Graph Neural Networks on Large Random Graphs: Convergence, Stability, Universality

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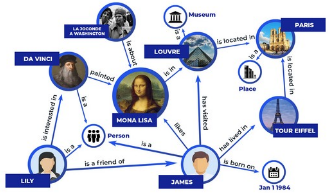
CNRS, GIPSA-lab

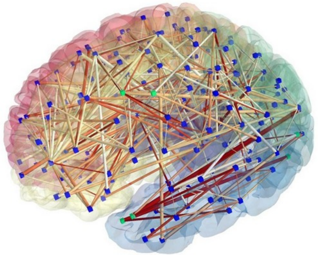
Joint work with Alberto Bietti (NYU) and Samuel Vaiter (CNRS, LJAD)

Graph Machine Learning

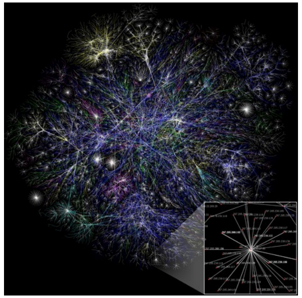
(Relatively) recent popularity of ML on graphs...



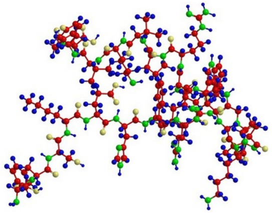
Knowledge graph



Brain connectivity network

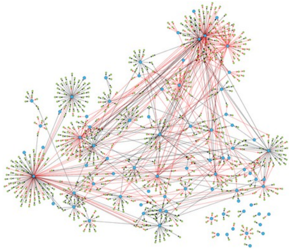


Internet

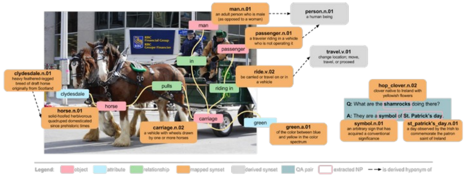


Molecule

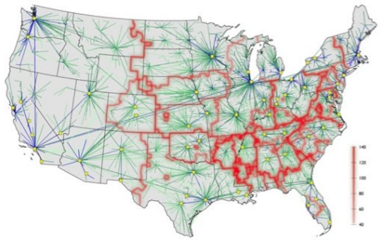
Social network



Gene regulatory network

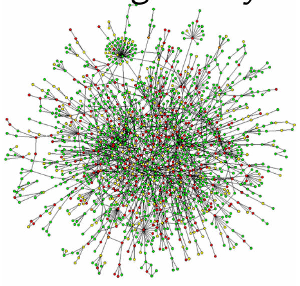


Scene understanding network

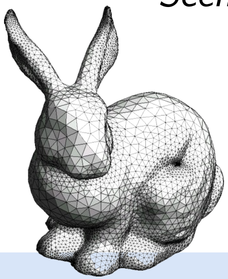


Transportation network

Computer network



Protein interaction network



3D mesh

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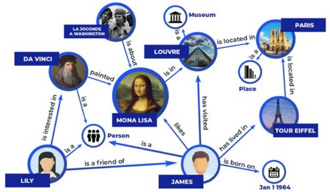

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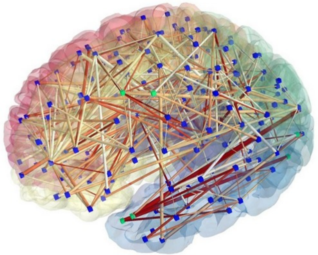

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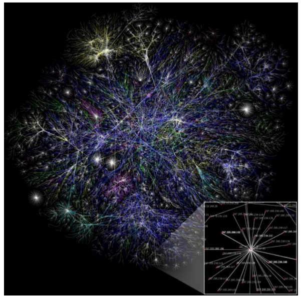

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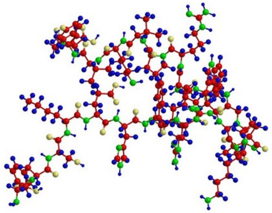

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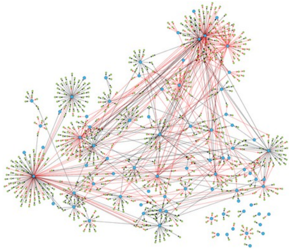

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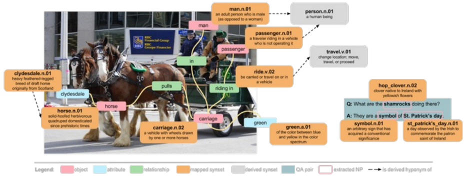

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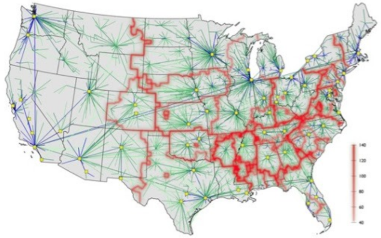

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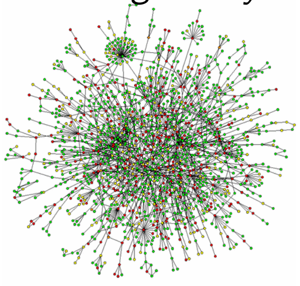

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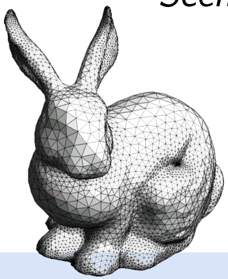

3D mesh

“if all you have is a hammer, everything looks like a nail”

ML on graphs: Graph Neural Networks

This talk: some **theoretical** properties of **Graph Neural Networks** on **large graphs.**

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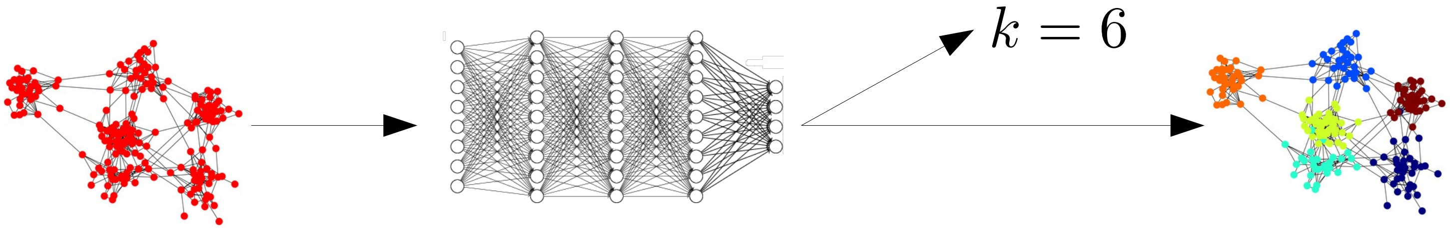

Graph Neural Networks (GNN) are "deep architectures" to do ML on graphs.

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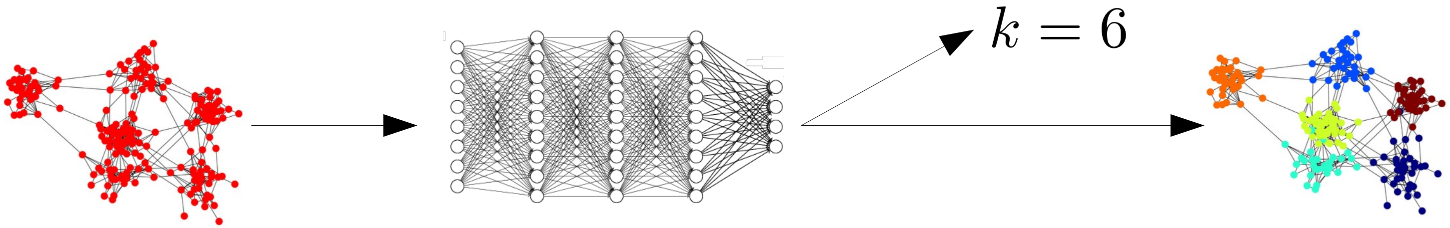

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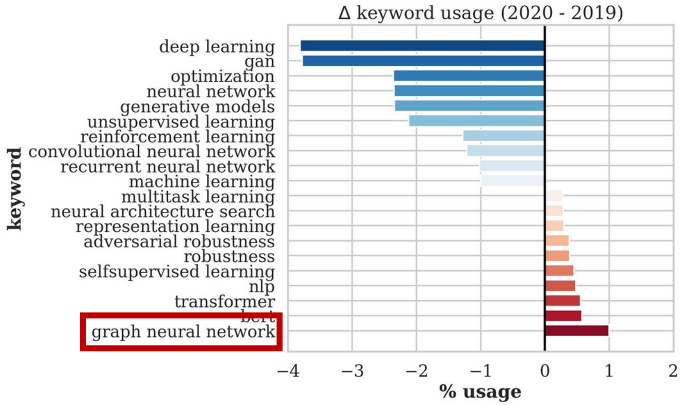

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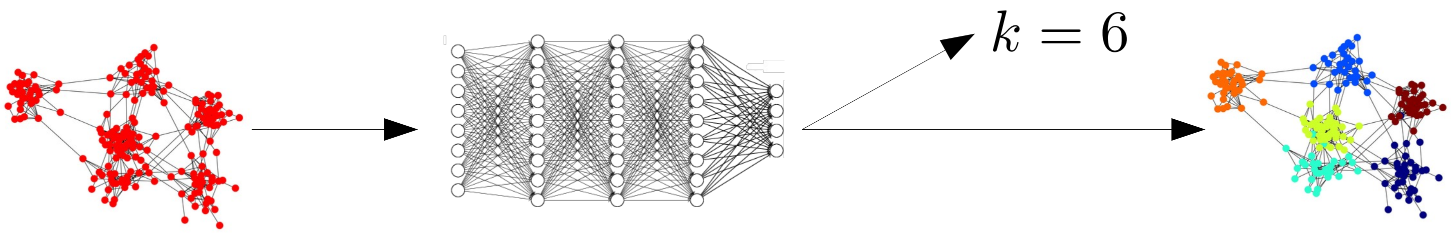
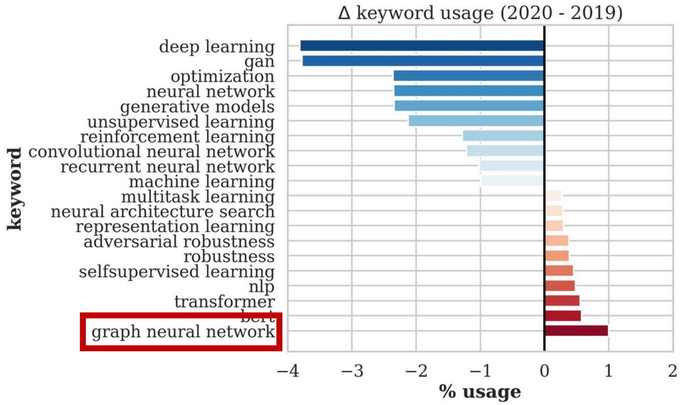


Graph Neural Networks (GNN) are "deep architectures" to do ML on graphs.

- Very (very) trendy right now!
- Work quite well, but...
  - Room for improvement! (compared to other "deep learning")
  - No "ImageNet moment" yet for GNNs (see *Open Graph Benchmark*)
  - The theory might be **actually useful** to design new architectures



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- (Even) compared to regular NNs, many properties of GNNs are still quite mysterious.
  - Eg: **universality** of NNs is known since the 90s, for GNNs it is still a very active field.

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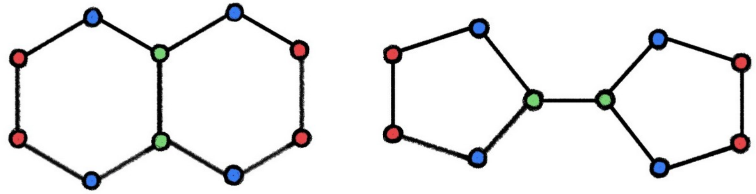
  - *Can a GNN distinguish two non-isomorphic graphs?*
  - *Can a GNN count triangles? compute the diameter of a graph? etc.*



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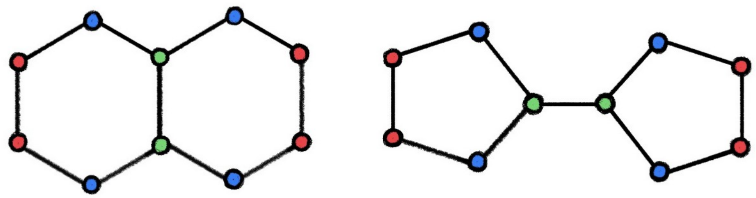

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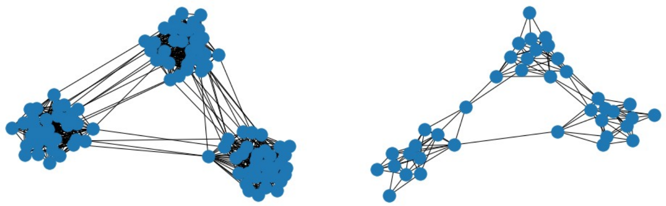

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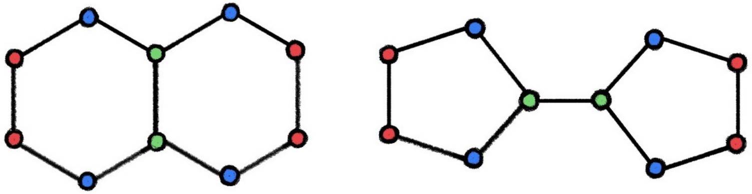

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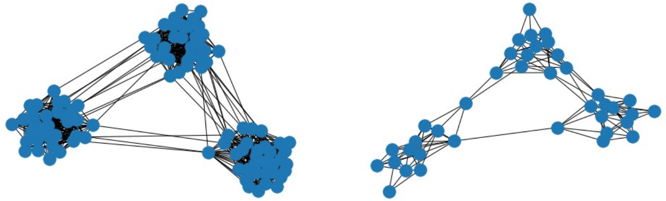

This talk: use random graph models to analyze GNN properties on large graphs

Outline

1. Convergence of GNNs
2. Stability of c-GNNs
3. Universality of c-GNNs

Random graphs models

Long history of modelling large graphs with **random generative models**

Chung and Lu. *Complex Graphs and Networks* (2004)
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Latent position models *(W-random graphs, kernel random graphs...)*

$x_i \overset{iid}{\sim} P \in \mathbb{R}^d \qquad a_{ij} \sim \mathrm{Ber}(\alpha_n W(x_i, x_j))$

Unknown *latent variables* — *Connectivity kernel*

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Relatively sparse $\alpha_n \sim (\log n)/n$

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$z_i = f(x_i)$ — *Node features (opt.)*

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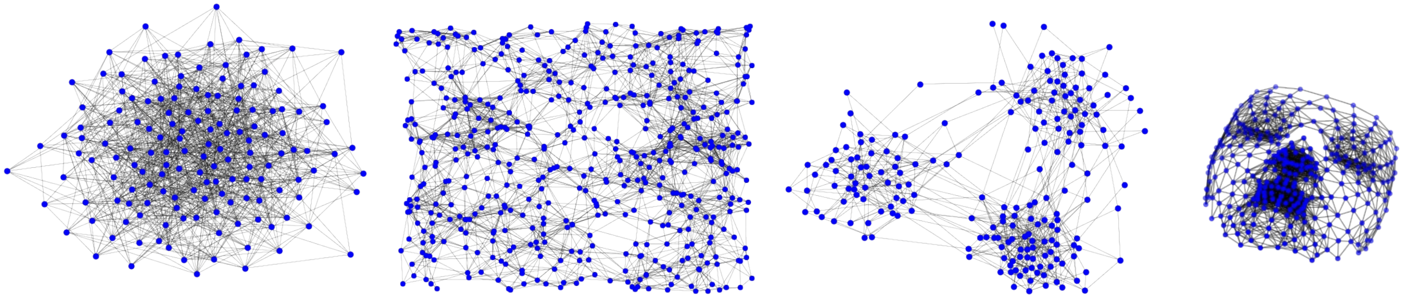

Includes Erdös-Rényi, Stochastic Block Models, Gaussian kernel, epsilon-graphs...

Filering on graphs

(Early-days) GNNs are based on **graph-convolutions** (filtering)

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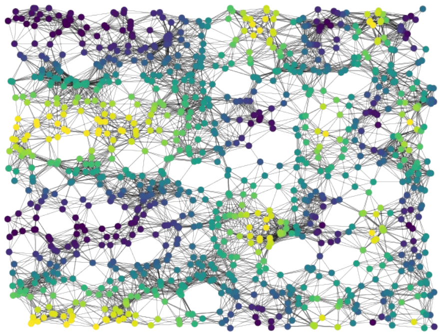

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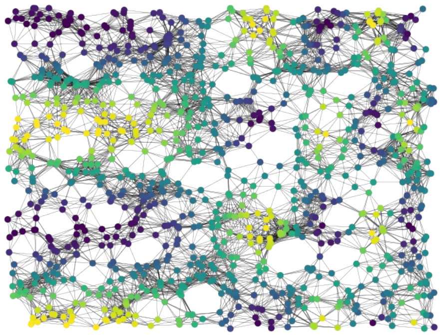

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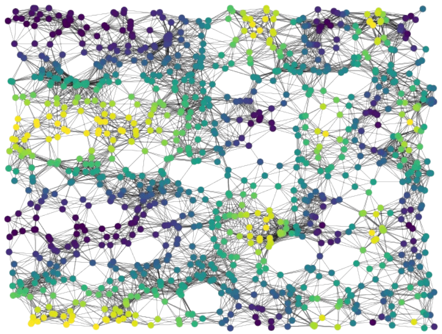

- Based on graph Fourier transform
- Defined by diagonalizing the graph Laplacian $L = Id - D^{-\frac{1}{2}}AD^{-\frac{1}{2}} = U^\top \Lambda U$

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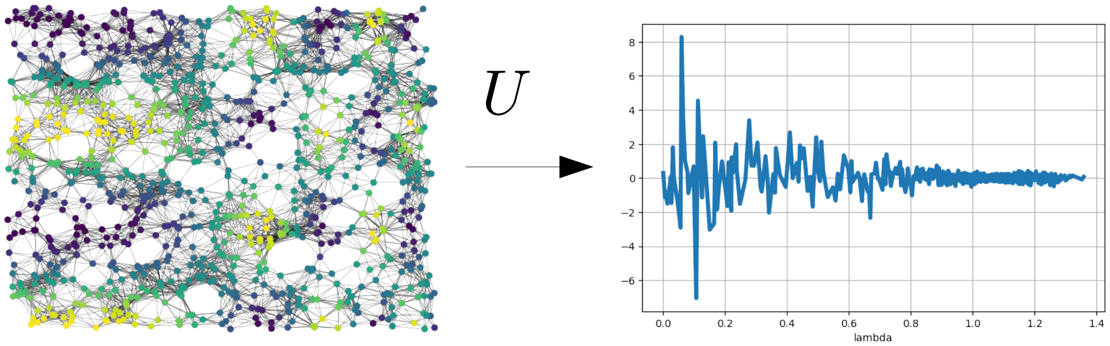

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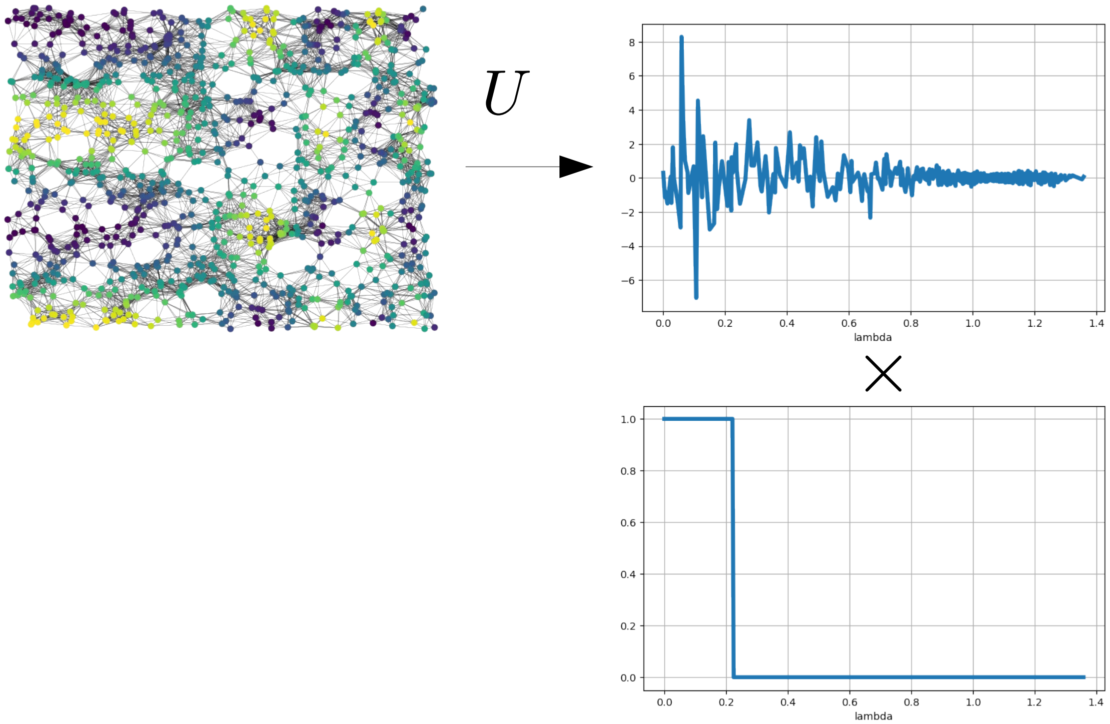

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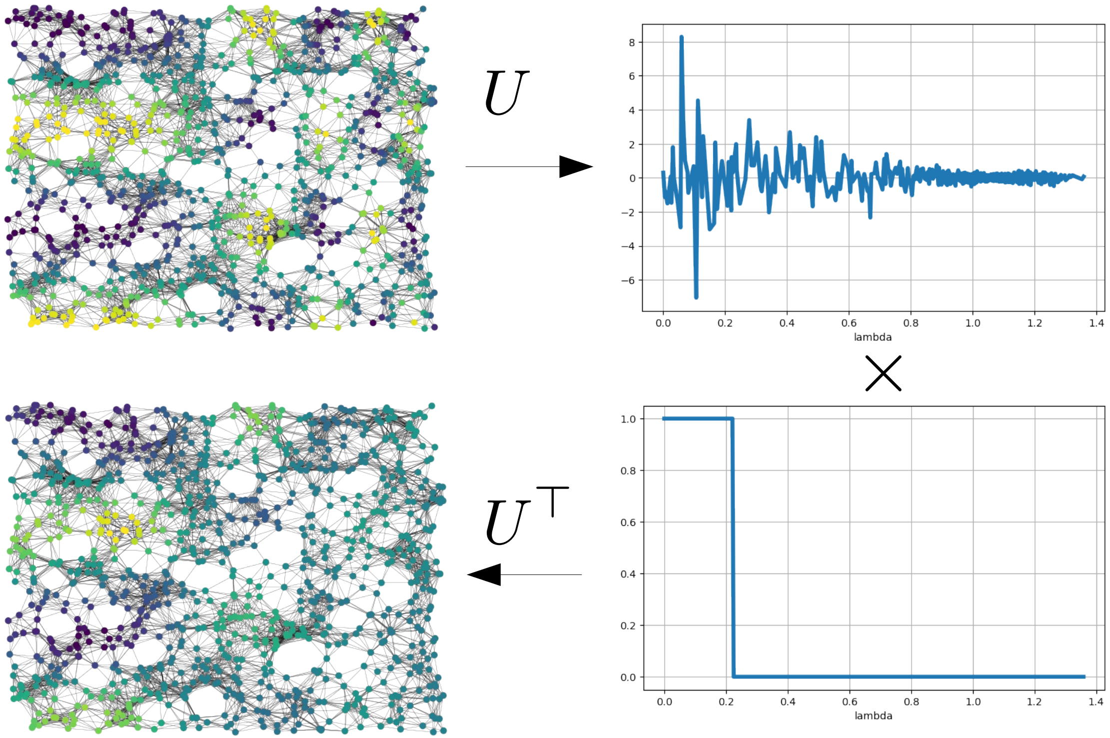

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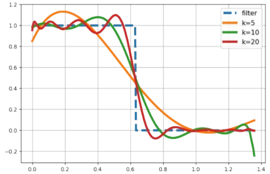
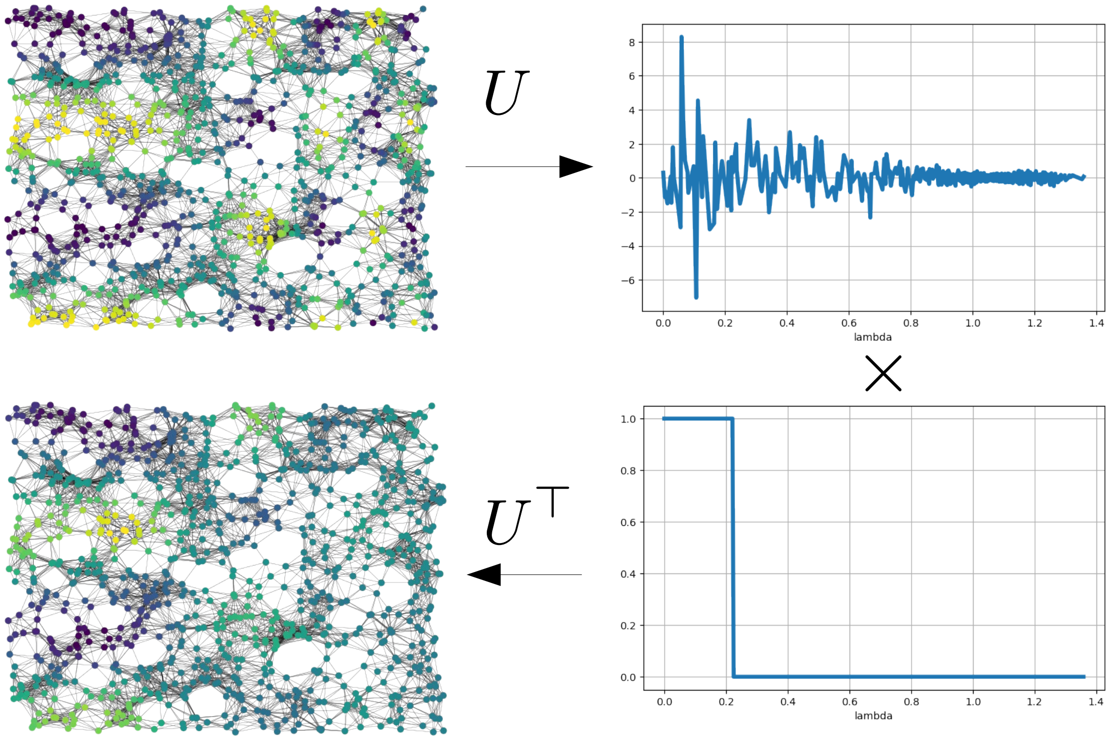
- Based on graph Fourier transform
- Defined by diagonalizing the graph Laplacian $L = Id - D^{-\frac{1}{2}} A D^{-\frac{1}{2}} = U^\top \Lambda U$
- Popular filters are polynomial filters

$$h \star z = \left(\sum_k \beta_k L^k\right) z$$





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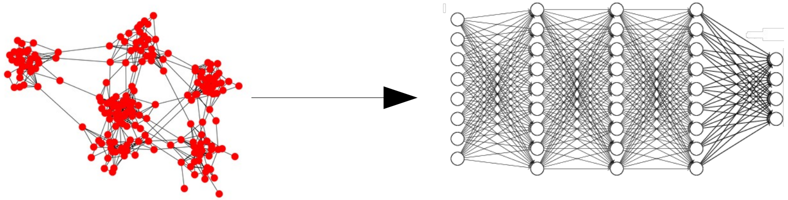

(Spectral) Graph Neural Networks

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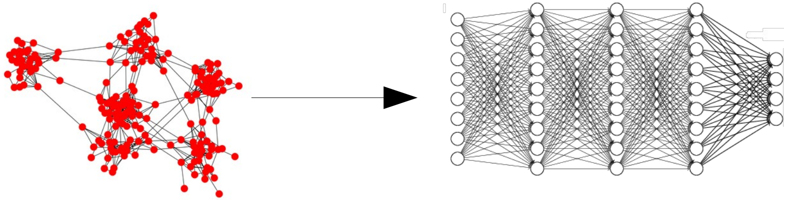
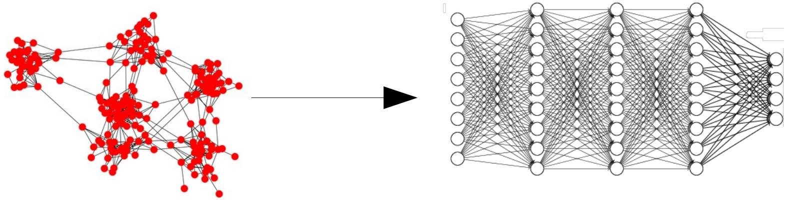


(Spectral) Graph Neural Networks

- Propagate **signal over nodes**

$$z_j^{(\ell+1)} = \rho\left(\sum\nolimits_i h_{ij}^{(\ell)}(L) z_i^{(\ell)} + b_j^{(\ell)} 1_n\right)$$

Discrete vs. continuous



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Trainable polynomial graph filters with normalized Laplacian $h(L) = \sum_k \beta_k L^k$, $L = D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$

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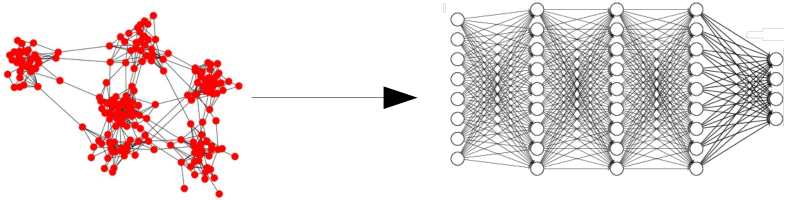

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ReLU

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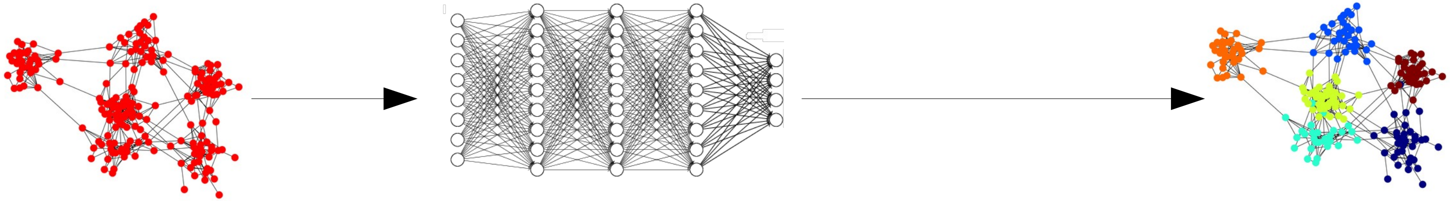

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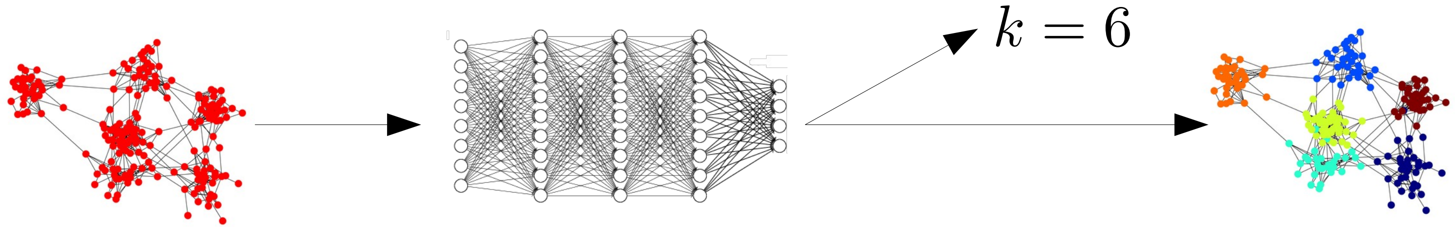
Output

- Signal over nodes (permutation-equivariant)

Discrete vs. continuous



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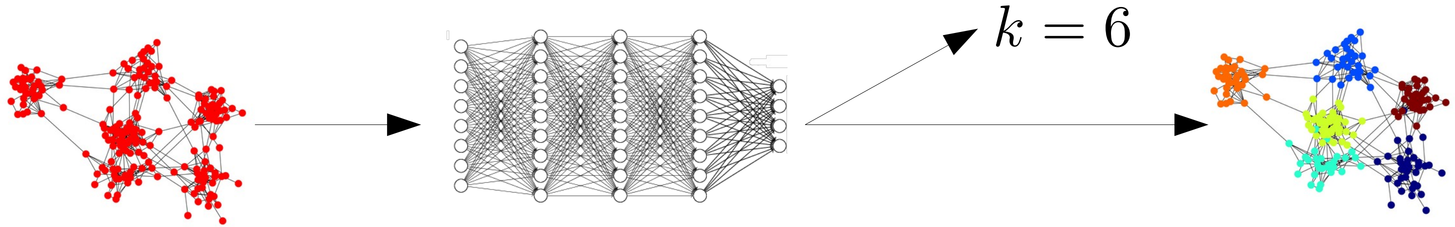
Output

- Signal over nodes (permutation-equivariant)
- Single vector with pooling (permutation-invariant)

Discrete vs. continuous



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Trainable polynomial graph filters with normalized Laplacian $h(L) = \sum_k \beta_k L^k$, $L = D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$

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Continuous Graph Neural Networks

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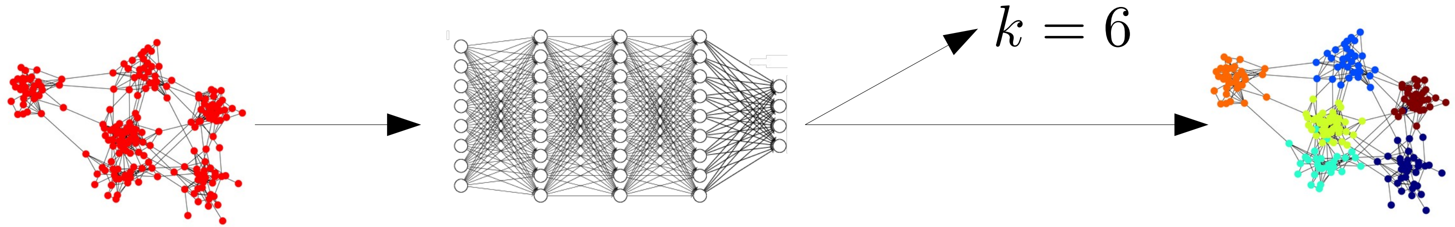
Discrete vs. continuous



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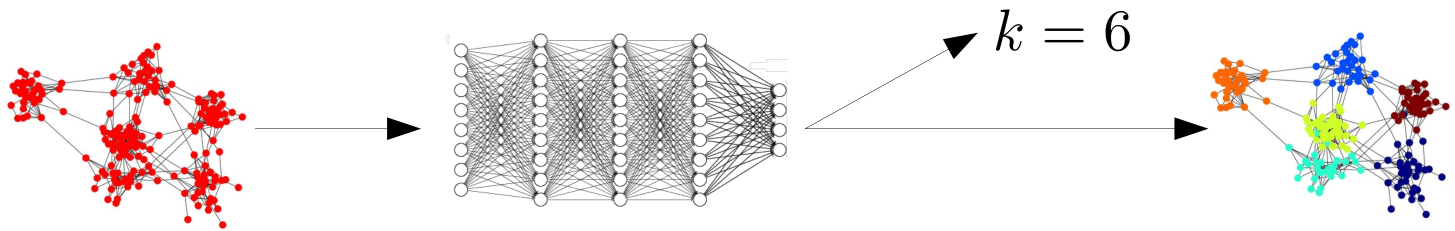

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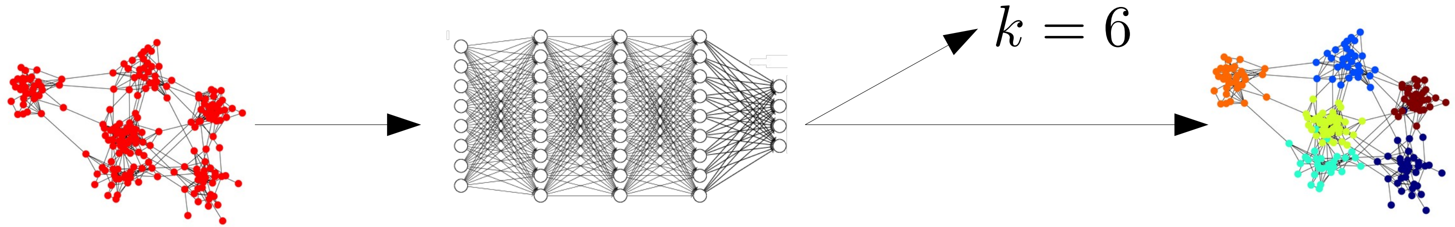

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Continuous limit of GNNs

Thm (Non-asymptotic convergence)

If $\alpha_n \gtrsim (\log n)/n$ *, with probability* $1 - n^{-r}$*, the deviation between the outputs of the discrete GNN and the continuous GNN is*

Perm-inv	$\|\Phi_G(Z) - \Phi_{W,P}(f)\|$	$\boxed{\lesssim \frac{d}{\sqrt{n}} + \frac{1}{\sqrt{\alpha_n n}}}$
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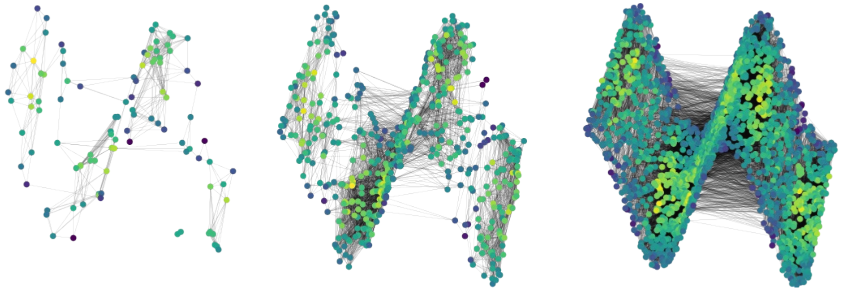

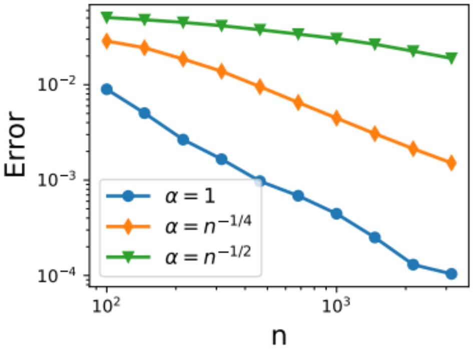

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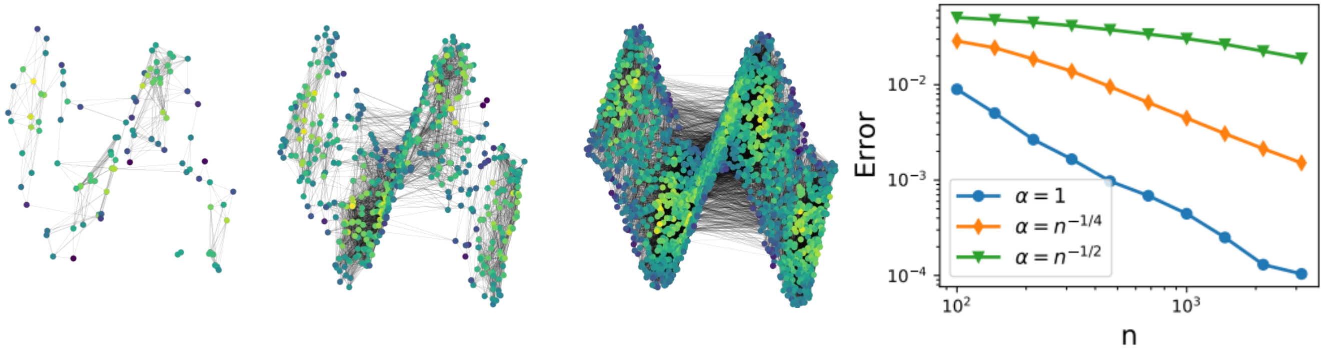

- Thanks to normalized Laplacian, the limit does ***not*** depend on α_n but the rate of convergence does...
- Could have used normalized adjacency $A/(n\alpha_n)$ with operator $\int W(x,y)f(y)dP(y)$

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2. Stability of c-GNNs

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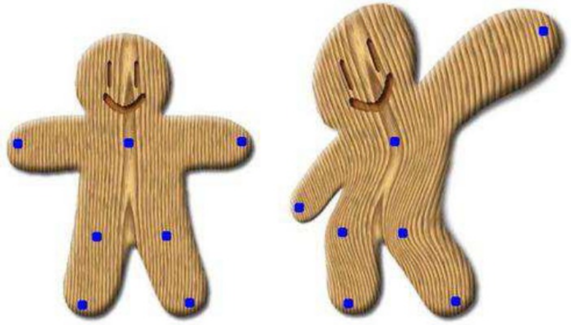
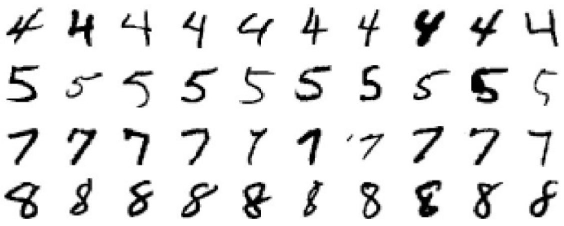
Large graphs?

- **CNN** (translation-invariant) are robust to spatial deformations

$$\|\Phi(f) - \Phi(f \circ (Id - \tau))\| \leq \|\nabla\tau\|_\infty$$





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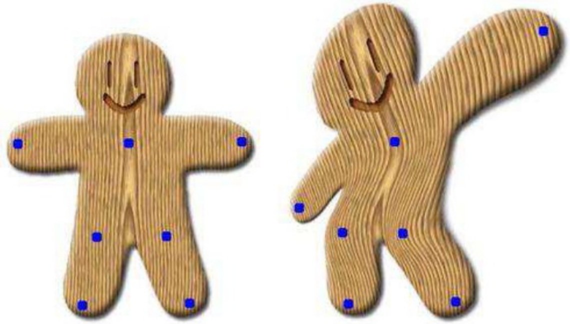

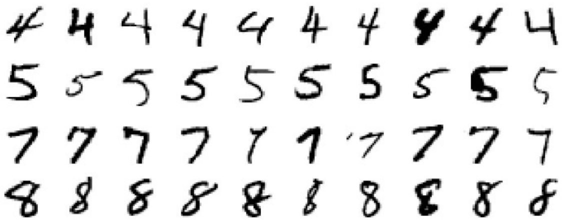

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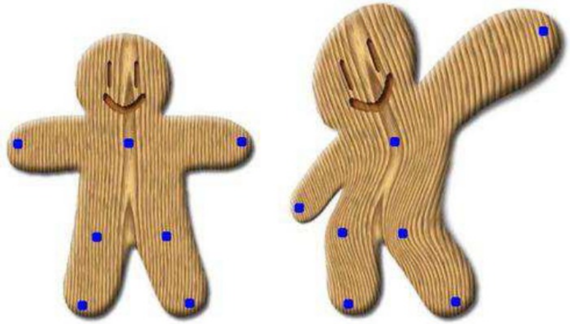

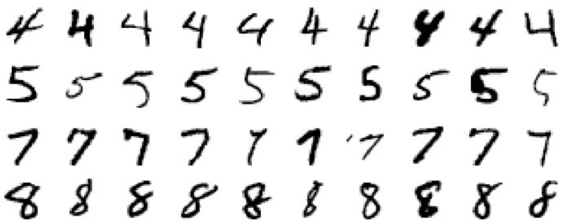

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  - *Difficult to interpret, difficult to define for different-sized graphs*
  - *What's a meaningful notion of deformation for a graph?*

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Continuous domain allows to define **intuitive geometric deformations**

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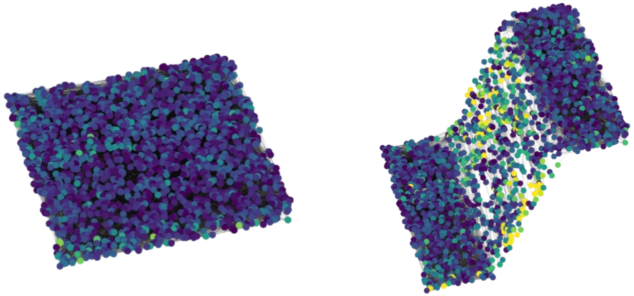

Deformation of distribution

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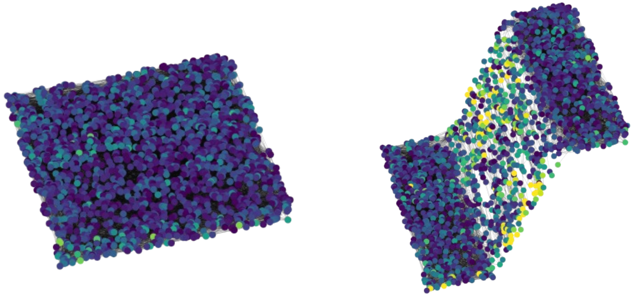

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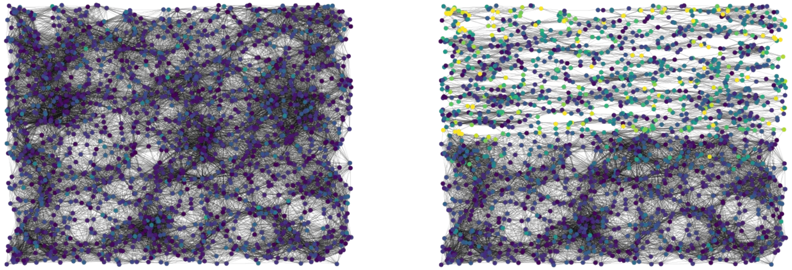

Deformation of kernel

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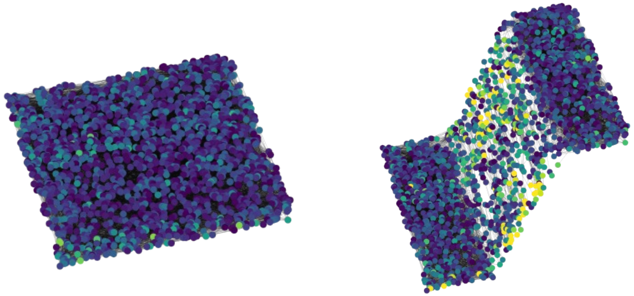

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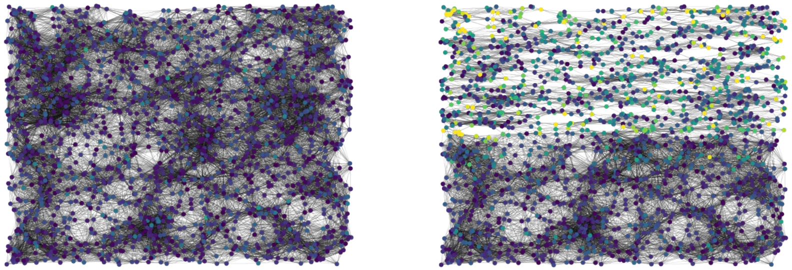


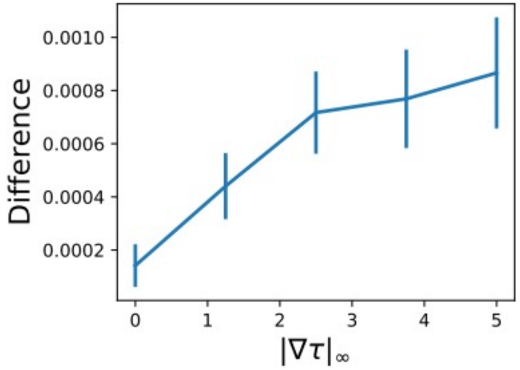
Deformation of kernel

Thm (Stability, simplified)

For *translation-invariant* kernels, if:

- W is replaced by $W(x-\tau(x), x'-\tau(x'))$
- P is replaced by $(Id-\tau)\sharp P$ (and f is translated)
- f is replaced by $f\circ(Id-\tau)$

Then, the deviation of c-GNN is bounded by $\|\nabla\tau\|_\infty$



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  - Works by propagating labels with injective message-passing function
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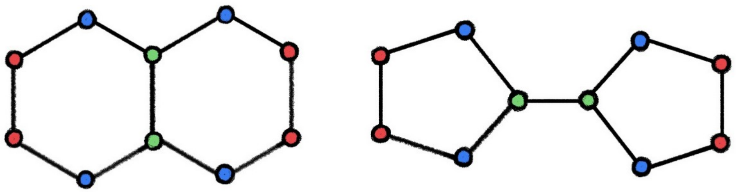
WL fails here...



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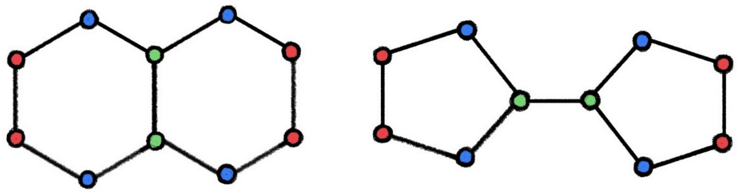

By construction, message-passing GNNs are not more powerful than WL test, and can be as powerful if the message-passing function is injective (sufficient number of neurons).

Xu et al. *How Powerful are Graph Neural Networks?* (2019)

Beyond WL

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- Using *higher-order tensors*
  - *Up until true universality!*

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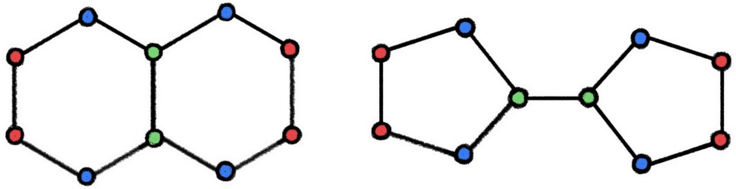

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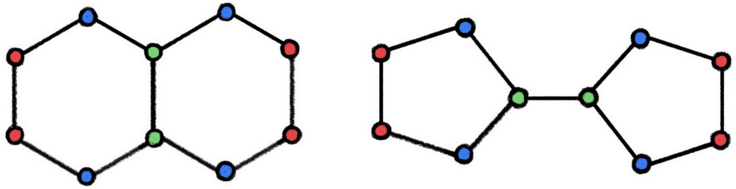

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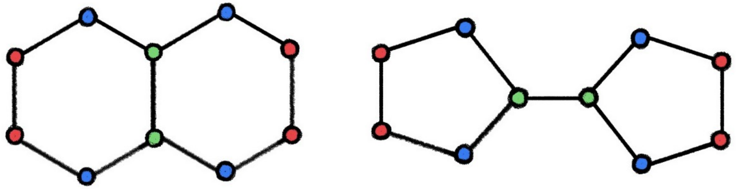

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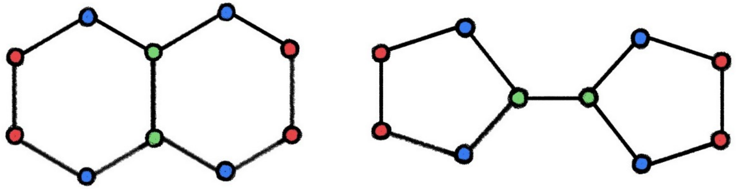

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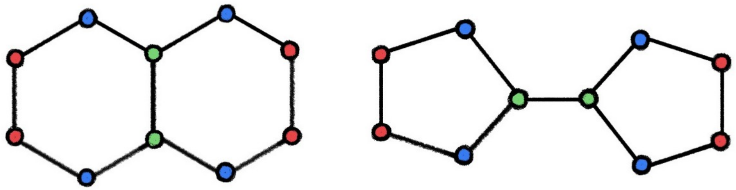

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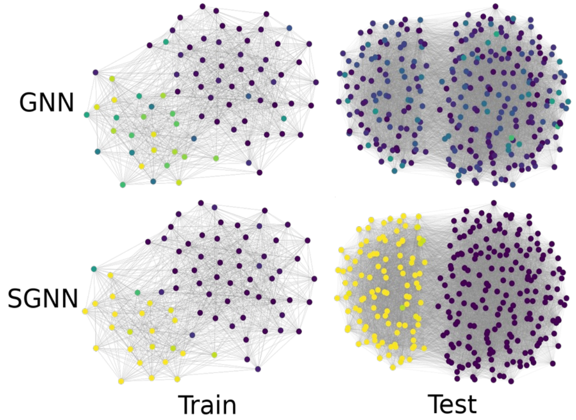

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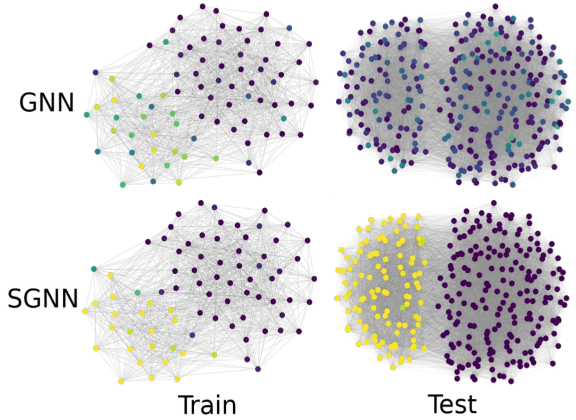

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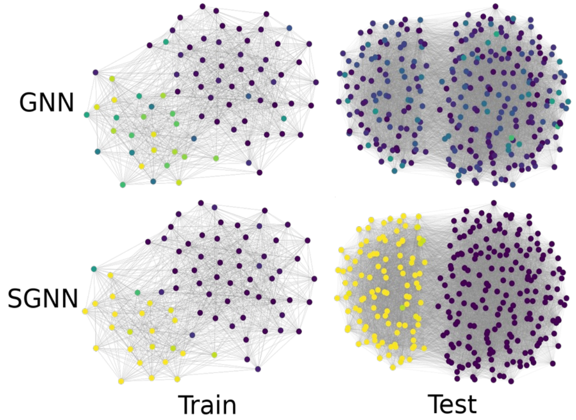

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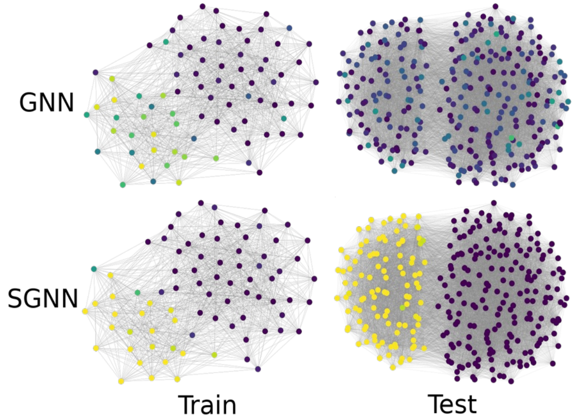

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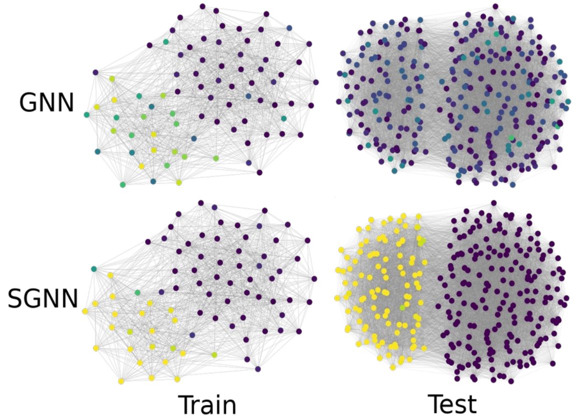

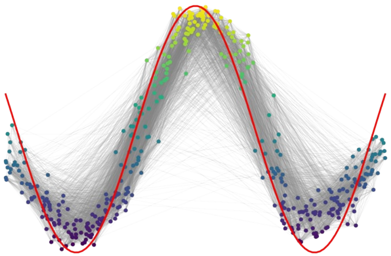

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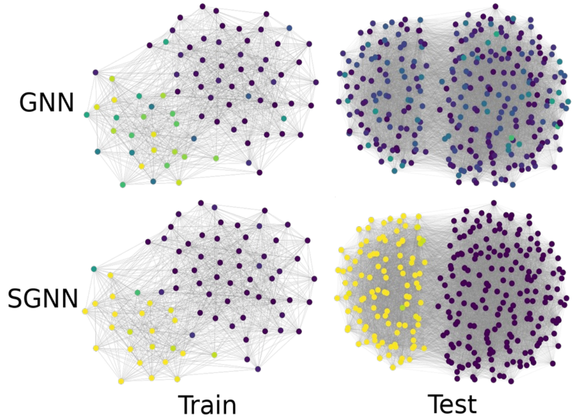

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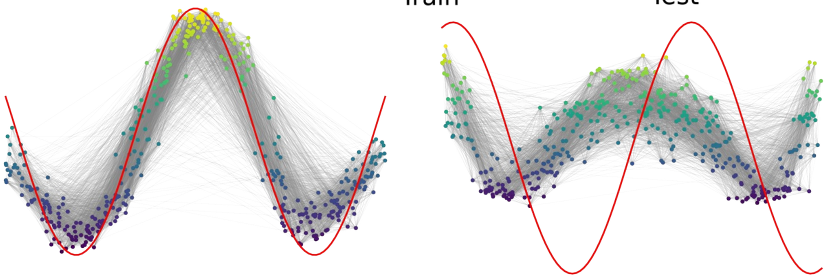

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- Thm. c-SGNNs are *strictly more powerful* than c-GNNs
- Thm. Using Stone-Weierstrass theorem, c-SGNNs are universal (both permutation-invariant/equivariant):
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  - Many "additive" kernels $W(x,y) = w(v(x) + v(y))$
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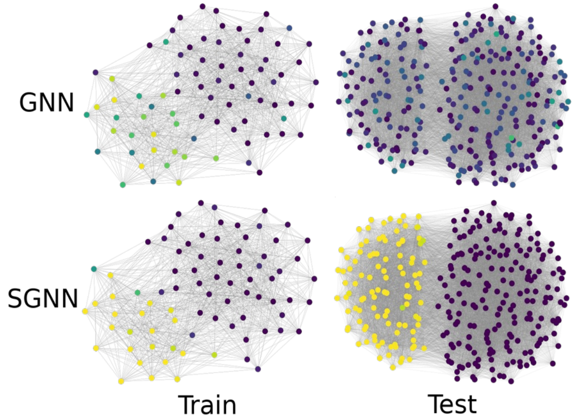

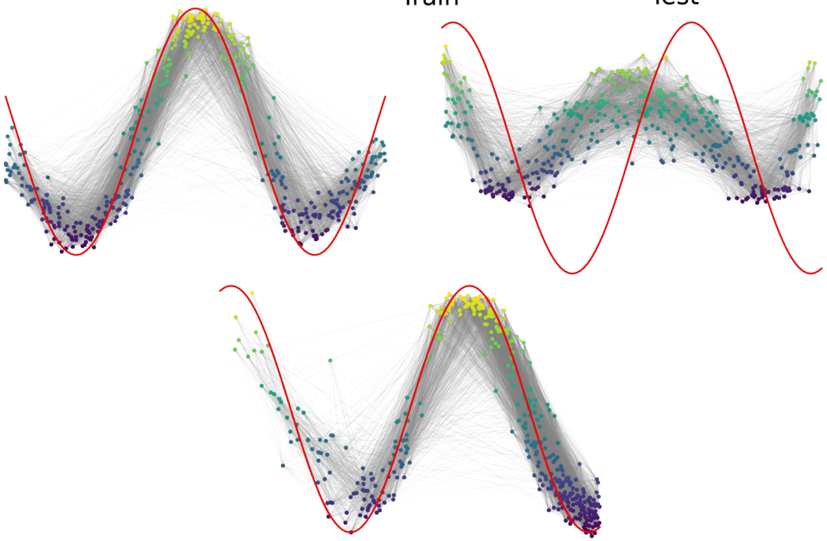

Continuous SGNN and universality

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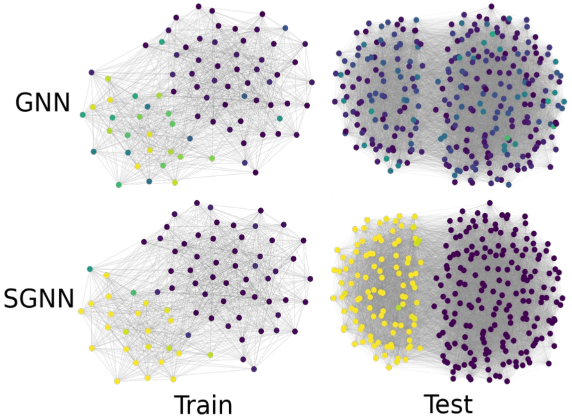

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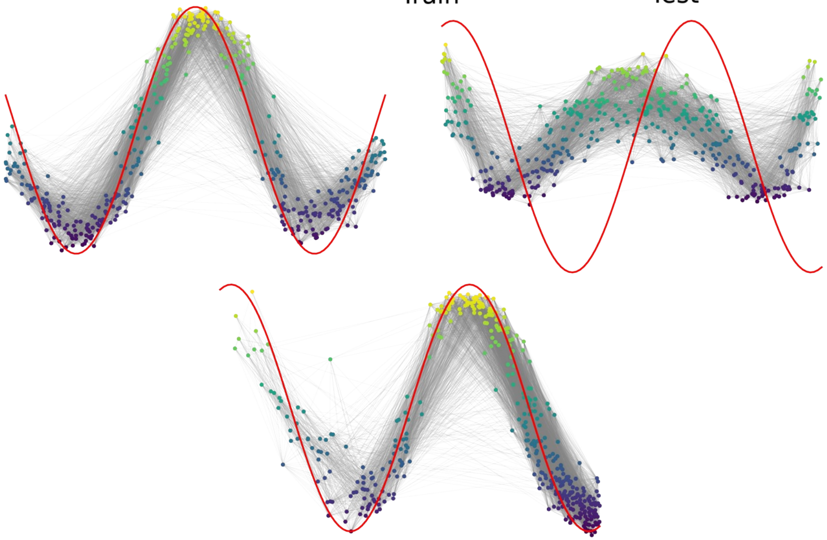

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