Geometric Deep Learning: An Introduction

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April 6, 2022

Outline

- Goal of Geometric Deep Learning
- Why Geometric Deep Learning?
- Groups and Symmetry
- Geometric Priors - Symmetry
- Geometric Priors - Scale Separation
- Geometric Deep Learning Blueprint
- Graph Neural Networks
- My Review of the "Proto Book"

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- Ideas from CNNs such as shift invariance can generalize to different types of data, hinting at a more general framework for Deep Learning.
- First occurrence of GDL is in the 2016 paper, "*Geometric deep learning: going beyond Euclidean data*" by Bronstein et al.

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3. GDL provides a common mathematical framework (Group Theory) from which to study and compare different DL architectures such as CNNs, RNNs, and Transformers.
4. Natural symmetries are commonplace in many branches of science including physics and chemistry (Conservation of Energy and Angular Momentum, Molecular Symmetry) and as such is a natural idea to bring into deep learning.

Preliminary Definitions - Domain and Signal

- Ω is our domain which is a set with (possible) additional structure.
- On Ω, we can define $\mathcal{X}(\Omega, \mathcal{C})$ to be the space of all $\mathcal{C}$-valued signals on Ω.
- Example: $\Omega = n \times n$ grid, then $v \in \mathcal{X}(\Omega, \mathbb{R}^3)$ is an RGB image.

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- **Examples**: The symmetry group of the circle is all rotations, the symmetry group of a set is all permutations of the elements.
- We can extend these ideas to our domains and signals by introducing the concept of a **Group Action** which gives a rule telling us how our domain and symmetry group interact.

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Invariant and Equivariant Functions

Once we have a specific domain, Ω and symmetry group, $\mathcal{G}$, we want to build our function by adding *layers* of functions that "respect" the symmetries of Ω. There are two types of functions that can do this:

- **Invariant Functions**: The output of an invariant function is equal for all symmetries of the input.

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- **Invariant Functions**: The output of an invariant function is equal for all symmetries of the input.
- **Equivariant Functions**: The change in the output of an equivariant function is proportional to the change of the input.

Invariance and Equivariance in CNNs

Invariant and equivariant layers are not new to Deep Learning and are incorporated into Convolutional Neural Networks (CNNs):

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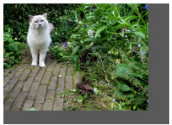
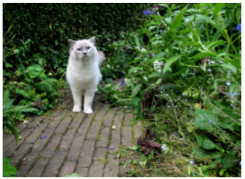
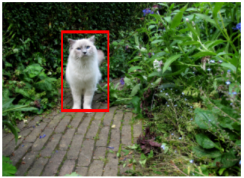
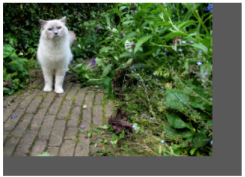
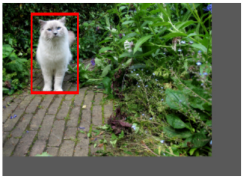
- Convolutional layers in CNNs are **equivariant** to translation of the input images.
- Adding global pooling after the convolutional layers (usually in the form of Global-Average Pooling) makes CNNs **invariant** to translations of the input images.

Invariance Visualized

$$\mathrm{F}(\text{  }) = \mathrm{F}(\text{  })$$

Equivariance Visualized

$$\mathbf{F}\left(\text{  }\right) = \text{  }$$

$$\mathbf{F}\left(\text{  }\right) = \text{  }$$

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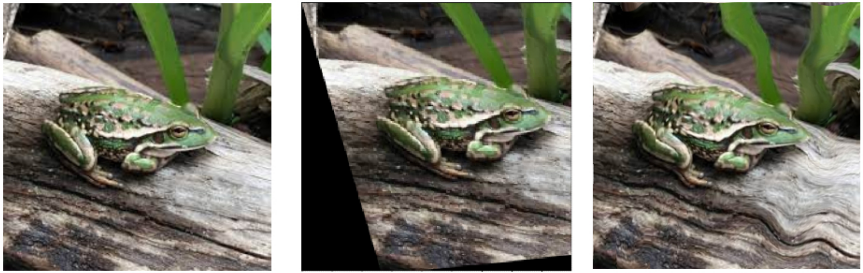
(4 frame difference)

Deformation Stability II

Instead of just considering global, exact symmetries, we want to build layers that are invariant (equivariant) to these local symmetries too. The authors call these **local deformations**:



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We can try to improve on this by exploiting the **multi-scale structure** of our learning problems, a popular approach in many domains of science.

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- Composing these operators allows us to build up equivariant functions that are computationally efficient while still respecting the symmetries and deformations of the signals.

Blueprint of Geometric Deep Learning

Let Ω be the domain and $\mathcal{G}$ be a symmetry group for Ω. We consider Ω' to be a coarsened version of Ω. We define the following building blocks:

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Using these blocks allows constructing $\mathcal{G}$-invariant functions, $f : \mathcal{X}(\Omega, \mathcal{C}) \to \mathcal{Y}$ of the form

$$f = A \circ \sigma_J \circ B_J \circ P_{J-1} \circ \cdots \circ P_1 \circ \sigma_1 \circ B_1$$

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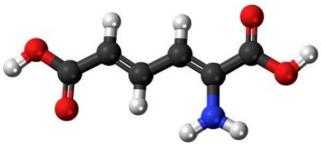

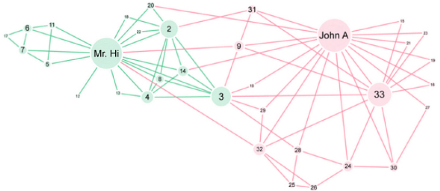

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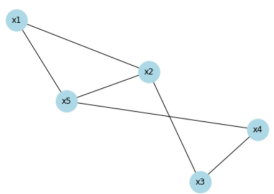
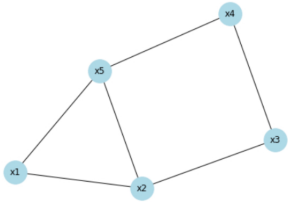
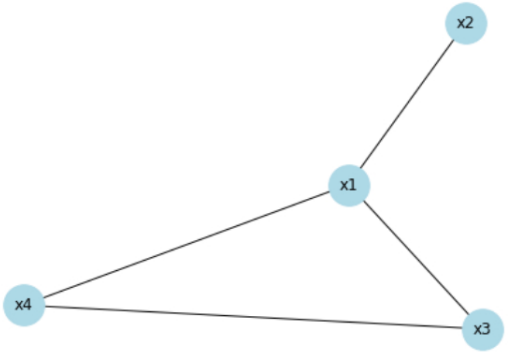




Graph and Adjacency Matrix



$$\begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

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- Example: $P = P_{(2413)} \in S_4$ maps 1 to 2, 2 to 4, etc.
- We can represent this transformation as a matrix multiplication:

$$PX = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} x_2 \\ x_4 \\ x_1 \\ x_3 \end{pmatrix}$$

- PAP^T is the adjacency matrix of the transformed graph, PX.

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- To ensure permutation equivariance of F, ϕ must be permutation **invariant**.

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- **Attentional**[5]: Neighbourhood features aggregated with **learned** weights:

$$\text{Ex: } \phi(x_j, X_{\mathcal{N}_j}) = \sum_{i \in \mathcal{N}(j)} \alpha(x_i, x_j) \psi(x_i)$$

Recipe for Graph Neural Networks II

- **Convolutional**[2]: Neighbourhood features aggregation is done with **fixed** weights:

$$\text{Ex: } \phi(x_j, X_{\mathcal{N}_j}) = \sum_{i \in \mathcal{N}(j)} c_{ij} \psi(x_i)$$

- **Attentional**[5]: Neighbourhood features aggregated with **learned** weights:

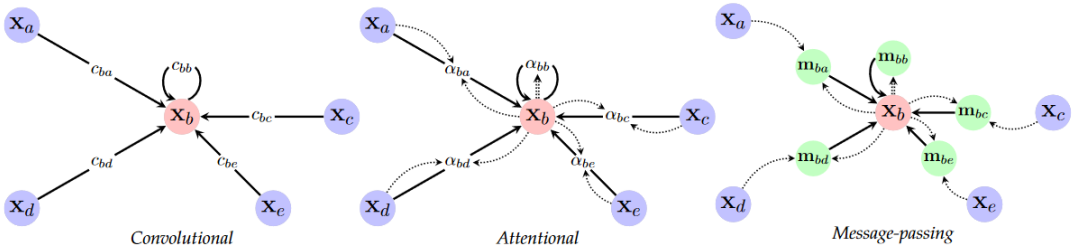
$$\text{Ex: } \phi(x_j, X_{\mathcal{N}_j}) = \sum_{i \in \mathcal{N}(j)} \alpha(x_i, x_j) \psi(x_i)$$

- **Message-Passing**[3]: Neighbourhood features aggregated through vector-valued function, φ:

$$\text{Ex: } \phi(x_j, X_{\mathcal{N}_j}) = \sum_{i \in \mathcal{N}(j)} \varphi(x_i, x_j)$$

Summary of Graph Neural Networks

- GNN layers are built by constructing locally equivariant functions operating on the 1-hop neighbourhoods of a node.
- Stacking GNN layers allows propagating of interactions across larger distances.
- **Connection**: Transformers are attentional GNNs on a complete graph.
- Increasing generality: convolutional $\subseteq$ attentional $\subseteq$ message-passing



GNNs in Practice

- Pinterest (Convolutional)
- Uber Eats (Convolutional)
- Google Maps (Attentional)

$$\mathbf{h}_v^0 = \mathbf{x}_v$$

initial layer 0 embeddings are equal to node features

$$\mathbf{h}_v^k = \sigma\left(\mathbf{W}_k \sum_{u \in N(v)} \frac{\mathbf{h}_u^{k-1}}{|N(v)|} + \mathbf{B}_k \mathbf{h}_v^{k-1}\right), \quad \forall k > 0$$

k^{th} layer embedding of v

non-linearity

average of neighbor's previous layer embeddings

previous layer embedding of v

$$z_v = \mathbf{h}_v^{last}$$

Review

The book was a bit of a mixed bag:

- **The Good**: Interesting concepts, clear presentation of CNNs, GNNs, good motivation.

Review

The book was a bit of a mixed bag:

- **The Good**: Interesting concepts, clear presentation of CNNs, GNNs, good motivation.
- **The Less-Good**: Authors make some large claims and don't expand/cite them. Claim book is useful for ML practitioners but do not expand on this.

Thanks for Listening!

More GDL Links

- Interactive article on GNNs
- GDL100 Lectures (By authors of the text)
- Practical GNN/GDL Tutorials: One, Two
- PyTorch Geometric Tutorials

[1] Y. Lecun et al. "Gradient-based learning applied to document recognition". In: *Proceedings of the IEEE* 86.11 (1998), pp. 2278–2324. DOI: 10.1109/5.726791.

[2] Thomas N. Kipf and Max Welling. *Semi-Supervised Classification with Graph Convolutional Networks*. 2017. arXiv: 1609.02907 [cs.LG].

[3] Justin Gilmer et al. *Neural Message Passing for Quantum Chemistry*. 2017. arXiv: 1704.01212 [cs.LG].

[4] Anna M M Scaife and Fiona Porter. "Fanaroff–Riley classification of radio galaxies using group-equivariant convolutional neural networks". In: *Monthly Notices of the Royal Astronomical Society* 503.2 (Feb. 2021), pp. 2369–2379. ISSN: 0035-8711. DOI: 10.1093/mnras/stab530. eprint: https://academic.oup.com/mnras/article-pdf/503/2/2369/36733567/stab530.pdf. URL: https://doi.org/10.1093/mnras/stab530.

[5] Petar Veličković et al. *Graph Attention Networks*. 2018. arXiv: 1710.10903 [stat.ML].