dortmund university

SFB 876 Providing Information
by Resource-Constrained Data Analysis

Relational Representation Learning with Graph Neural Networks

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Roadmap

1. Motivation & Introduction
2. Common Operators
3. Efficient Computation of Graph Neural Networks
4. Relation to the Weisfeiler-Lehman Algorithm
5. Recent Extensions
    - Hierarchical Models
    - Deep(er) Models
    - Unsupervised Models
    - Generative Models
6. Conclusion

Motivation & Introduction

Motivation

Enable **learning on irregularly structured data**, *e.g.*, graphs, point clouds, and manifolds:

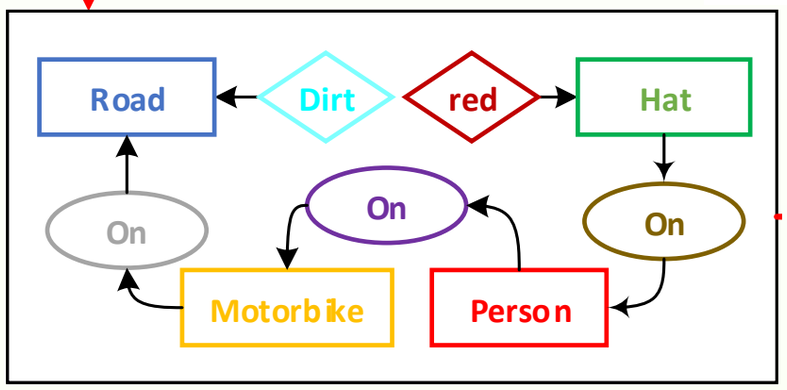
borrow from/**generalize** successful concepts on Euclidean domains, *e.g.*, **convolution**

Enforce **relational inductive biases** into the model: enable learning about **entities**, **relations**, and rules for **composing** them

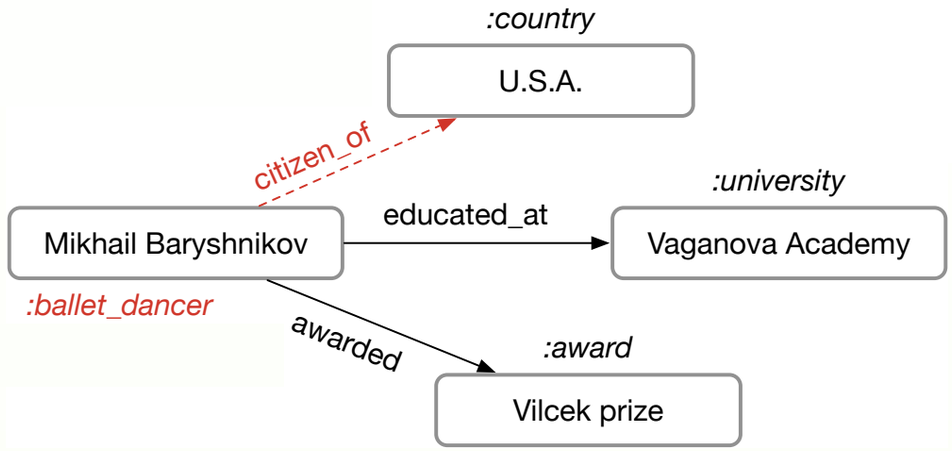
known as either Geometric Deep Learning or Relational Representation Learning

Bronstein et al.: **Geometric Deep Learning: Going Beyond Euclidean Data** (IEEE Sig. Proc. Mag. 2017)
Battaglia et al.: **Relational Inductive Biases, Deep Learning, and Graph Networks** (arXiv/1806.01261)

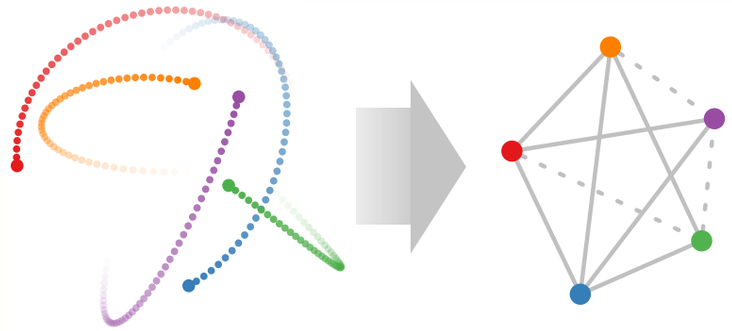
A Non-Exhaustive List of Applications



Visual Scene Understanding

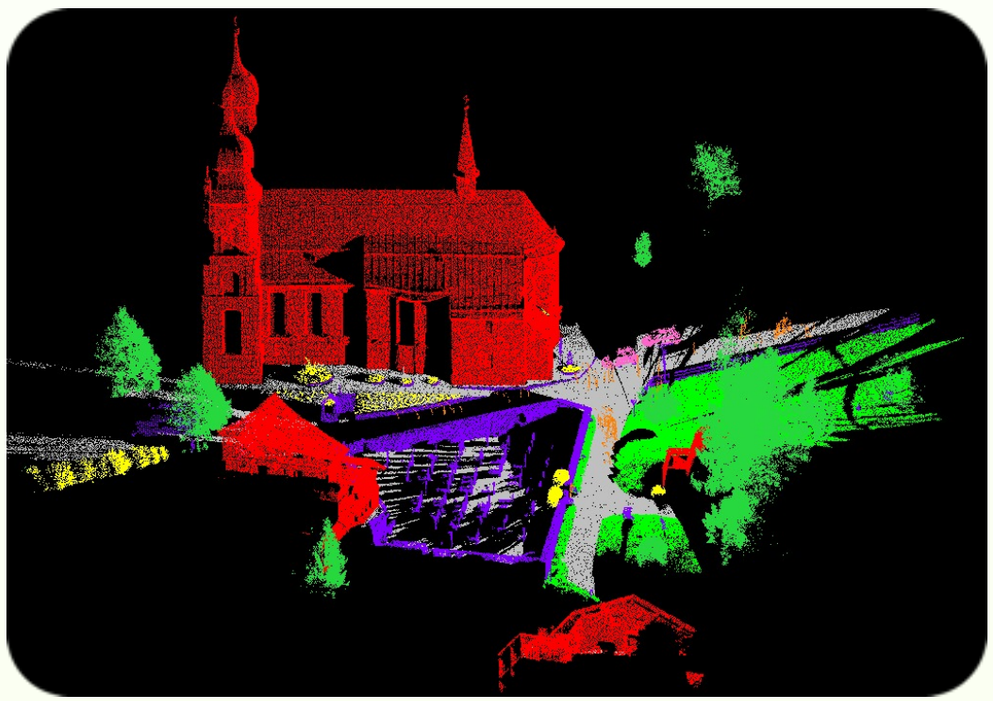


Reasoning in
Knowledge Graphs



Dynamics in
Physical Systems

Autonomous Driving

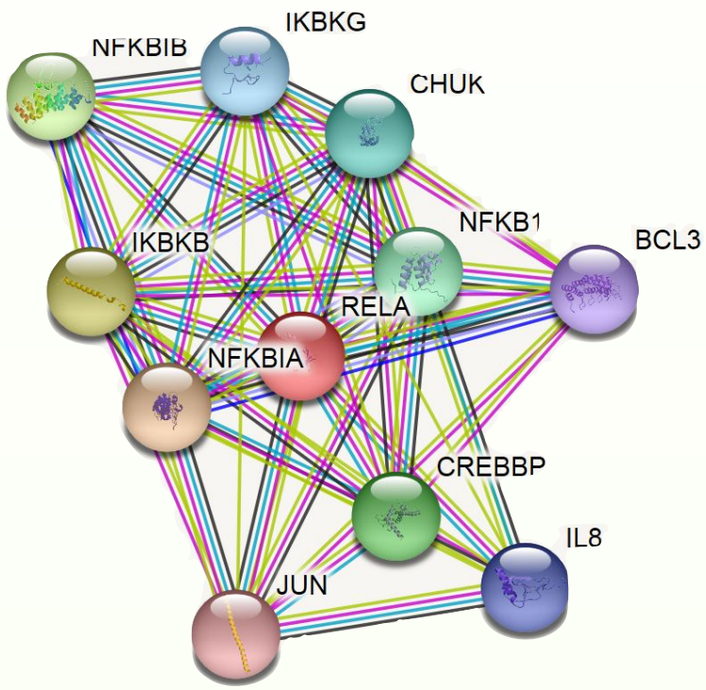


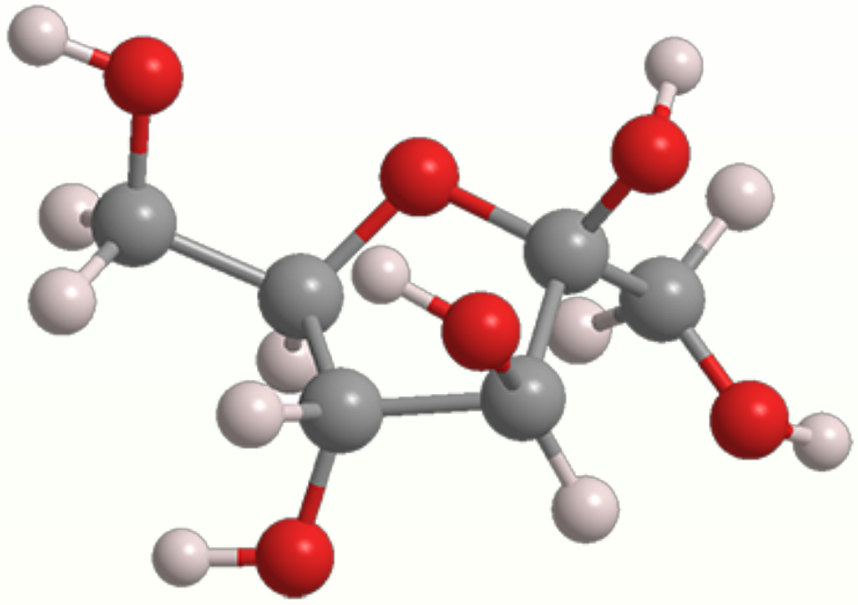
Point Cloud Analysis

A Non-Exhaustive List of Applications

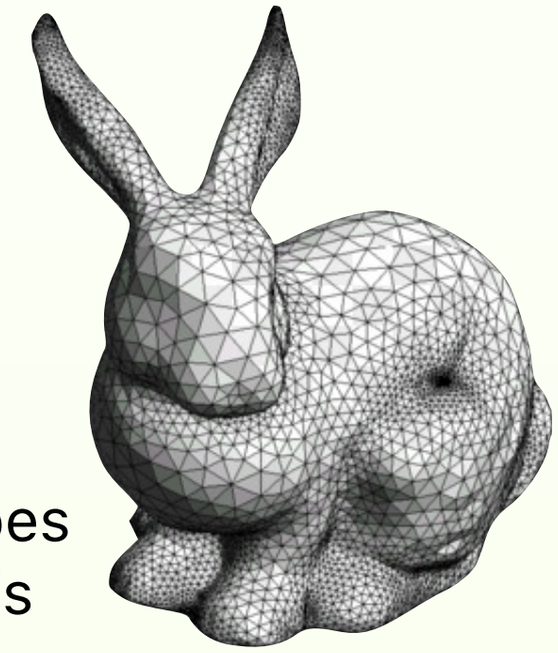
Social Networks

Protein-Protein-Interactions





Prediction of molecular properties and drug discovery

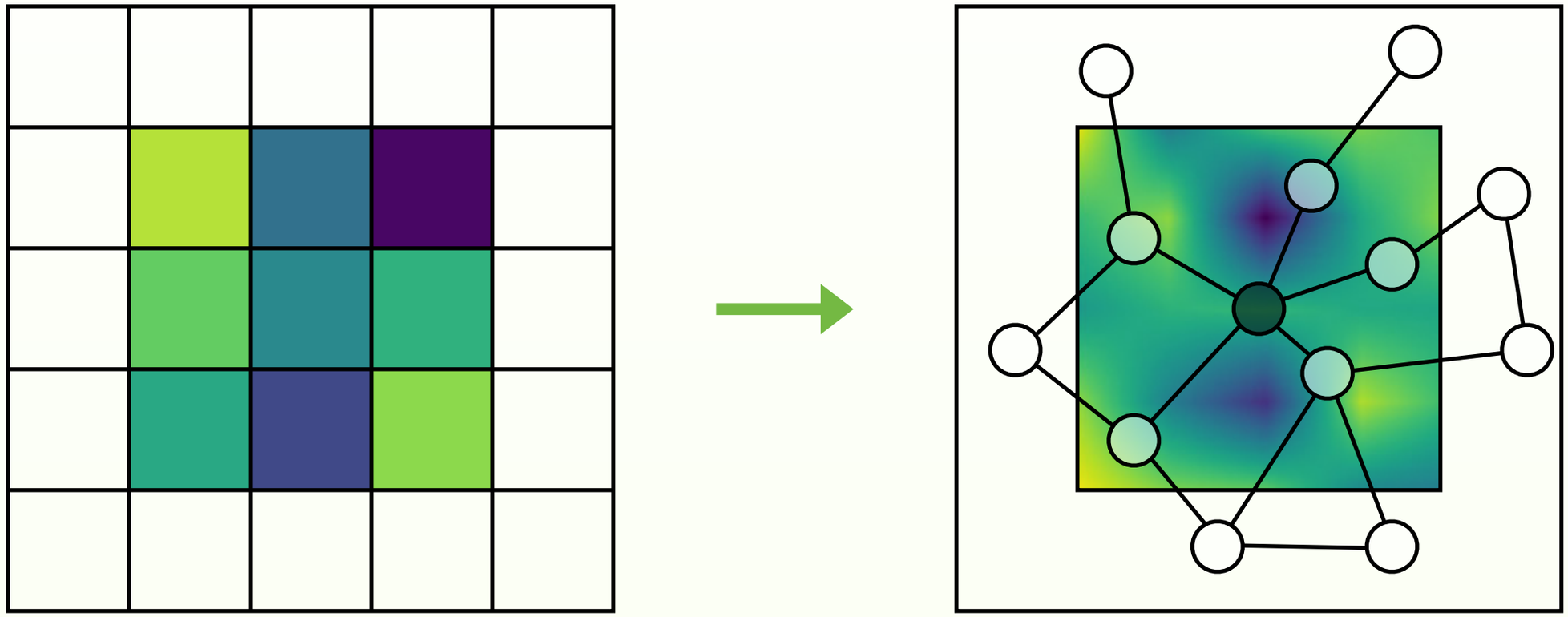


3D Shapes Analysis

Human Pose Estimation

Graph Neural Networks (GNN)

Generalization of the convolution operator to graphs



dynamic positions

dynamic number of neighbors

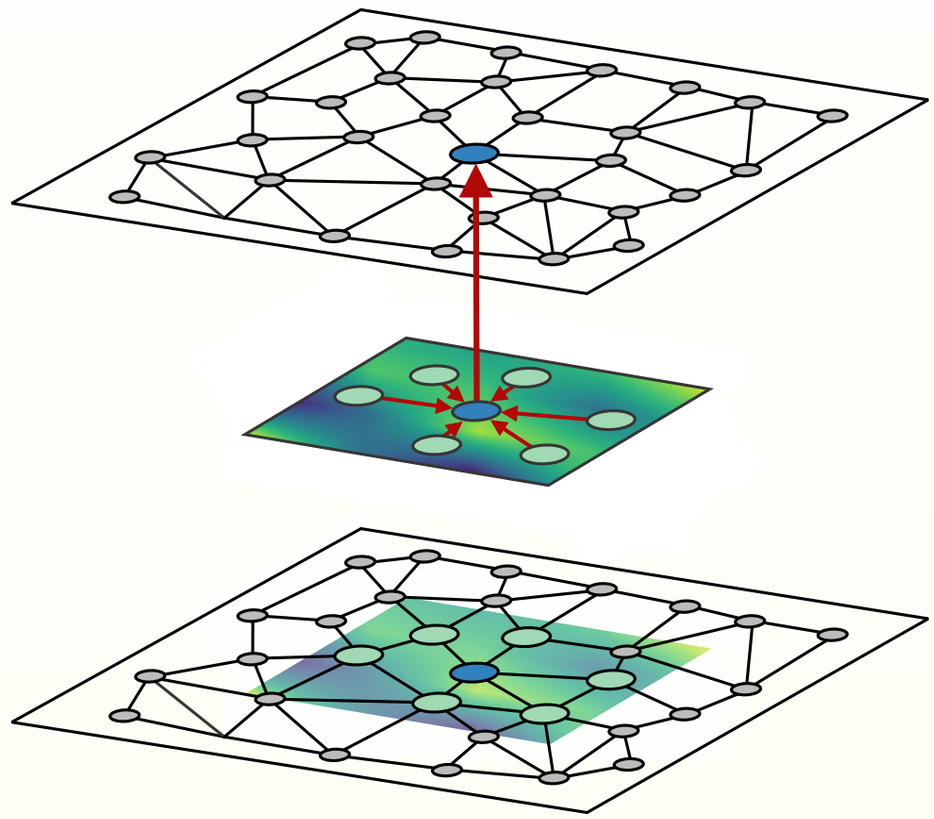
→ From **discrete** to **continuous filters**

Fey et al.: **SplineCNN: Fast Geometric Deep Learning with Continuous B-Spline Kernels** (CVPR 2018)

Graph Neural Networks (GNNs)

Graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$

Node features $\vec{h}_v^{(t)} \in \mathbb{R}^F$ in layer t



GNNs can be expressed as a **neighborhood aggregation** or **message passing** scheme:

$$\vec{m}_v^{(t)} = \text{AGGREGATE}^{(t)}\left(\left\{\vec{h}_w^{(t-1)} : w \in \mathcal{N}(v)\right\}\right)$$

permutation-invariant

$$\vec{h}_v^{(t)} = \text{COMBINE}^{(t)}\left(\vec{h}_v^{(t-1)}, \vec{m}_v^{(t)}\right)$$

Gilmer et al.: **Neural Message Passing for Quantum Chemistry** (ICML 2017)
Xu et al.: **How Powerful are Graph Neural Networks?** (ICLR 2019)

Common Operators

Operators for Learning on Graphs

$$\vec{h}_v^{(t)} = \sigma\left(\Theta^{(t)} \sum_{w \in \mathcal{N}(v) \cup \{v\}} C_{v,w}^{(t-1)}\, \vec{h}_w^{(t-1)}\right)$$

Non-Linearity

Trainable parameters

Added self-loops

Normalization coefficient

Normalization can be either ...

... static: $C_{v,w}^{(t)} := 1$

... structure-dependent: $C_{v,w}^{(t)} := |\mathcal{N}(v)|^{-1}$

... data-dependent, aka **Attention**

Xu et al.: **How Powerful are Graph Neural Networks?** (ICLR 2019)
Hamilton et al.: **Inductive Representation Learning on Large Graphs** (NIPS 2017)
Kipf and Welling: **Semi-Supervised Classification with Graph Convolutional Networks** (ICLR 2017)
Velickovic et al.: **Graph Attention Networks** (ICLR 2018)

Operators for Learning on Point Clouds

PointNet(++):

$$\vec{h}_v^{(t)} = \max_{w \in \mathcal{N}(v) \cup \{v\}} \phi_{\mathbf{\Theta}}^{(t)} \left(\vec{h}_w^{(t-1)}, \vec{p}_w - \vec{p}_v \right)$$

trainable function, *e.g.*, MLP

relative Cartesian coordinates

Neighborhood is typically given by **ball query** or ***K* nearest neighbor search.**

Formulation can be easily extended to handle **arbitrary edge features!**

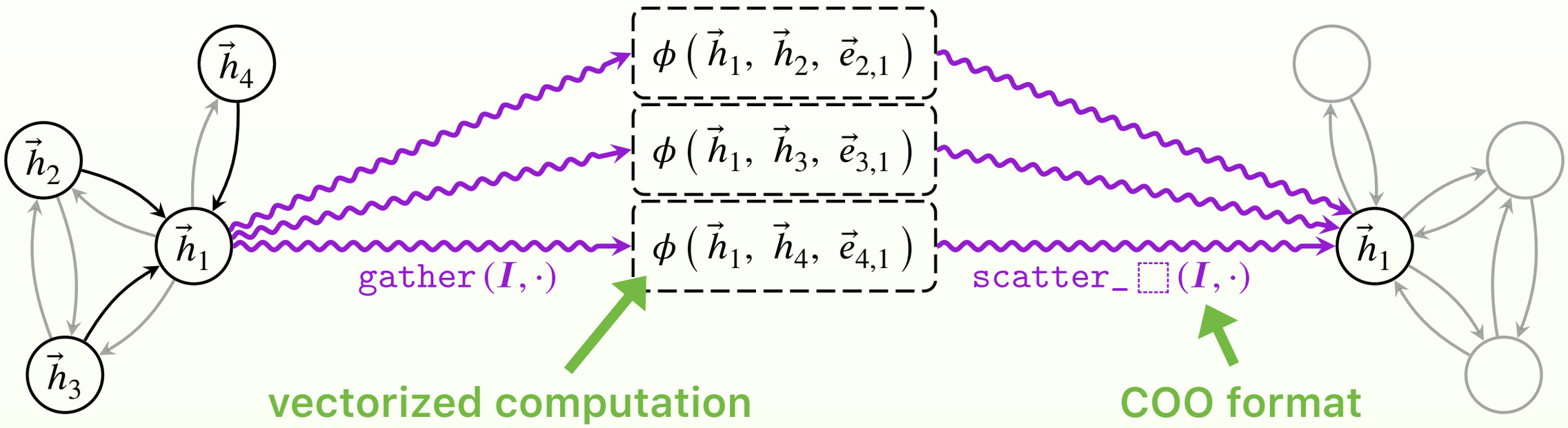
Qi et al.: **Deep Learning on Point Sets for 3D Classification and Segmentation** (CVPR 2017)
Qi et al.: **PointNet++: Deep Hierarchical Feature Learning on Point Sets in a Metric Space** (NIPS 2017)
Fey et al.: **SplineCNN: Fast Geometric Deep Learning with Continuous B-Spline Kernels** (CVPR 2018)

Efficient Computation of Graph Neural Networks

Efficient Parallelization of GNNs

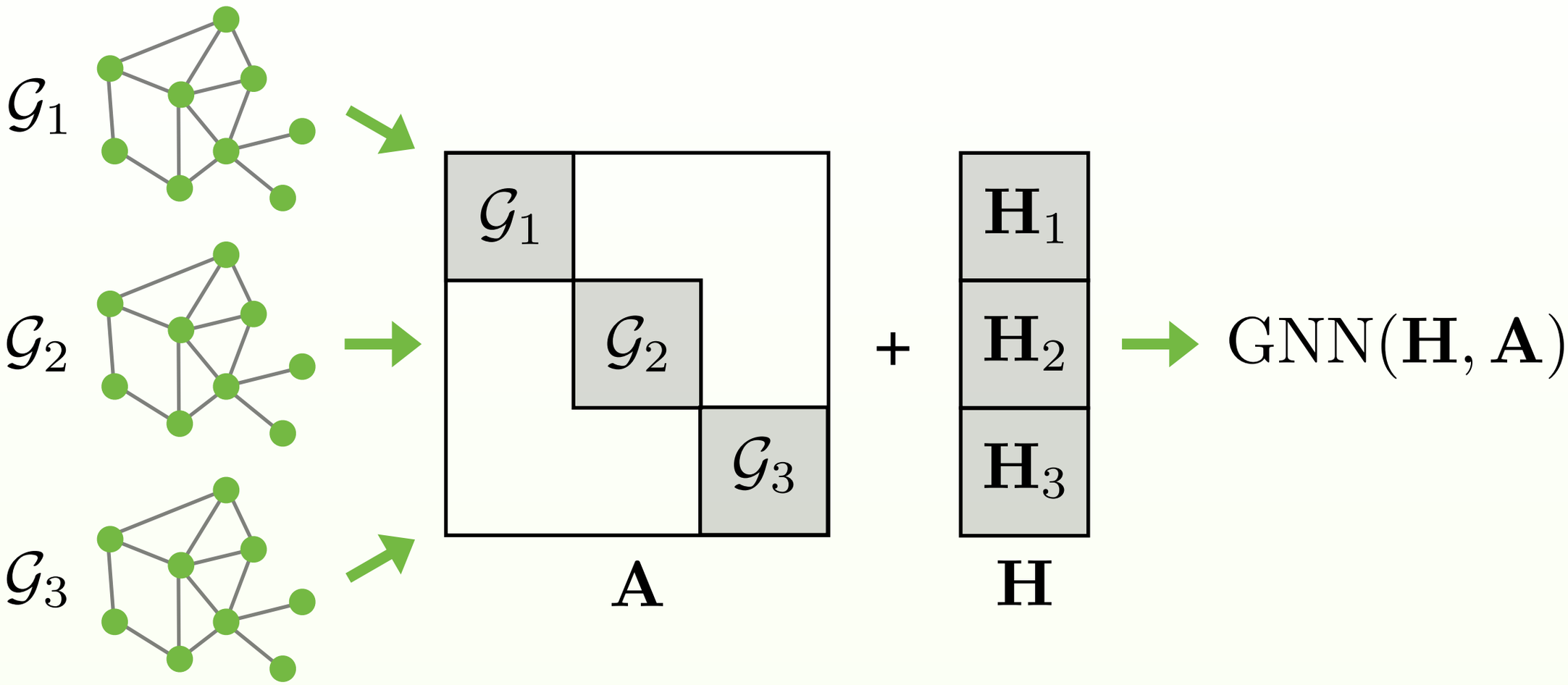
$$\text{AGGREGATE}^{(t)}(v) = \square_{w \in \mathcal{N}(v)} \phi_{\mathbf{\Theta}}^{(t)} \left(\vec{h}_v^{(t-1)}, \vec{h}_w^{(t-1)}, \vec{e}_{w,v}^{(t-1)} \right)$$

$\square$ is placeholder for either `sum`, `mean`, or `max`



1. **Gather node** information into **edge** parallel space
2. **Scatter edge** information into **node** parallel space

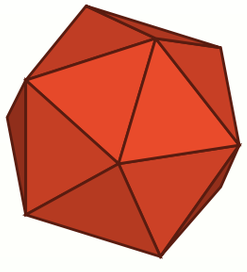
Mini-Batching in GNNs



No additional overhead due to **sparse layout!**

Input examples can have **different size!**

PyTorch Geometric: A Fast GNN Library

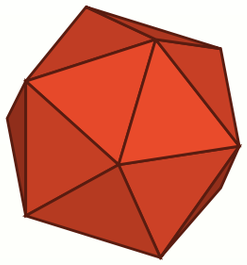


PyTorch
geometric

- ✓ provides over **25 GNN** implementations
- ✓ access to over **100 benchmark datasets**
- ✓ extendable via a **simple Message Passing API**
- ✓ leverages **dedicated CUDA kernels**
- ✓ supports **multi-GPUs**
- ✓ thoroughly **documented**

`https://github.com/rusty1s/pytorch_geometric`

PyTorch Geometric: A Fast GNN Library



PyTorch
geometric

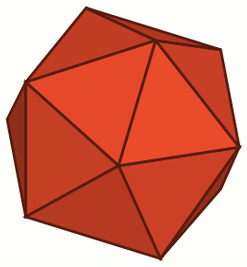
```
class MyOwnNet(Module):
    def __init__(self, in_channels, out_channels):
        self.conv1 = GCNConv(in_channels, 16)
        self.conv2 = GCNConv(16, out_channels)

    def forward(self, x, edge_index):
        x = self.conv1(x, edge_index)
        x = relu(x)
        x = self.conv2(x, edge_index)
        x = softmax(x, dim=1)
        return x
```

layer initialization

network execution flow

PyTorch Geometric: A Fast GNN Library



PyTorch
geometric

```
class MyOwnConv(MessagePassing):
    def __init__(self, ...):
        super(MyOwnConv, self).__init__('add')

    def forward(self, x, edge_index):
        return self.propagate(edge_index, x=x)

    def message(self, x_i, x_j):
        # Construct messages to aggregate.
```

add, mean or max aggregation

pass every-thing needed to construct messages

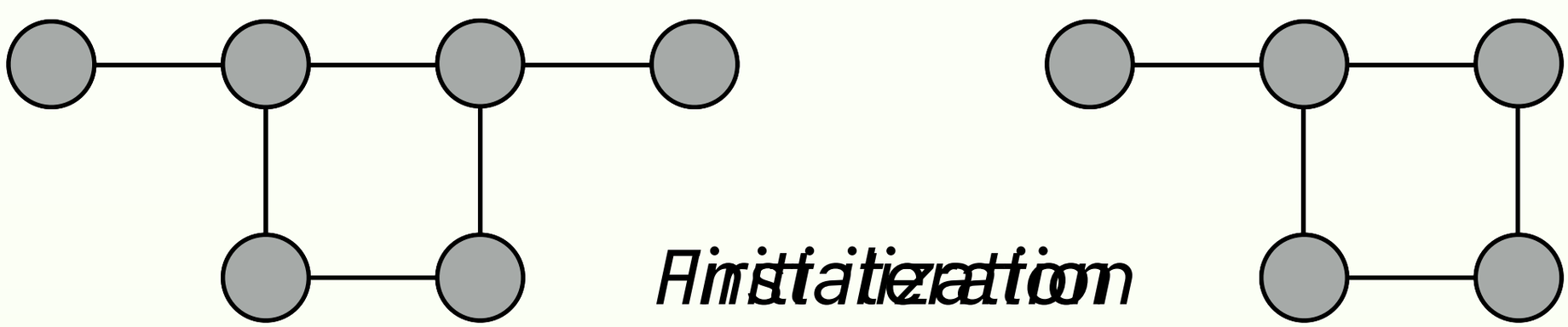
Features get automatically mapped to respective source and target nodes

Relation to the Weisfeiler-Lehman Algorithm

How Powerful are Graph Neural Networks?

WL-Test - A Graph Isomorphism Heuristic via **iterative color refinement:**

1. Aggregate colors from neighboring nodes
2. Hash aggregated colors into unique new colors



3. Graphs are non-isomorphic if color histograms differ after T rounds

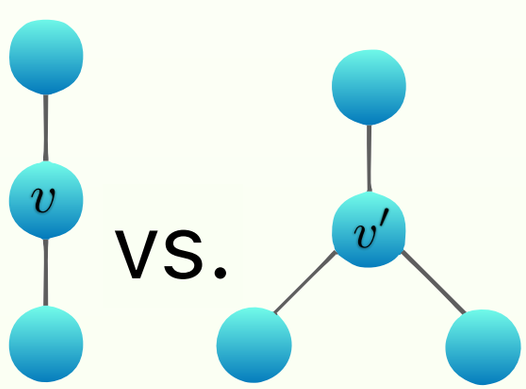
Xu et al.: **How Powerful are Graph Neural Networks?** (ICLR 2019)
Morris et al.: **Weisfeiler and Leman Go Neural: Higher-order Graph Neural Networks** (AAAI 2019)

How Powerful are Graph Neural Networks?

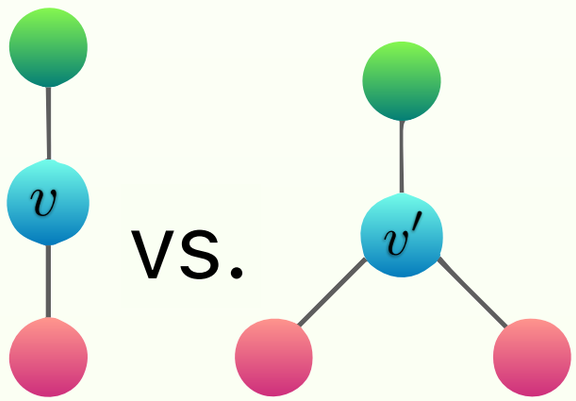
→ GNNs are **at most as powerful** as the WL-Test in distinguishing graph structures

→ GNNs **are as powerful** as the WL-Test *iff* $\mathrm{AGGREGATE}$ and $\mathrm{COMBINE}$ are **injective**

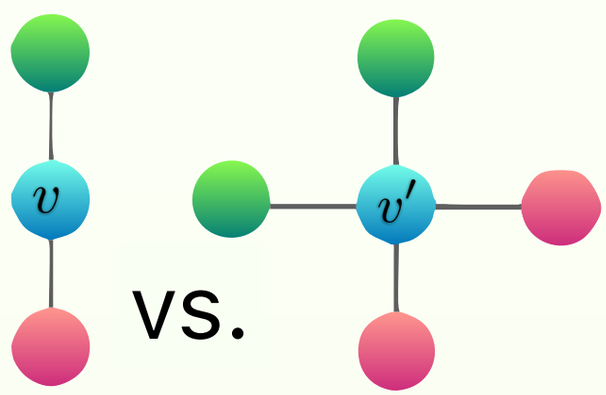
→ Use `sum` instead of `mean` or `max` aggregation



mean/max fail



max fails



mean/max fail

Xu et al.: **How Powerful are Graph Neural Networks?** (ICLR 2019)
Morris et al.: **Weisfeiler and Leman Go Neural: Higher-order Graph Neural Networks** (AAAI 2019)

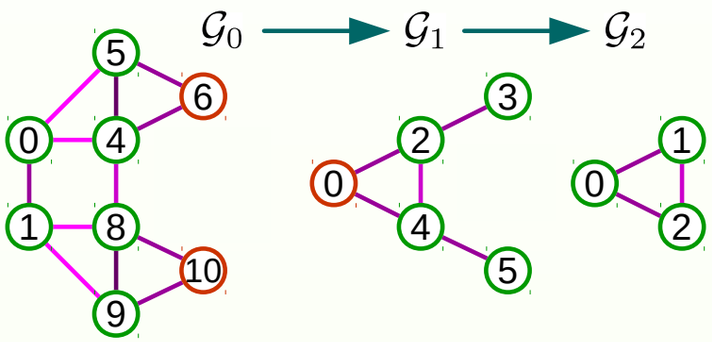
Recent GNN Extensions

Hierarchical Models

Either via **deterministic coarsening** methods...

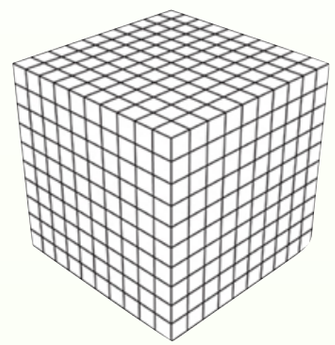
Graclus

(greedy pair matching)



Voxel Grids

(`pool_2d` generalisation)

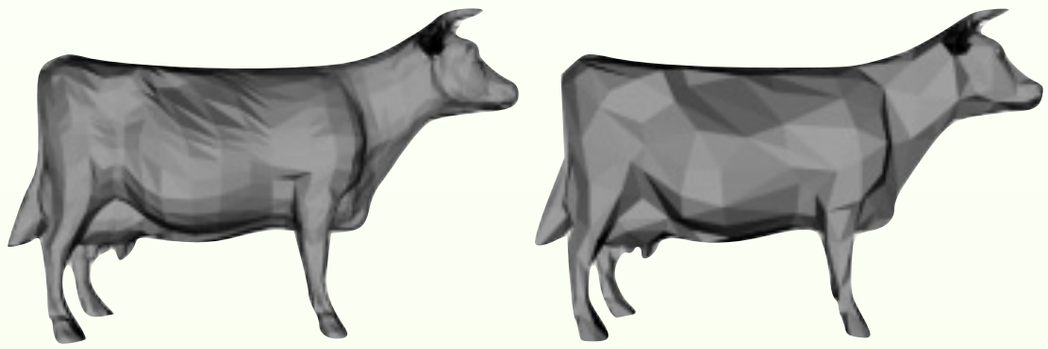


Iterative Sampling

of the most distant points

Mesh Downsampling

via quadric matrices



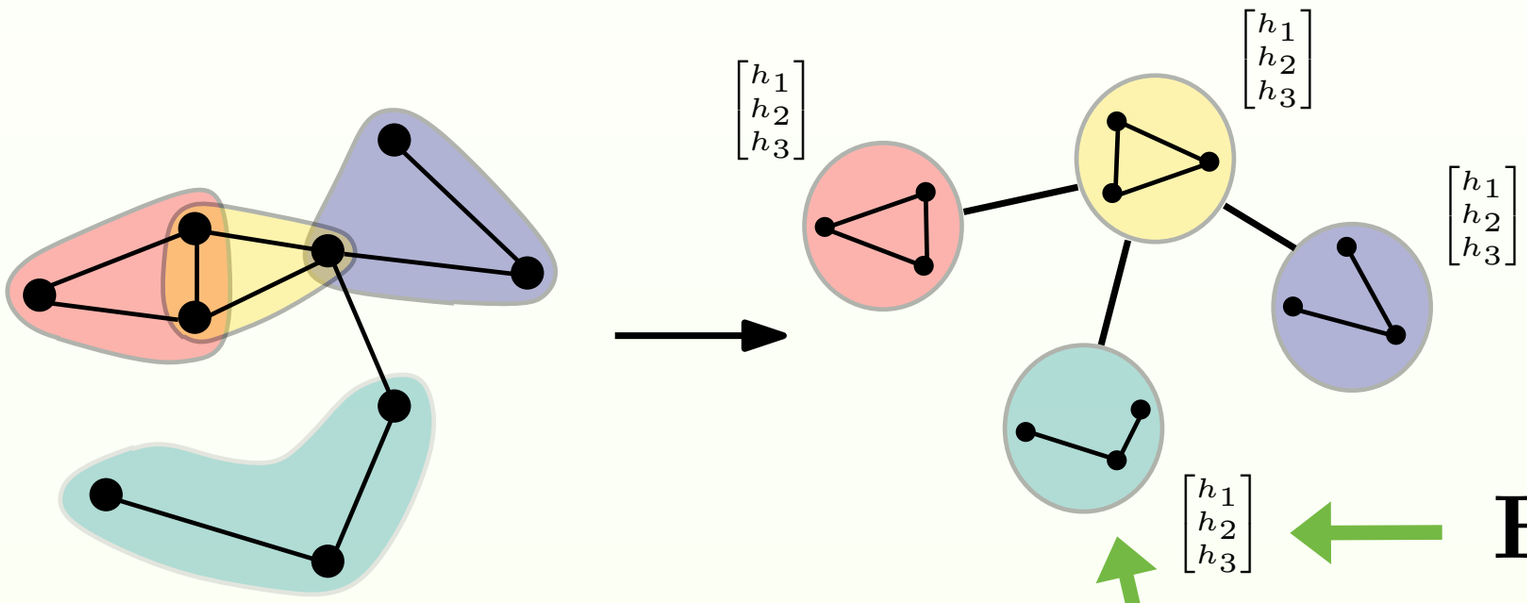
Defferrard et al.: **Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering** (NIPS 2016)
Simonovsky and Komodakis: **Dynamic Edge-Conditioned Filters in CNNs on Graphs** (CVPR 2017)
Qi et al.: **PointNet++ Deep Hierarchical Feature Learning on Point Sets in a Metric Space** (NIPS 2017)
Ranjan et al.: **Generating 3D Faces using Convolutional Mesh Autoencoders** (ECCV 2018)

Hierarchical Models

... or **differentiable pooling modules**

DiffPool:

One GNN learns **node embeddings**
Another GNN learns **cluster assignments**



soft assignment matrix

$$\mathbf{H} = \mathbf{S}^\top \mathbf{H}$$

$$\mathbf{H} = \mathrm{GNN}_1(\mathbf{H}, \mathbf{A})$$

$$\mathbf{A} = \mathbf{S}^\top \mathbf{A}\mathbf{S}$$

$$\mathbf{S} = \mathrm{softmax}(\mathrm{GNN}_2(\mathbf{H}, \mathbf{A}))$$

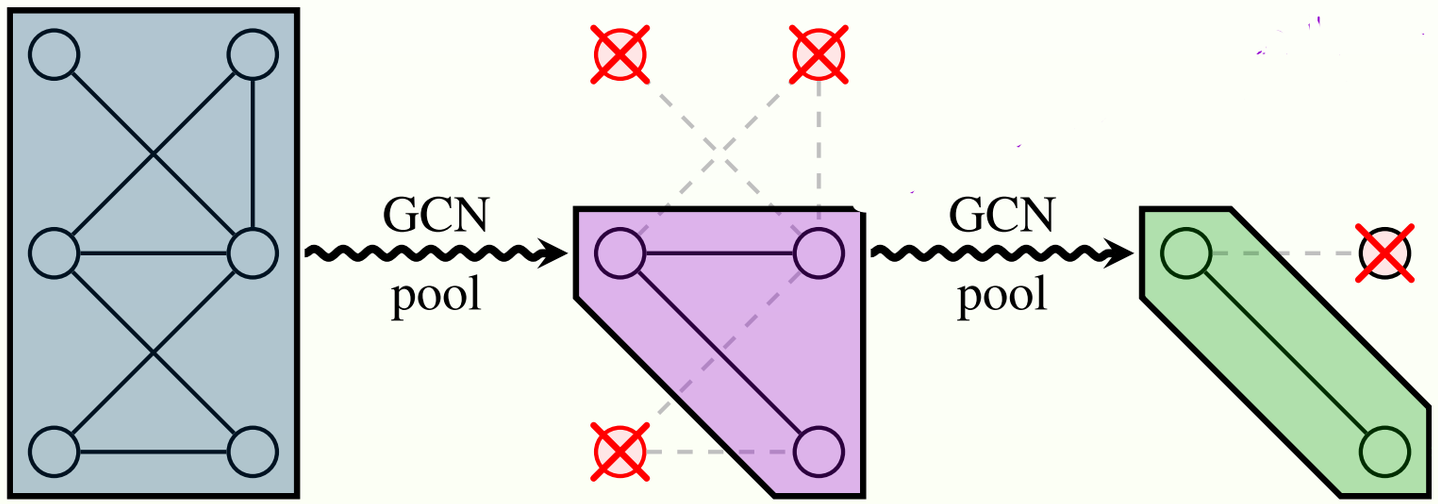
Ying et al.: **Hierarchical Graph Representation Learning with Differentiable Pooling** (NeuriPS 2018)

Hierarchical Models

... or **differentiable pooling modules**

Top-k Pooling:

Filter nodes based on **scoring function**



$$\vec{y} = \tanh(\mathbf{H} \cdot \vec{\theta})$$

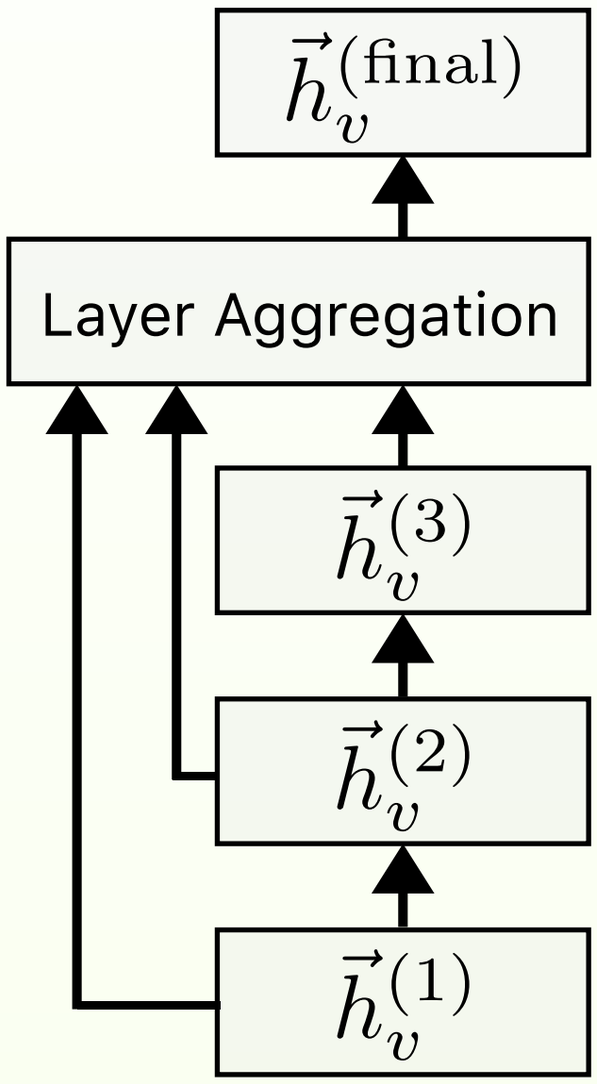
ensure gradient computation

$$\vec{i} = \text{top}_k(\vec{y}) \qquad \mathbf{H} = (\mathbf{H} \odot \vec{y})_{\vec{i}}$$

Deep(er) Models

"Washed out" representations after just a few layers

Idea: "Jump back" to earlier representations



Concatenation: $\vec{h}_v^{(1)} \parallel \ldots \parallel \vec{h}_v^{(T)}$

Pooling: $\max\left(\vec{h}_v^{(1)}, \ldots, \vec{h}_v^{(T)}\right)$

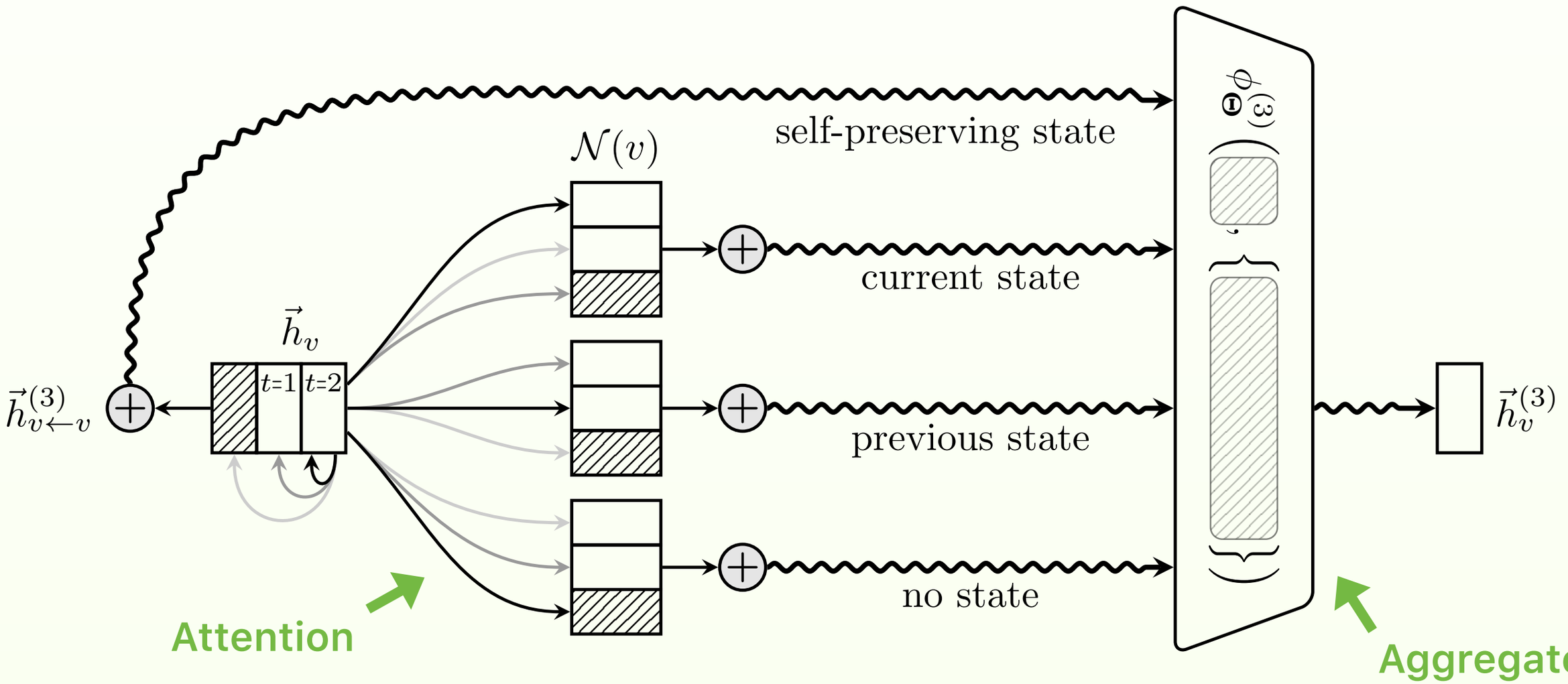
Weighted Sum: $\sum_{t=1}^{T} \alpha_v^{(t)} \vec{h}_v^{(t)}$

Attention

Deep(er) Models

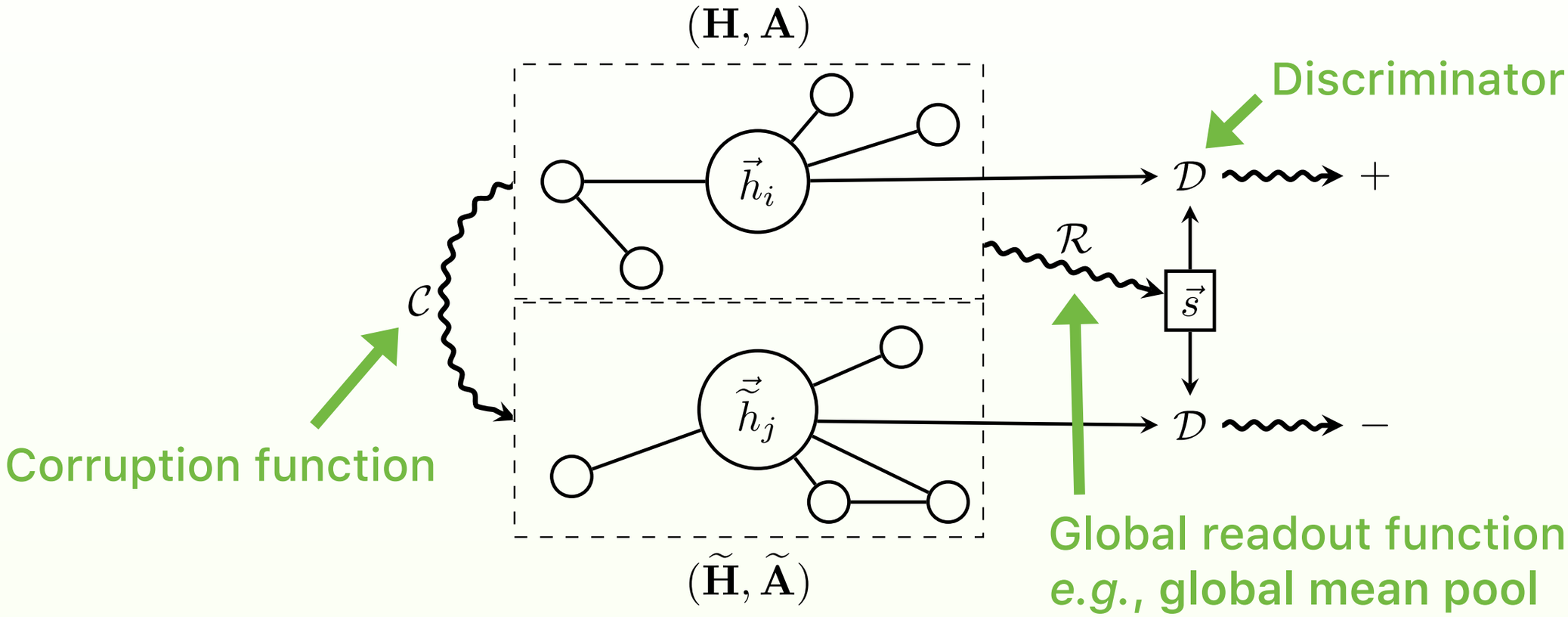
Extension: Allow jumps directly *while* aggregating

→ Aggregate more **global** information **in one branch** while falling back to more **local** information **in others**



Unsupervised Models

based on Message Passing-based models



Maximize mutual information:

$$\sum_{v \in \mathcal{V}} \mathbb{E}_{(\mathbf{H},\mathbf{A})} \left[\log \mathcal{D}\left(\vec{h}_v, \vec{s} \right) \right] + \mathbb{E}_{(\tilde{\mathbf{H}},\tilde{\mathbf{A}})} \left[\log \left(1 - \mathcal{D}\left(\tilde{\vec{h}}_v, \vec{s} \right) \right) \right]$$

Velickovic et al.: **Deep Graph Infomax** (ICLR 2019)

Generative Models

(Variational/Adversarially Regularized) Autoencoder:
GNN encoder and inner product/MLP decoder

→ expensive graph matching procedure, prefixed size

Generative Adversarial Nets for Graphs:
MLP generator and GNN discriminator

→ likelihood-free, but still prefixed in size

Auto-regressive Graph Generation:
Decomposing of graph generation into a sequence of node and edge formations

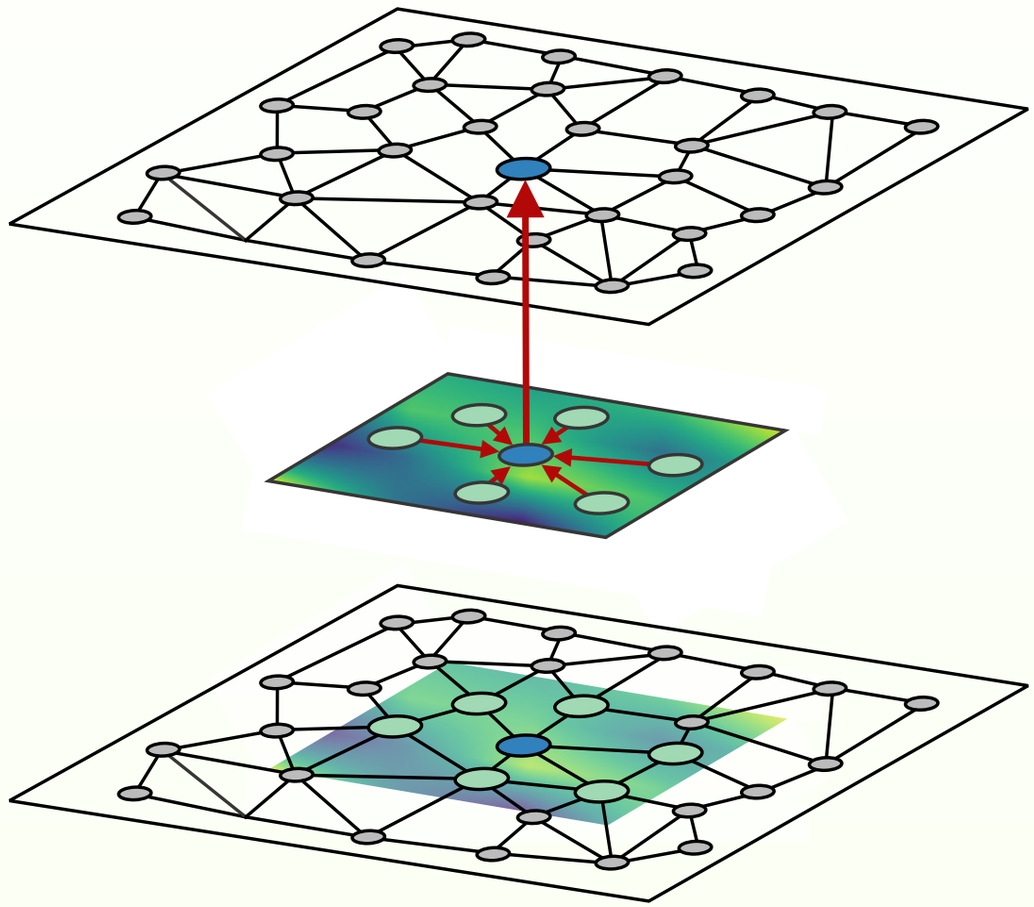
→ not prefixed in size, but inherently sequential

Kipf and Welling: **Variational Graph Auto-Encoders** (NIPS-W 2016)
Pan et al.: **Adversarially Regularized Graph Autoencoder for Graph Embedding** (IJCAI 2018)
Simonovsky and Komodakis: **GraphVAE: Towards Generation of Small Graphs Using VAEs** (arXiv/1802.03480)
Cao and Kipf: **MolGAN: An Implicit Generative Model for Small Molecular Graphs** (ICML-W 2018)
You et al.: **Generating Realistic Graphs with Deep Auto-regressive Models** (ICML 2018)

Conclusion

GNNs have interesting applications in many different areas

GNNs follow a simple message passing scheme to learn *localized* embeddings



GNNs can be very efficiently implemented

GNNs can be enhanced by and used for various concepts

GNNs are really hot right now 🔥🔥🔥