Graph Neural Networks: Applications & Open challenges

Dr Dorina Thanou

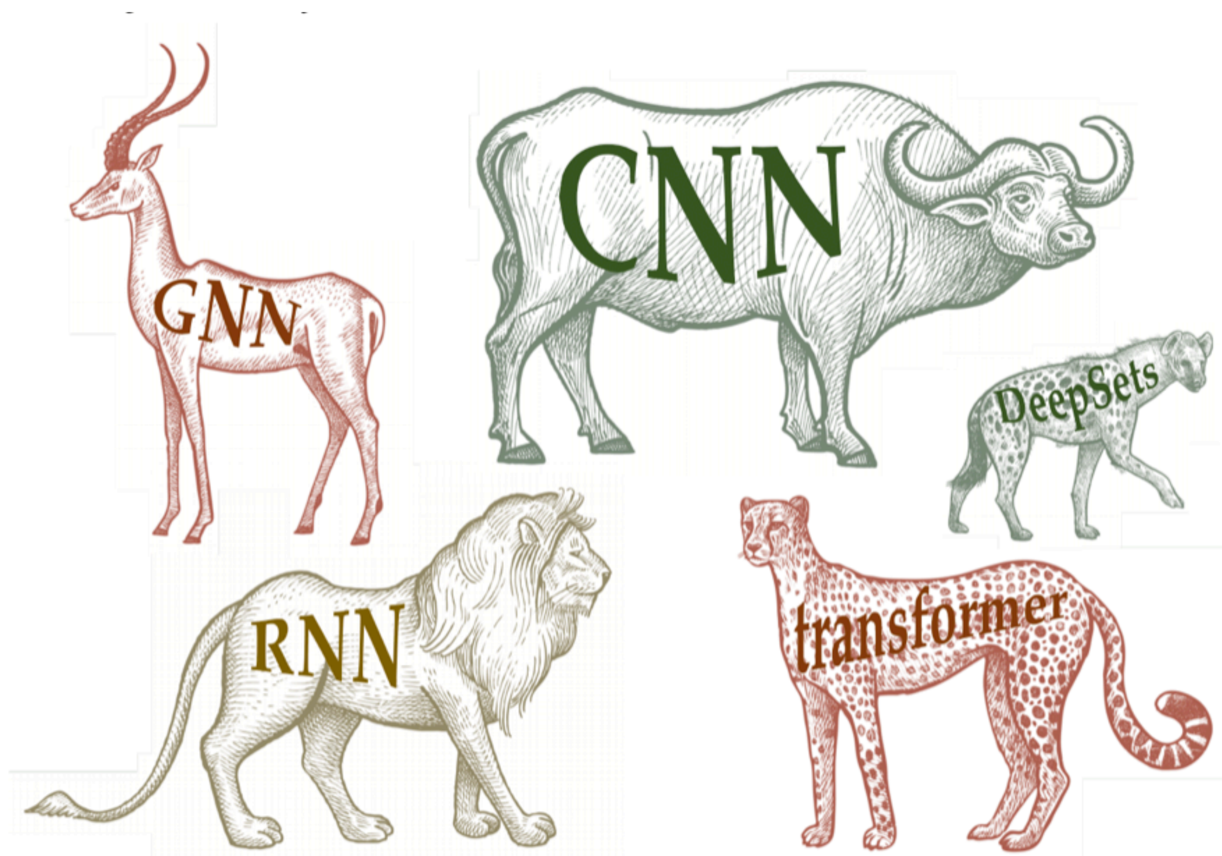
May 22, 2023

Today's lecture

- **A glimpse of geometric deep learning**
- Applications
- Open research questions
- Wrap up of the class
- Feedback on the class

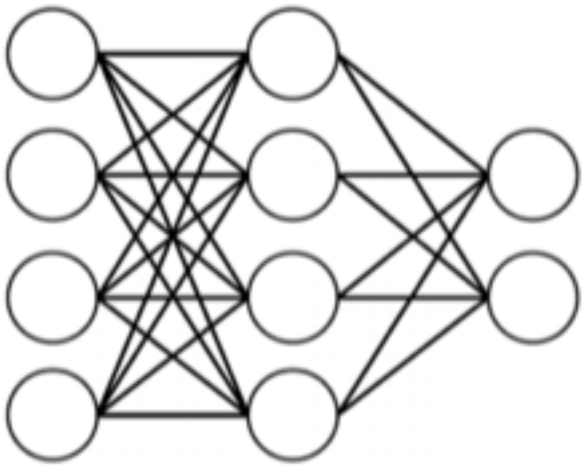
Geometric Deep Learning

- An attempt to unify deep learning architectures under a common mathematical framework

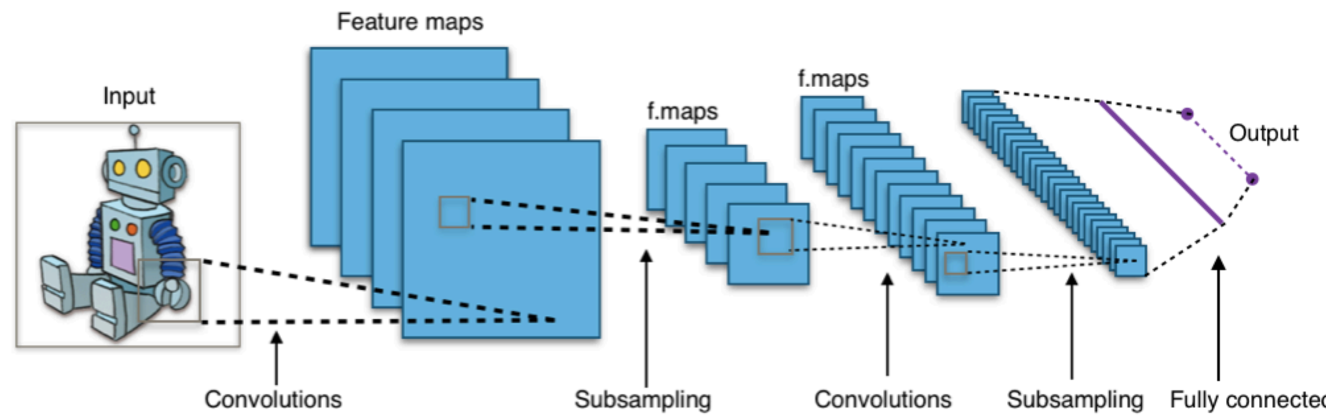


What is the one true architecture?

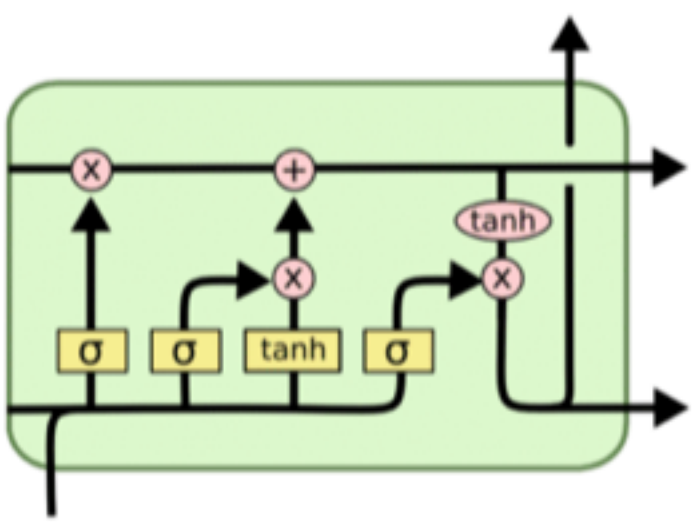
All architectures derive from geometric priors



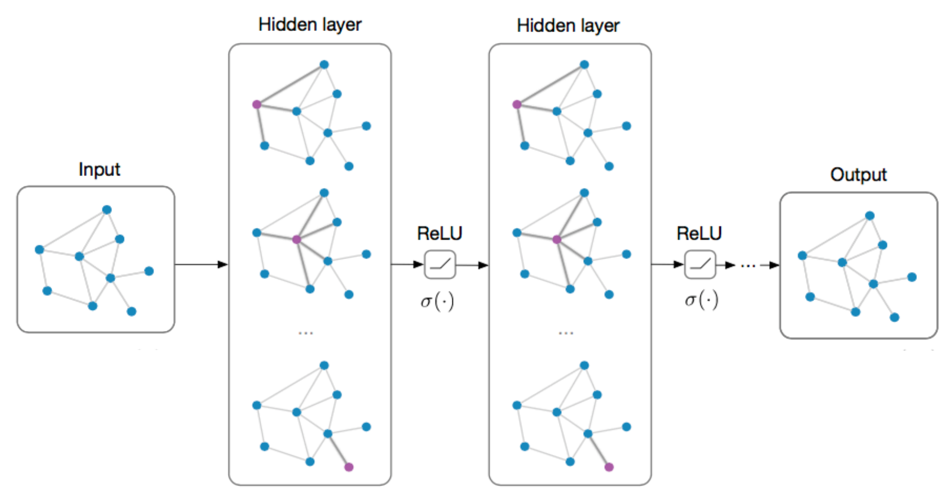
Perceptrons:
Function regularity



CNNs:
Translation invariance



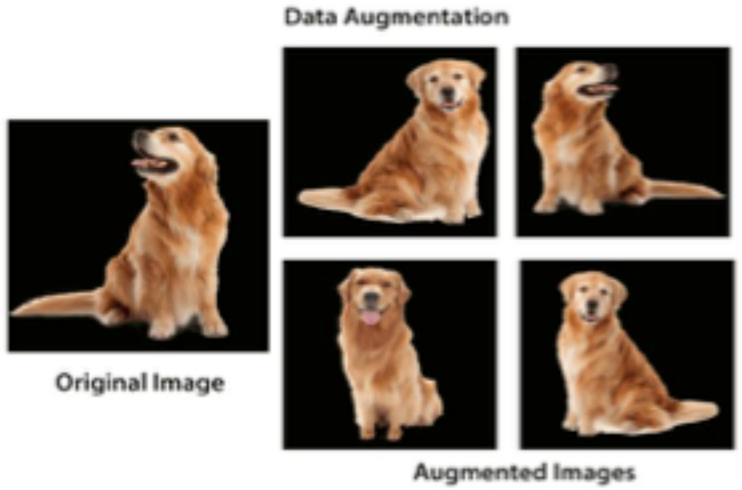
RNNs:
Time warping

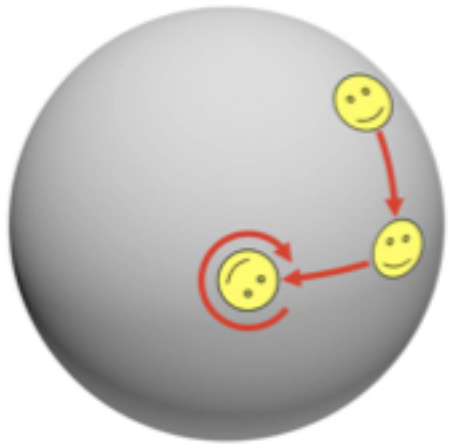


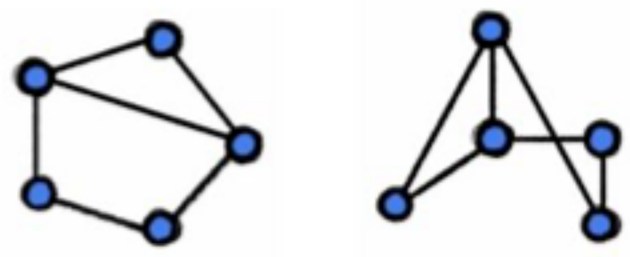
GNNs:
Permutation invariance

Prior 1: Symmetries

- Symmetry is a transformation that leaves an object **invariant**
  - Images should be processed independently of **shifts**
  - Spherical data should be processed independently of **rotation**
  - Graph data should be processed independently of **isomorphism**



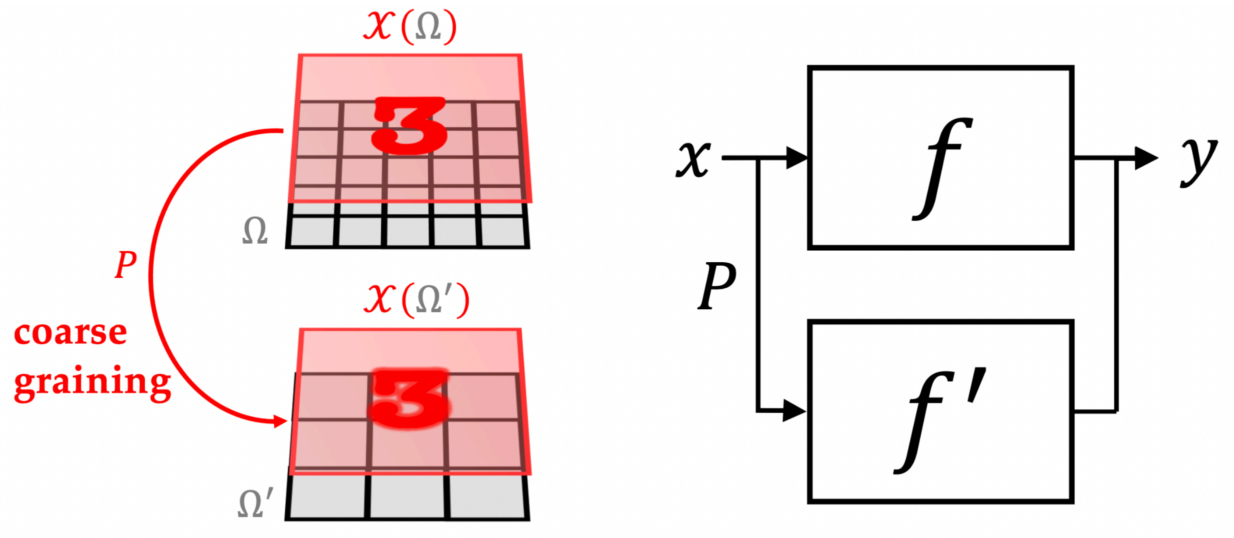




Prior 2: Scale separation

- We can extract sufficient statistics at a lower spatial resolution by downsampling demodulated localized filter responses

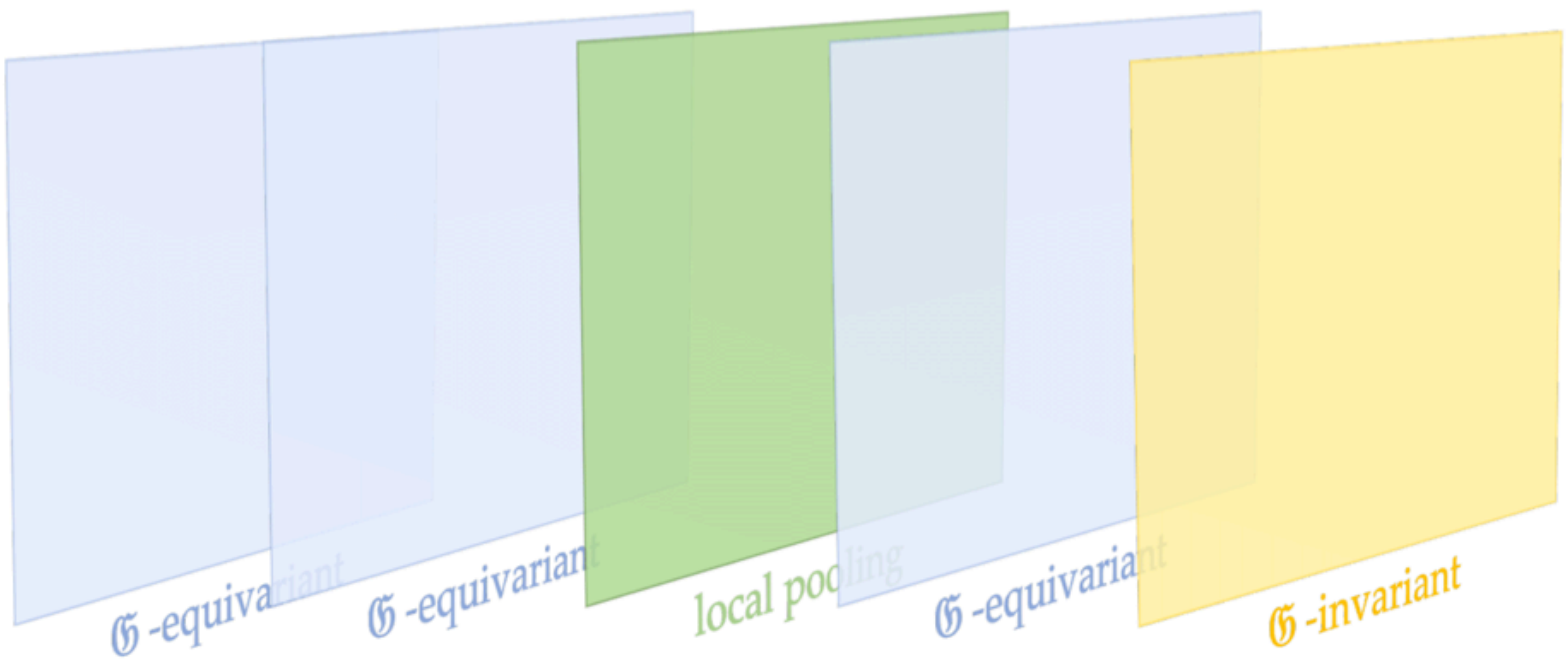
- Long range dependencies can be broken into multi-scale local interaction terms



$$f \approx f' \circ P$$

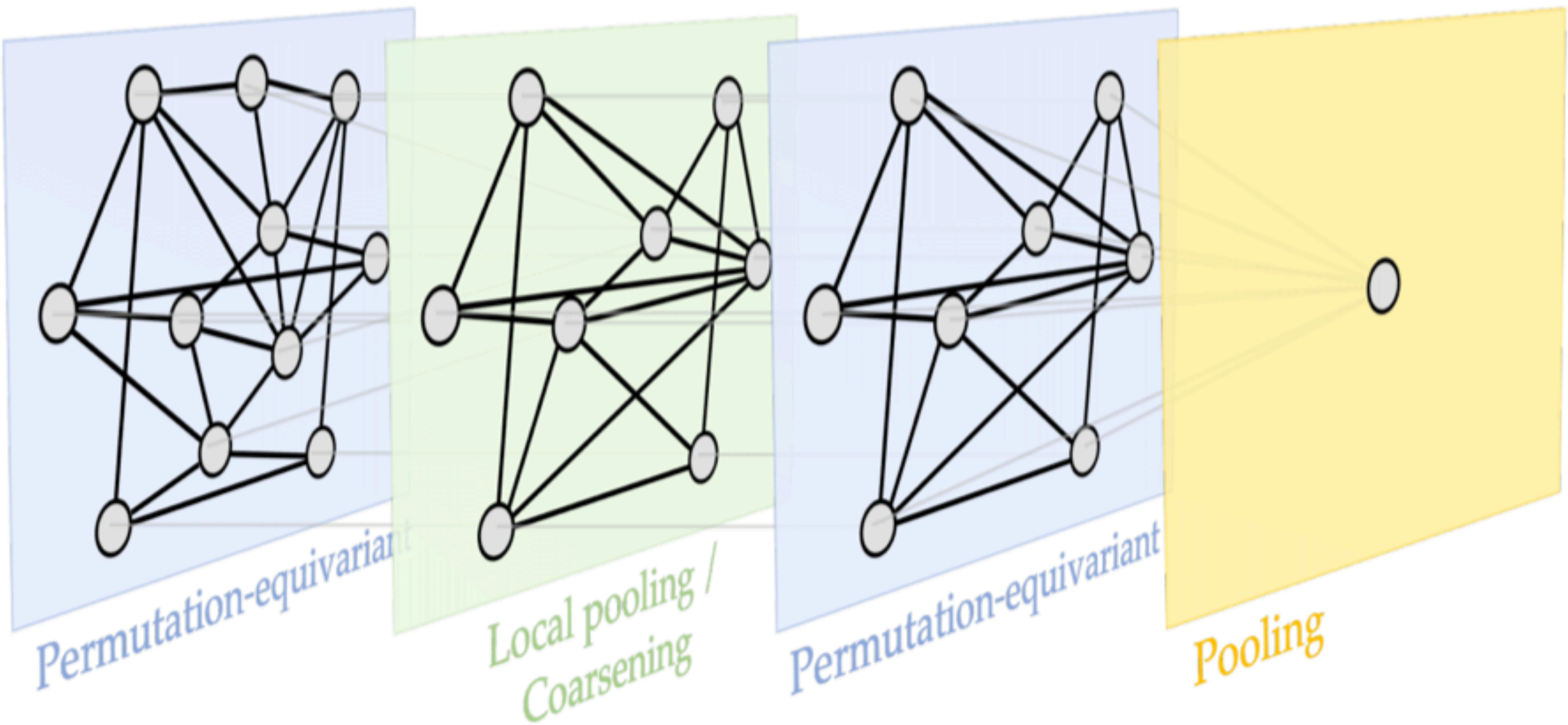
Geometric deep learning blueprint

- We can apply a sequence of equivariant layers that preserve the symmetries of the domain
- Local pooling defines a hierarchy of domains
- Invariant global pooling aggregates features into a single output



Graph neural networks

- They can be considered a specific instance of geometric deep learning



Examples of architectures and their priors

Architecture	**Domain** Ω	**Symmetry group** $\mathfrak{G}$
CNN	Grid	Translation
Spherical CNN	Sphere / SO(3)	Rotation SO(3)
Intrinsic / Mesh CNN	Manifold	Isometry Iso(Ω) / Gauge symmetry SO(2)
GNN	Graph	Permutation Σ_n
Deep Sets	Set	Permutation Σ_n
Transformer	Complete Graph	Permutation Σ_n
LSTM	1D Grid	Time warping

For a deeper understanding

Geometric Deep Learning
Grids, Groups, Graphs,
Geodesics, and Gauges

Michael M. Bronstein[1], Joan Bruna[2], Taco Cohen[3], Petar Veličković[4]

May 4, 2021

[1]Imperial College London / USI IDSIA / Twitter
[2]New York University
[3]Qualcomm AI Research. Qualcomm AI Research is an initiative of Qualcomm Technologies, Inc.
[4]DeepMind

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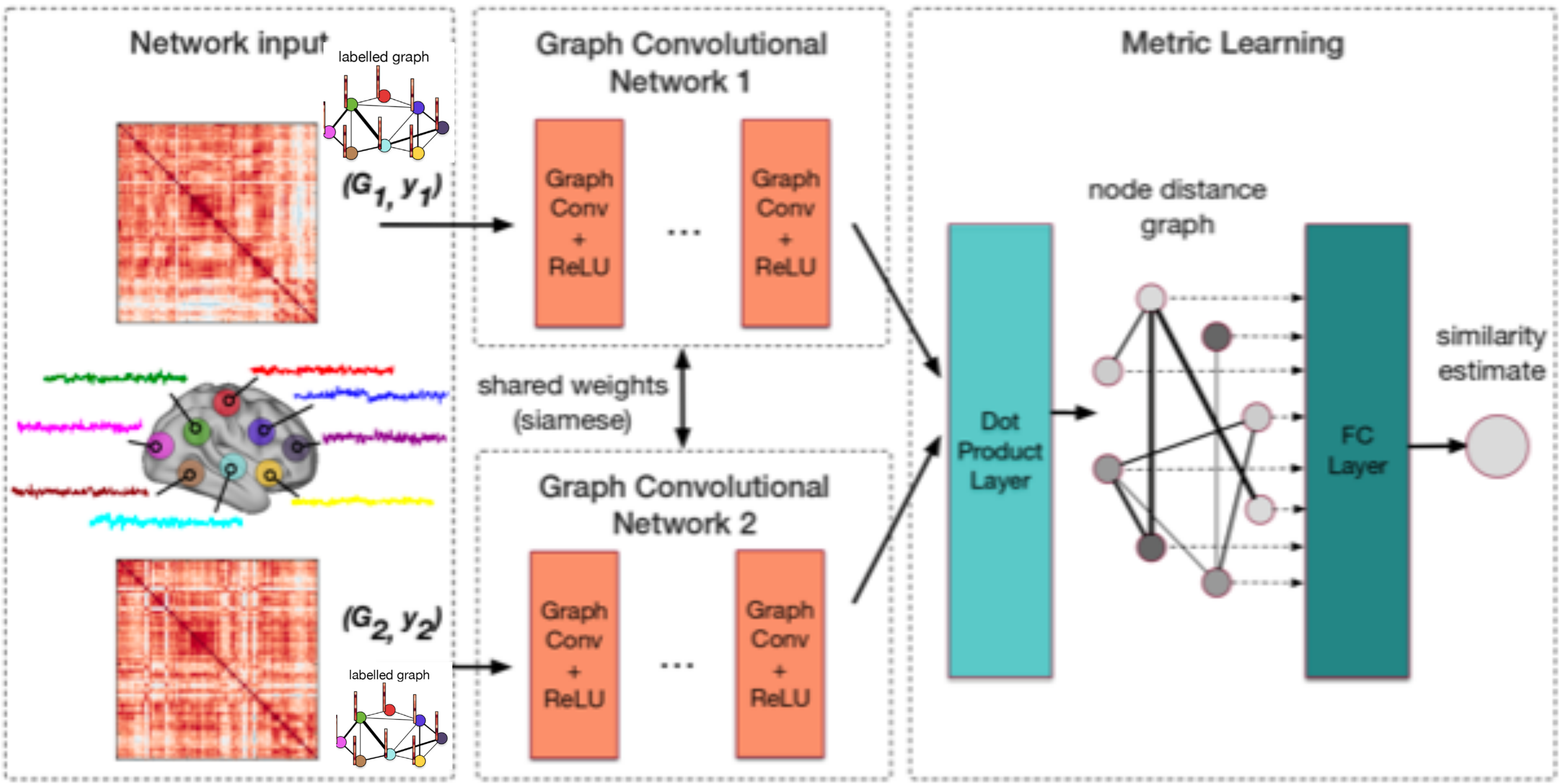
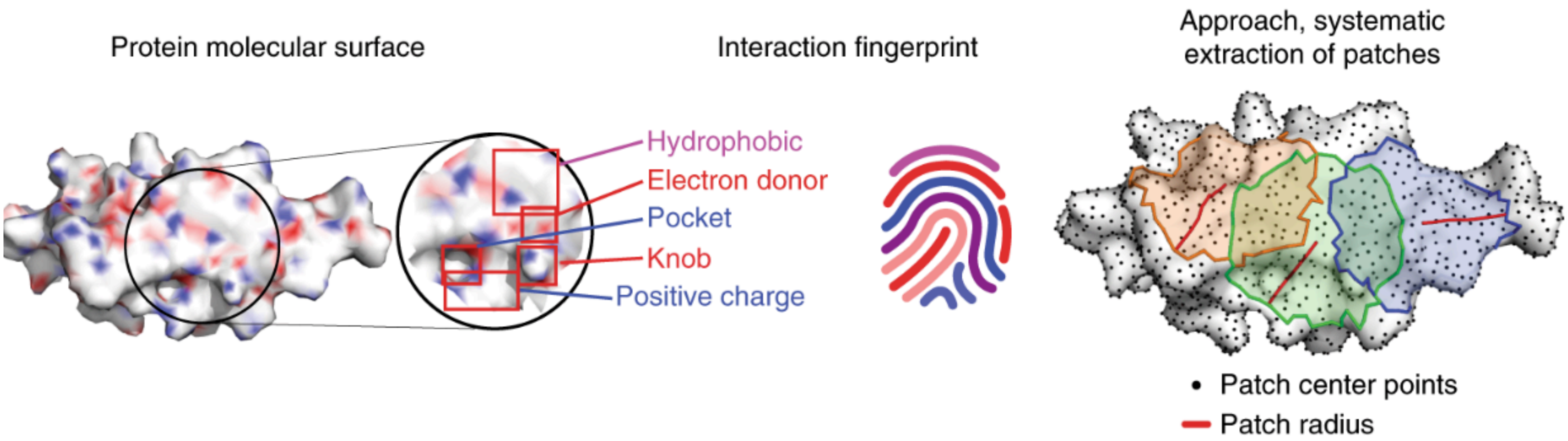
Neuroscience: learn to compare brain networks



[Ktena et al., Metric learning with spectral graph convolutions on brain connectivity networks, NeuroImage, 2018]

Protein-protein interactions

- Predicting interactions between proteins and other biomolecules solely based on structure remains a challenge in biology
- Exploit GNNs to learn interaction fingerprints in protein molecular surfaces that determine protein interactions



[Gainza et al, Deciphering interaction fingerprints from protein molecular surfaces using geometric deep learning, Nature methods, 2019]

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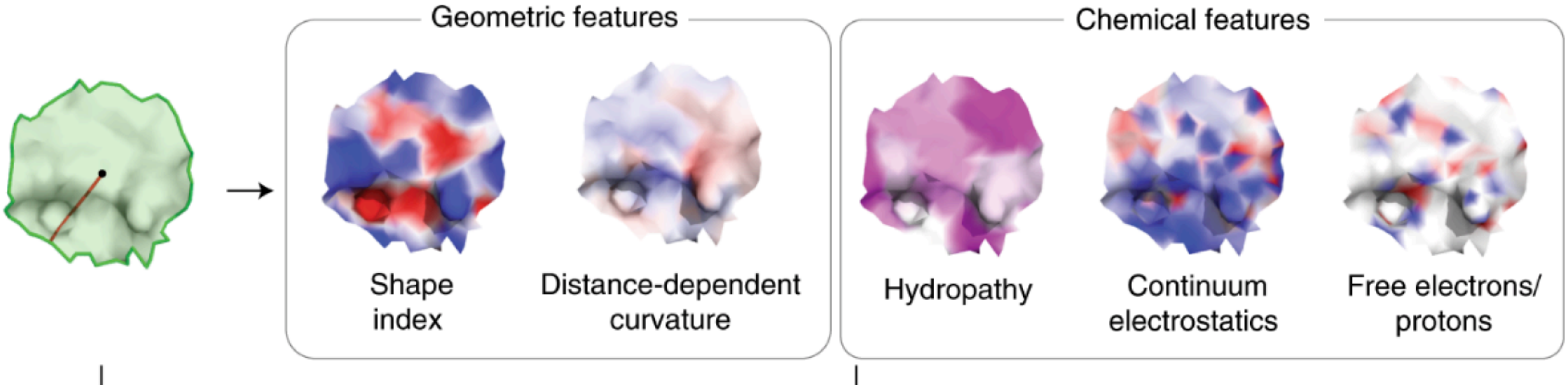

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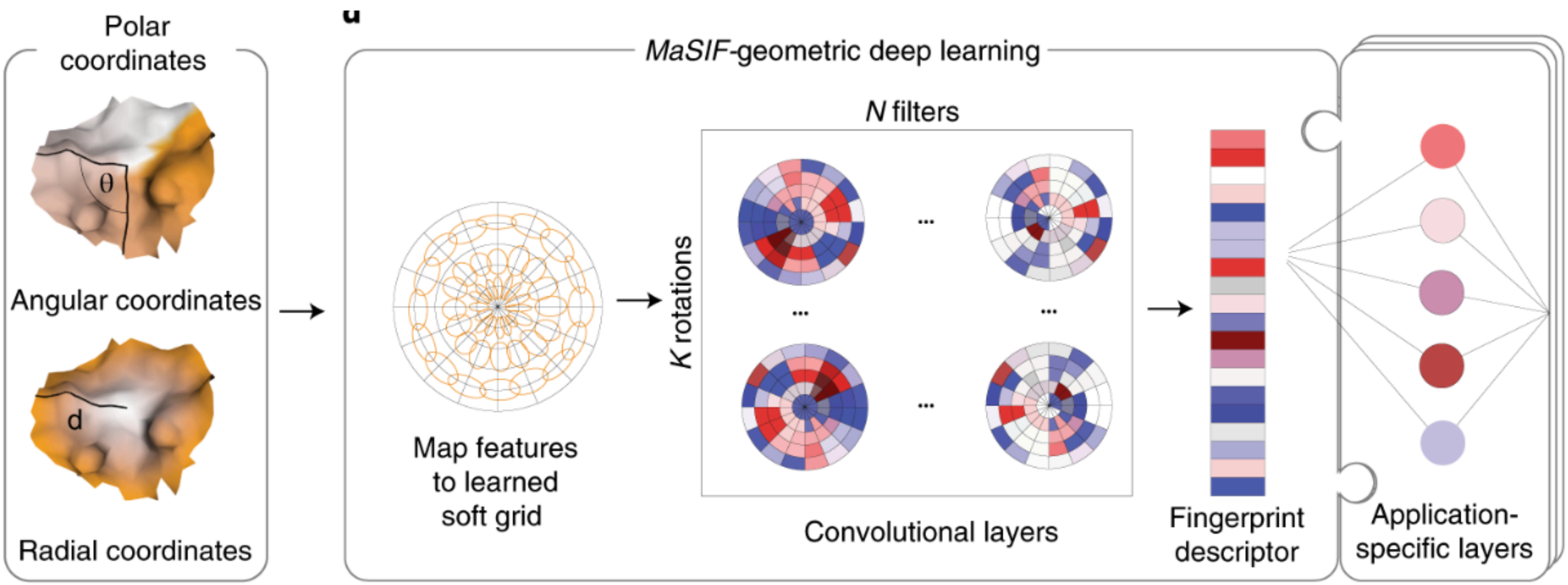

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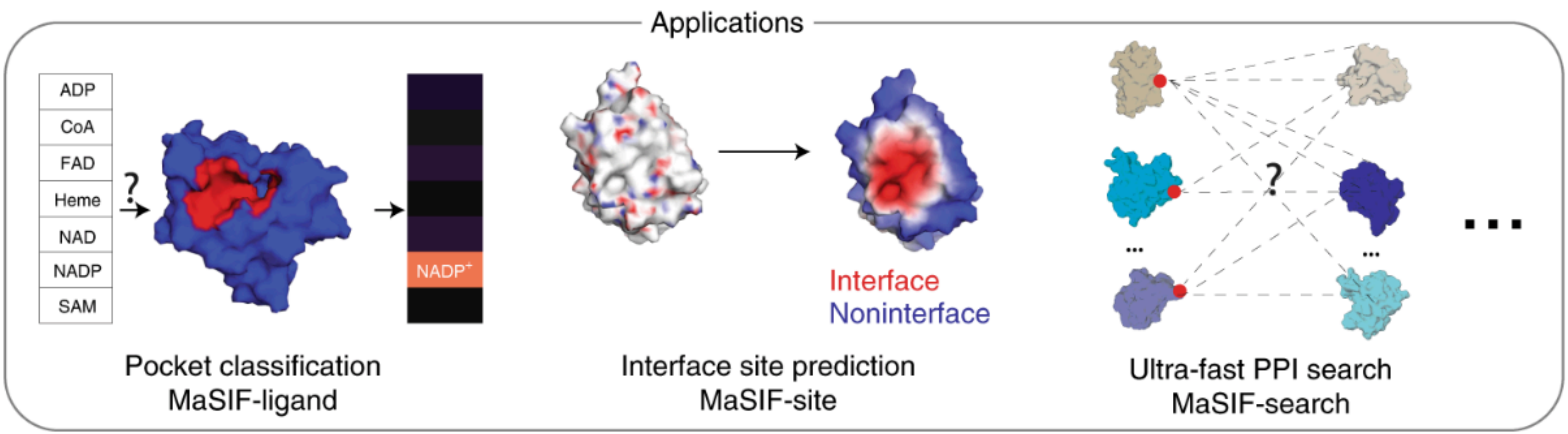
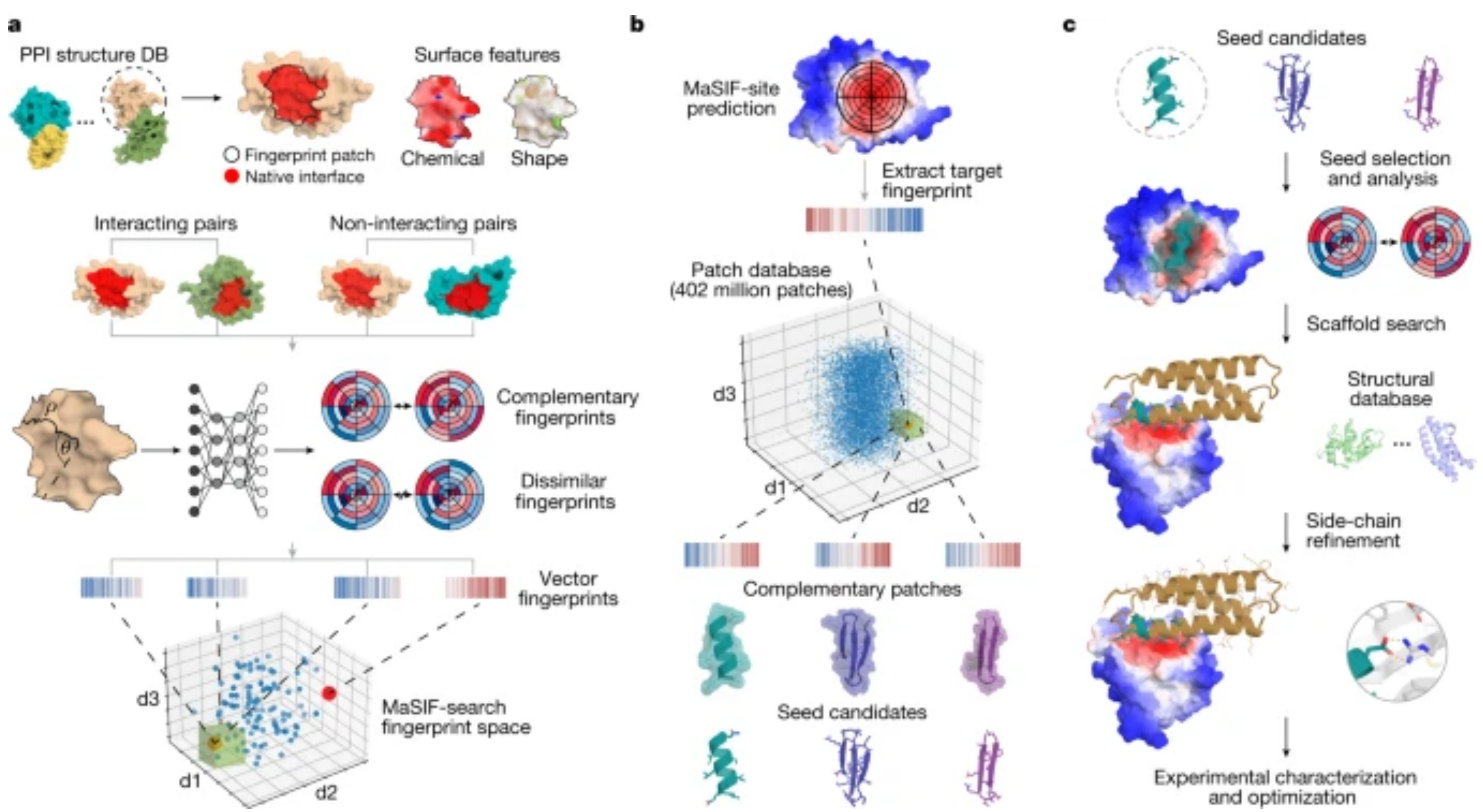


[Gainza et al, Deciphering interaction fingerprints from protein molecular surfaces using geometric deep learning, Nature methods, 2019]

De novo design of protein-protein interactions

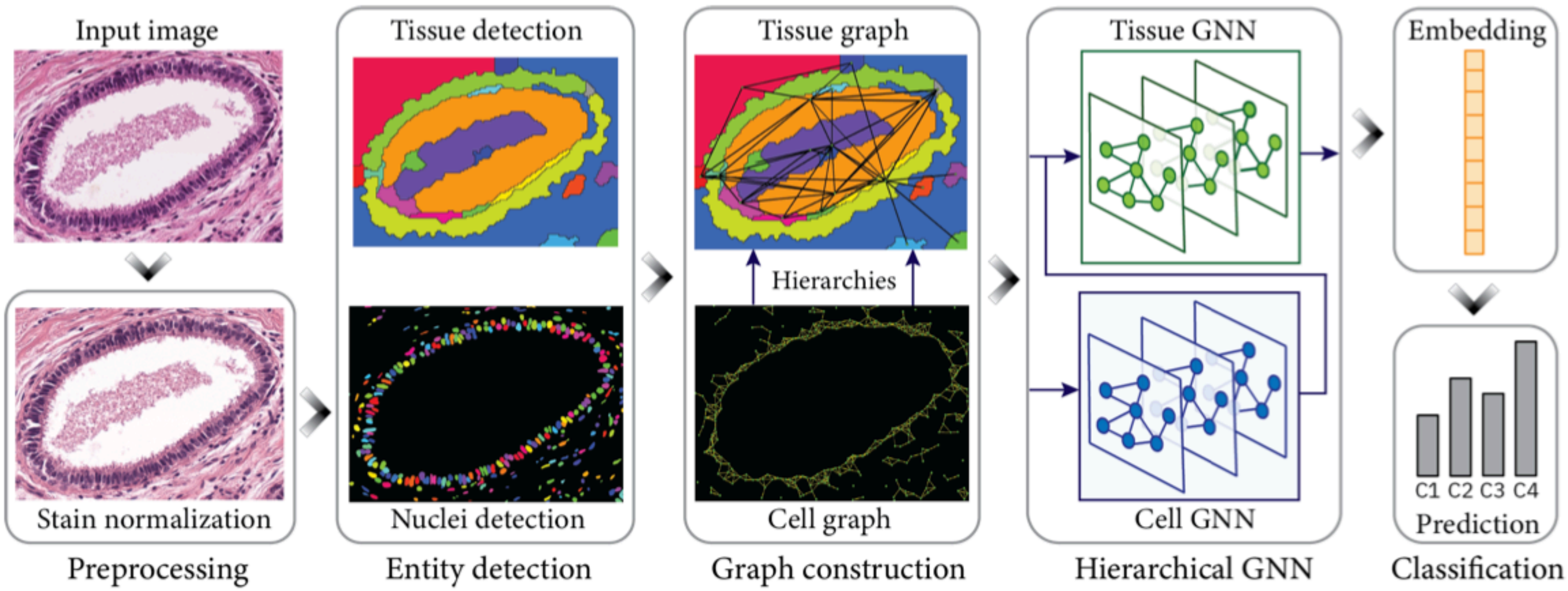
- Design PPIs by targeting sites using only structural information from the target protein



[Gainza et al, De novo design of protein interactions with learned surface fingerprints, Nature, 2023]

Medical imaging

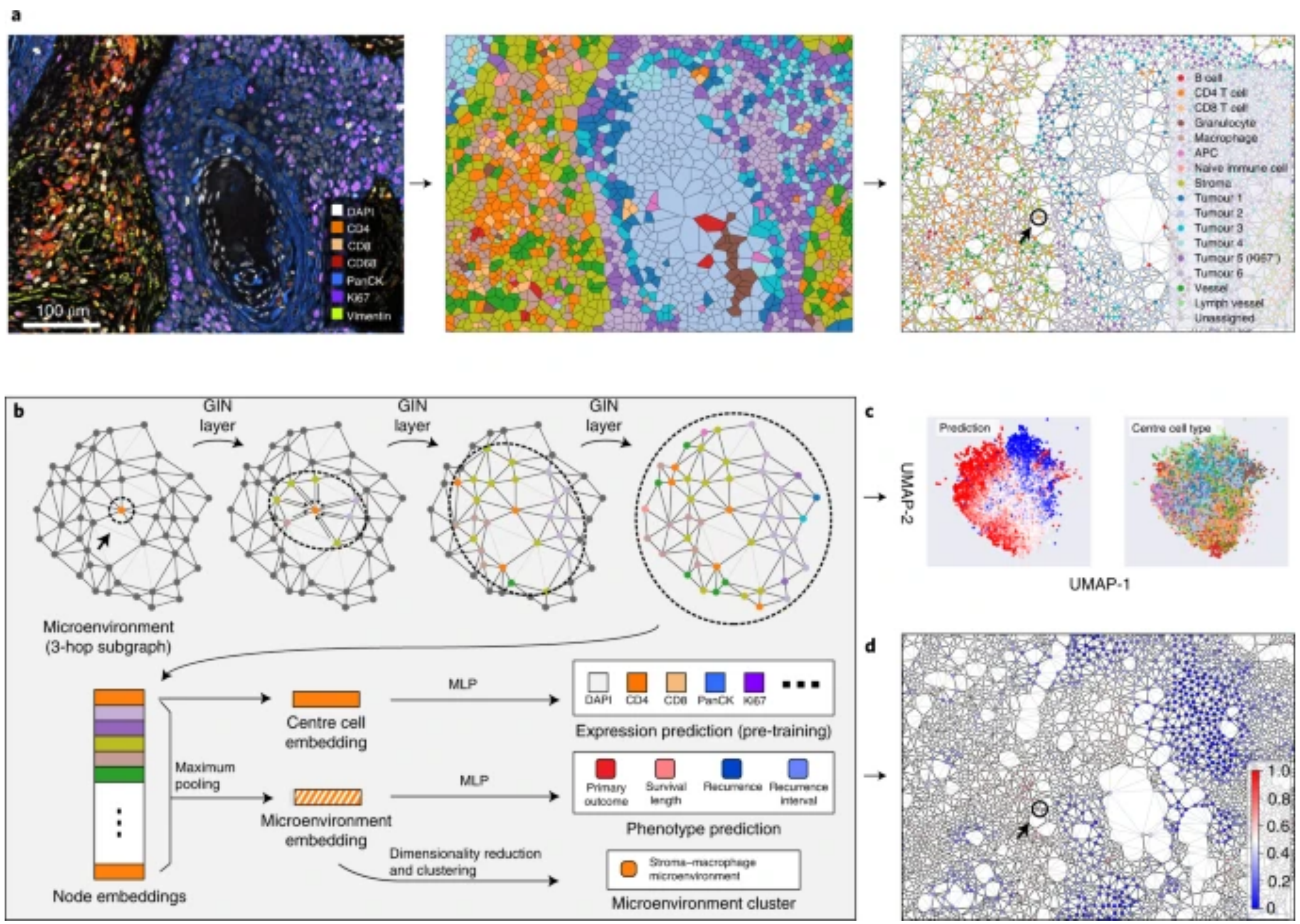
- Digital pathology: Graph based representations provide a flexible tool for modelling complex dependencies at different levels of hierarchy (e.g., cells, tissues)



[Pati et al, “Hierarchical graph representation in digital pathology,” MEDIA, 2022]

[Li et al, Representation learning for networks in biology and medicine: Advancements, challenges, and opportunities, arXiv, 2021]

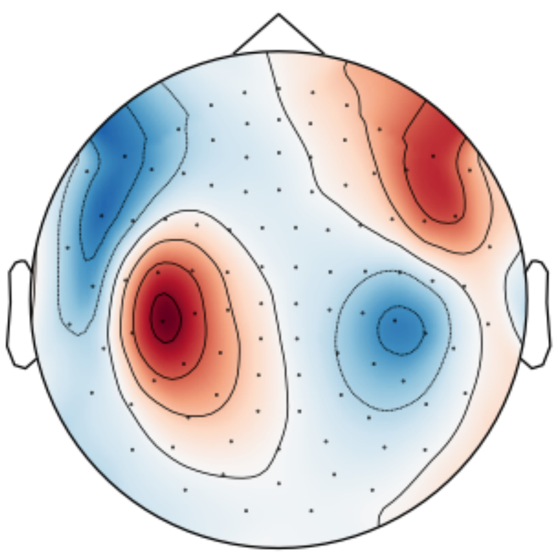
Geometric deep learning models cellular microenvironment



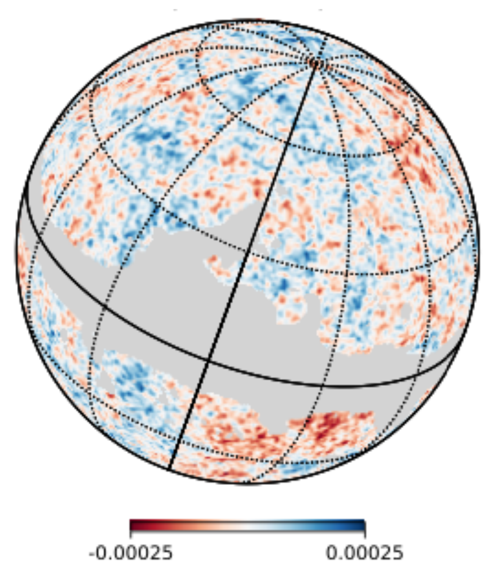
[Wu et al, Graph deep learning for the characterization of tumour microenvironments from spatial protein profiles in tissue specimens, Nature Biomedical Engineering, 2022]

Spherical imaging

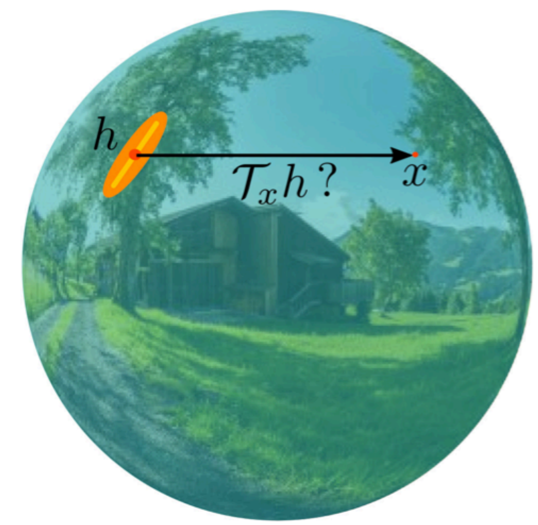
- Spherical data has specific spatial and statistical properties that cannot be captured by regular CNN models



Brain activity (MEG)



Cosmic microwave background temperature



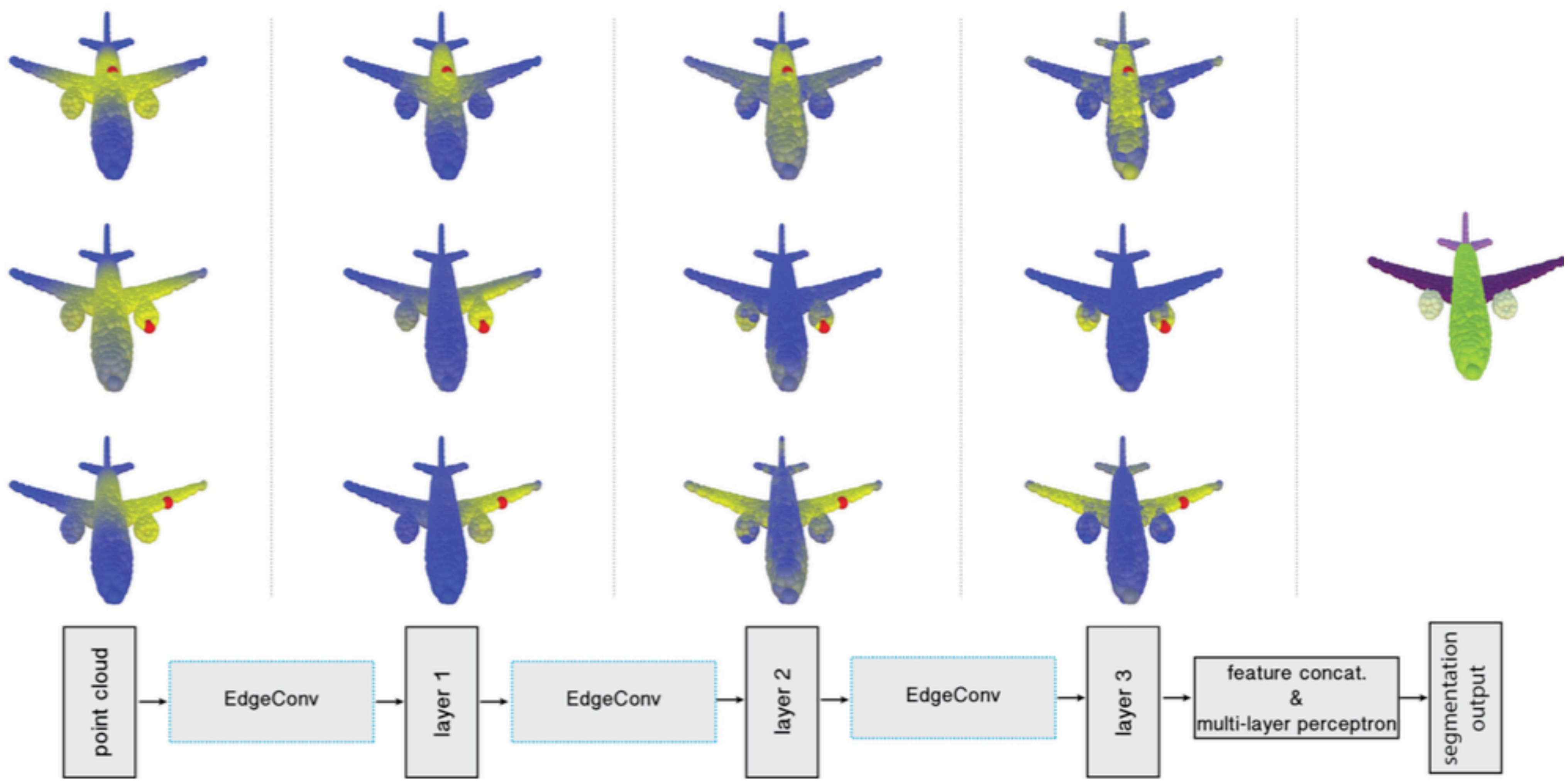
Omnidirectional images

- Sphere is modelled as a graph and classical operation (convolution, translation, pooling…) are performed on the graph

[Perraudin et al., “DeepSphere”, Astronomy and Computing, 2019]
[Bidgoli et al, OSLO: On-the-Sphere Learning for Omnidirectional images and its application to 360-degree image compression, arXiv, 2021]

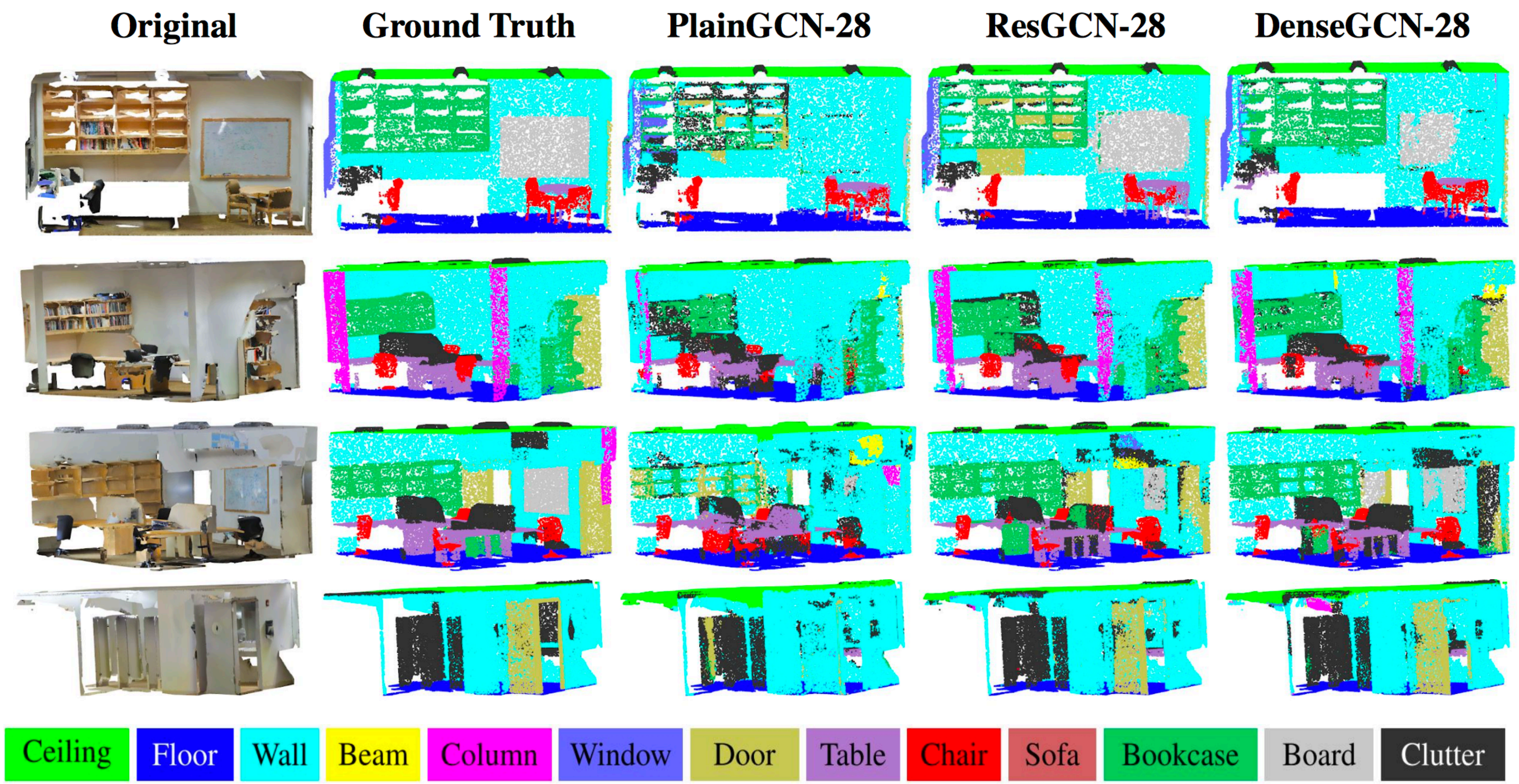
Point cloud semantic segmentation

- Graph attention convolution are successful in capturing specific shapes that adapt to the structure of an object



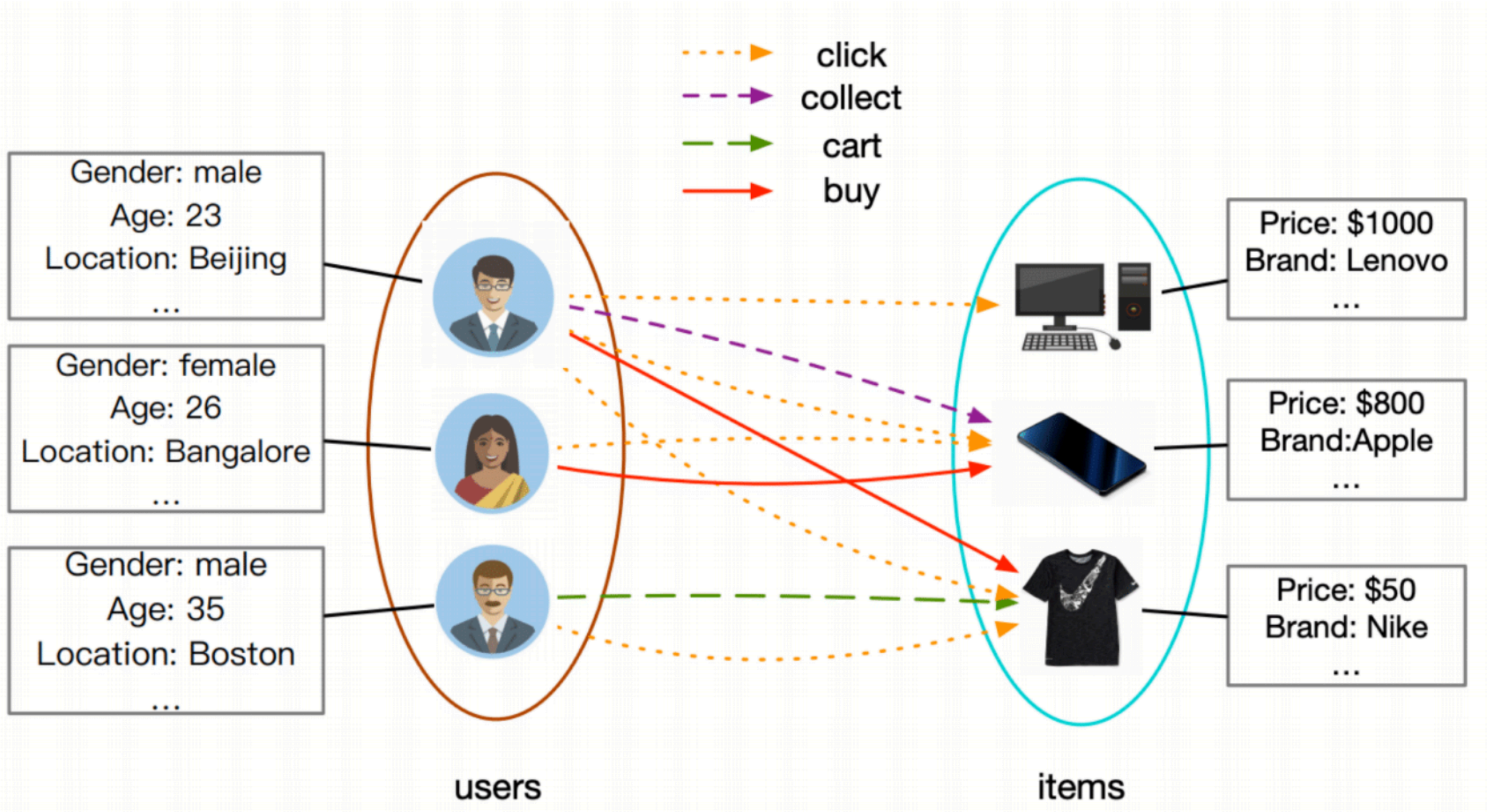
[Wang et al., Graph Attention Convolution for Point Cloud Semantic Segmentation, CVPR, 2019]

Point clouds semantic segmentation



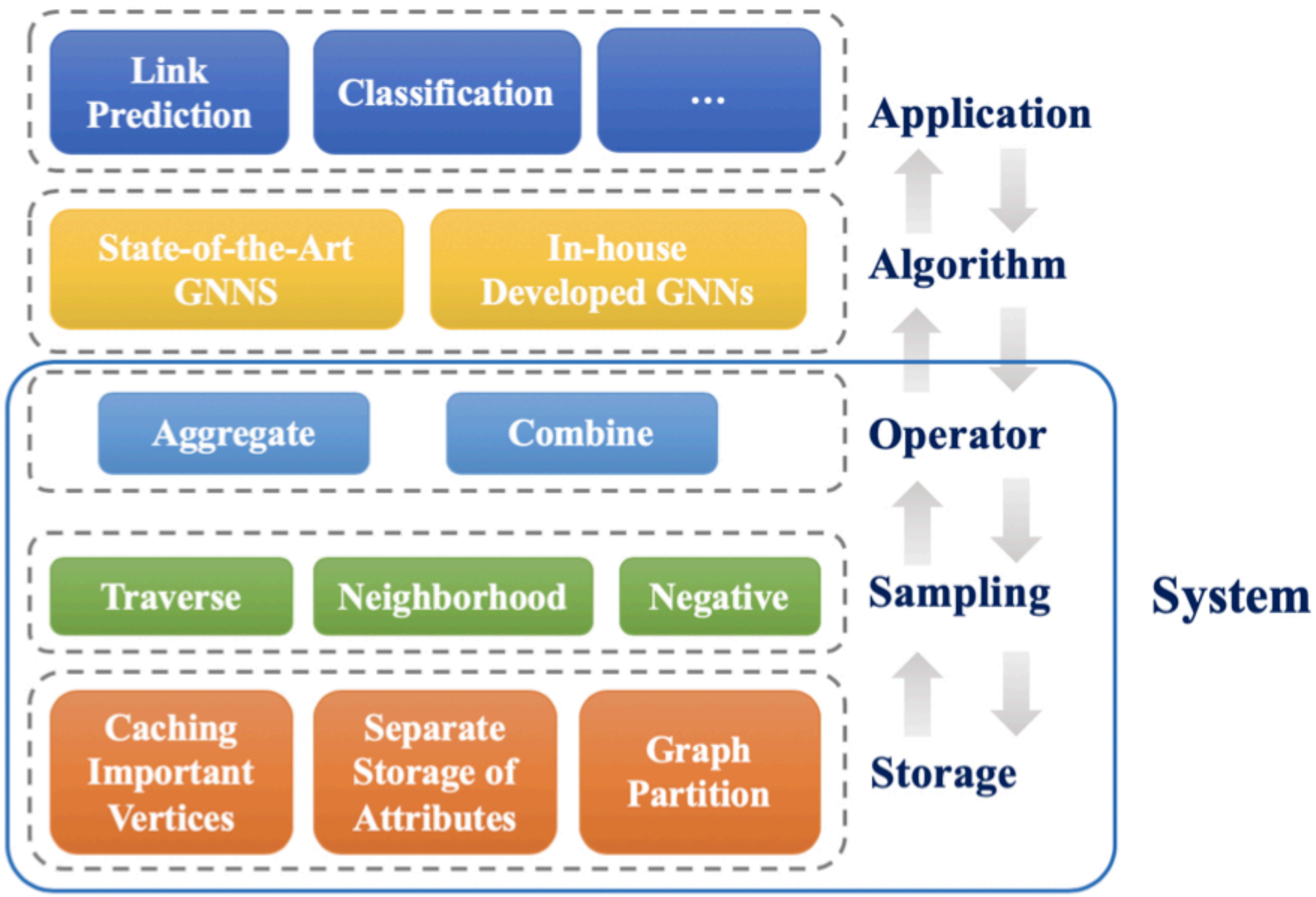
[Li et al., DeepGCNs: Can GCNs Go as Deep as CNNs?, ICCV 2019]

Recommender systems



Recommender systems: Aligraph

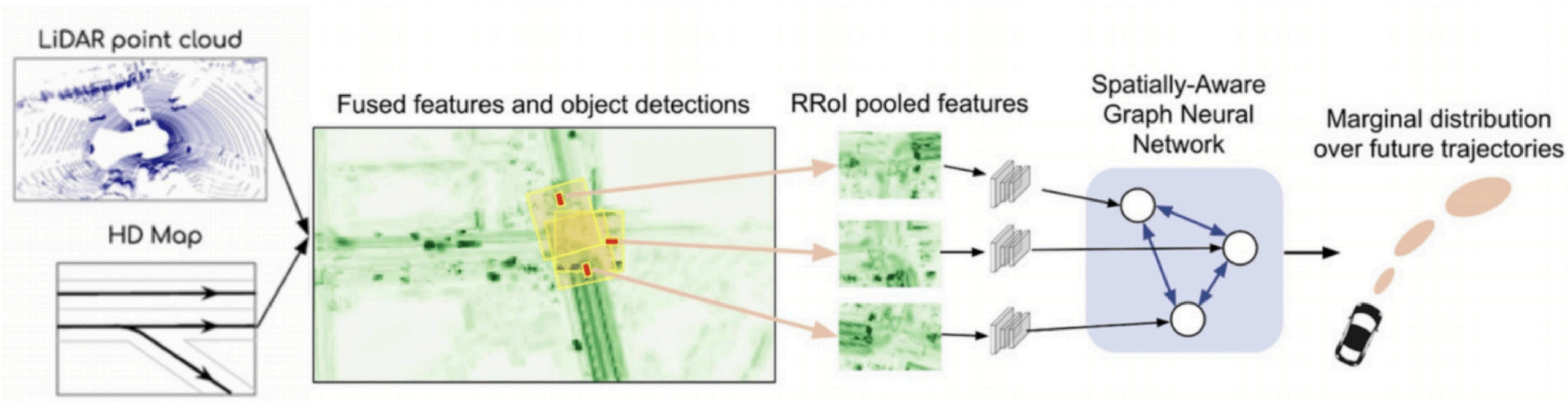
- The system is currently deployed at Alibaba to support product recommendation and personalized search at Alibaba's E-Commerce platform



[Zhu et al., *AliGraph*: A Comprehensive Graph Neural Network Platform, 2019]

Self driving cars

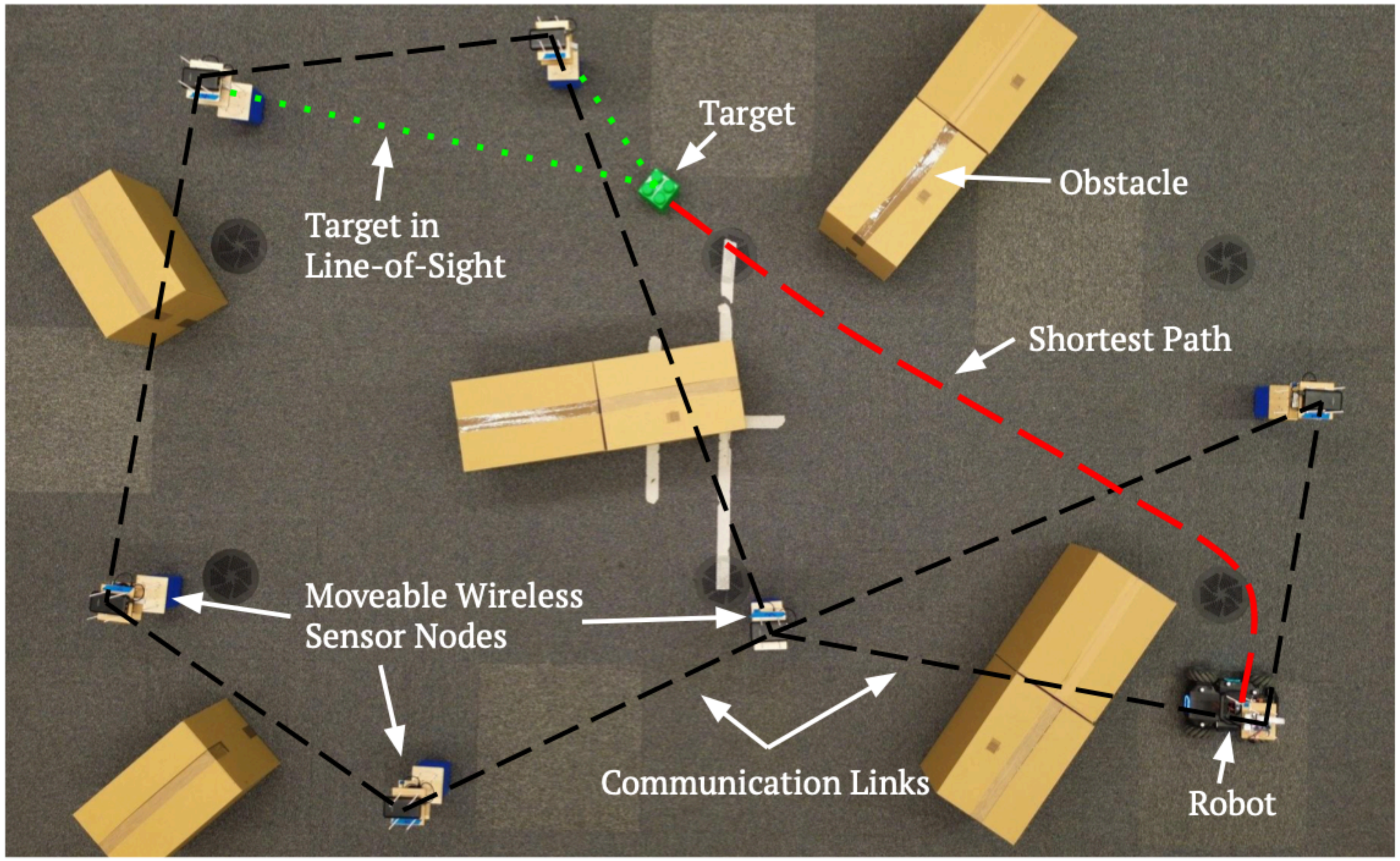
- GNNs provide probabilistic estimates of future trajectories
  - A CNN detects objects
  - A GNN captures interactions between objects and predicts behaviors



[Casas et al, Spatially aware graph neural networks for relational behaviour forecasting for sensor data, ICRA, 2020]

Learning cooperative perception

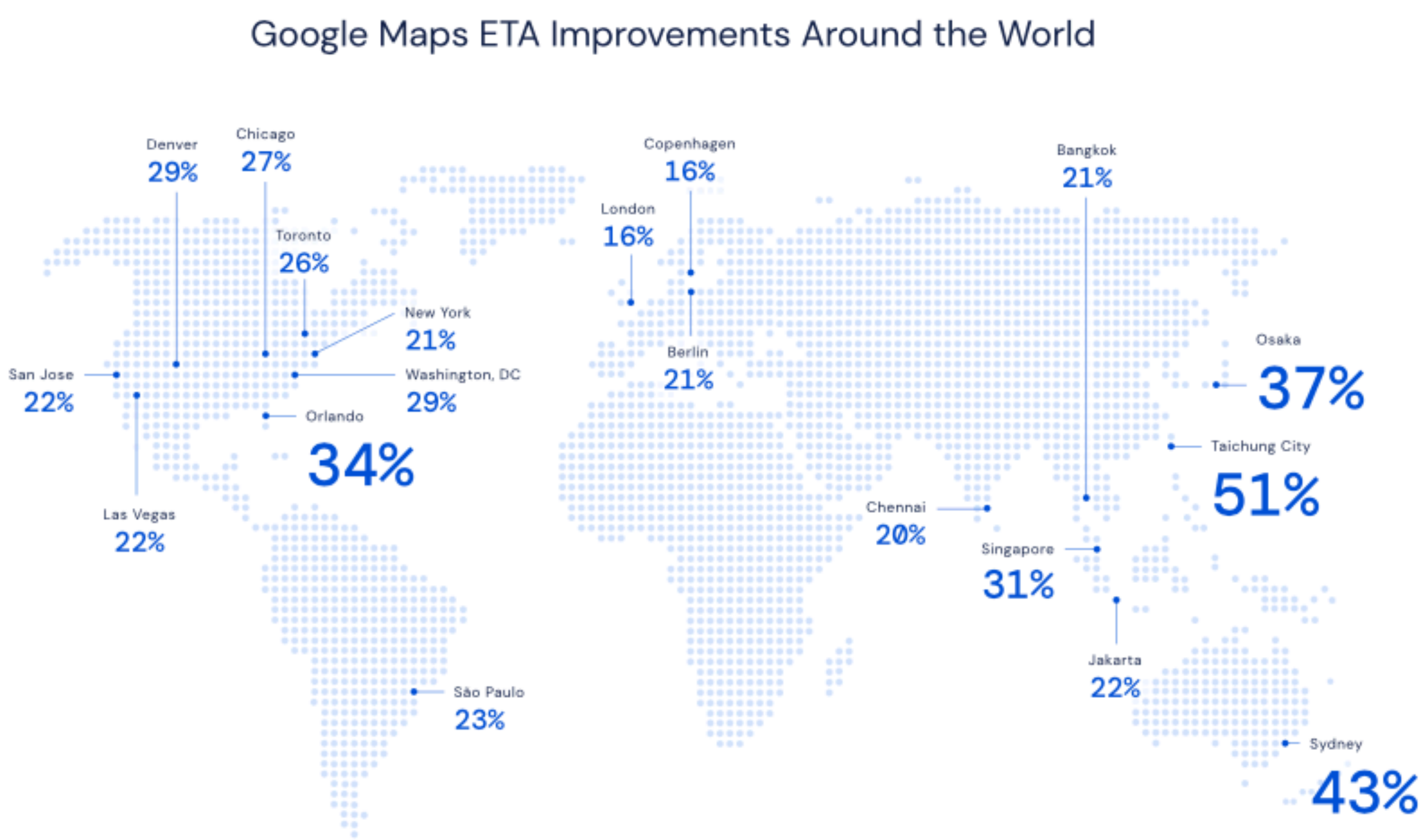
- GNNs can learn to guide the robot to its target under the guidance of a visual sensor network



[Blumenkamp et al, See What the Robot Can't See: Learning Cooperative Perception for Visual Navigation, arXiv 2023]

Traffic prediction

- As the road network is naturally modelled by a graph of road segments and intersections, ETA prediction can be improved with graph representation learning



[Derrow-Pinion et al., ETA Prediction with Graph Neural Networks in Google Maps, 2021]

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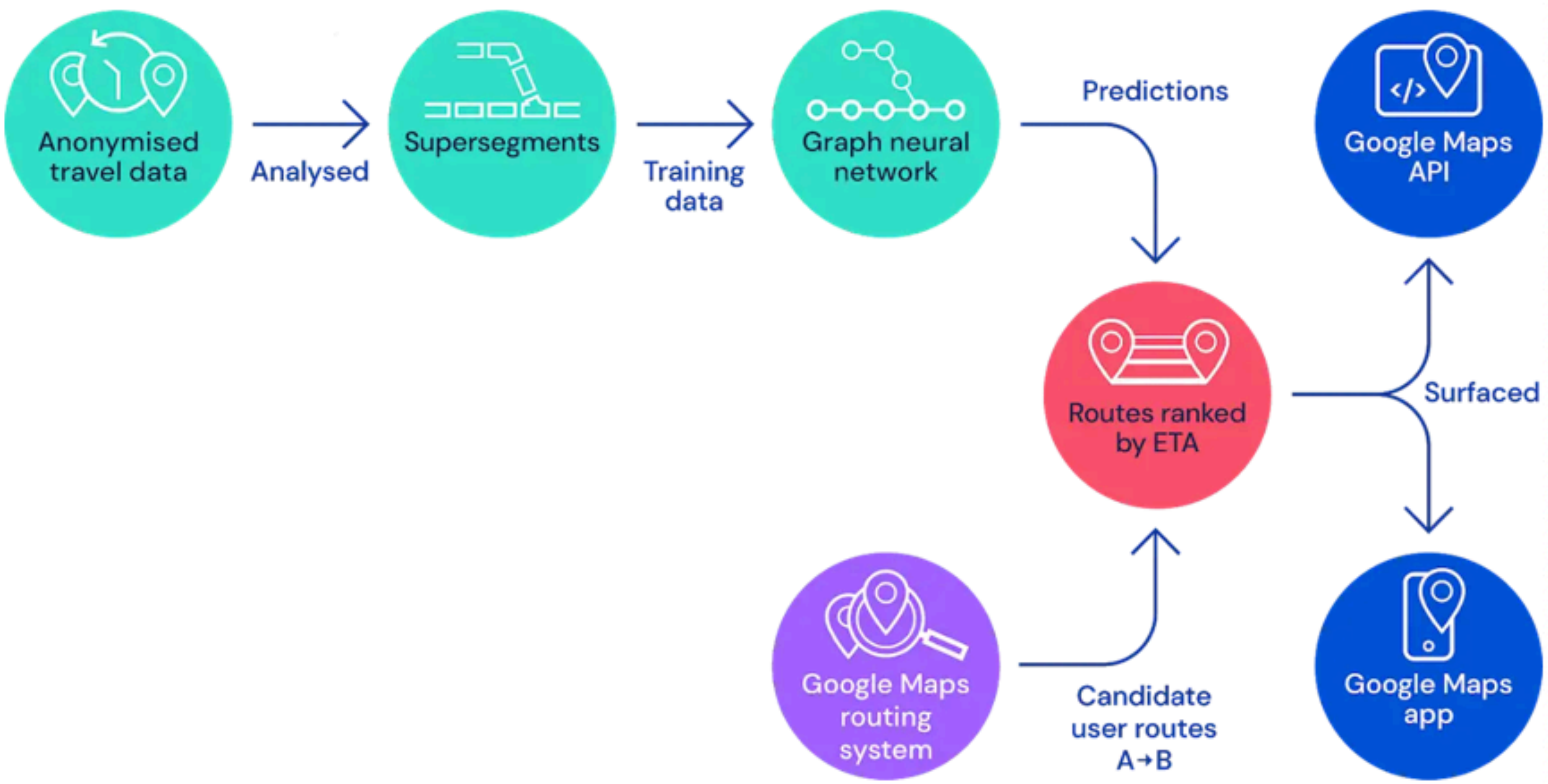
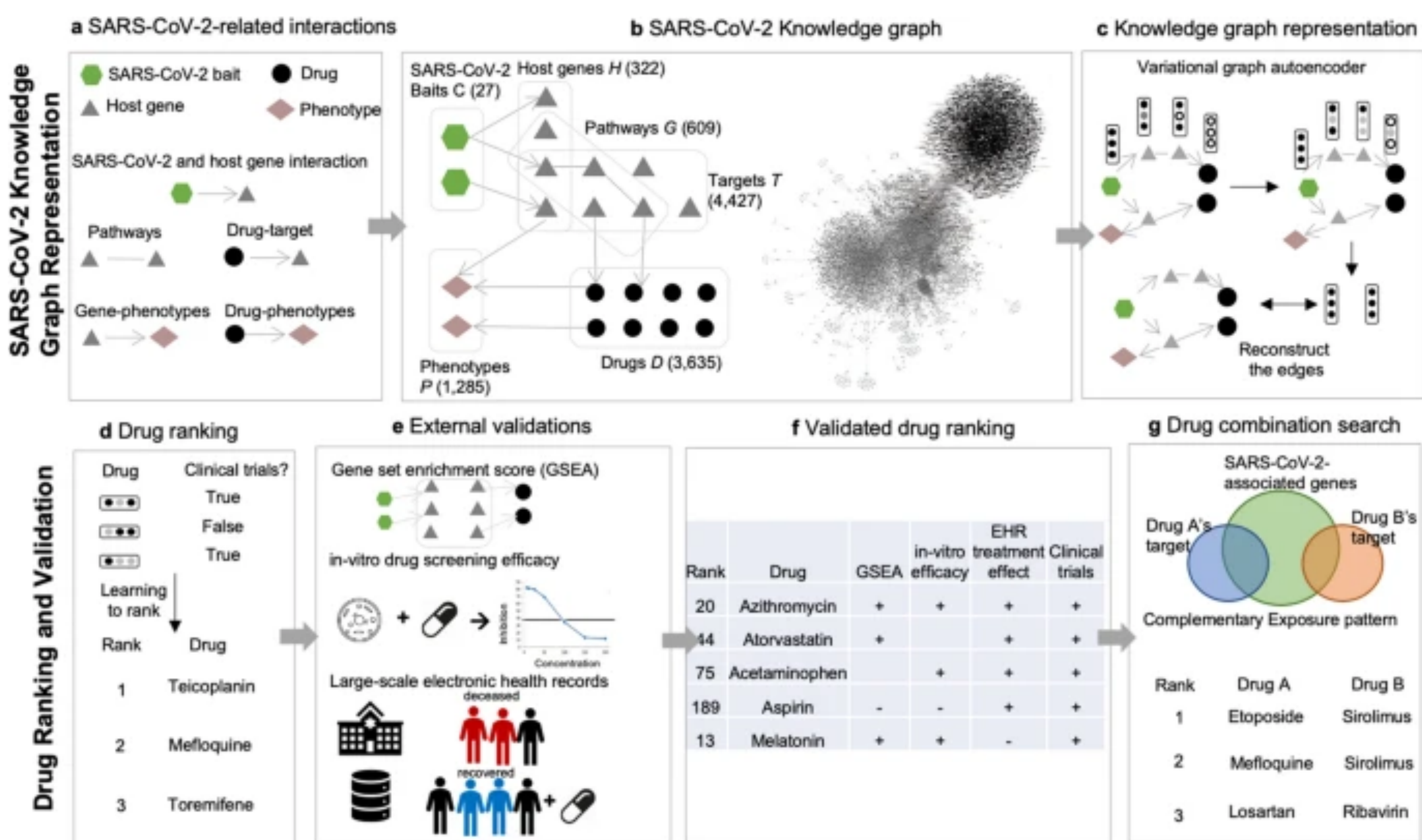


[Derrow-Pinion et al., ETA Prediction with Graph Neural Networks in Google Maps, 2021]

Drug repurposing for COVID-19

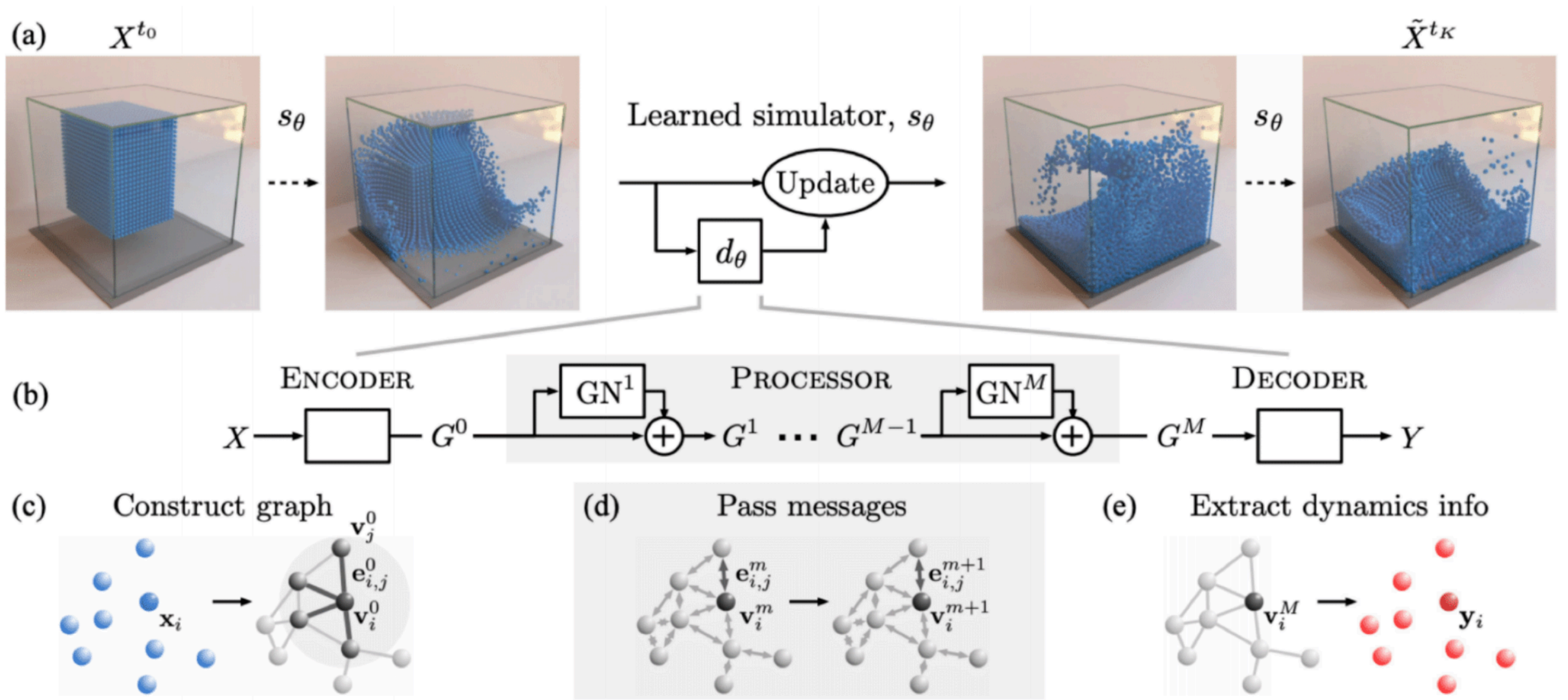
- Deep GNN approaches have been used to derive the candidate drug’s representation based on the biological interactions



[Hsieh et al, Drug repurposing for COVID-19 using graph neural network and harmonizing multiple evidence, Nature Sc. Rep., 2021]

Learning physical simulations

- Mesh-based simulations are central to modeling complex physical systems
- High-dimensional scientific simulations are very expensive
- GNNs have been used to learn mesh-based simulations and predict the dynamics of physical systems



[Sanchez-Gonzales et al, Learning to Simulate Complex Physics with Graph Networks, ICML 2020]
[Pfaff et al, Learning mesh-based simulation with Graph Networks, ICML 2021]

Learning physical simulations

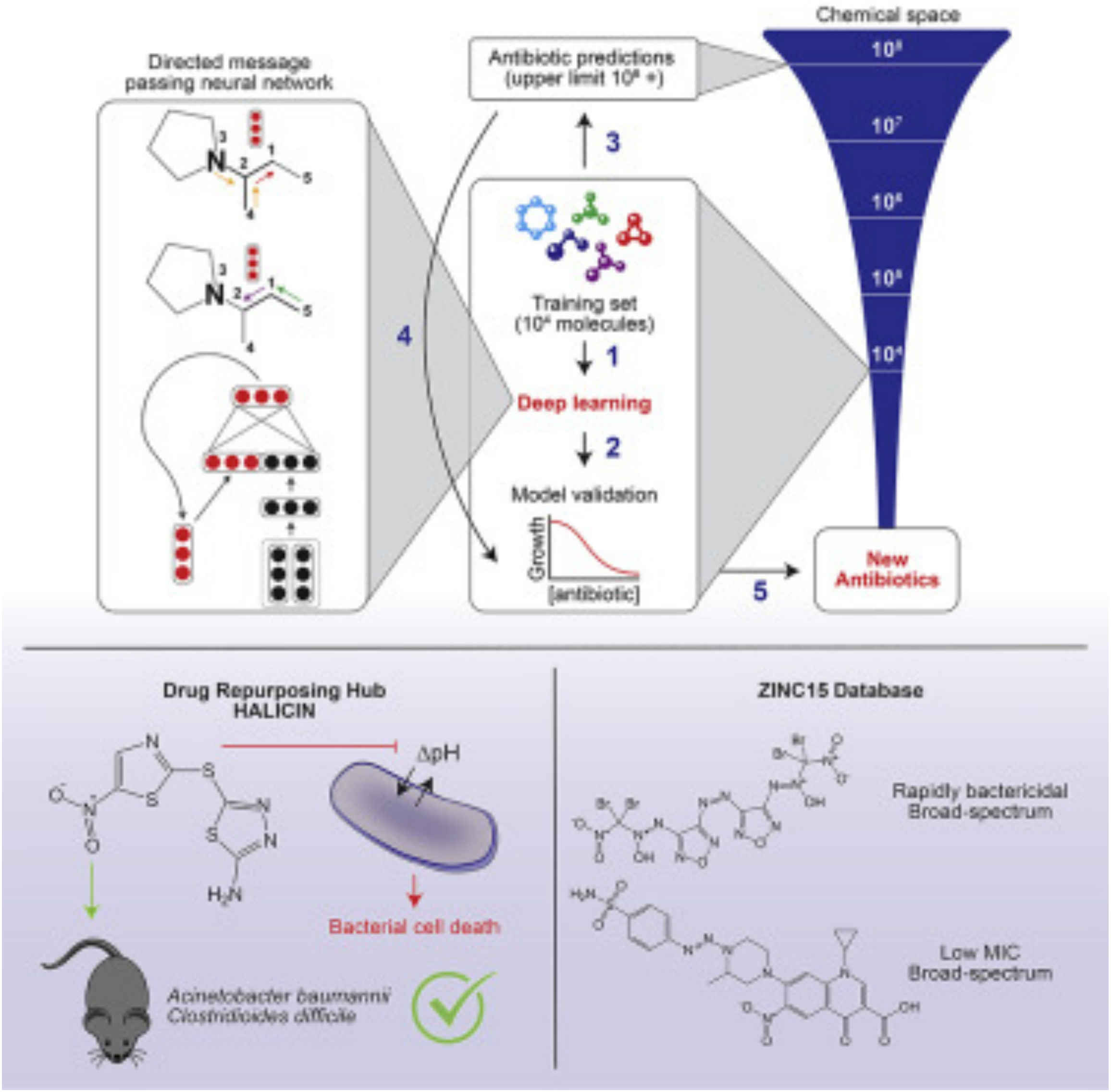
- Some examples:

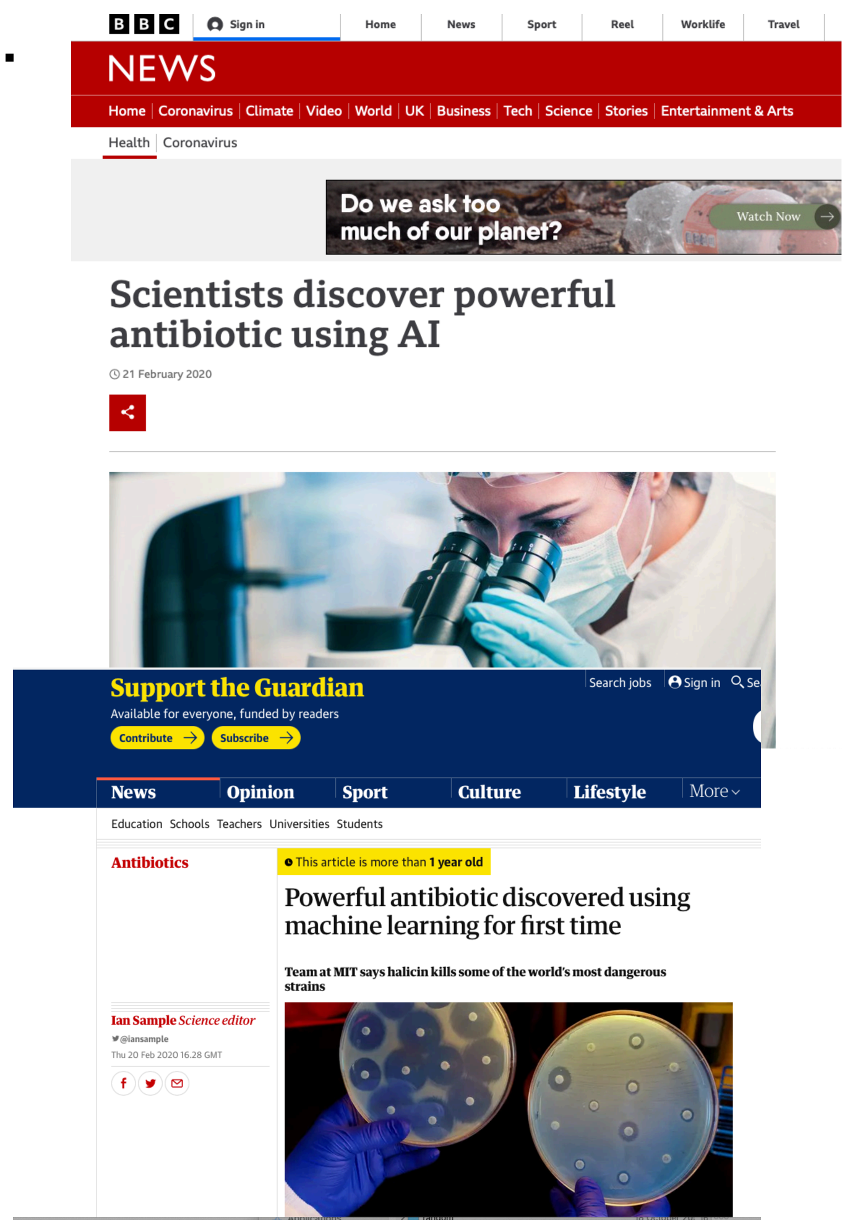
https://sites.google.com/view/learning-to-simulate

https://sites.google.com/view/meshgraphnets

Molecular graph generation

- Recent advances in antibiotic discovery …





[Simonovsky et al, 2017, De Cao et al 2018, Stokes et al 2020]

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- Applications
- **Open research questions**
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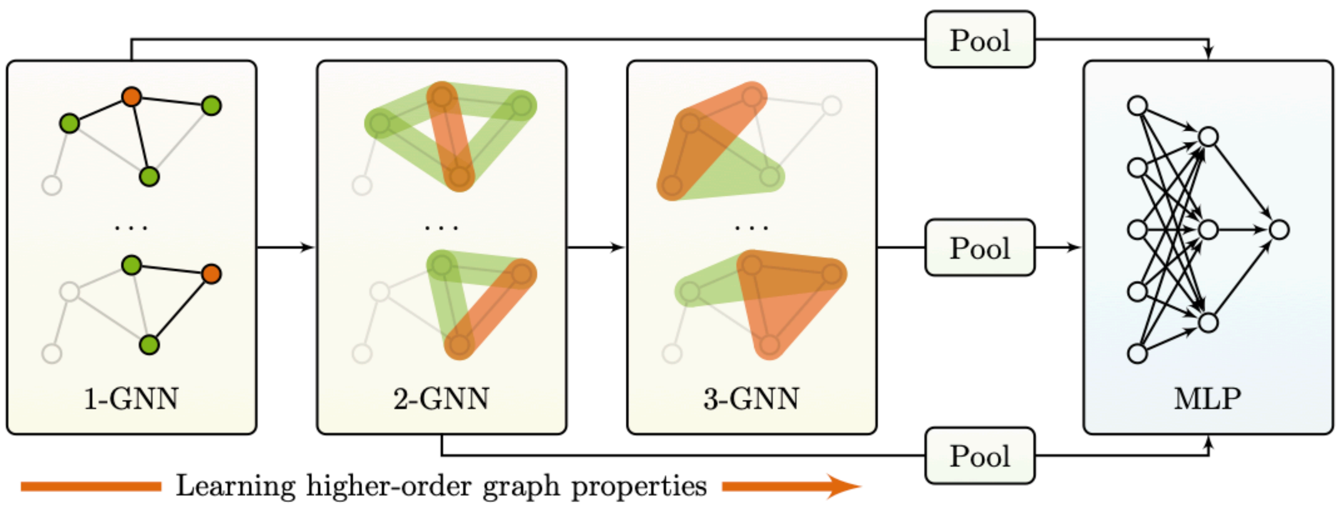
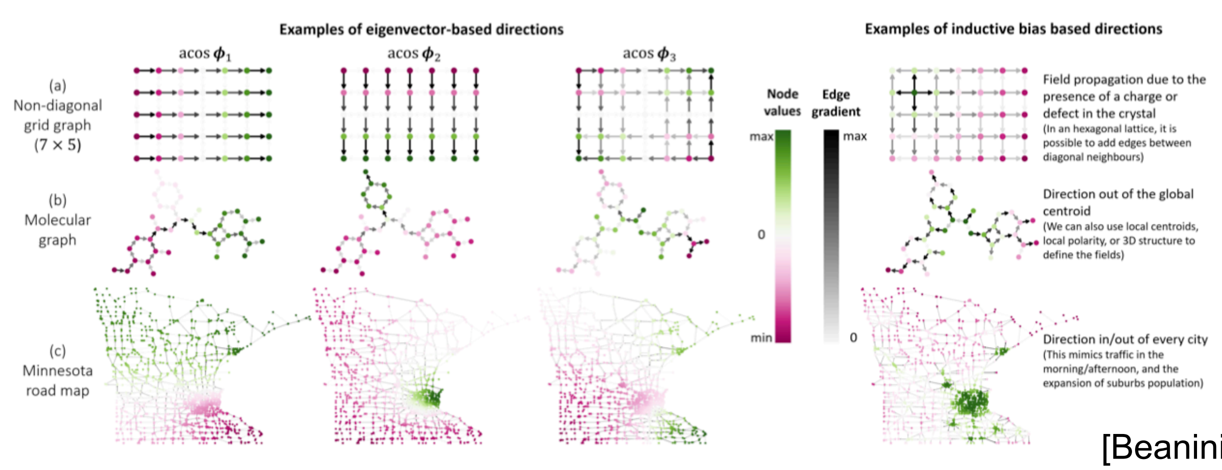
Towards more expressive GNNs

- How can we go beyond the message passing framework?
  - Higher order structures (simplicial /cell complexes)



[Morris et al., Weisfeiler and Leman Go Neural: Higher-Order Graph Neural Networks, AAAI 2019]

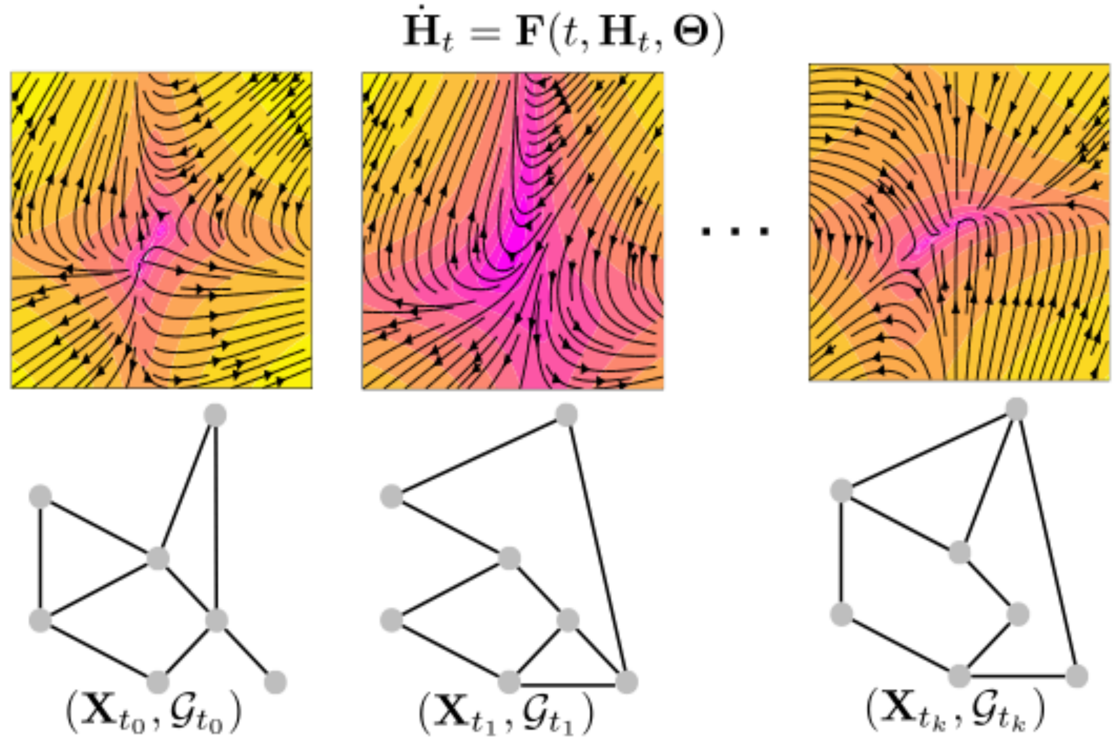
  - Use notions from spectral theory/graph signal processing



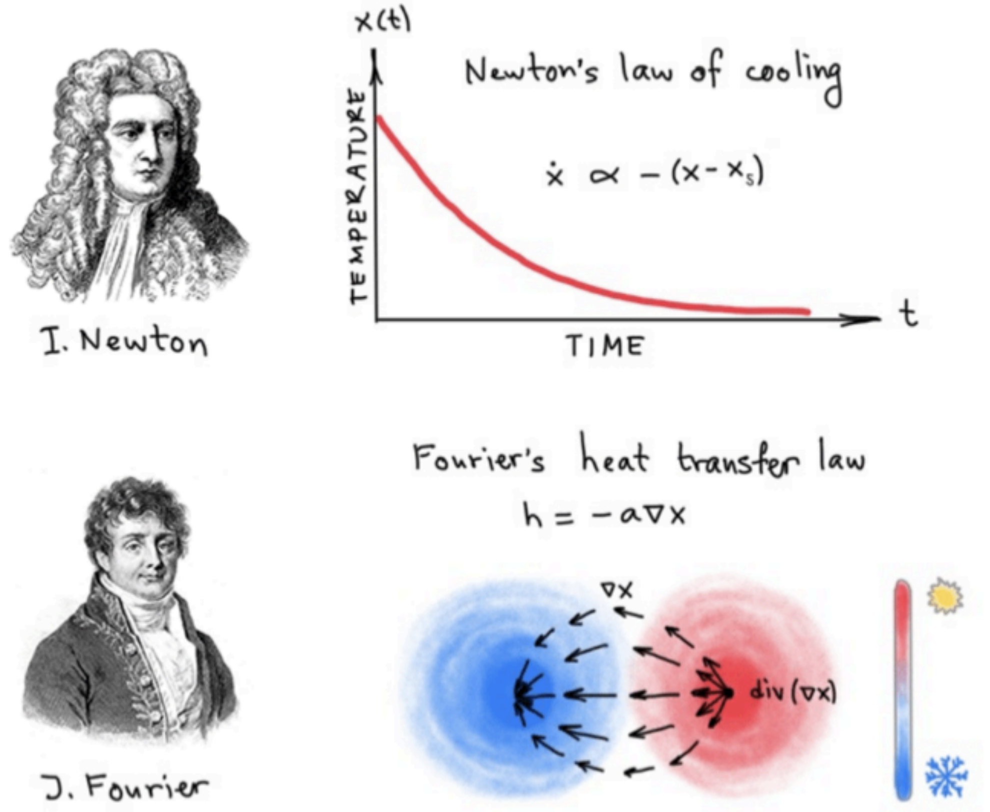
[Beanini et al., Directional graph networks, PMLR, 2021]

A neural PDE viewpoint of GNNs

- GNNs can be seen as discretised diffusion PDEs
  - Instead of several layers of message passing, we consider a continuous -time physical process
- Deep links to differential geometry



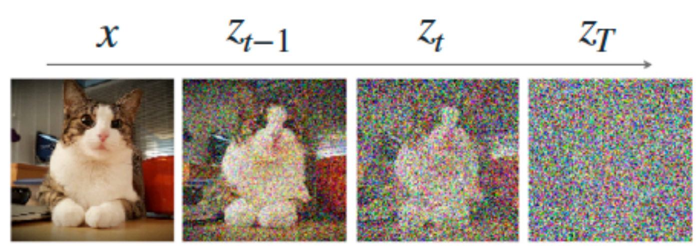
[Poli et al., Graph Neural Ordinary Differential Equations, AAAI 2021]



[Chamberlain et al., GRAND: Graph Neural Diffusion, NeurIPS 2021]

Generative models: denoising diffusion

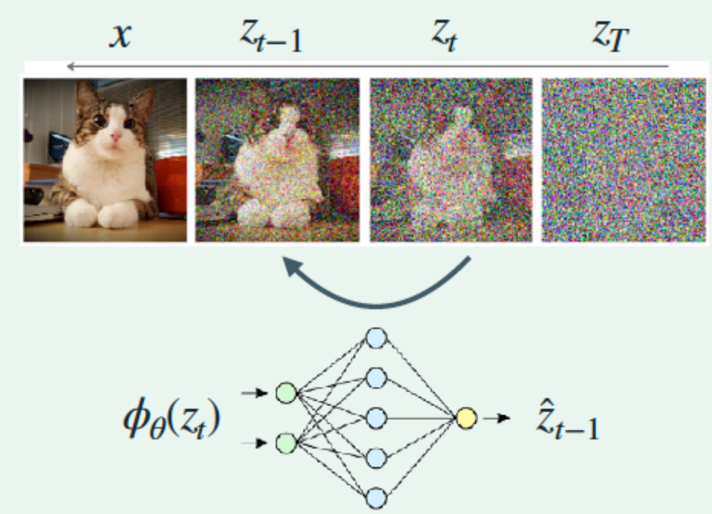
- Diffusion models have gained significant interest



$$q(z_1, \ldots, z_T \mid x) = q(z_1 \mid x) \prod_{t=2}^{T} q(z_t \mid z_{t-1})$$

Noise model

Generate **diffusion trajectories** by recursively adding noise to a data point.

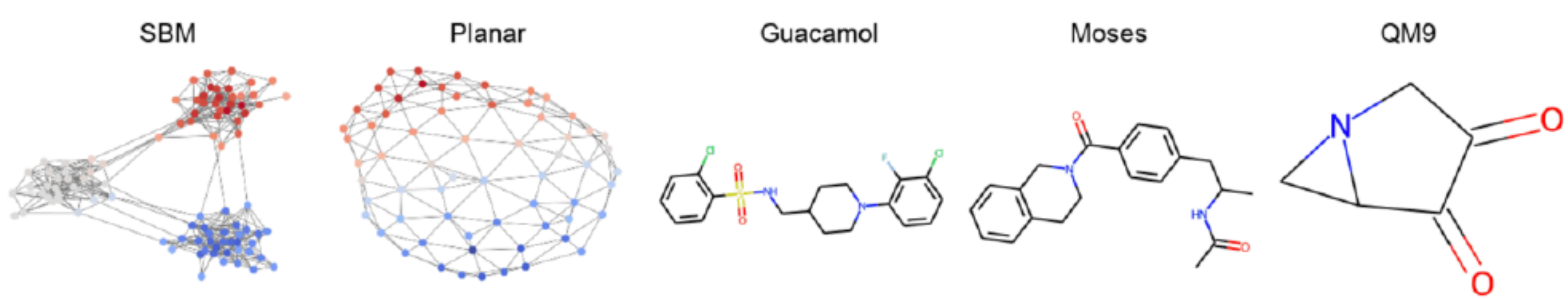


Denoising network

Train a network to predict the **inverse** diffusion iterations.

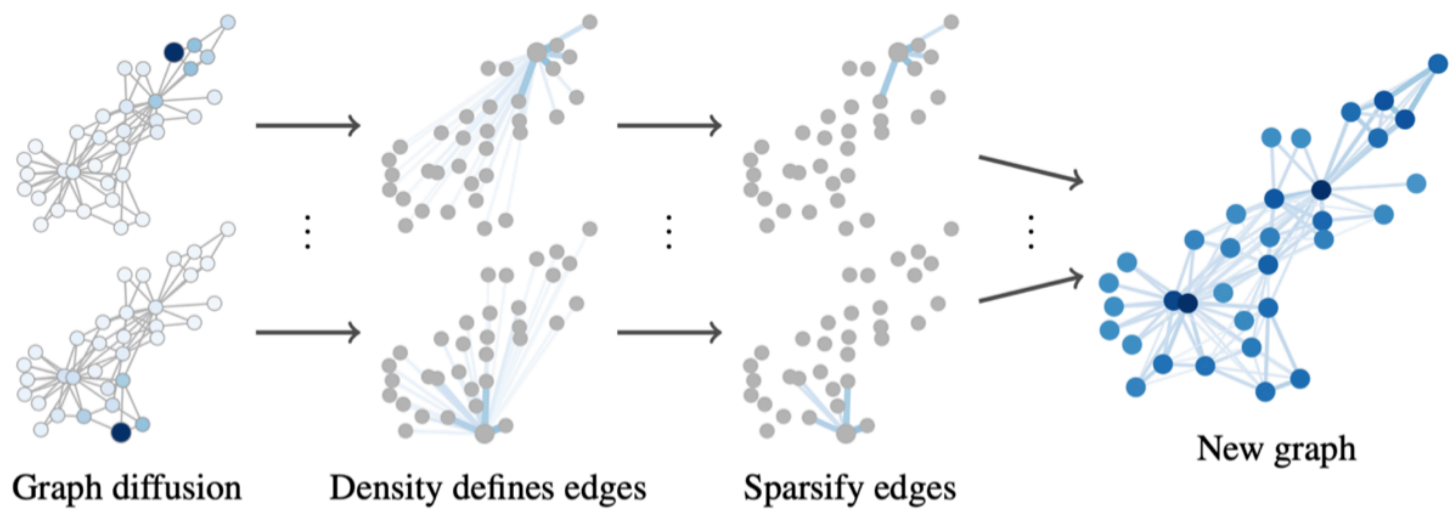
Generative models: denoising diffusion for molecules and proteins

- Diffusion models on graphs generate sets and graphs that look like the objects in a training set (e.g., DiGress, GeoDiff)
  - How can we improve performance (faster sampling, efficient solvers)
  - How can we achieve conditional generation?
  - How can we apply diffusion in real world applications (e.g., data augmentation)?



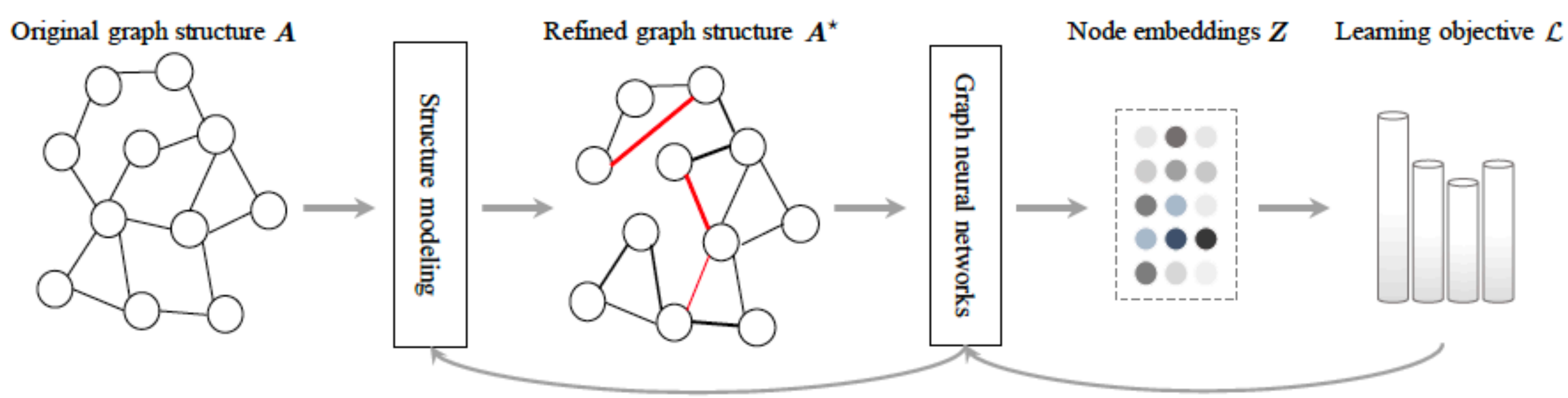
What is the right graph for my data?

- Graph rewiring: Data versus computational graph



[Gasteiger et al., Diffusion improves graph learning, NeurIPS 2019]

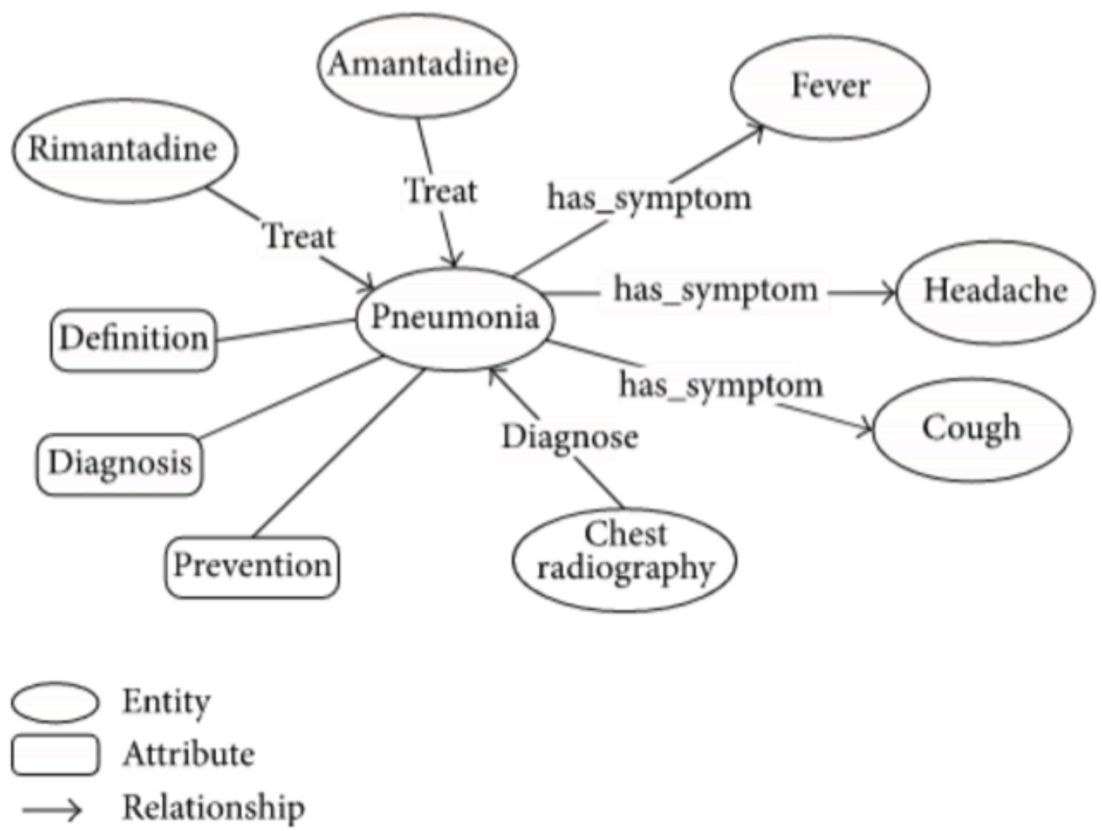
- Graph learning



[Zhu et al., Deep Graph Structure Learning for Robust Representations: A Survey, arXiv, 2021]

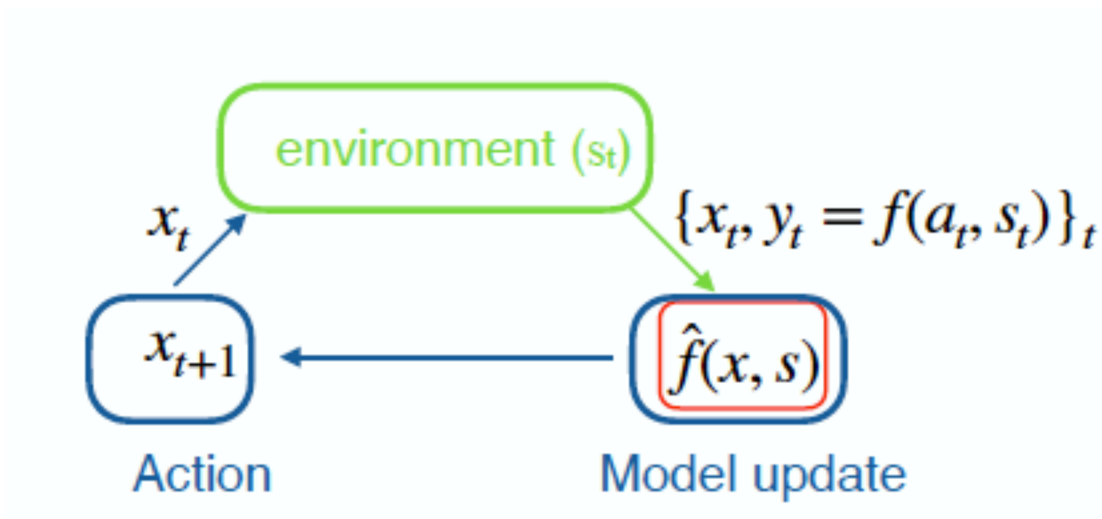
Knowledge graphs

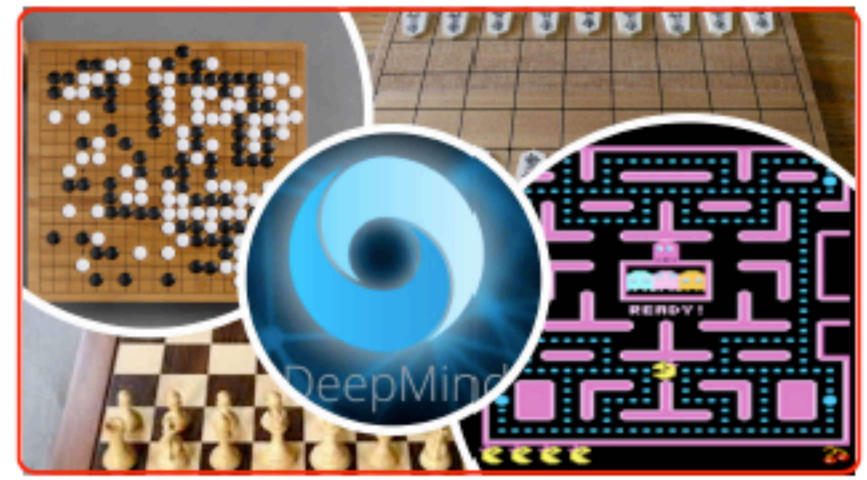
- Graphs often consist of nodes/edges of different types
- Reasoning and generalization in heterogenous graphs is an open question



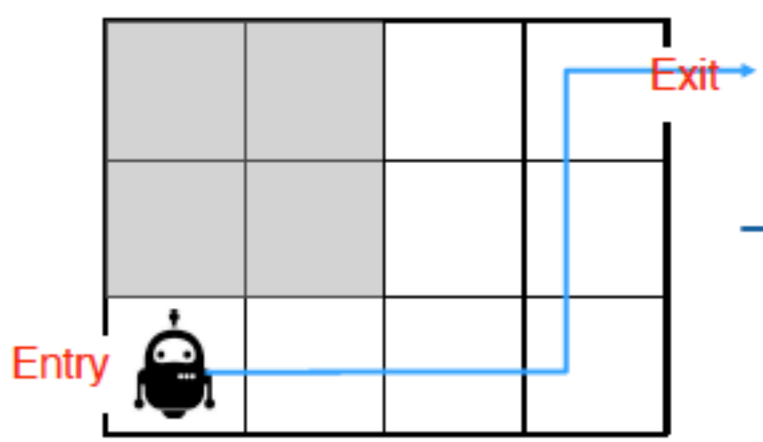
[Ji et al., A Survey on Knowledge Graphs: Representation, Acquisition and Applications, arXiv, 2021]

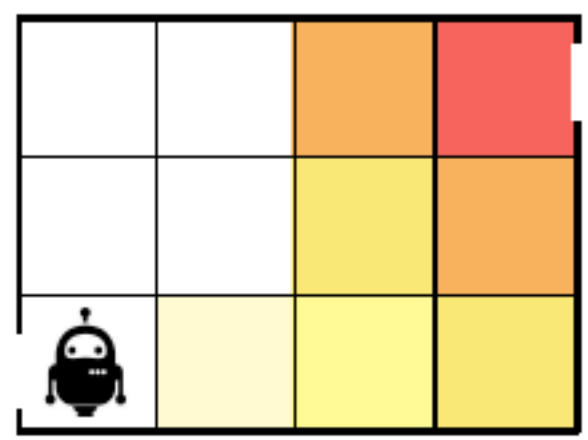
GNNs for Reinforcement Learning



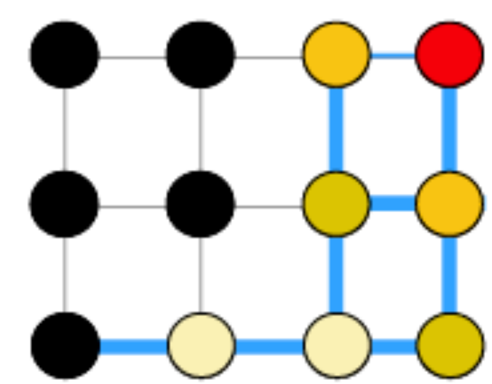


High-dimensional state-action space





Learning model / value function



Learning graph edge weights / signal on graph

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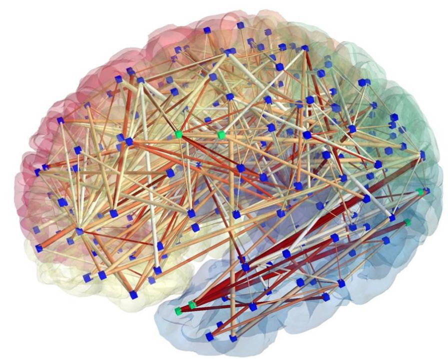
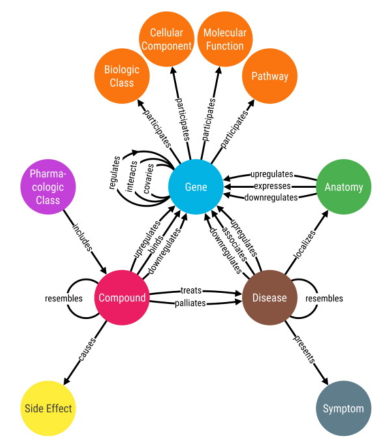
Network data is everywhere

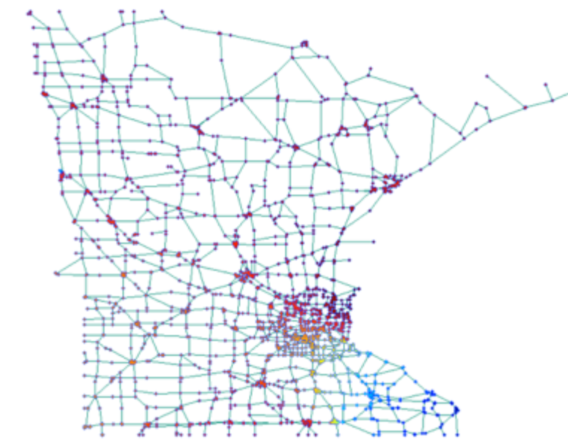
Social networks



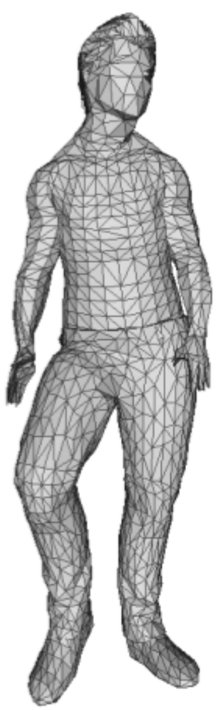
Biological networks



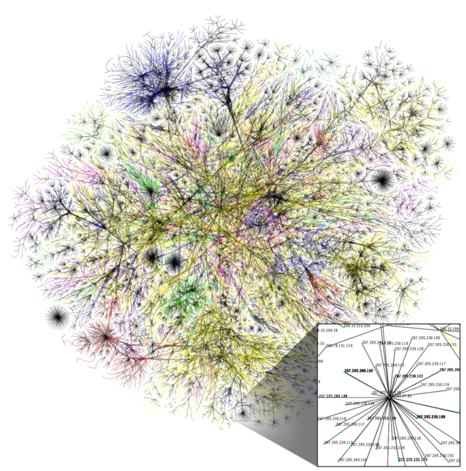
Knowledge graphs



Transportation networks

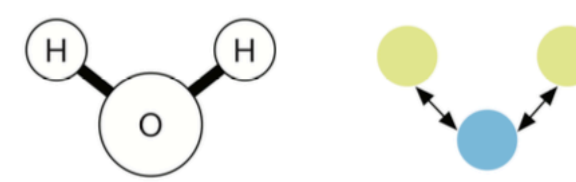


3D shapes



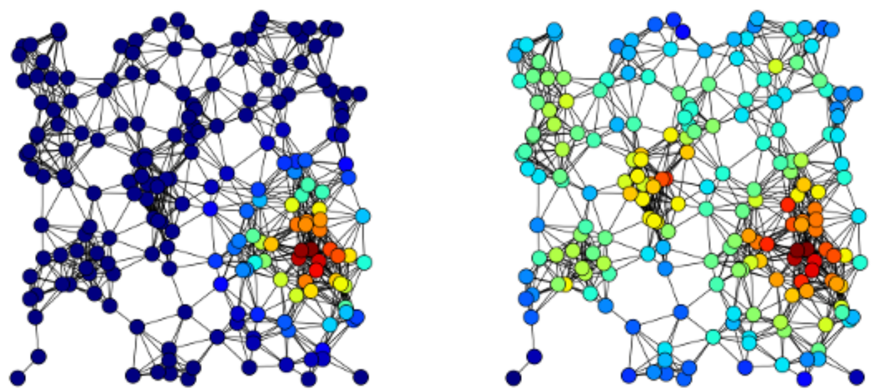
Communication networks

n-body system

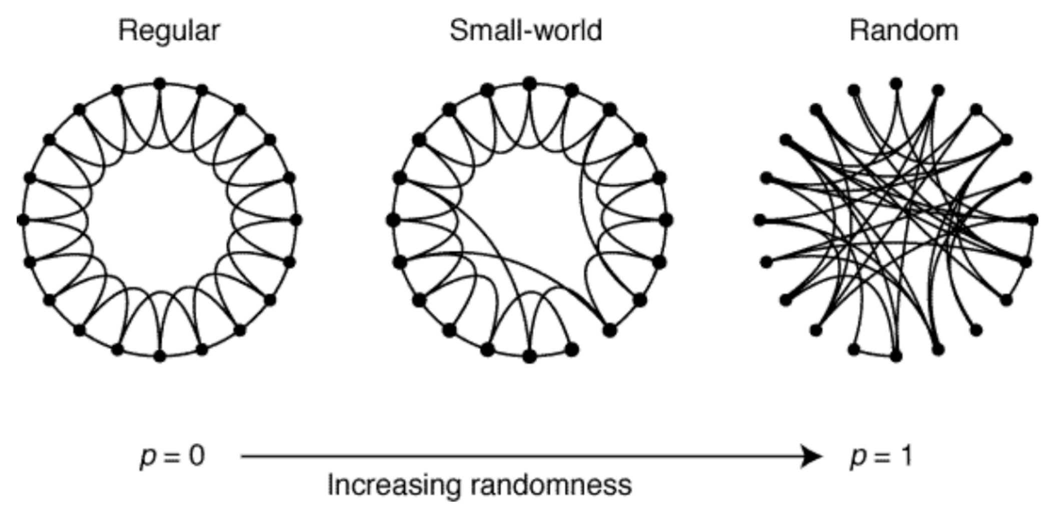


molecule

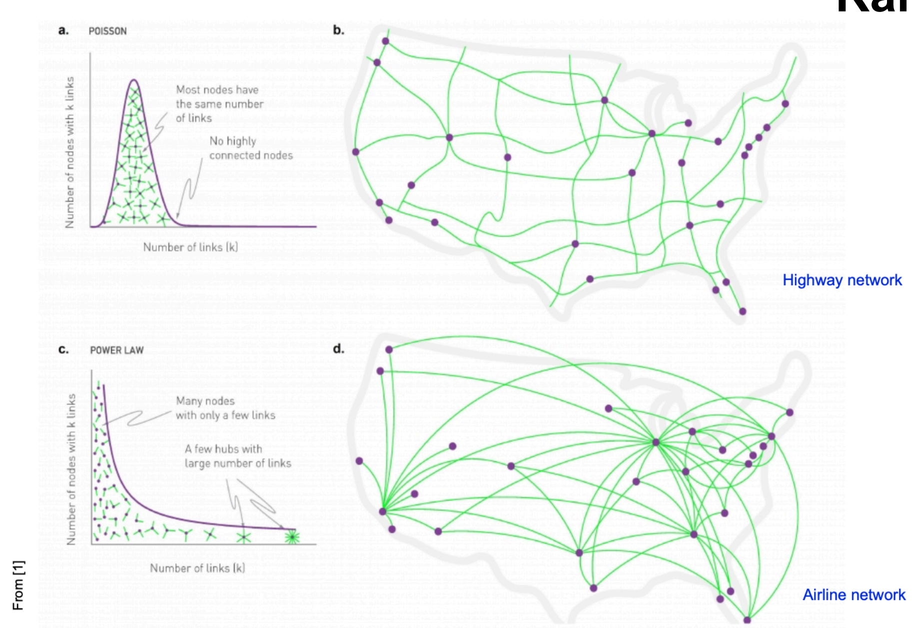
Wrap up: Network analysis



Node centrality



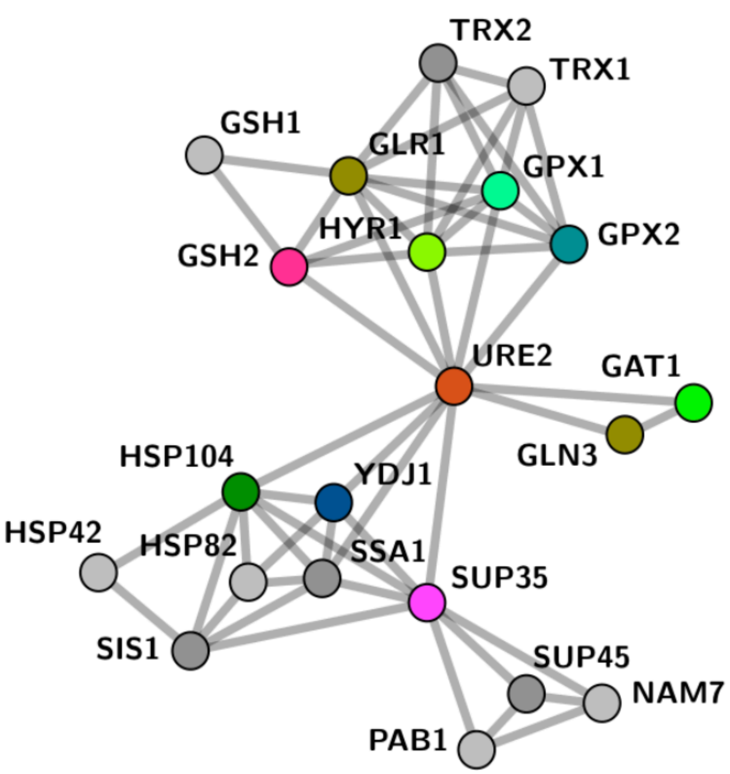
Random graph models



Random versus scale free models

Wrap up: Inference on networks

- How can we infer useful information from data that live on a network or graph?
  - Graphs could be weighted or unweighted
  - Nodes could have attributes



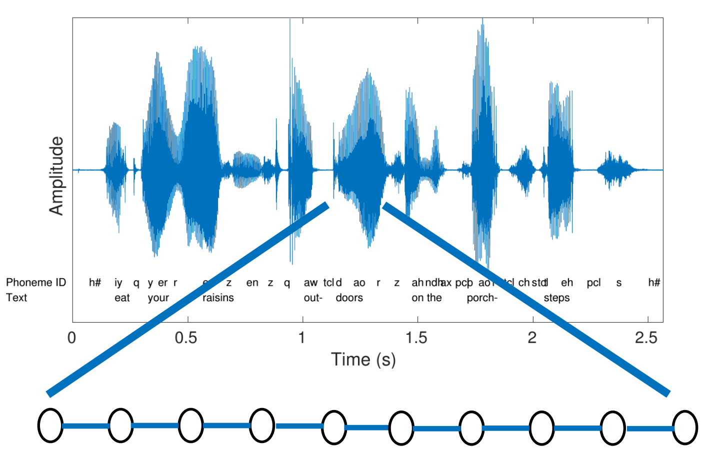
→ **Machine learning (ML)/ Signal processing (SP) on graphs** → **Actionable knowledge**

e.g., node/graph classification, signal inpainting/denoising

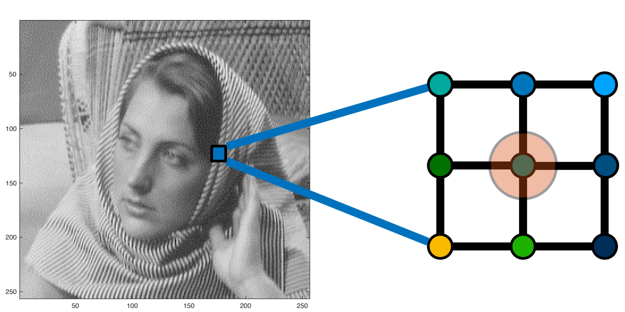
$$X, \mathcal{G} \rightarrow f(X, \mathcal{G}) \rightarrow Y$$

Why learning from graphs is hard?

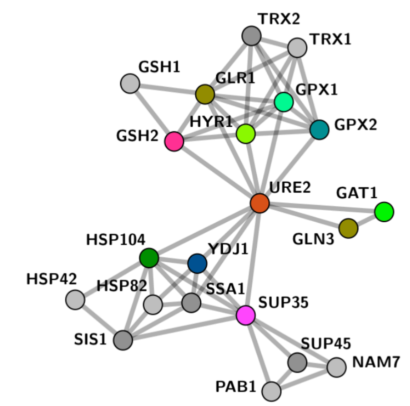
- Contrary to traditional modalities:
  - Graphs capture complex and irregular connections
  - There is no explicit notion of ordering
  - Nodes can have multiple attributes



Domain: line



Domain: grid



Domain: irregular graph

Graph-structured features/embeddings: A high level overview

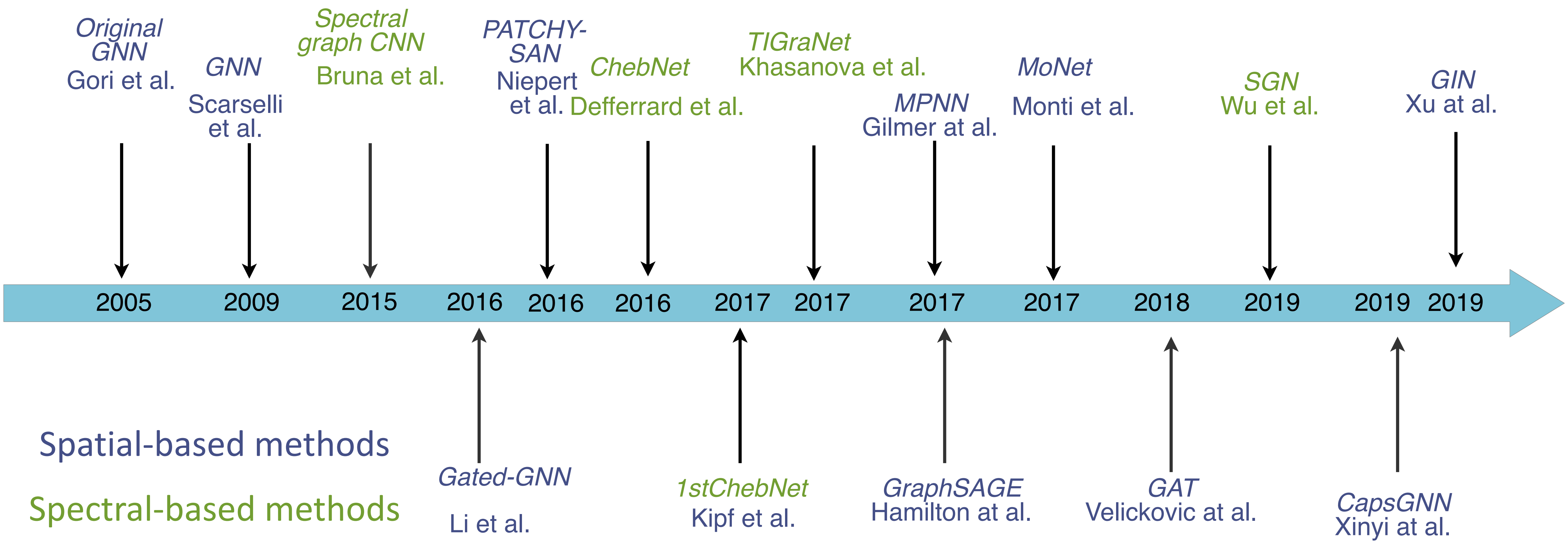
- **Hand-crafted features:** Capture some structural properties of the graph, followed by some statistics (signatures)
- **Graph kernel methods:** Design similarity functions in an embedding space
- **Spectral features:** Capture the graph properties through spectral graph theory

Model-driven

- **Learned features:** Learn graph features directly from data by designing models based on meaningful assumptions
  - **Unsupervised embeddings:** Learn features based on different ways of preserving information from the original graph (without node attributes)
  - **Graph neural network features:** Learn features from the data using a well-designed family of neural networks (with node attributes)

Data-driven

First GNN architectures



- Recent trends
  - Spectrally-inspired architectures: GraphHeat (Xu’19), GWNN (Xu’19), SIGN (Frasca’20), DGN (Beaini’20), Framelets (Zheng’21), FAGCN (Bo’21)
  - More expressive GNNs: higher order WL test (Maron’19, Morris’20), physics-inspired GNNs (Chamberlain’21), and many more!

Other topics

- Learning on dynamic graphs
- Learning connectivity matrix
- Self-supervised learning
- Applications
- Open challenges

Today's lecture

- A glimpse of geometric deep learning
- Applications
- Open research questions
- **Feedback on the class**

Suggestions for next year?

- Class material
- Assignments/Labs
- Organisational aspects
- Anything else….

Please share your thoughts with us!

Thank you!