An introduction to geometric deep learning

Who Am I

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Interested in: Statistical machine learning, Geometric deep learning

Deep Learning

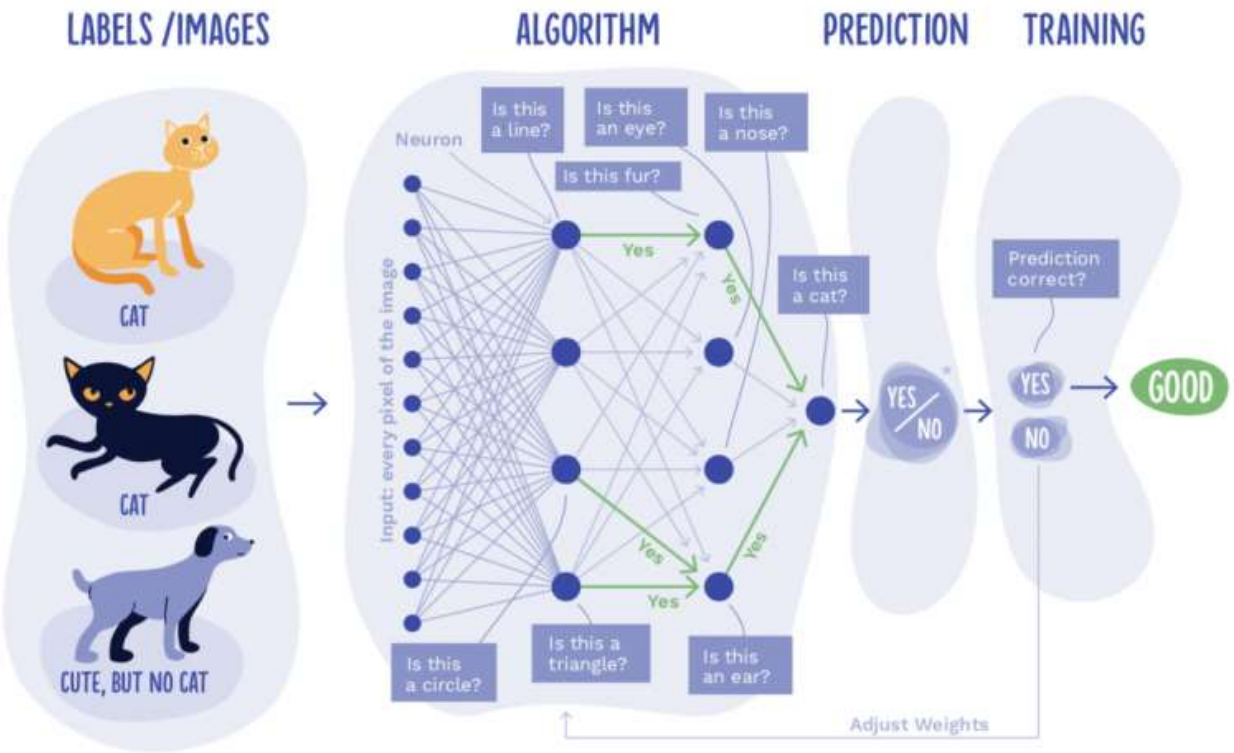


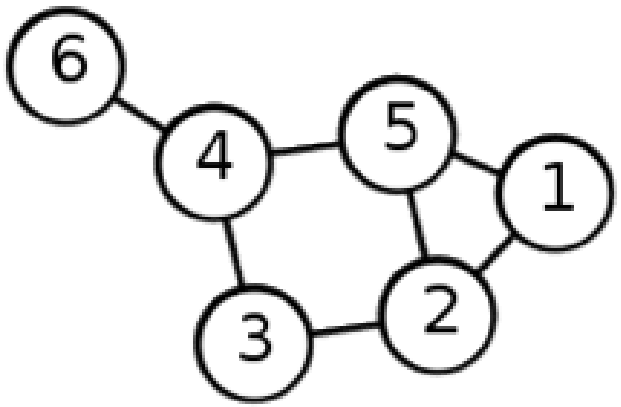
Image source: https://karmaadvisory.com/wp-content/uploads/2018/11/Screen-Shot-2018-11-04-at-2.38.34-PM-768x499.png

Goal

What is the one true architecture?

As in times past, this makes it difficult to understand the relations between various methods,
inevitably resulting in the reinvention and re-branding of the same concepts in different application domains[1]

We could consider Graphs as a starting point



Go Back in Time


Erlangen Programme, Klein proposed approaching geometry as the study of invariants, i.e. properties unchanged under some class of transformations, called the symmetries of the geometry[1]

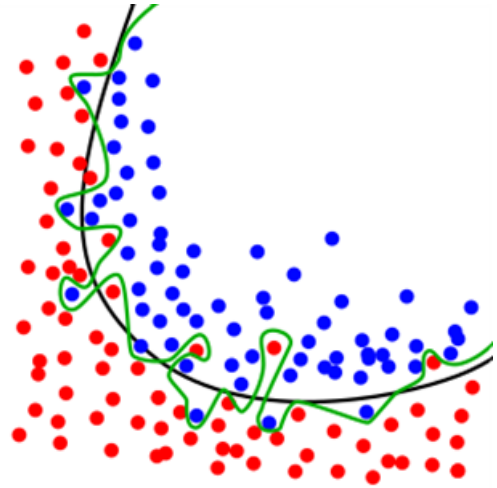
Image sources:
https://en.wikipedia.org/wiki/File:Scuola_di_atene_23.jpg
https://en.wikipedia.org/wiki/File:Lobachevsky_03_crop.jpg
https://en.wikipedia.org/wiki/File:Georg_Friedrich_Bernhard_Riemann.jpeg
https://en.wikipedia.org/wiki/File:Felix_Klein,_ante_1897_-_Accademia_delle_Scienze_di_Torino_0078_B.jpg

Why we’re interested in geometry?

*Almost everything is curve fitting

We’ve got high dimensional data
- Curse of dimensionality/ dimensionality reduction

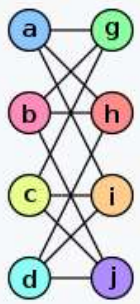
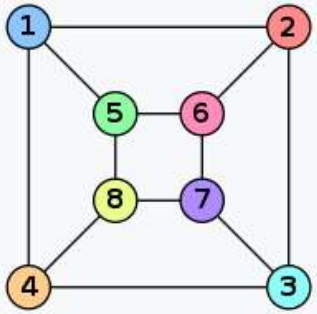
We need to restrict the definition of our function under certain assumptions -> Inductive Biases



https://en.wikipedia.org/wiki/File:Overfitting.svg

Inductive biases

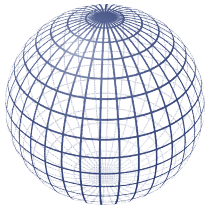
- Shifts do not affect image processing
- Rotations do not affect spherical data
- Graphs does not have order

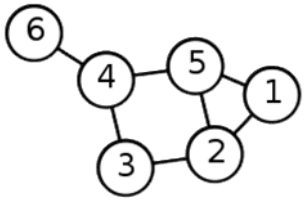
Graph G	Graph H	An isomorphism between G and H
		$f(a) = 1$ $f(b) = 6$ $f(c) = 8$ $f(d) = 3$ $f(g) = 5$ $f(h) = 2$ $f(i) = 4$ $f(j) = 7$

https://en.wikipedia.org/wiki/Graph_isomorphism

5G

Grids / Groups / Graphs / Geodesic & Gauges





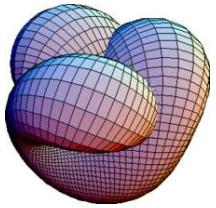


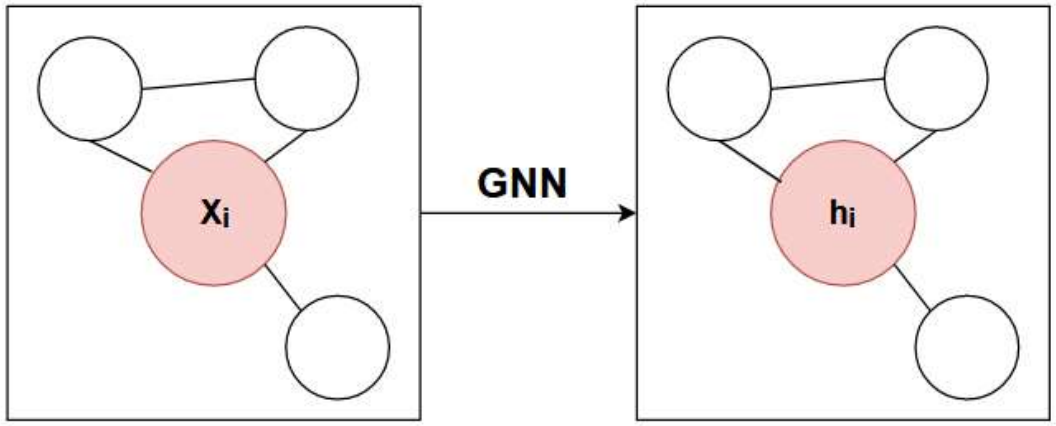
Image sources:
https://en.wikipedia.org/wiki/File:BoysSurfaceTopView.PNG
https://en.wikipedia.org/wiki/File:6n-graf.svg
https://en.wikipedia.org/wiki/Sphere#/media/File:Sphere_wireframe_10deg_6r.svg

Invariance & Equivariance

Considering graphs with no edges:
Permutation invariance: $f(PX) = f(X)$
Permutation equivariance: $f(PX) = Pf(X)$

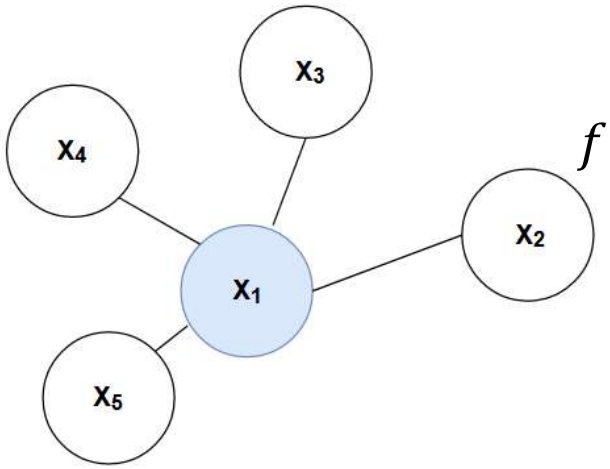
Considering normal graphs:
Permutation invariance: $f(PX, PAP^t) = f(X, A)$
Permutation equivariance: $f(PX, PAP^t) = Pf(X, A)$

Graphs in action



Node Classification / Graph Classification / Link prediction

Convolutional GNN



$$f(x_1) = x_1 + x_2 + x_3 + x_4 + x_5$$
$$f(x_1) = c_{11}x_1 + c_{12}x_2 + c_{13}x_3 + c_{14}x_4 + c_{15}x_5$$
$$f(x_1) = c_{11}x_1W + c_{12}x_2W + c_{13}x_3W + c_{14}x_4W + c_{15}x_5W$$
$$f(x_1) = \sigma(c_{11}x_1W + c_{12}x_2W + c_{13}x_3W + c_{14}x_4W + c_{15}x_5W)$$

$$f(x_i) = \phi(x_i \bigoplus_{j \in N_i} c_{ij}\psi(x_j)$$

Domains & Symmetry group

Architecture	Domain	Symmetry Group
CNN	Grid	Translation
Spherical CNN	Sphere/SO(3)	Relation SO(3)
Intrinsic/Mesh CNN	Manifold	Isometry Iso/Gauge symmetry SO(2)
GNN	Graph	Permutation
Deep Sets	Set	Permutation
Transformer	Complete Graph	Permutation
LSTM	1D Grid	Time wrapping

References

[1] Bronstein, Michael M., et al. "Geometric deep learning: Grids, groups, graphs, geodesics, and gauges.“ *arXiv preprint arXiv:2104.13478* (2021).
[2] Bronstein, Michael M., et al. "Geometric deep learning: going beyond euclidean data.“ *IEEE Signal Processing Magazine* 34.4 (2017): 18-42.