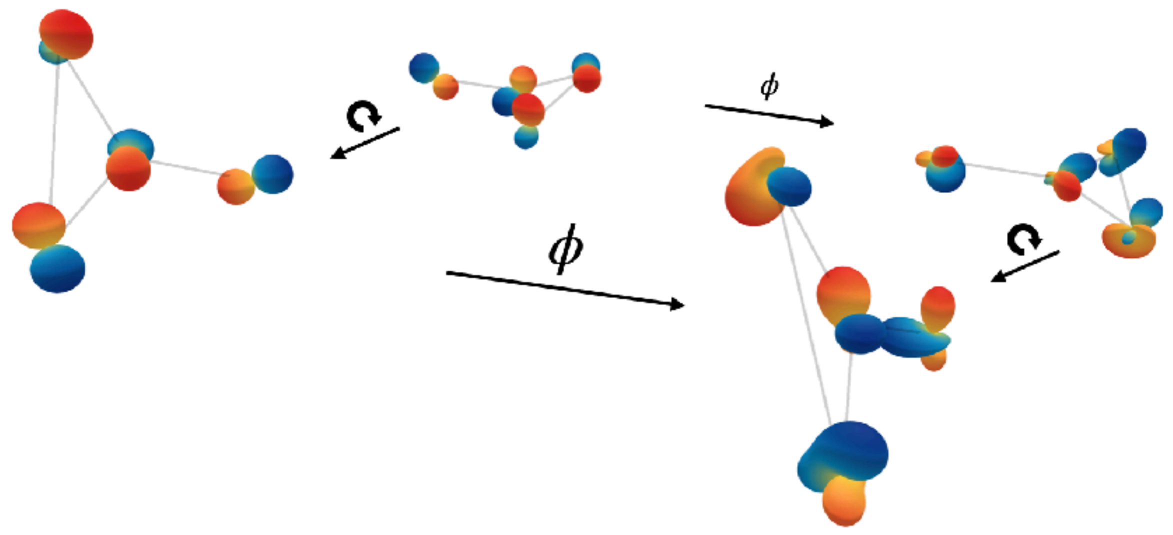


Group equivariant deep learning

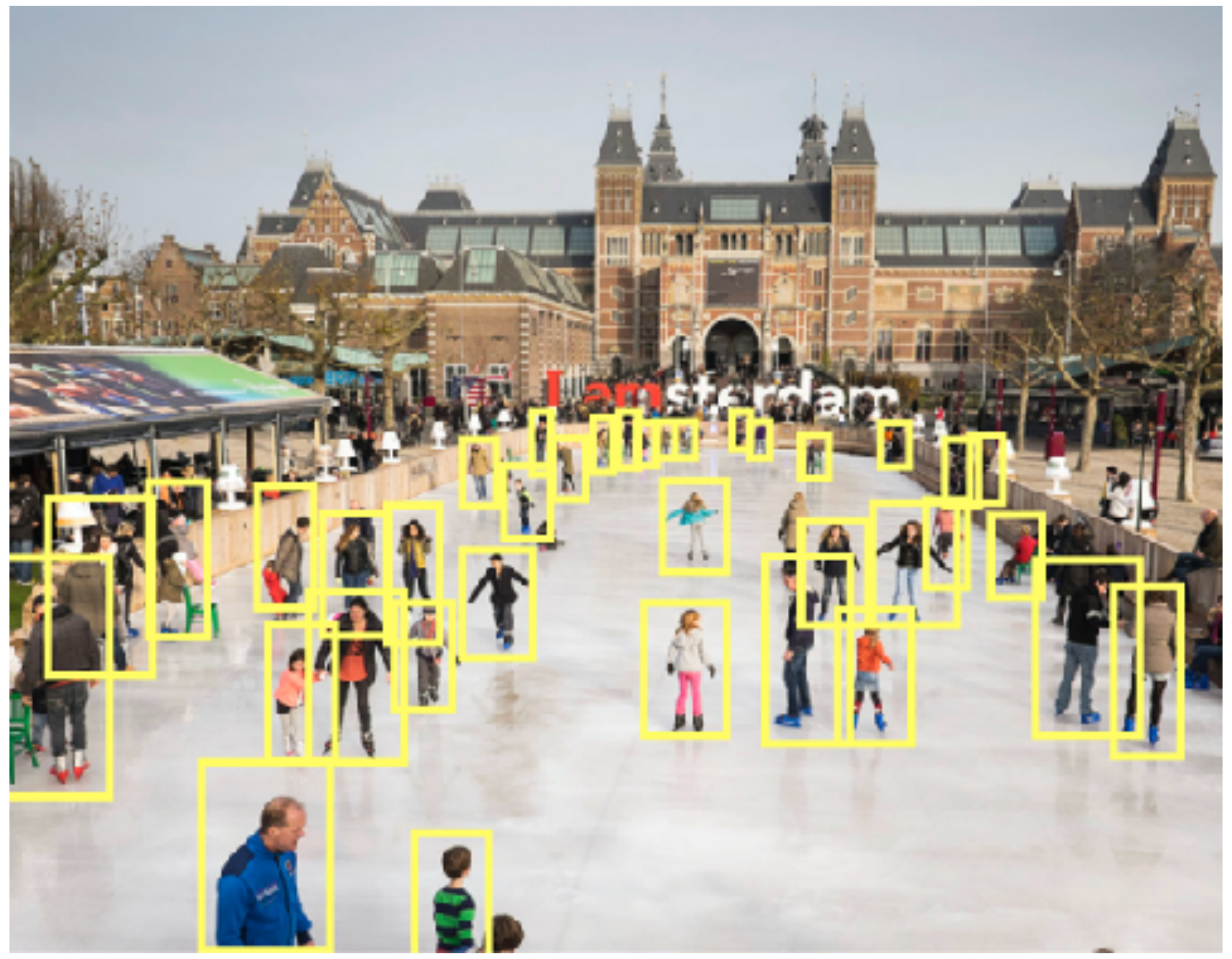
Create architectures with guarantees of invariance or equivariance
(often demanded by problems)



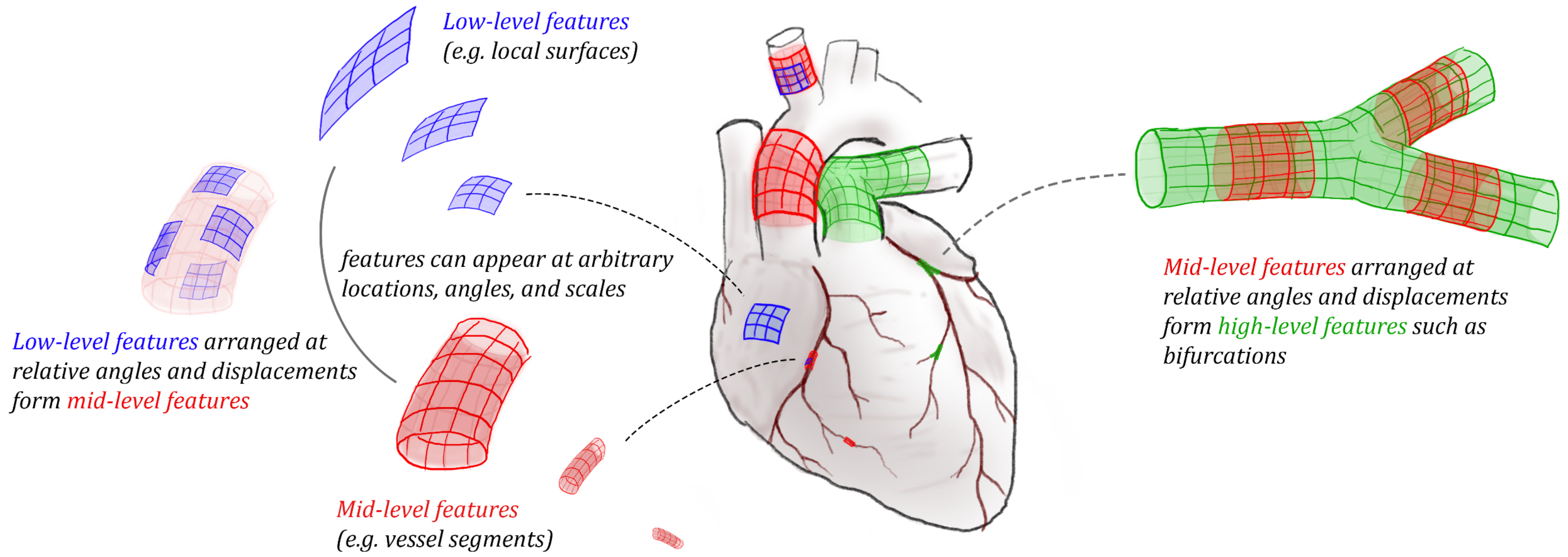




Equivariance allows for
increased weight sharing



Psychology of vision
(recognition by components)



Efficient representation learning
(leverage symmetries)