Deep Learning for Graphs - Fundamentals

Generative and Deep Learning (GDL)

Davide Bacciu (davide.bacciu@unipi.it)

IN SUPREMÆ DIGNITATIS 1343
UNIVERSITÀ DI PISA

Lecture Outline

- Motivations
- Formalization of the learning task: graph prediction, induction, transduction and generation
- Historical perspective: contractive and contextual models
- A view on modern deep learning for graphs
  - Convolutional, feedforward, recurrent and attention-based approaches

Introduction

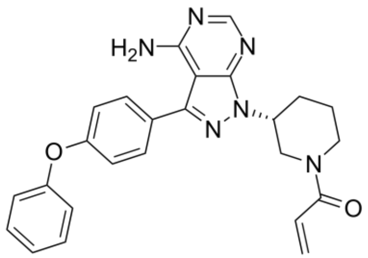
Why graphs?

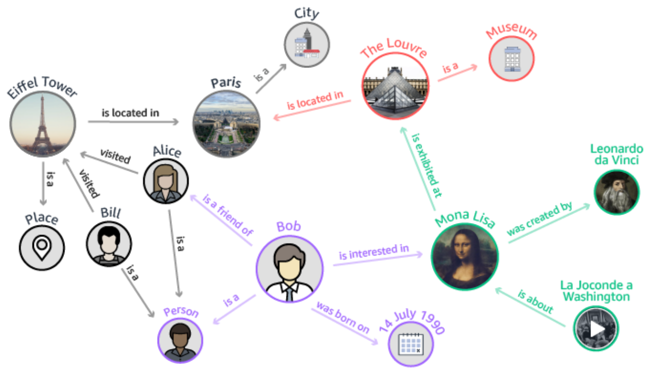
Why graphs?

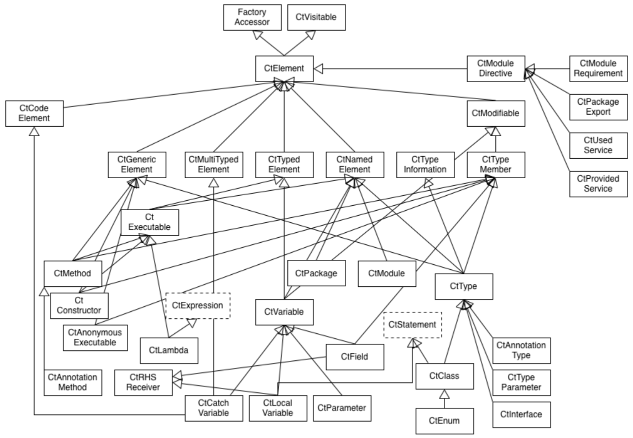
Context is fundamental for the correct interpretation of information

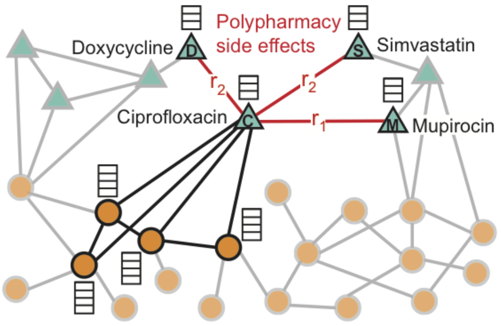
...well also for the plenty of applications

- Chemistry & Physics
- Knowledge graphs
- (Bio/social) networks
- Recommender systems
- Point clouds
- Code & ICT systems







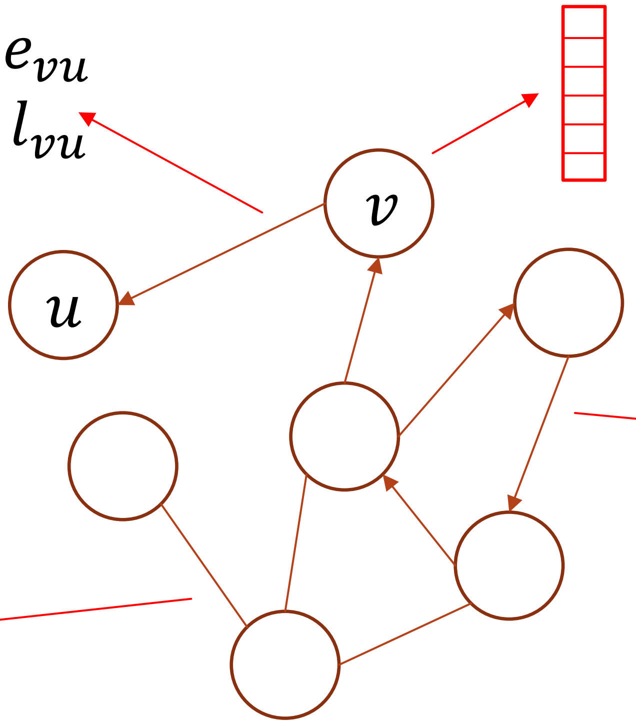


Graph Structured Data

Oriented edge/arc e_{vu}
possibly with label l_{vu}

Vectorial node label
x_v

Node/vertex u



Cycle

Undirected edge

Structures are useful because allow to represent relationships in the data

A Nomenclature Nightmare

Neural networks for graphs

Deep learning for graphs

CNN for/on graphs

Graph neural networks

Deep Graph Networks

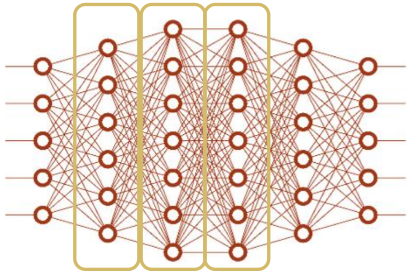
Graph CNN

Learning graph/node embedding

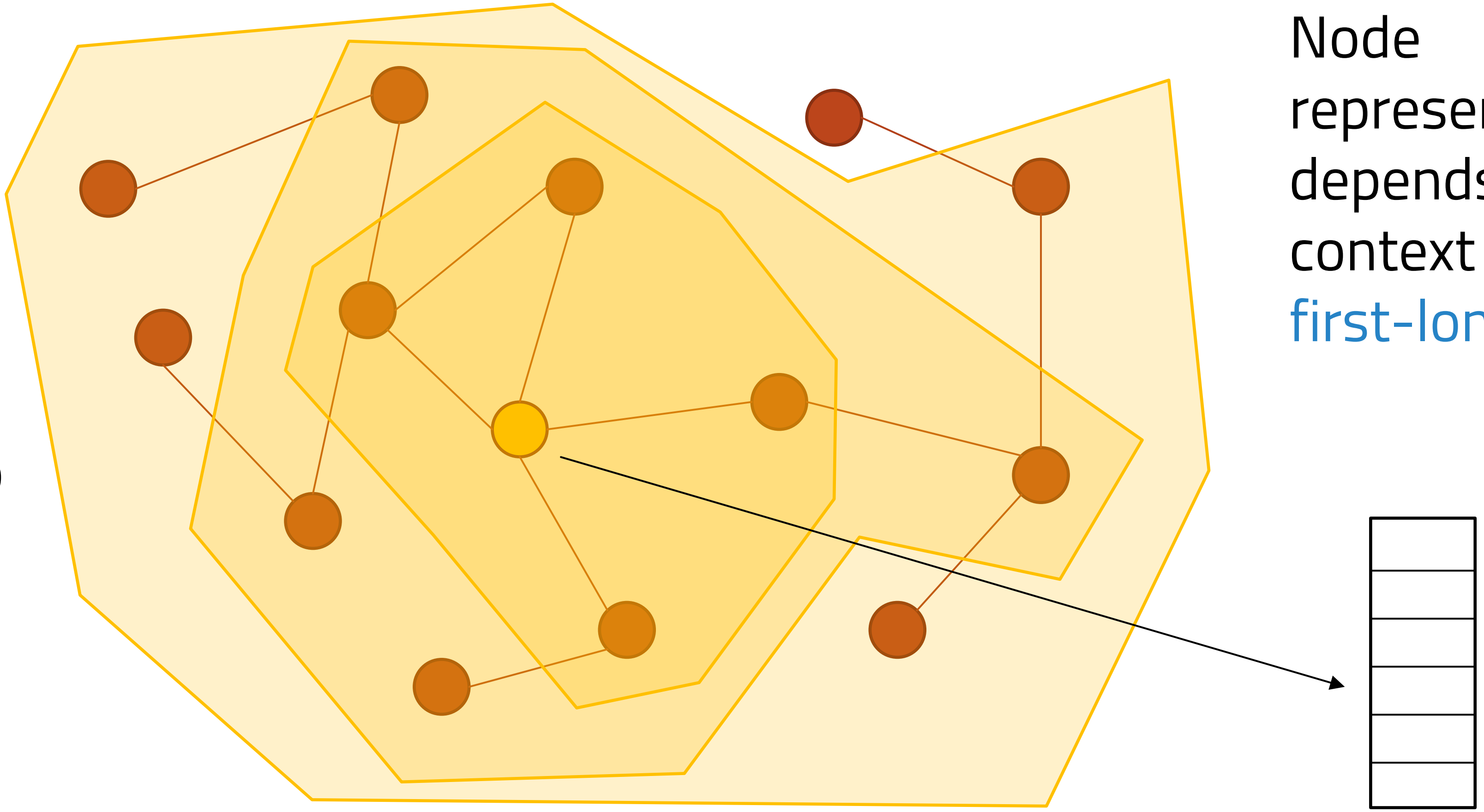
Geometric deep learning

Graph Convolutional Networks

Deep Learning with graphs

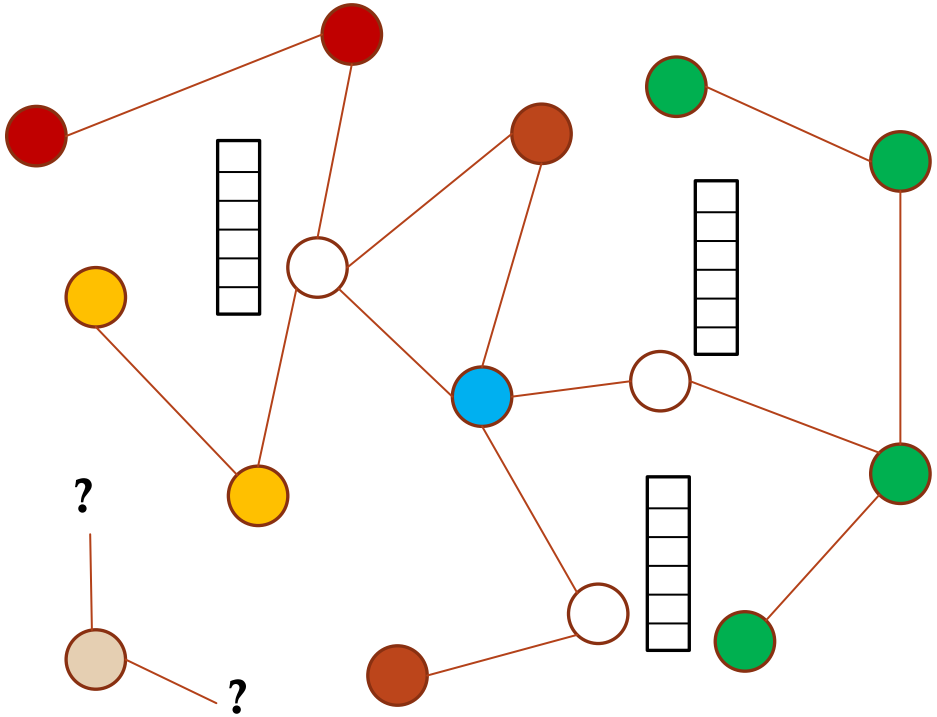


Hierarchical representation learning allows to efficiently diffuse information through graph structure



Node representation depends on its context (shorter first-longer later)

Predictive Tasks – Network data

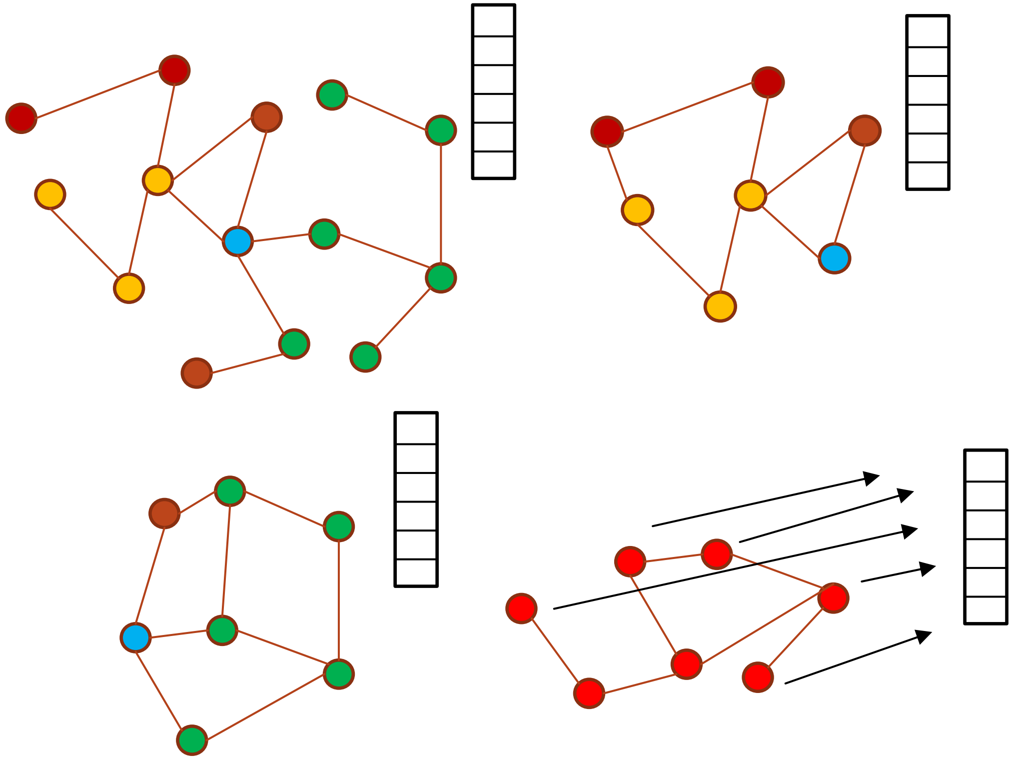


Node predictions
Predict a type or a continuous value for a given node

Link prediction
Predict whether two nodes are linked

Community/module detection
Identify clusters of linked nodes that are alike

Predictive Tasks – Graph Level



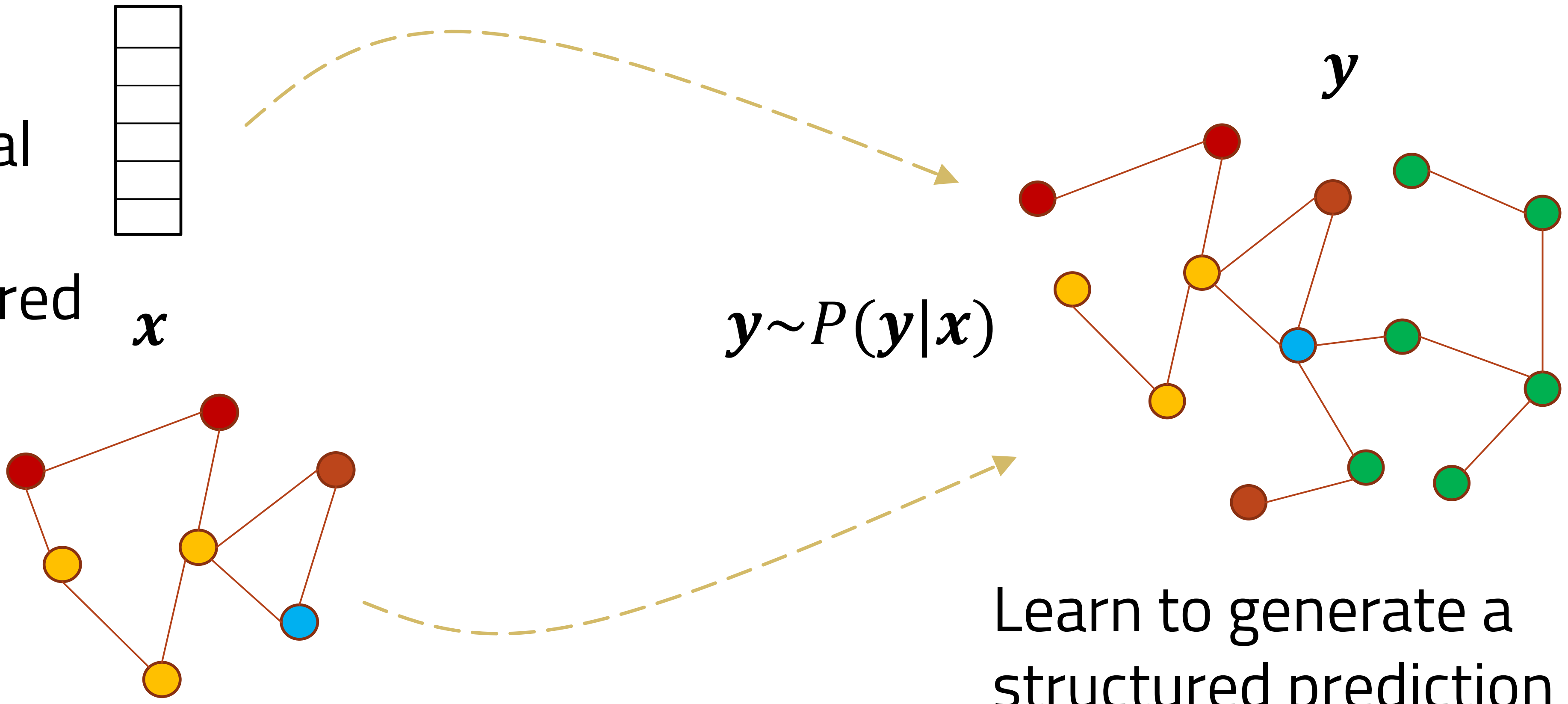
A dataset of i.i.d graphs

Graph classification
Assign whole structure to a specific class

Graph regression
Regress a structure to a value (or a vector of values)

Transductive tasks

Given a vectorial and/or structured input



Learn to generate a structured prediction

An Hystorical (and Geographical) Perspective

Early neural network approaches to deal with cyclic graphs of varying topology date back to 2005-2009

(Sperduti & Starita, TNN 1997)

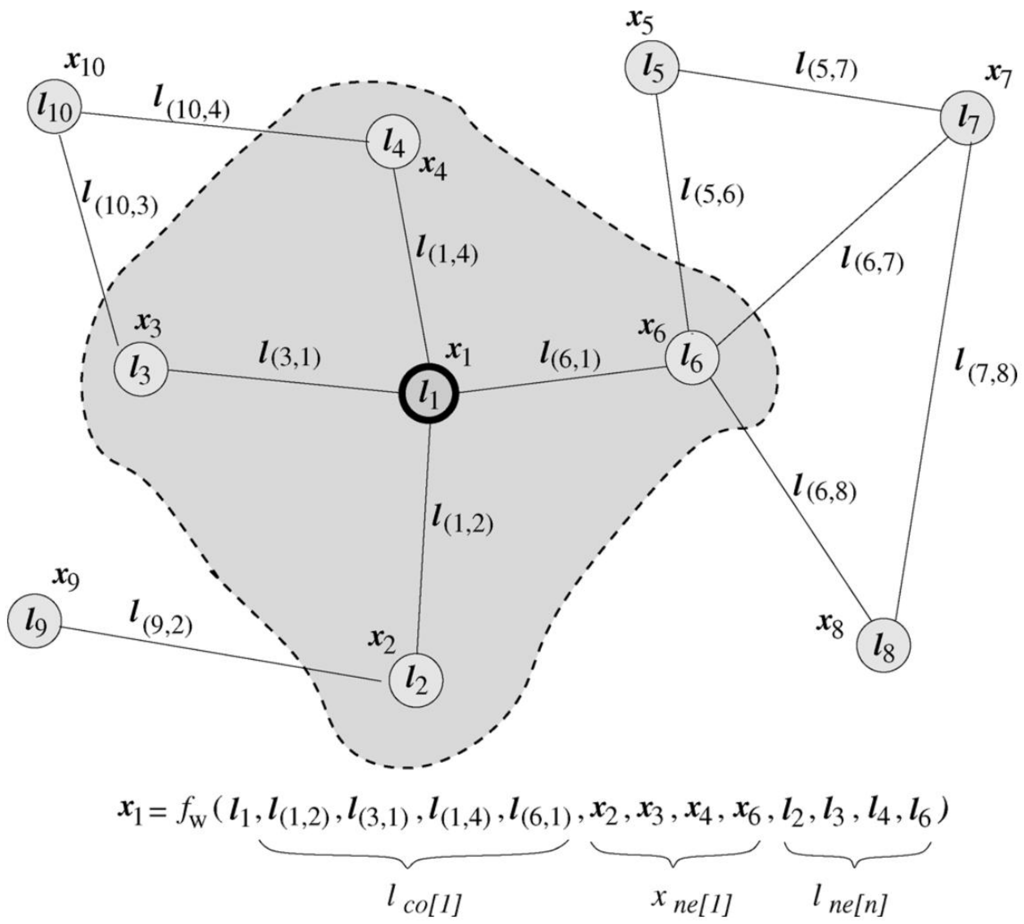
A. Micheli, TNN 2009

UNIVERSITÀ DI PISA

Scarselli et al, TNN 2009

UNIVERSITÀ DI SIENA 1240

Contractive - Graph Neural Networks (GNN)

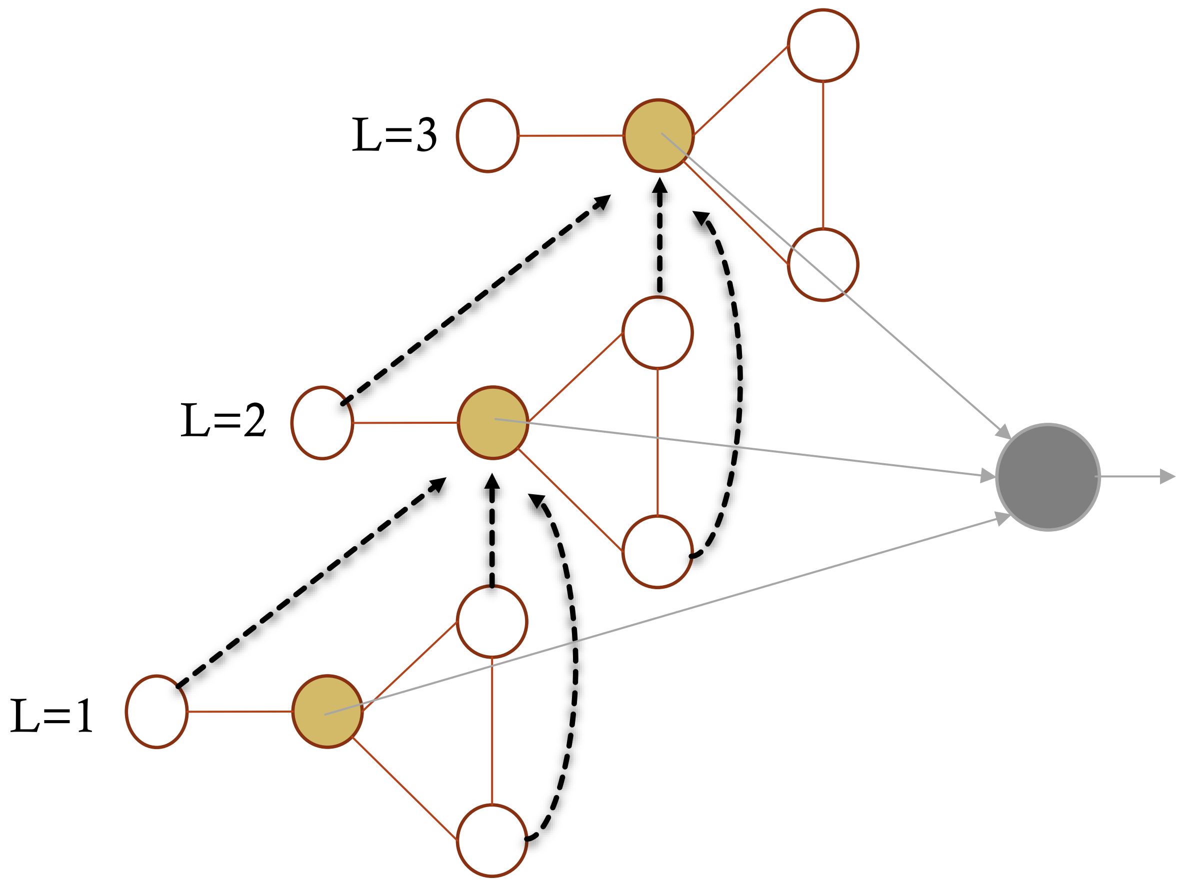


- Extend the Recurrent/Recursive Neural Network approach to cyclic graphs
- Handle loops through fixed points
- Impose dynamic weight constraints to yield a contractive state mapping

Scarselli et al, TNN 2009

https://sailab.diism.unisi.it/gnn/

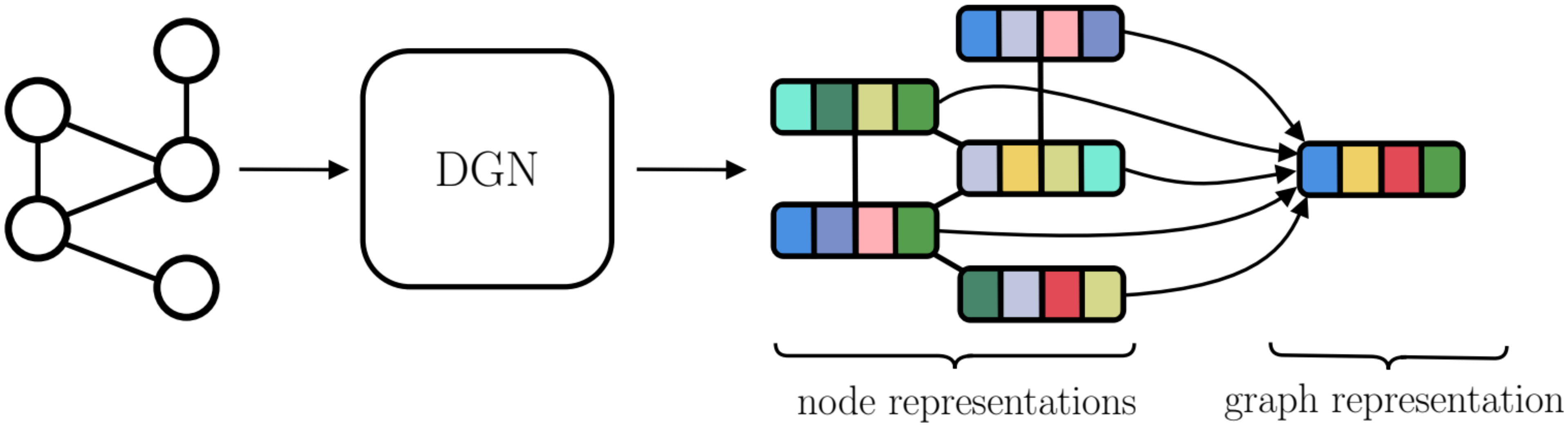
Contextual - Neural Networks for Graphs (NN4G)



- A feedforward approach to process graphs
- Handle loops through layering
- Uses context from frozen earlier layers compute the state on the node at current layer
- Layerwise training

A. Micheli, TNN 2009

Deep Graph Networks



- Encode vertices and the graph itself into a vector space by means of an adaptive (learnable) mapping
- Use the learned encodings to solve predictive and explorative tasks

A Survey of Recent Approaches

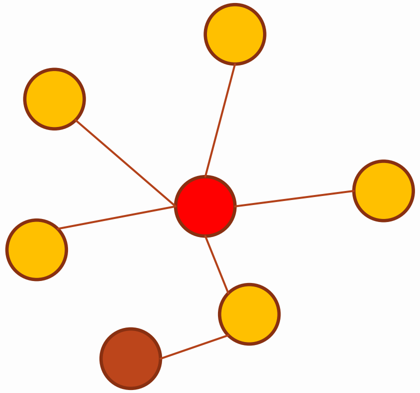
- Convolutional Neural Networks for Graphs
  - Spectral
  - Spatial
- Message Passing Graph Processing
  - The message passing paradigm
  - Overview of relevant feedforward approaches
- Graph reduction
- Recurrent (randomized) graph processing
- Attention-based graph processing (Graph Transformers)

Convolutional Neural Networks for Graphs

How to Perform Convolutions on Graphs?

Spatial DOMAIN

- What is the equivalent of sliding a kernel to aggregate local spatial information?



Spectral DOMAIN

$$\mathcal{F}(f * g) = \mathcal{F}(f) \times \mathcal{F}(g)$$

- Exploit the Convolution Theorem and Fourier analysis to perform convolutions in the spectral domain
- Decompose a function f as a combination of vectors $\boldsymbol{e}_k$ from an orthonormal basis

Spectral Graph Convolution in 1 Slide

- Given a graph G, the eigendecomposition of its Laplacian provides an orthonormal basis U which allow to compute the graph convolution of its node signals $\boldsymbol{f}$ with a filter

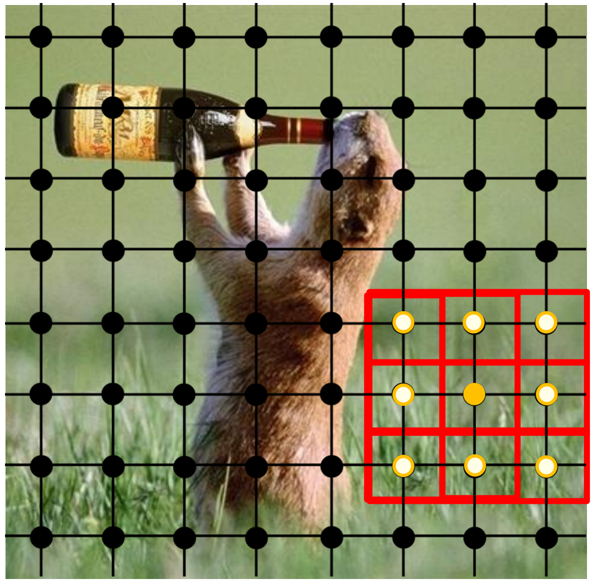
$$(\boldsymbol{f} *_G \boldsymbol{g}) = \mathcal{F}^{-1}\big(\mathcal{F}(\boldsymbol{f})\,\mathcal{F}(\boldsymbol{g})\big) = U\mathbf{W}(\lambda)U^T\boldsymbol{f}$$

Convolutional filter **g** in spectral domain

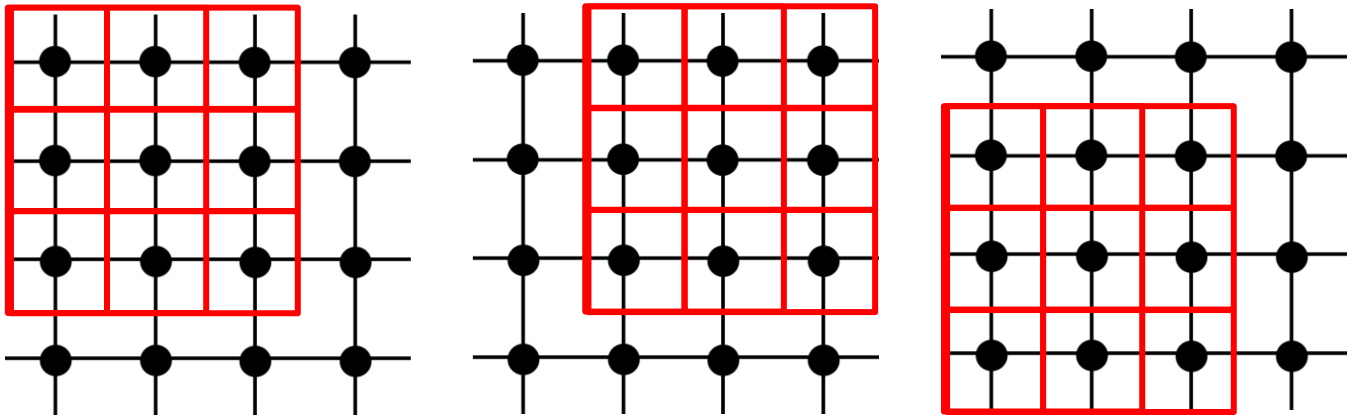
Graph equivalent of the learnable CNN filter matrix **W**

Spectral convolution matrix **W** contains information on the graph Laplacian

A Graph View on (Image) Convolutions



Visual convolutions are graph convolutions on a regular grid

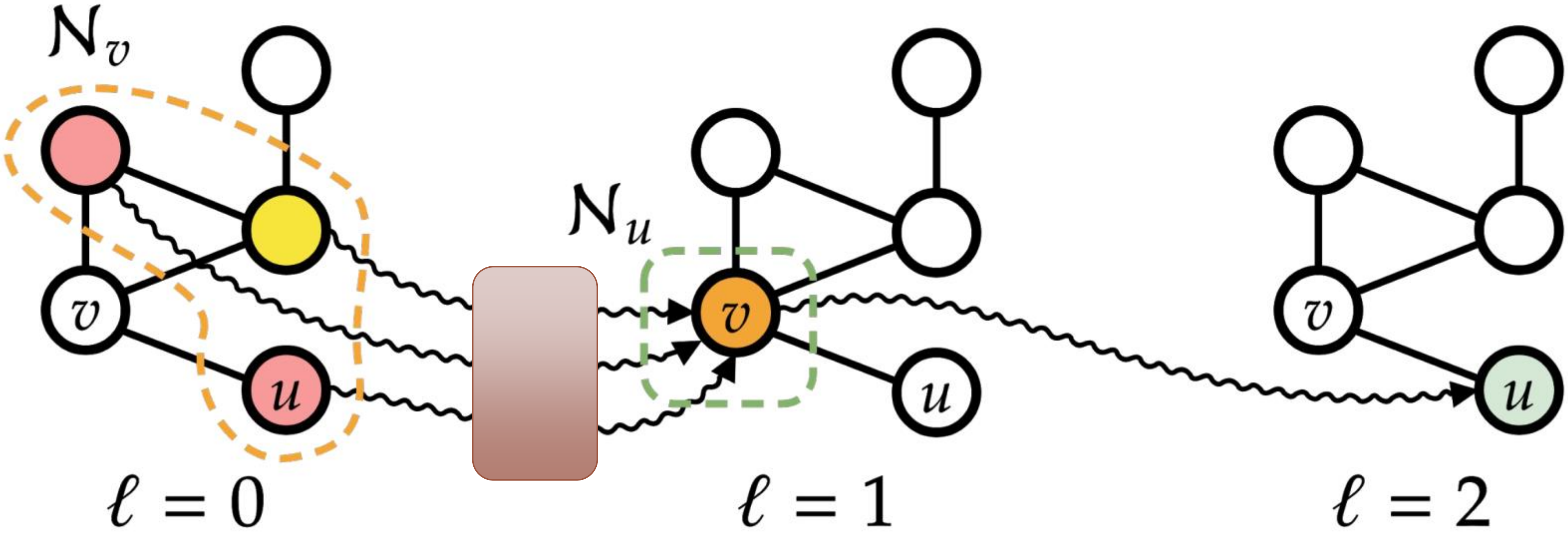


Plus some key assumptions which make it difficult to directly apply them to graphs

- Regular neighborhood
- Existence of a total node ordering

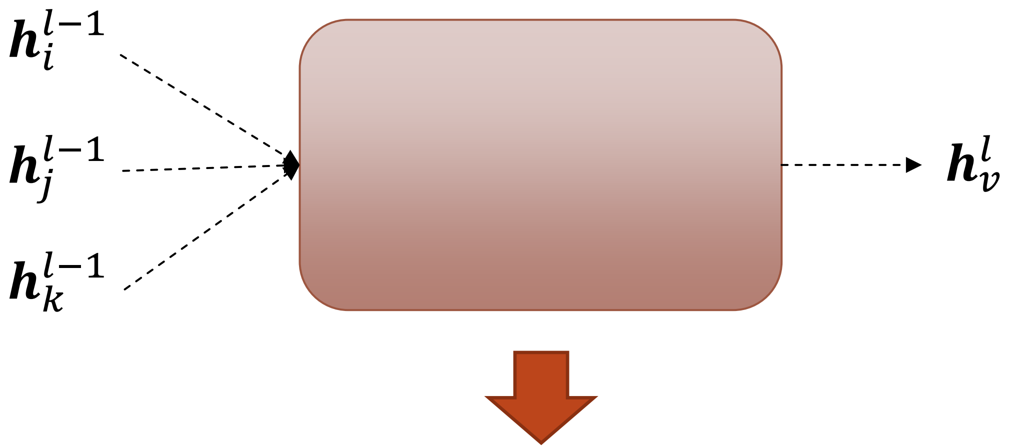
Message Passing Graph Processing

Neighborhood Aggregation & Layering



What is inside of the Box?

A learning model of course (e.g. a neural network) including an aggregation function to handle size-varying neighborhoods



A simple model

$$\boldsymbol{h}_v^{l} = \sigma\left(\boldsymbol{W}_l AGG\left(\left\{\boldsymbol{h}_i^{l-1} : i \in N(v)\right\}\right), \widehat{\boldsymbol{W}}_l \boldsymbol{h}_v^{l-1}\right)$$

The graph convolutional layer

$$\underbrace{\mathbf{h}_v^{\ell+1}}_{\text{state}} = \overbrace{\phi^{\ell+1}}^{\text{MLP/Linear}}\Big(\mathbf{h}_v^{\ell},\ \underbrace{\Psi}_{\text{perm. invariant function}}(\{\overbrace{\psi^{\ell+1}}^{\text{MLP/Linear}}(\mathbf{h}_u^{\ell}) \mid u \in \mathcal{N}_v\})\Big)$$

MLP/Linear

MLP/Linear

state

perm. invariant function

Variants/extensions:

- Edge-aware convolution
- Attention over neighbours
- Laplacian-normalized

Model	Neighborhood Aggregation $\mathbf{h}_v^{\ell+1}$
NN4G [88]	$\sigma\Big(\mathbf{w}^{\ell+1^T}\mathbf{x}_v + \sum_{i=0}^{\ell}\sum_{c_k\in\mathcal{C}}\sum_{u\in\mathcal{N}_v^{c_k}} w_{c_k}^i * \mathbf{h}_u^i\Big)$
GNN [104]	$\sum_{u\in\mathcal{N}_v} MLP^{\ell+1}\Big(\mathbf{x}_u, \mathbf{x}_v, \mathbf{a}_{uv}, \mathbf{h}_u^{\ell}\Big)$
GraphESN [44]	$\sigma\Big(\mathbf{W}^{\ell+1}\mathbf{x}_u + \hat{\mathbf{W}}^{\ell+1}[\mathbf{h}_{u_1}^{\ell}, \dots, \mathbf{h}_{u_{\mathcal{N}_v}}^{\ell}]\Big)$
GCN [72]	$\sigma\Big(\mathbf{W}^{\ell+1}\sum_{u\in\mathcal{N}(v)}\mathbf{L}_{vu}\mathbf{h}_u^{\ell}\Big)$
GAT [120]	$\sigma\Big(\sum_{u\in\mathcal{N}_v}\alpha_{uv}^{\ell+1} * \mathbf{W}^{\ell+1}\mathbf{h}_u\Big)$
ECC [111]	$\sigma\Big(\frac{1}{\lvert\mathcal{N}_v\rvert}\sum_{u\in\mathcal{N}_v} MLP^{\ell+1}(\mathbf{a}_{uv})^T\mathbf{h}_u^{\ell}\Big)$
R-GCN [105]	$\sigma\Big(\sum_{c_k\in\mathcal{C}}\sum_{u\in\mathcal{N}_v^{c_k}}\frac{1}{\lvert\mathcal{N}_v^{c_k}\rvert}\mathbf{W}_{c_k}^{\ell+1}\mathbf{h}_u^{\ell} + \mathbf{W}^{\ell+1}\mathbf{h}_v^{\ell}\Big)$
GraphSAGE [54]	$\sigma\Big(\mathbf{W}^{\ell+1}(\frac{1}{\lvert\mathcal{N}_v\rvert}[\mathbf{h}_v^{\ell}, \sum_{u\in\mathcal{N}_v}\mathbf{h}_u^{\ell}])\Big)$
CGMM [3]	$\sum_{i=0}^{\ell} w^i * \Big(\sum_{c_k\in\mathcal{C}} w_{c_k}^i * (\frac{1}{\lvert\mathcal{N}_v^{c_k}\rvert}\sum_{u\in\mathcal{N}_v^{c_k}}\mathbf{h}_u^i)\Big)$
GIN [131]	$MLP^{\ell+1}\Big((1+\epsilon^{\ell+1})\mathbf{h}_v^{\ell} + \sum_{u\in\mathcal{N}_v}\mathbf{h}_u^{\ell}\Big)$

A Message-Passing view on Deep Graph Networks

Algorithm 13.1: Simple message-passing neural network

Input: Undirected graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$
Initial node embeddings $\{\mathbf{h}_n^{(0)} = \mathbf{x}_n\}$
$\mathrm{Aggregate}(\cdot)$ function
$\mathrm{Update}(\cdot, \cdot)$ function

Output: Final node embeddings $\{\mathbf{h}_n^{(L)}\}$

```
// Iterative message-passing
```

for $l \in \{0, \ldots, L-1\}$ **do**

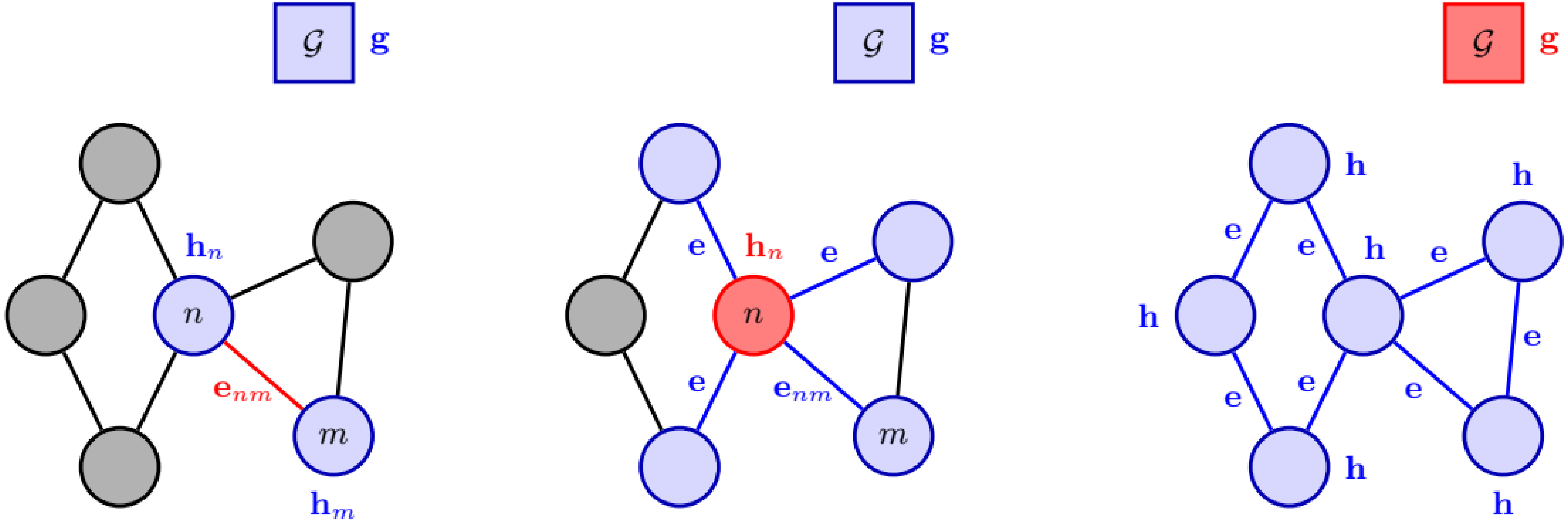
$\quad \mathbf{z}_n^{(l)} \leftarrow \mathrm{Aggregate}\left(\left\{\mathbf{h}_m^{(l)} : m \in \mathcal{N}(n)\right\}\right)$

$\quad \mathbf{h}_n^{(l+1)} \leftarrow \mathrm{Update}\left(\mathbf{h}_n^{(l)}, \mathbf{z}_n^{(l)}\right)$

end for

return $\{\mathbf{h}_n^{(L)}\}$

Different kinds of message-passing updates



Edge **Node** **Graph**

Graph Isomorphism Network (a.k.a. sum is better)

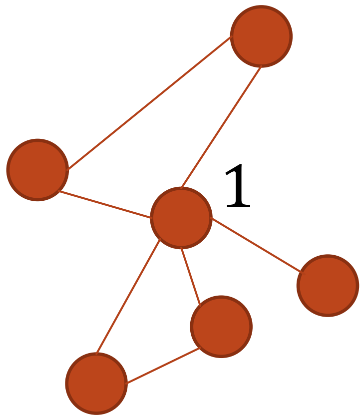
- A study of GNN expressivity w.r.t. WL test of graph isomorphism
- Choice of aggregation functions influences what structures can be recognized
- Propose a simple aggregation and concatenation model

$$h_v^{(k)} = \mathrm{MLP}^{(k)}\left(\left(1 + \epsilon^{(k)}\right) \cdot h_v^{(k-1)} + \sum_{u \in \mathcal{N}(v)} h_u^{(k-1)} \right)$$

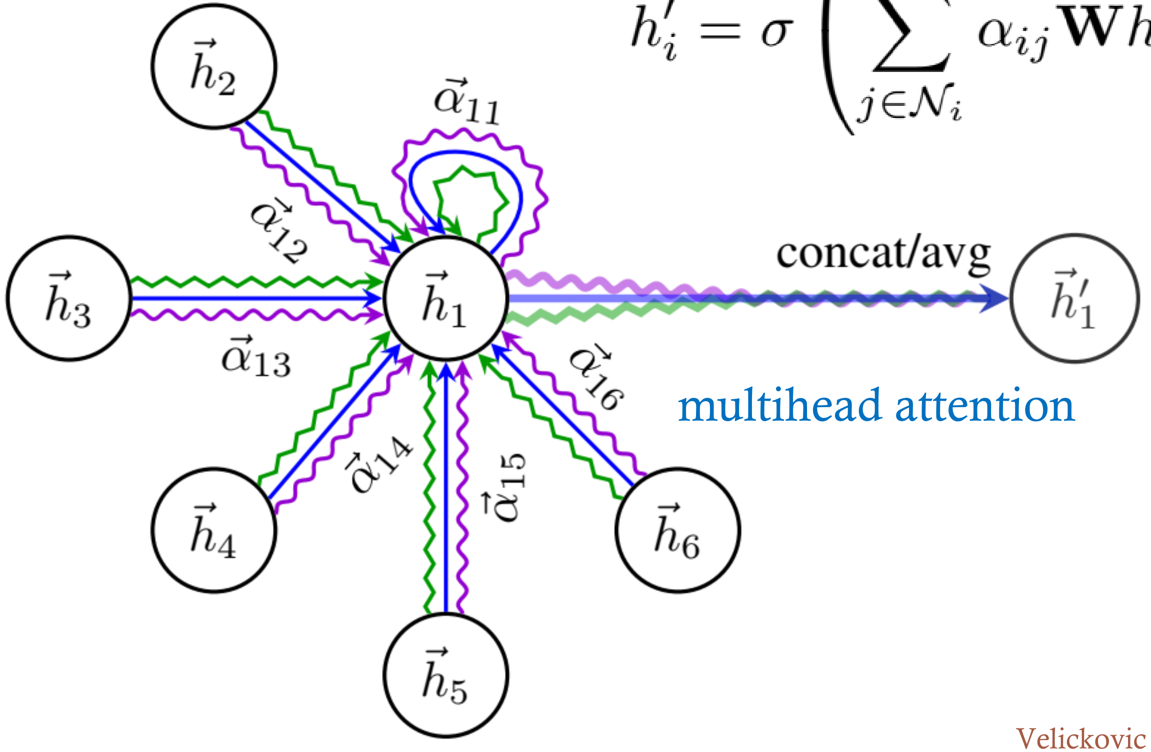
$$h_G = \mathrm{CONCAT}(\mathrm{READOUT}\left(\{h_v^{(k)} | v \in G\} \right) | k = 0, 1, \cdots, K)$$

Xu et al, ICLR 2019

Graph Attention



$$\vec{h}'_i = \sigma\left(\sum_{j \in \mathcal{N}_i} \alpha_{ij} \mathbf{W} \vec{h}_j\right)$$

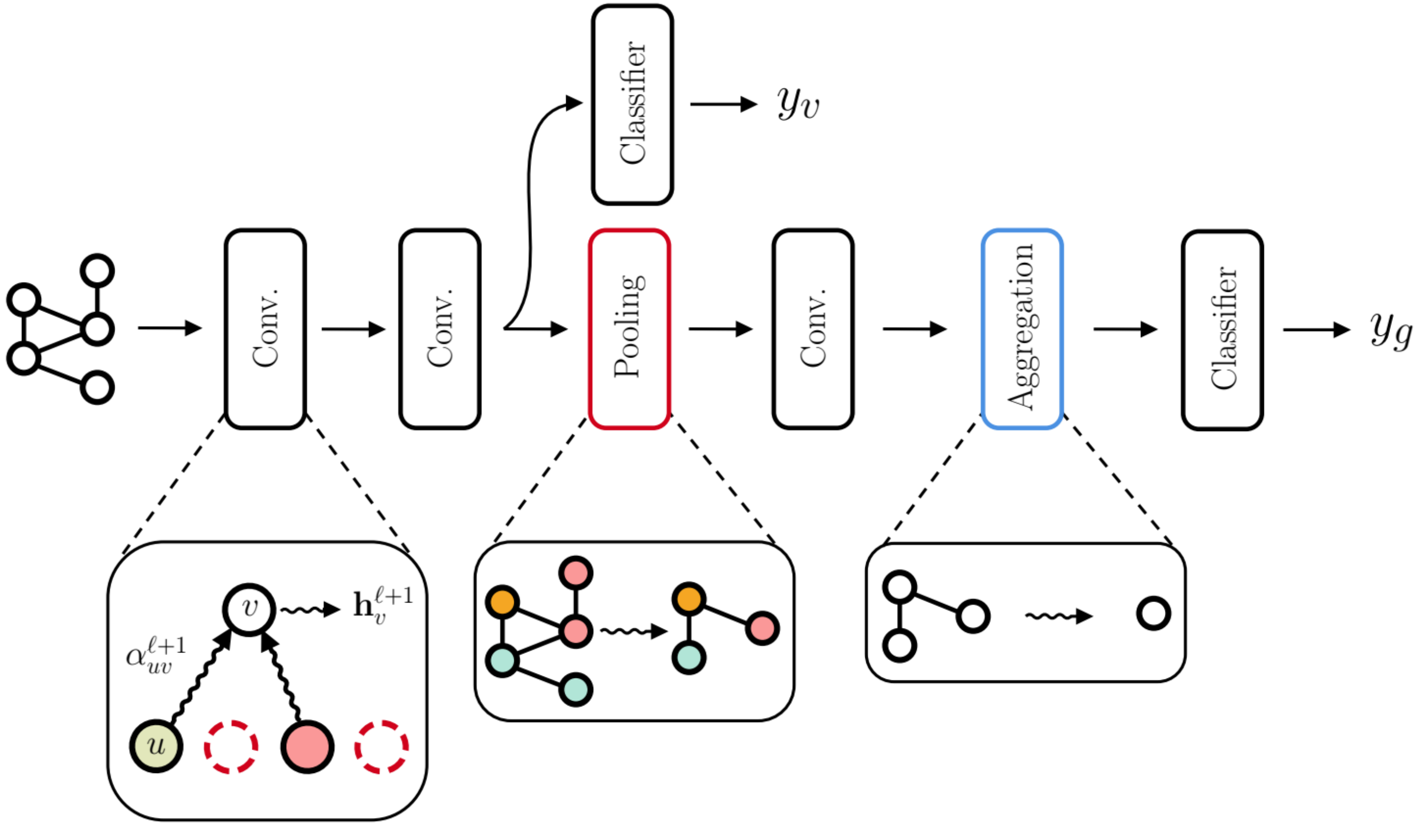


multihead attention

Learning to weight contribution of other nodes when aggregating to form the node embedding

Velickovic et al, ICLR 2018

Deep Graph Networks - The Complete Picture

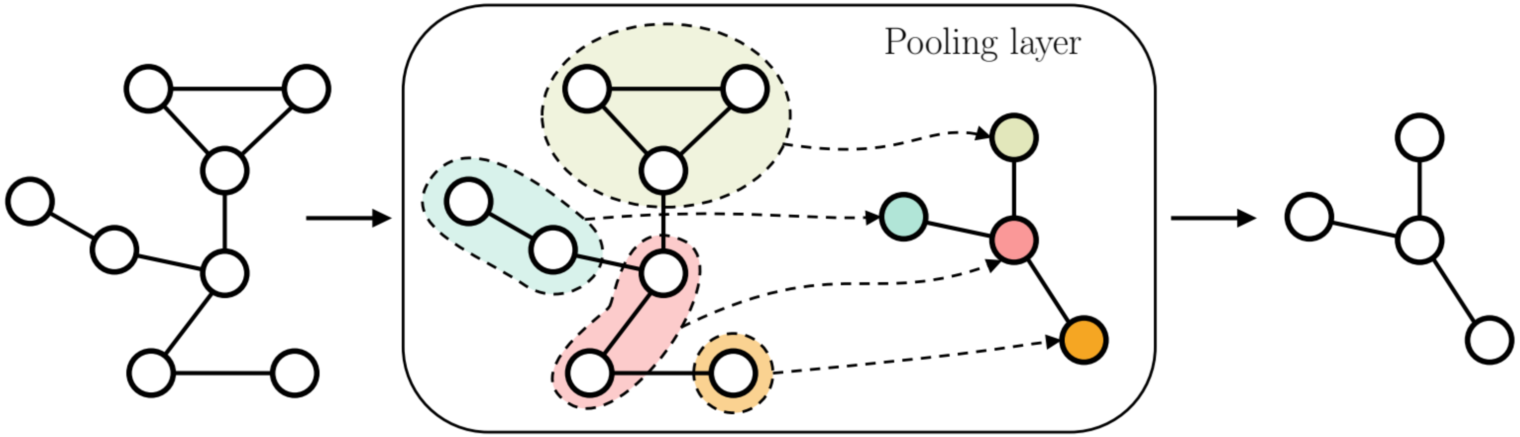


What About Pooling?

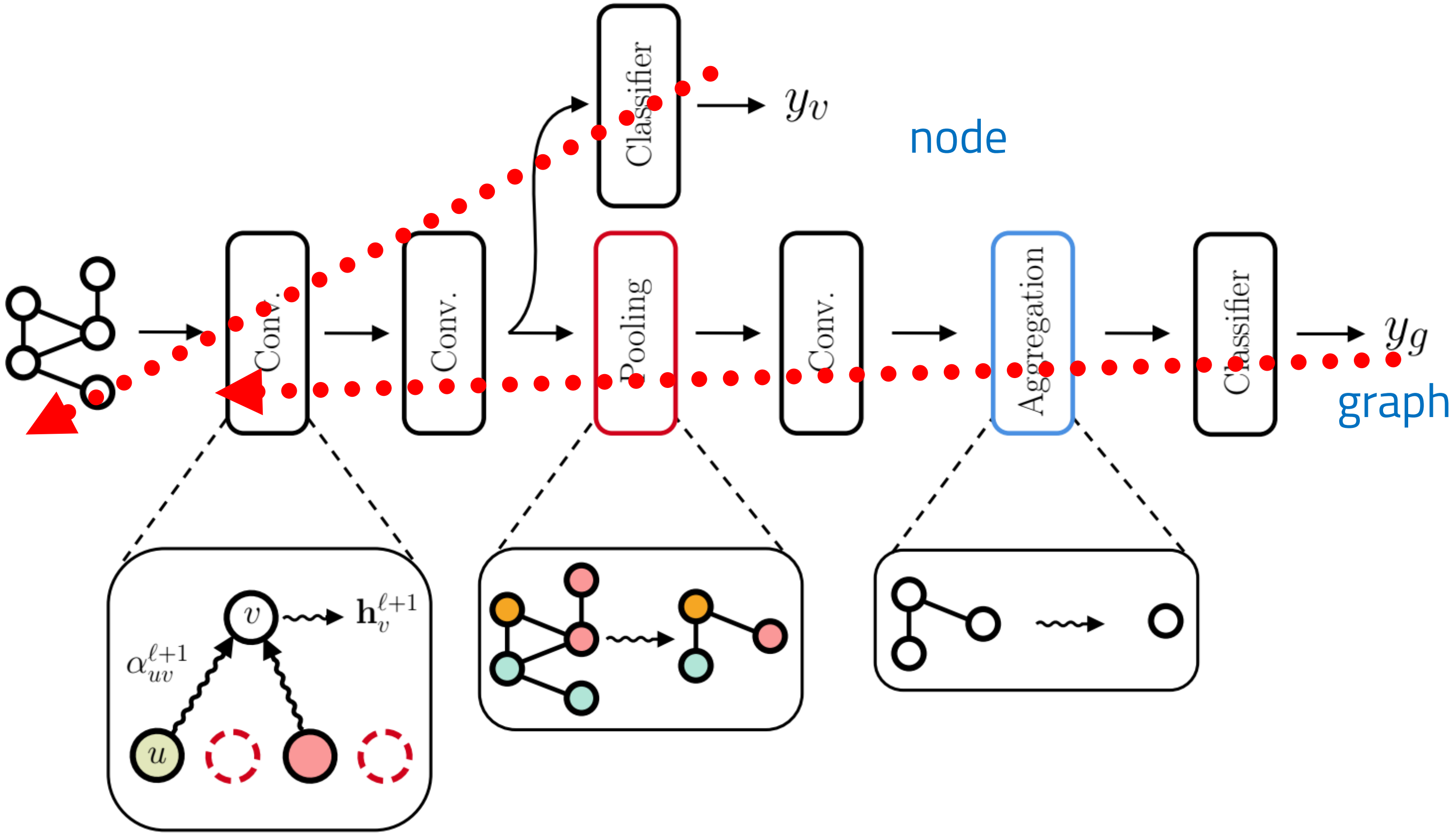
- Standard aggregation operates of predefined node subsets
- Ignore community/hierarchical structure in the graph
- Need graph coarsening (pooling) operators
  - Differentiable
  - Graph theoretical
  - Graph signature

Rex Ying et al, NIPS 2018

Bacciu et al, AAAI 2023



Training the Embedding

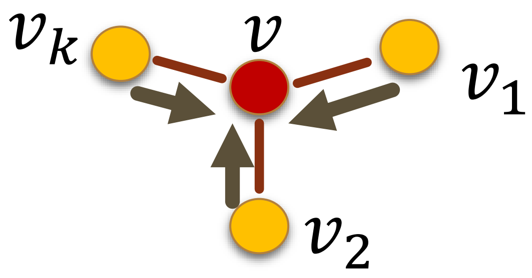


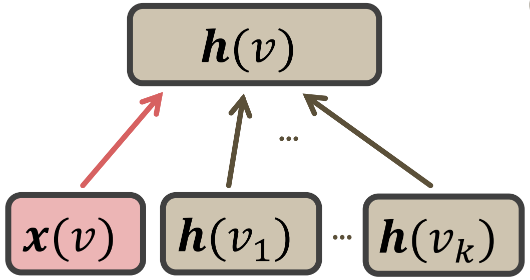
Backpropagate from the (graph or node level) error computed from the top layer embeddings to the early layers

Recurrent Graph Processing

Graph embedding by learning-free neurons

Each vertex in an input graph is encoded by the hidden layer





$$\mathbf{h}(v) = \tanh\left(\mathbf{V}\,\mathbf{x}(v) + \sum_{v' \in N(v)} \mathbf{W}\,\mathbf{h}(v')\right)$$

input weight matrix

hidden weight matrix

embedding (state) of vertex v

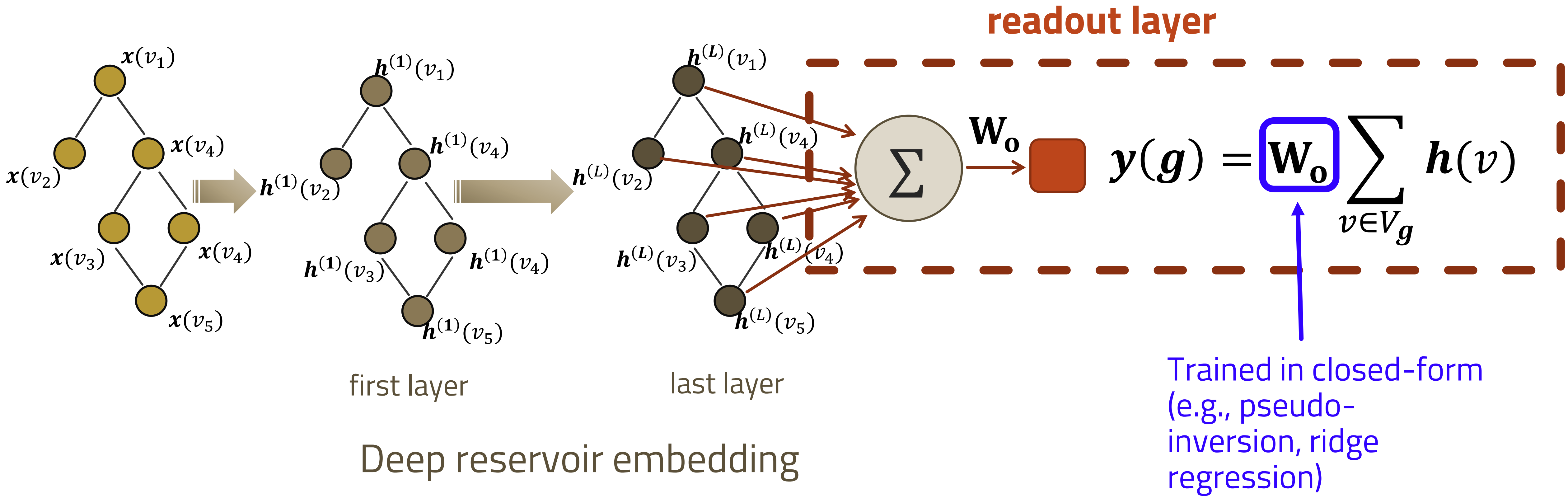
input feature of vertex v

embedding (state) of neighbors of vertex v

Need this to be contractive to ensure convergence of embedding

Deep Reservoirs for Graphs

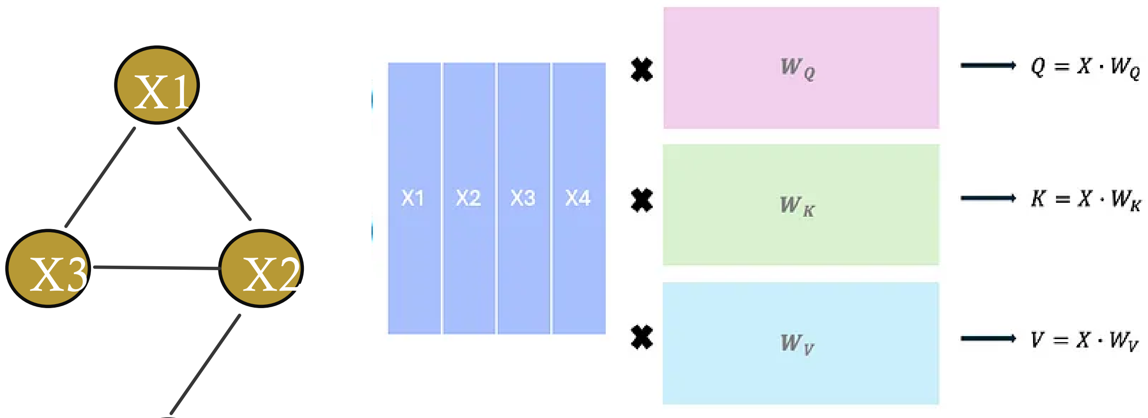
Gallicchio & Micheli. *AAAI* 2020.



Graph Transformers

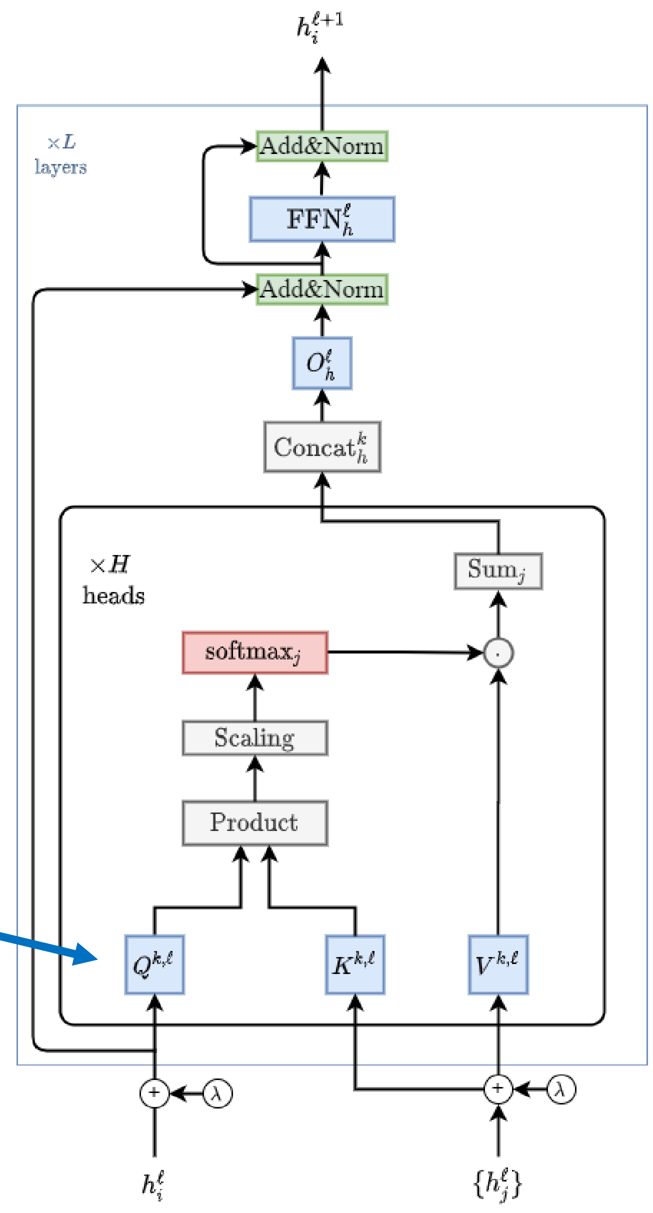
Global Graph Attention

A direct generalization of standard attention from sequence tokens to nodes



$$Attention(Q, K, V) = \text{softmax}\left(\frac{Q\,K^T}{\sqrt{d_k}}\right)V$$

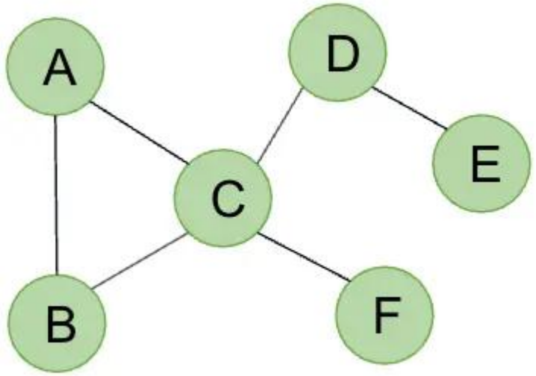
Img adapted from Medium



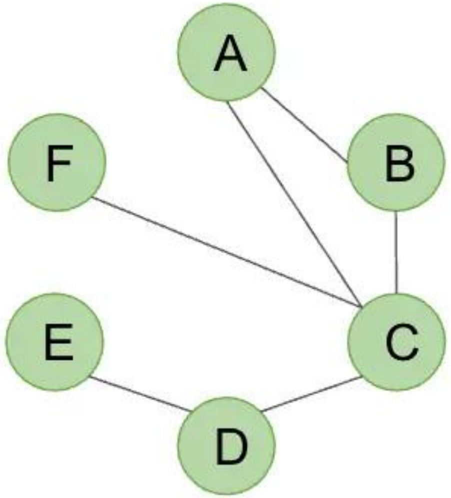
Graph Transformer Layer

Dwivedi & Bresson, AAAI-WS 2021

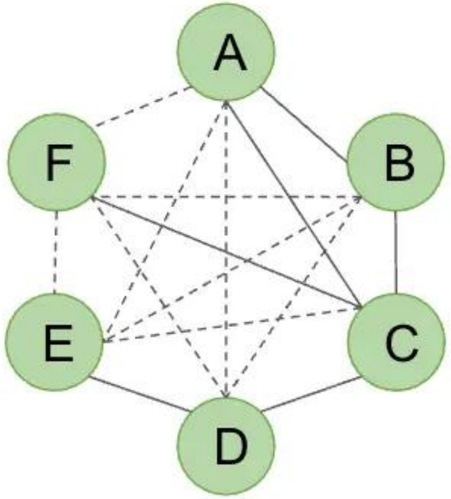
Wait! What is the inductive bias here?



Original graph



GAT Model

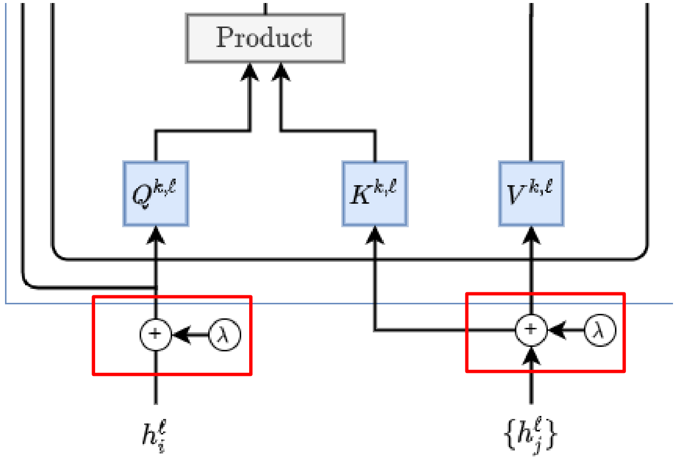


Graph Transformer

Img source: [Kumo AI]

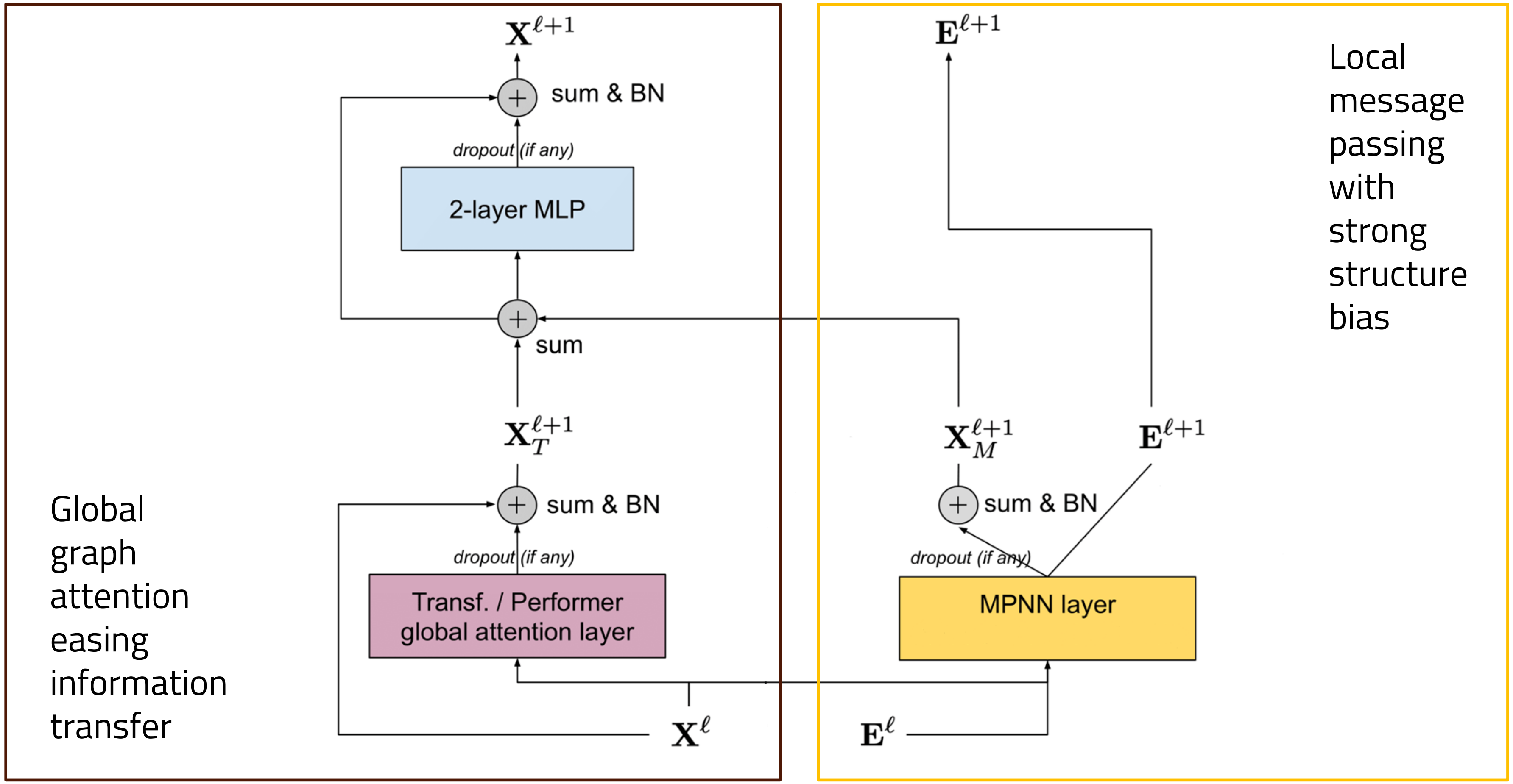
The return of positional encodings

- Transformers incorporate positional encodings to provide directional sense in a sequence (complete ordering)
- Graph have no complete ordering, but positional encodings can be used to reintroduce structural bias
  - Local PEs (Node-Level): Reflect a node's position relative to a specific substructure or cluster within the graph (e.g. reachability in random walks)
  - Global PEs (Node-Level): Node's position w.r.t. entire graph (e.g. Laplacian eigenvectors)
  - Relative PEs (Edge-Level): Represent the positional relationship between pairs of nodes (e.g. pairwise distances in random walks)
- Can be complemented with structural encodings providing insights into the local and global architecture of the graph



Graph Transformer Layer

GPS – Best of 2 worlds



Rampášek et al, NeurIPS 2022

Wrap-up

Software

You can find most of the foundational models in this lecture implemented here

PyTorch geometric

DeepGraphLibrary

Take-home messages

- Deep learning for graphs is a now a consolidated research area
  - DGNs as natural extensions of convolutional and recurrent architectures to graphs
- A candidate integrative paradigm for AI
  - Symbolic knowledge, numerical data and reasoning
  - Discrete, continuous and time-evolving
- First wave of works (now over?) focusing mainly on
  - Different ways of implementing message passing and aggregation on static graphs
  - Graph reductions and pooling
  - Expressivity properties associated with different aggregation functions
  - Efficiency and efficacy of context creation and propagation by mixing local and global message passing

Next Lecture

- Generative graph learning
  - Probabilistic models on graphs
  - Graph VAE, graph language models and graph diffusion models
- Issues with information propagation on graphs
  - Oversmoothing, oversquashing and undereaching
  - Topological approaches
  - Dynamical systems approaches
- Spatio-temporal and dynamic graphs
- Applications