Geometric Deep Learning Self-Study Group

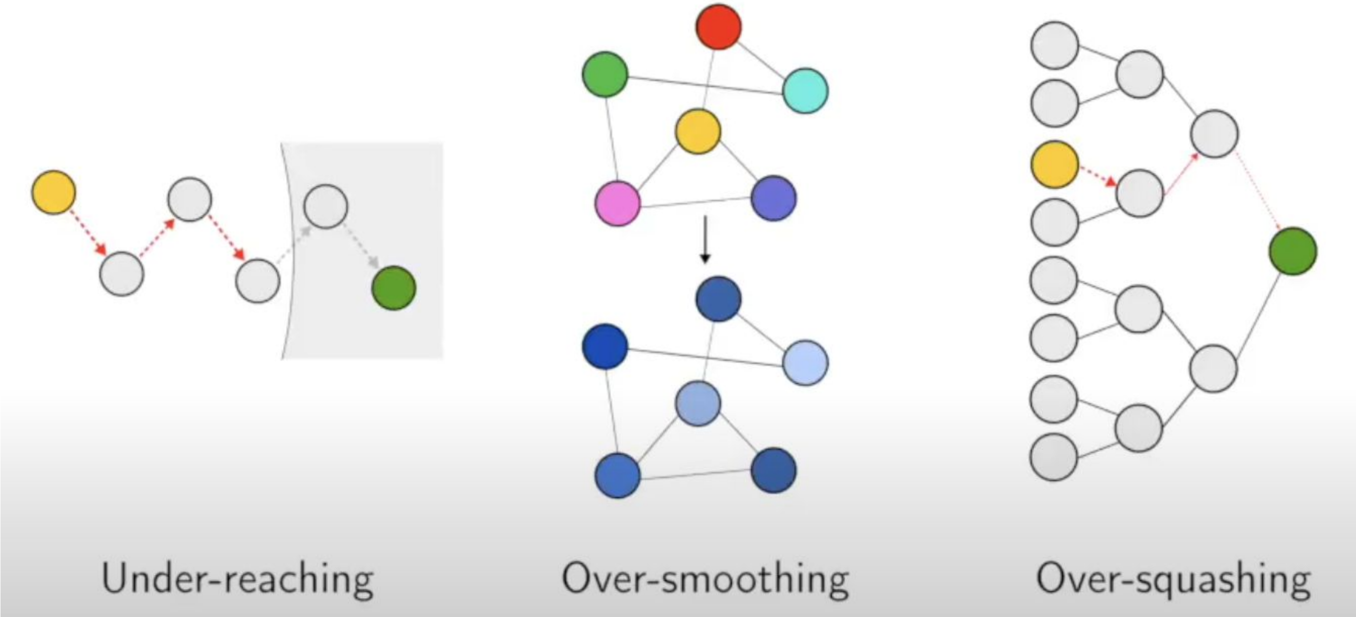
Session 4

October 13, 2025

Aaron Margolis
https://armargolis.github.io/

Session Outline

Expressivity/
Under-reaching



Tutorials

Group Discussion - Possible Project

Remaining Sessions:

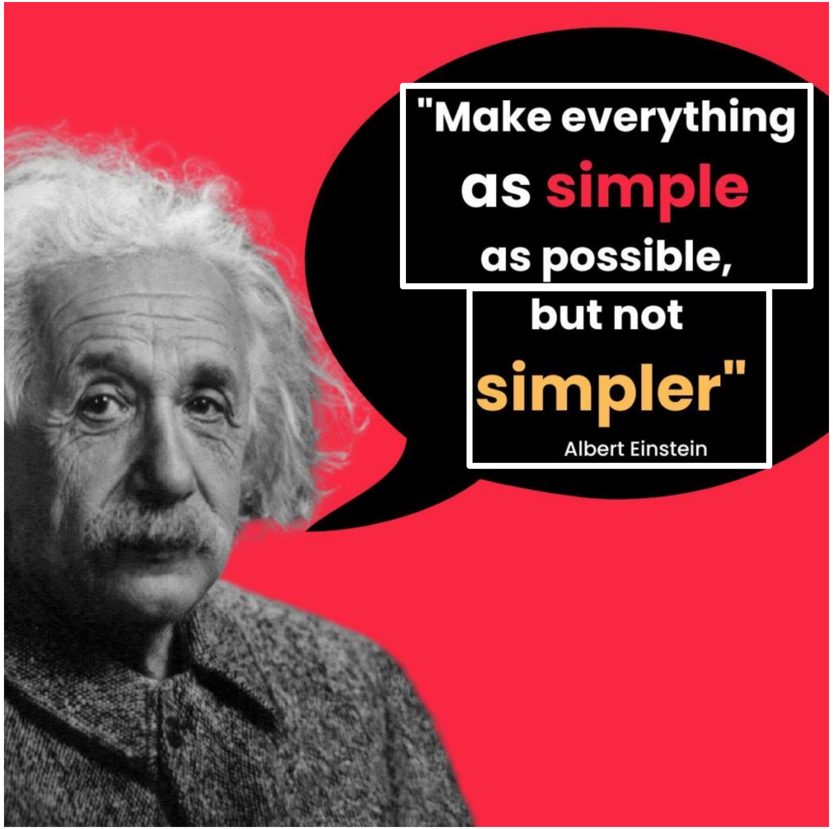
Oct 13: Expressivity

Nov 3: Over-smoothing, Over-squashing and Curvature

Nov 17: Equivariance

Dec 1: Manifolds

Expressivity and Oversquashing



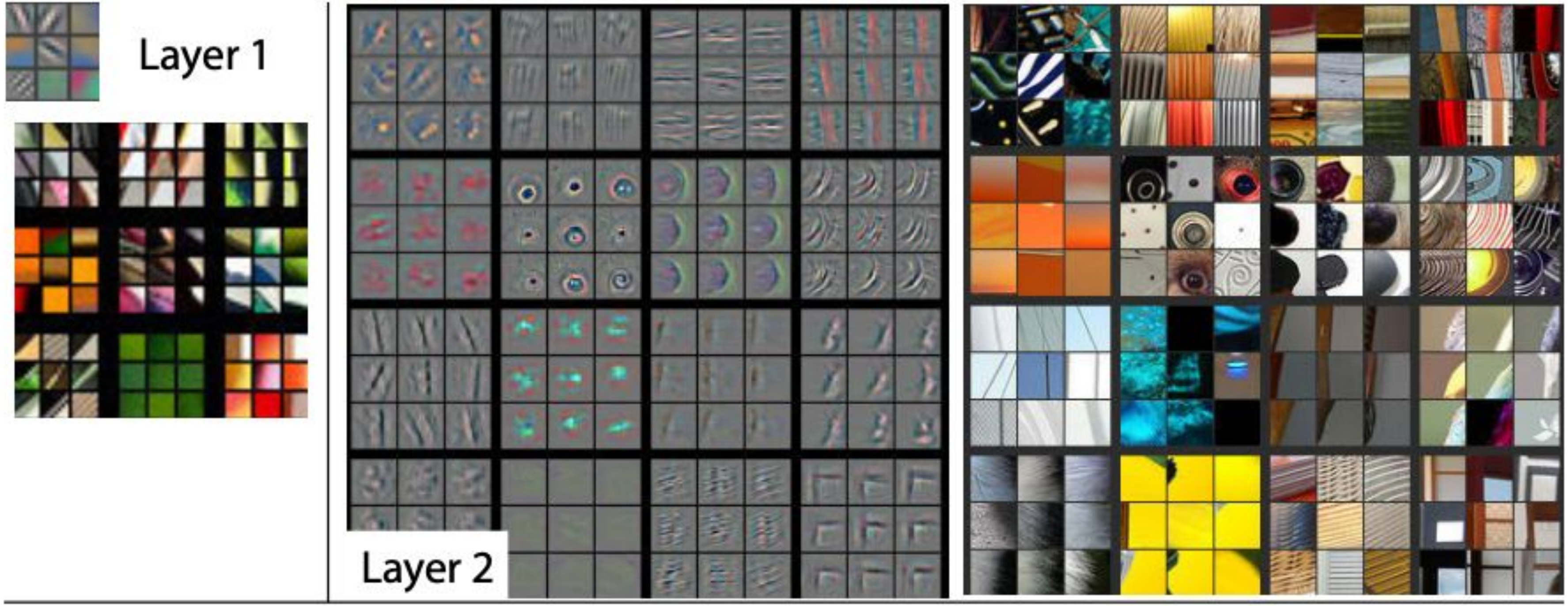
Avoid Oversmoothing and oversquashing

Why dense layers at the beginning don't work

Achieve Minimum Expressivity

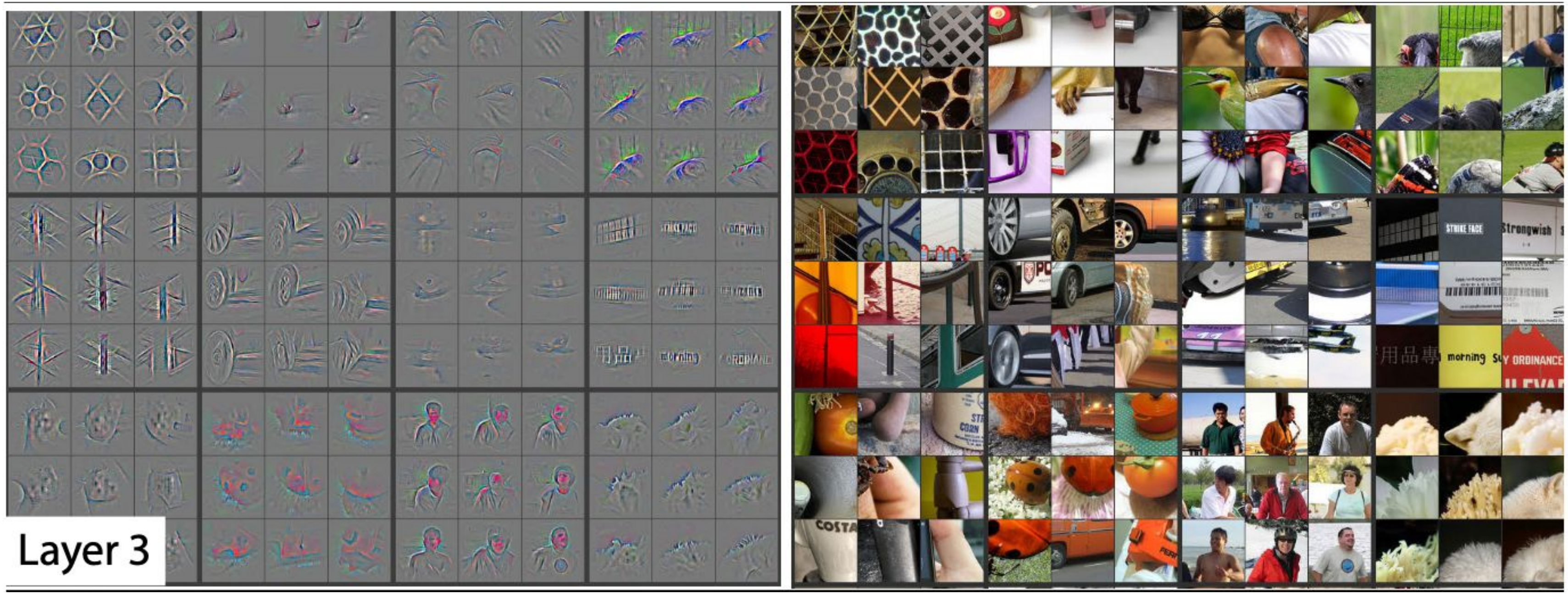
Why you need multiple convolutional layers

Expressivity



Source: Visualizing and Understanding Convolutional Networks
By Matthew D. Zeiler, Rob Fergus

Expressivity



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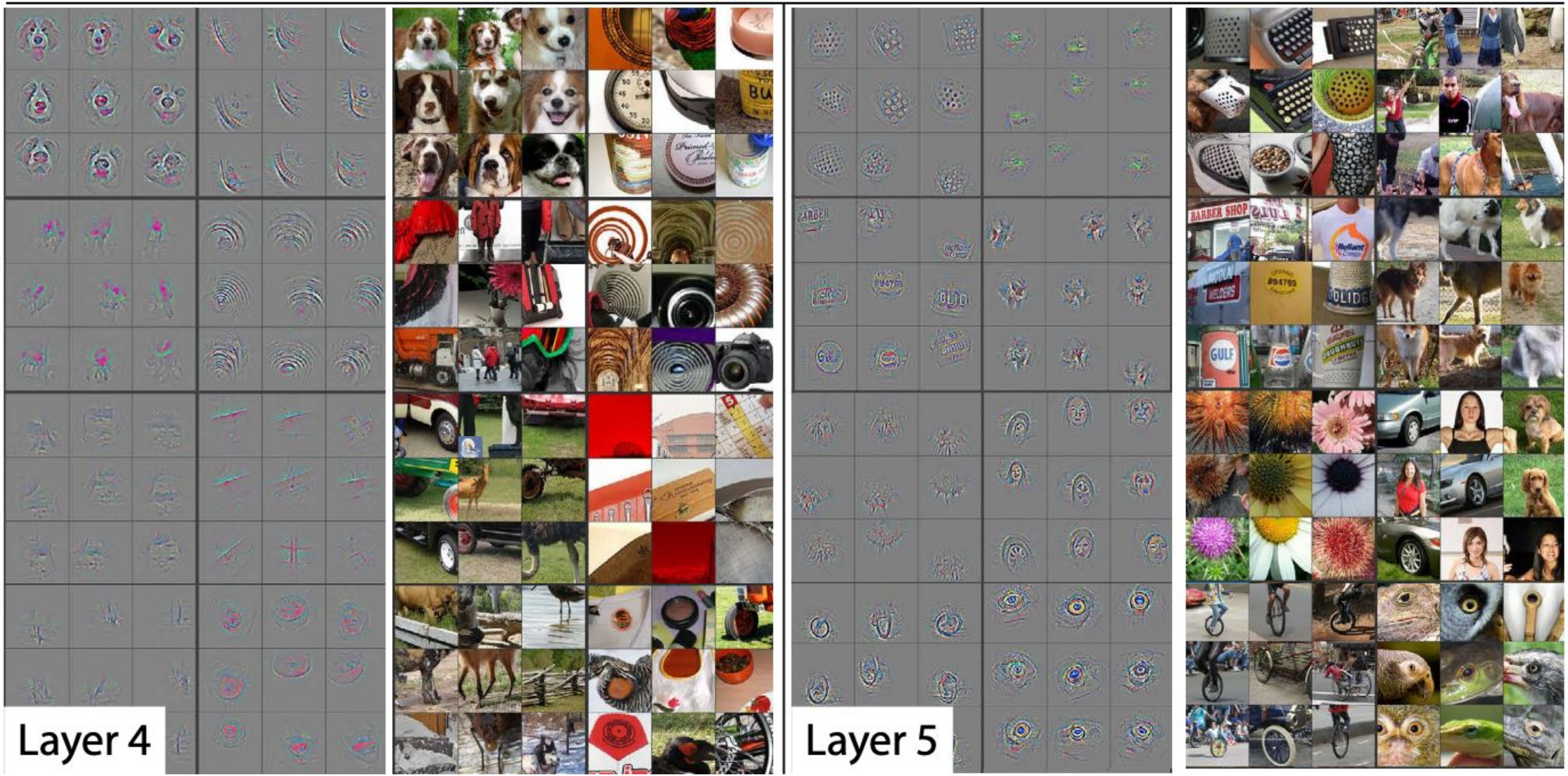
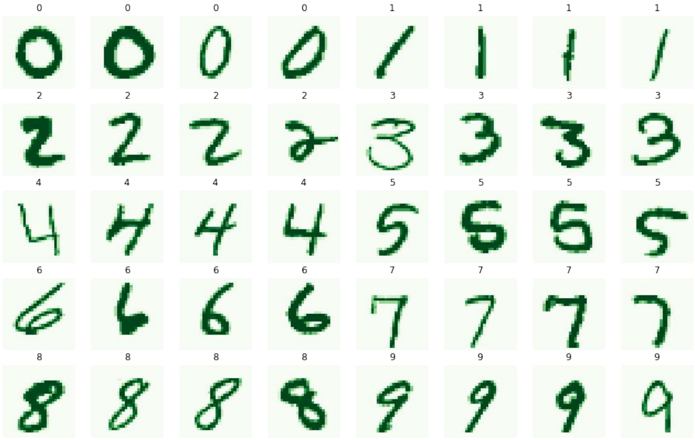

Layer 4
Layer 5
BARBER SHOP
GULF

5,000 images 28 by 28 images = 3,920,000 data points

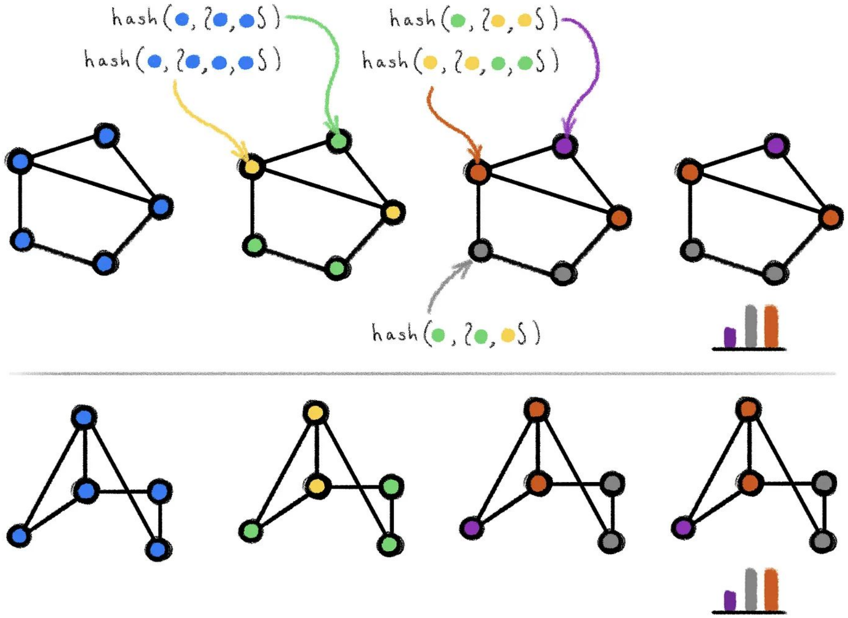
Input images (28 by 28)

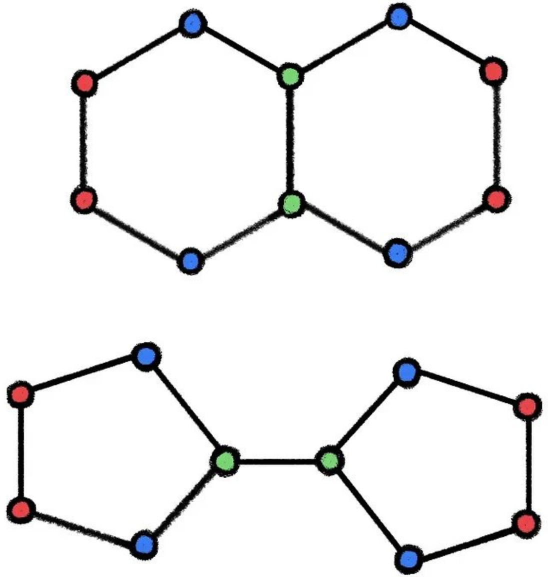


https://www.kaggle.com/code/gpreda/simple-introduction-to-cnn-for-mnist-99-37

```
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
conv2d (Conv2D)              (None, 28, 28, 32)        320
batch_normalization (BatchNo (None, 28, 28, 32)        128
conv2d_1 (Conv2D)            (None, 26, 26, 32)        9248
batch_normalization_1 (Batch (None, 26, 26, 32)        128
conv2d_2 (Conv2D)            (None, 13, 13, 32)        25632
max_pooling2d (MaxPooling2D) (None, 6, 6, 32)          0
batch_normalization_2 (Batch (None, 6, 6, 32)          128
dropout (Dropout)            (None, 6, 6, 32)          0
conv2d_3 (Conv2D)            (None, 3, 3, 64)          18496
max_pooling2d_1 (MaxPooling2 (None, 1, 1, 64)          0
batch_normalization_3 (Batch (None, 1, 1, 64)          256
conv2d_4 (Conv2D)            (None, 1, 1, 64)          36928
dropout_1 (Dropout)          (None, 1, 1, 64)          0
flatten (Flatten)            (None, 64)                0
dense (Dense)                (None, 128)               8320
dropout_2 (Dropout)          (None, 128)               0
dense_1 (Dense)              (None, 10)                1290
=================================================================
Total params: 100,874
Trainable params: 100,554
Non-trainable params: 320
```

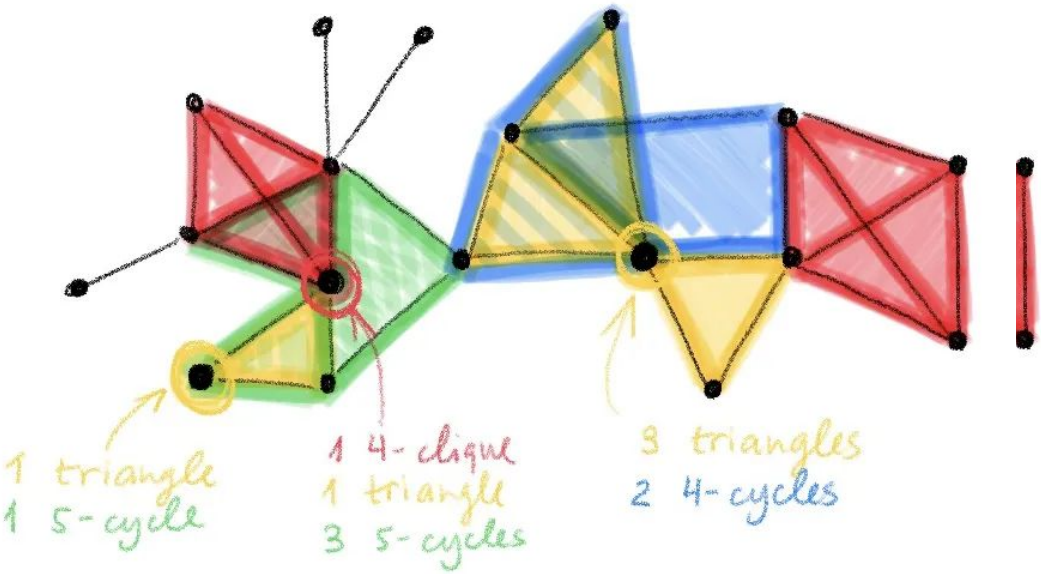
Node Embeddings, Expressive Power and Limitations





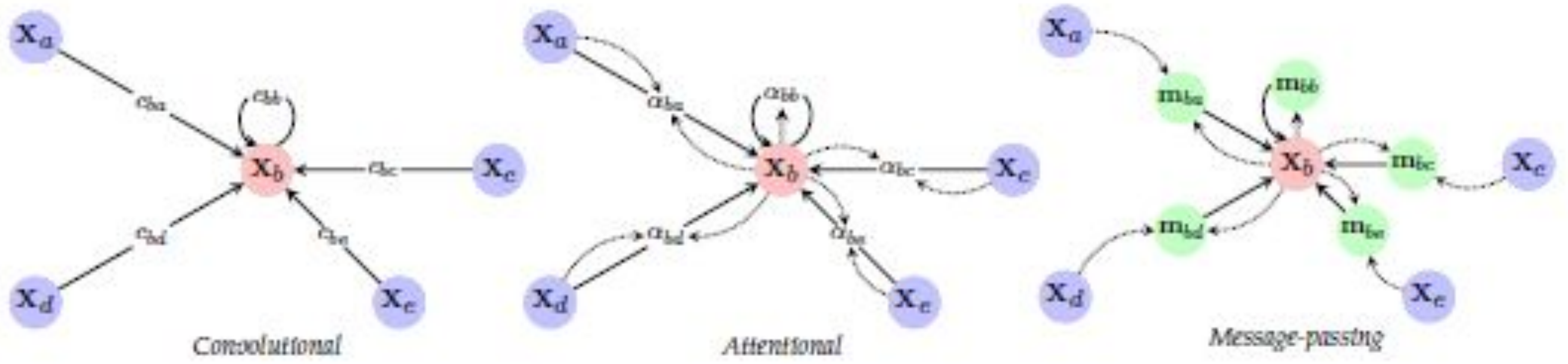
Source: Bronstein
https://medium.com/data-science/expressive-power-of-graph-neural-networks-and-the-weisefeiler-lehman-test-b883db3c7c49?sk=5c2a28ccd38db3a7b6f80f161e825a5a

We need something more powerful than GNNs

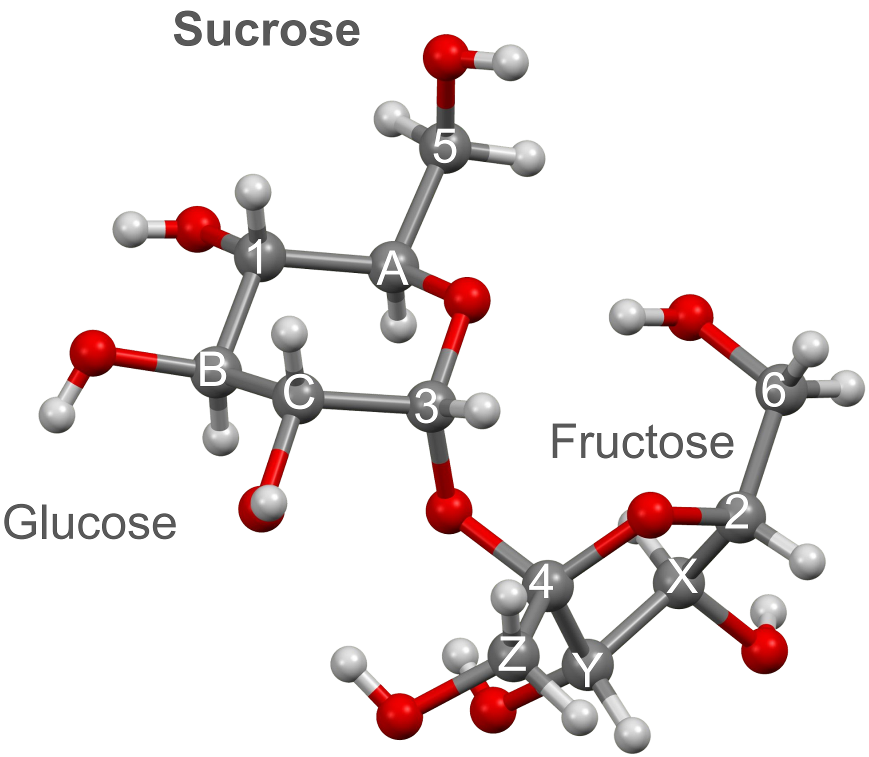


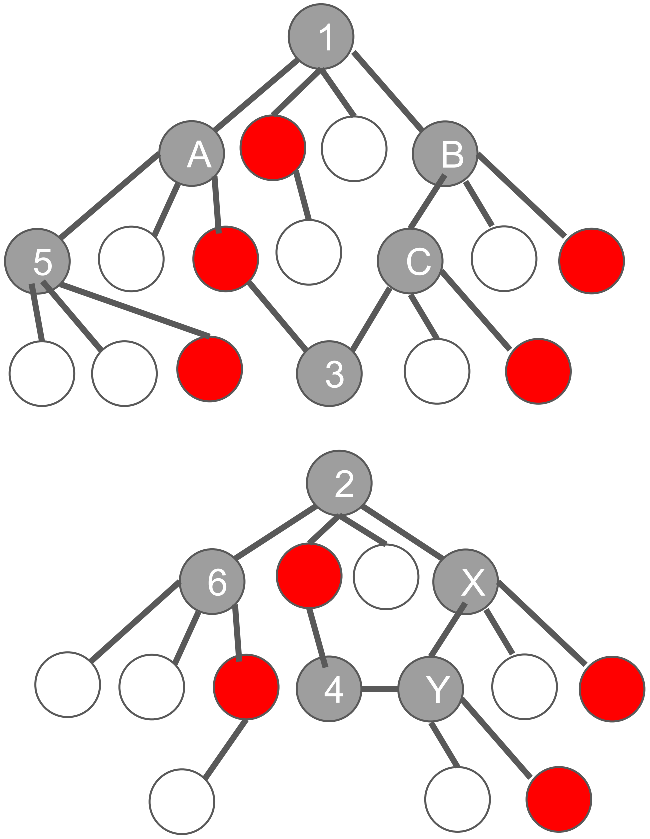
Source:
https://medium.com/data-science/beyond-weisfeiler-lehman-using-substructures-for-provably-expressive-graph-neural-networks-d476ad665fa3?sk=bc0d14c28a380b4d51debc4935345b73

More powerful techniques

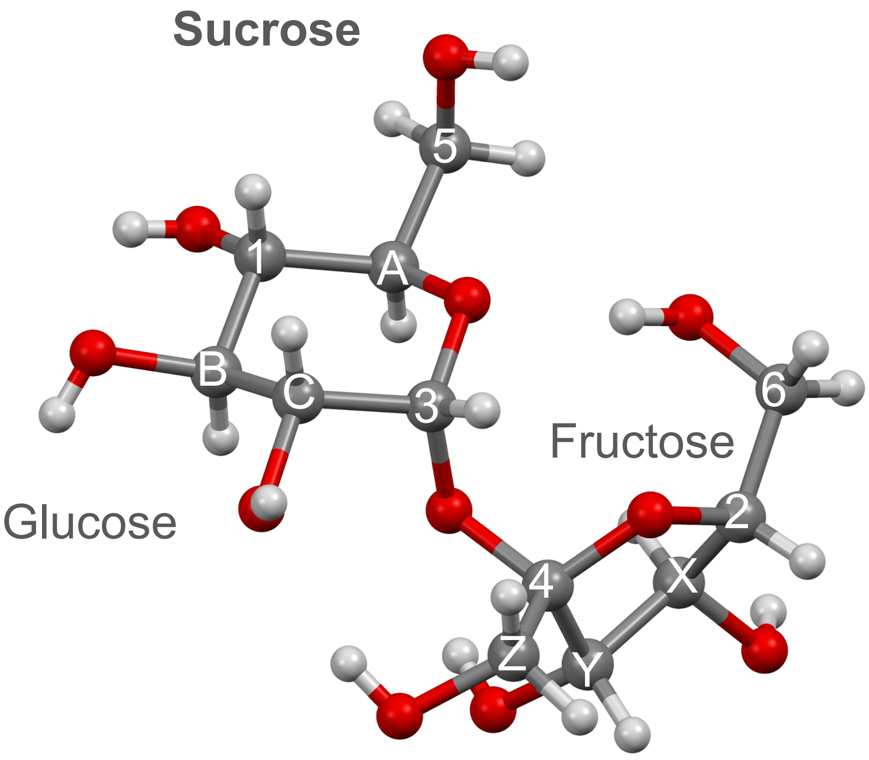


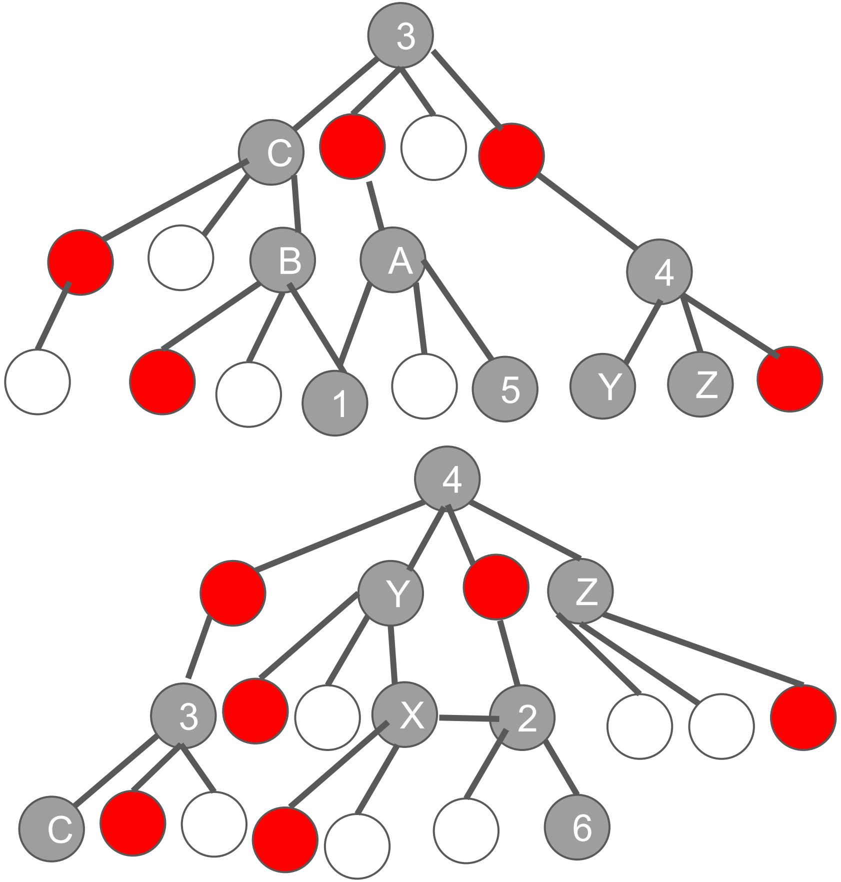
Trees as Inputs: Real World Example





Trees as Inputs: Real World Example





Next Meeting Nov 3

Readings (blogs by Bronstein and collaborators):
Expressive power of graph neural networks and the Weisfeiler-Lehman test
Beyond Weisfeiler-Lehman: using substructures for provably expressive graph neural networks
GNNs through the lens of Differential Geometry and Algebraic Topology
Over-squashing, Bottlenecks, and Graph Ricci curvature

Lectures:
Discrete Ollivier-Ricci curvature for data visualization and analysis by Abigail Hickok Watch the first 10 minutes to understand discrete curvature
Curvature and Over-Squashing in GNNs by Francesco Giovanni You can skip the first 10 minutes
Tutorials: Molecular Property Prediction with GNNs, Parts 2-5

To present, fill out this form:
https://docs.google.com/forms/d/e/1FAIpQLSfjuvRWuHfQ9M11uz9PUnq_3j_trOAcTyDG2a5yPoMvMWgfLQ/viewform?usp=header

References and Resources

Main Reference:
Geometric Deep Learning: Grids, Groups, Graphs, Geodesics, and Gauges
Michael M. Bronstein, Joan Bruna, Taco Cohen, Petar Veličković
https://geometricdeeplearning.com/book/ We'll use the chapters rather than the big pdf

Additional References:
Mathematical Foundations of Geometric Deep Learning by Borde and Bronstein
https://www.arxiv.org/abs/2508.02723
Introduction to Geometric Deep Learning by Patrick Nicolas
https://patricknicolas.substack.com/p/introduction-to-geometric-deep-learning

Further Reading:
Valence Labs
https://portal.valencelabs.com

Graph Learning on Wednesdays
https://sites.google.com/view/graph-learning-on-weds