Graph Neural Networks

A constraint-based formulation [a]

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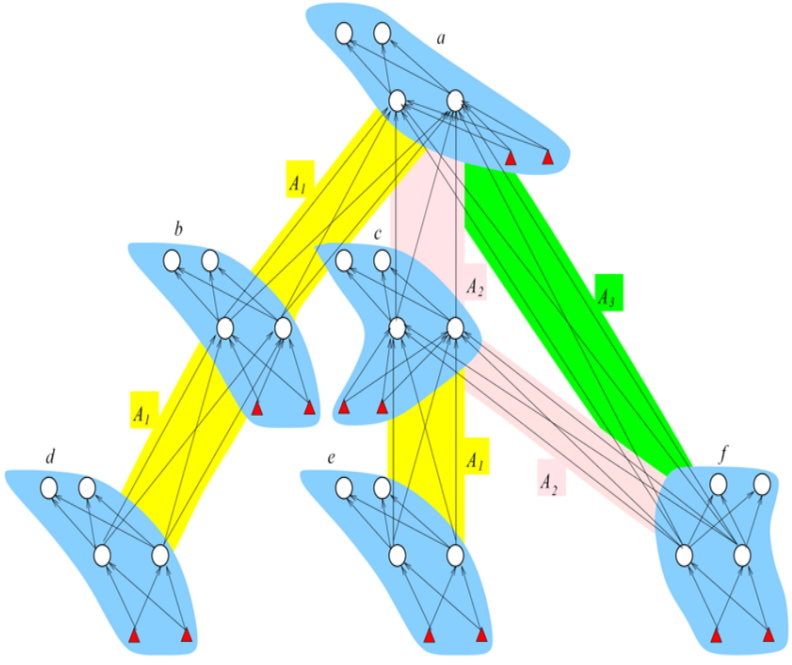

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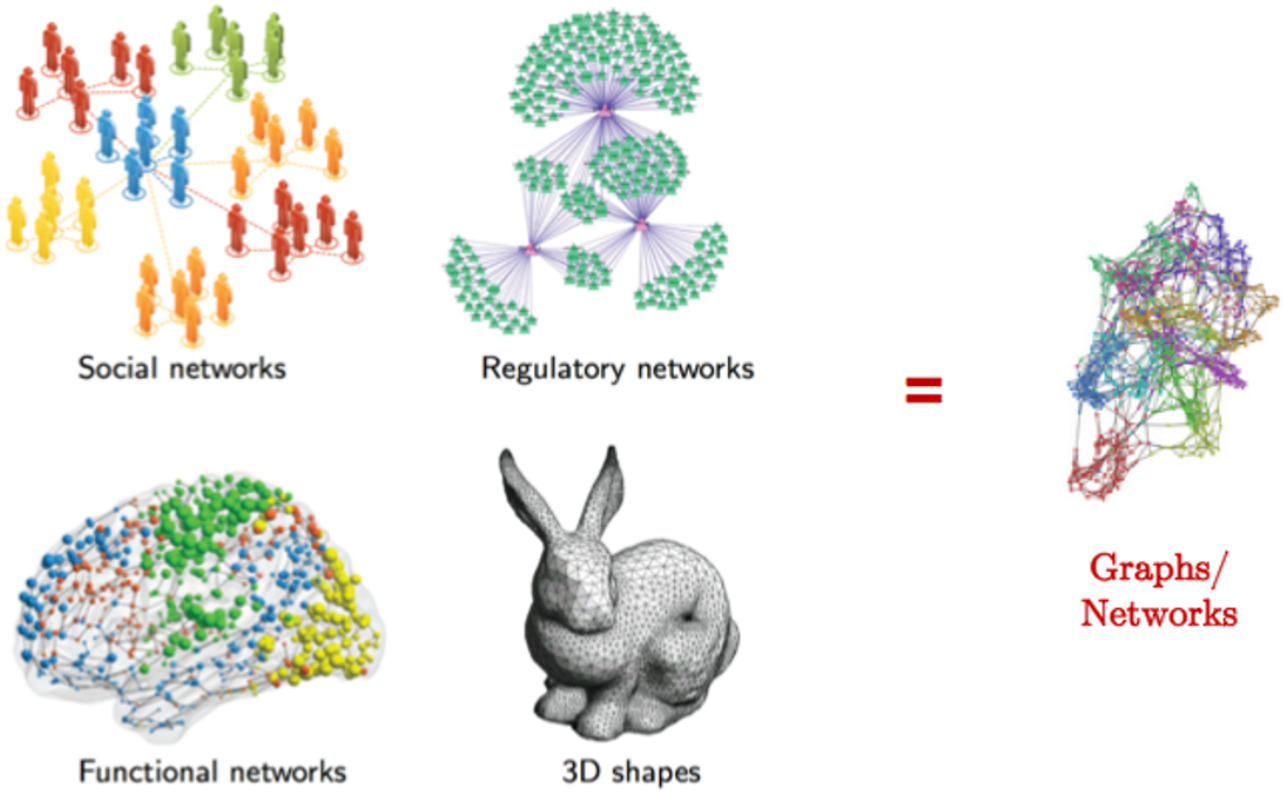
ACDL Satellite Workshop on Graph Neural Networks

Learning in structured domains



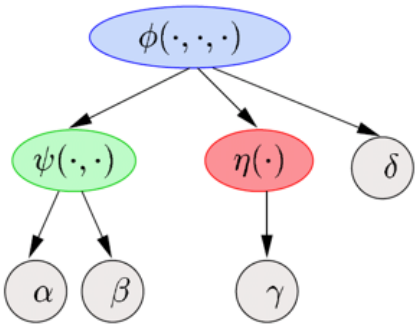
- Non-Euclidean (graph or manifold-structured) data such as social networks, molecular graphs and 3D point clouds in computer vision

Graph-focused Tasks

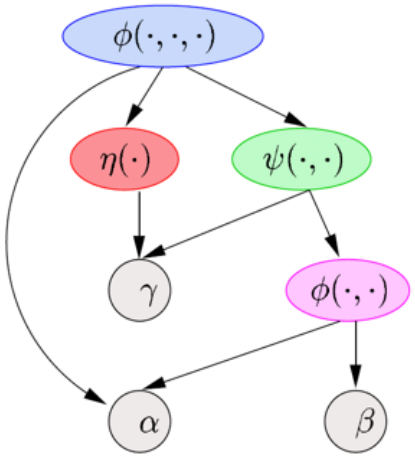
$$\tau(G)$$

On the truth of logic statements

$\phi(\psi(\alpha,\beta),\eta(\gamma),\delta)$

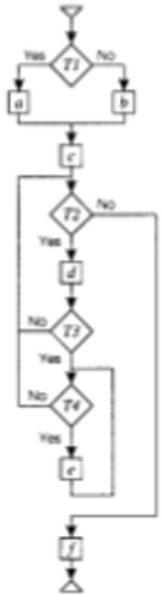


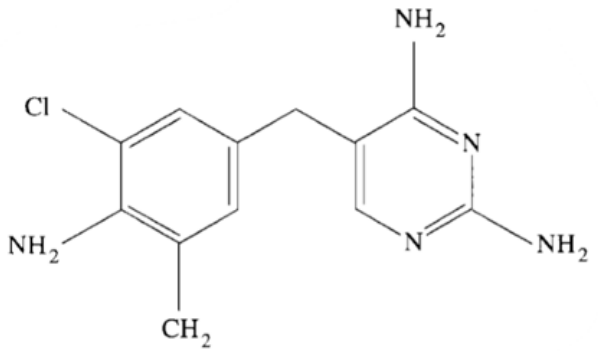
$\phi(\alpha,\eta(\gamma),\psi(\gamma,\phi(\alpha,\beta)))$



Program behavior

```
program name (list);
var
...
begin
if T1 then
        a
else
        b;
c;
while T2 do
        begin
        d;
        if T3 then
        while T4 do
                e
        end;
f
end.
```





Physicochemical behavior

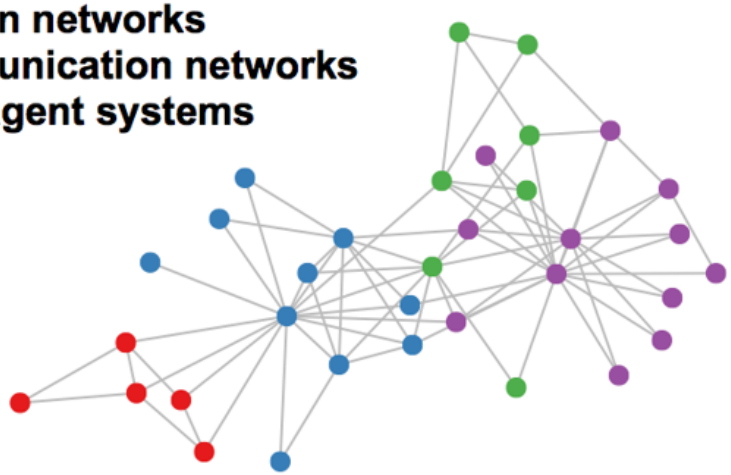
Node-focused Tasks

$$\tau(G, n)$$

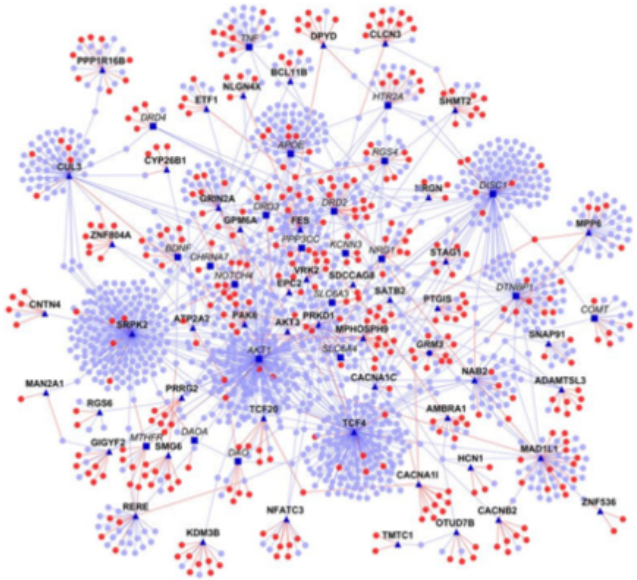
Social nets

here we need to make prediction at node level!

Social networks
Citation networks
Communication networks
Multi-agent systems



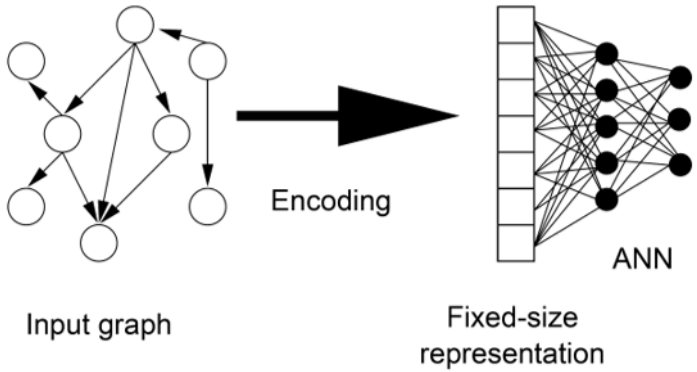
Karate club network



Protein Interaction Network

Graph Representation

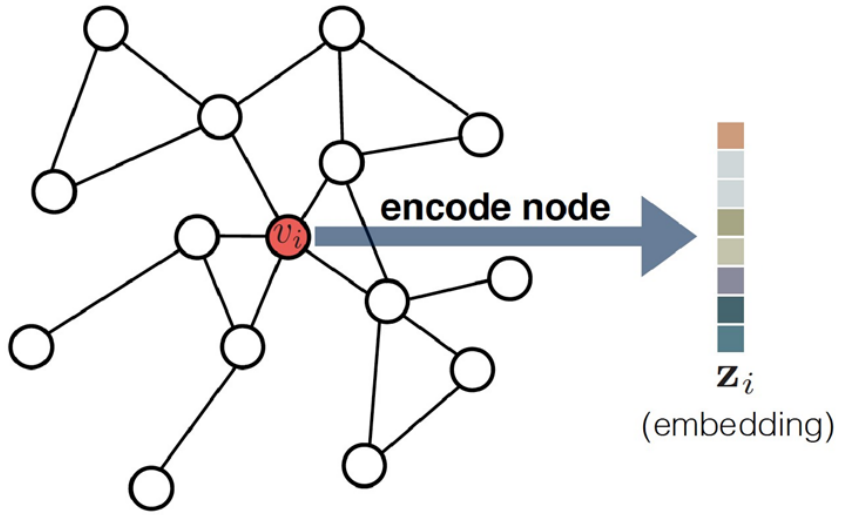
- Traditional machine learning approaches assume to deal with *flat data*
- Aim at obtaining simple representations from complex data structures, relying on summary graph statistics, kernel functions, graph traversals procedures etc.

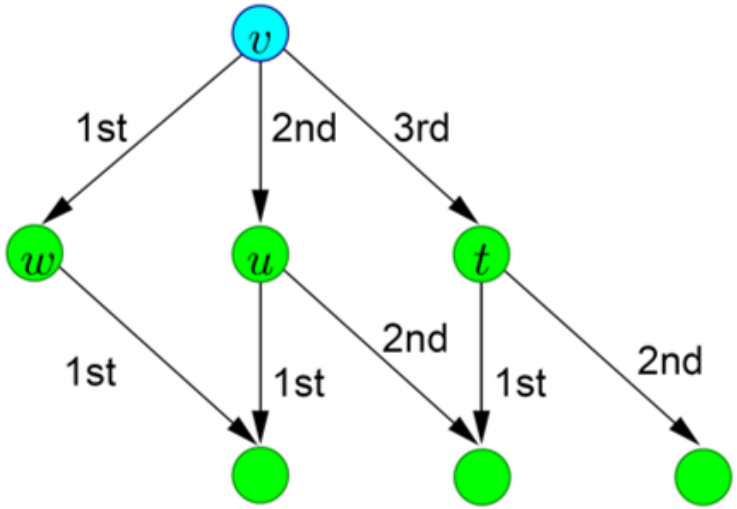


- **Pre-processing step**, using hand-engineered statistics to extract structural information into simpler encodings
- Limited approaches – **loosing useful information, not able to adapt during learning**

Embedding a graph

- Mapping a graph to a real valued vector – concatenating the features stored in each node, following an order derived from the connection topology





- The encoding of the topology by the position of the node inside the vector is not well defined for any category of graph – it holds for Directed Ordered Acyclic Graphs (DOAGs), this does not hold for generic cyclic graphs

The Graph Neural Network Model

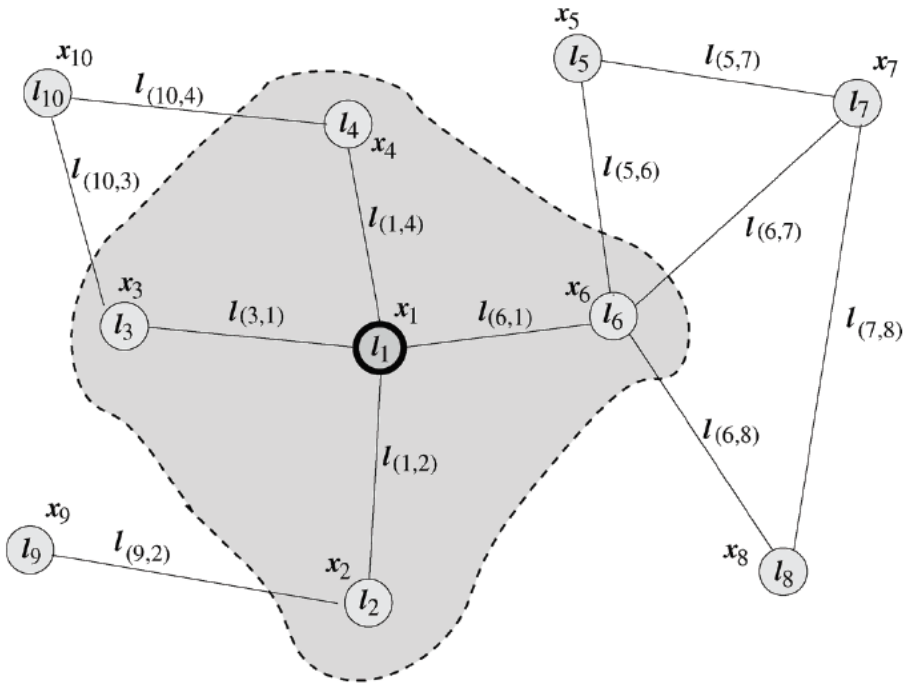
The Graph Neural Network Model (GNN)

- Introduced in [Scarselli et al. 2009], it is able to process graphs directly, without the need of a preprocessing step and without any limitation on the graph type (more general w.r.t Recursive nets, [Frasconi et al. 1998])
- This model exploits neural networks to learn how to encode nodes of a graph for a given task taking into account both the *information local* to each node and the whole *graph topology*.
- The learning process requires, for each epoch, an iterative **diffusion mechanism** up to convergence to a **stable fixed point**

The Graph Neural Network Model

- Given an input graph $G = (V, E)$, where V is a finite set of *nodes* and $E \subseteq V \times V$ collects the *arcs*, GNNs apply a two-phase computation on G
- **Encoding (aggregate) phase** the model computes a state vector for each node in V by (iteratively) combining the states of neighboring nodes (i.e. nodes $u, v \in V$ that are connected by an arc $(u, v) \in E$) – exploiting the **state transition function** f_w
- **Output (readout) phase** the latent representations encoded by the states stored in each node are exploited to compute the model output – exploiting the **output function** g_w

Neighbor-based computation



$$x_1 = f_w(l_1, l_{(1,2)}, l_{(3,1)}, l_{(1,4)}, l_{(6,1)}, x_2, x_3, x_4, x_6, l_2, l_3, l_4, l_6)$$

$l_{co[1]}$ $x_{ne[1]}$ $l_{ne[n]}$

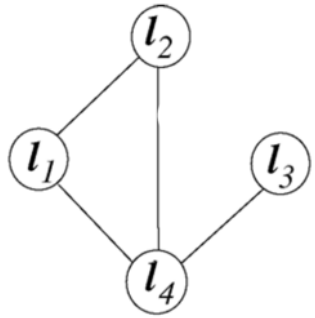
node label connection label neighbor state neighbor label

$$x_n = f_w(l_n, l_{co[n]}, x_{ne[n]}, l_{ne[n]}) \qquad x = F_w(x, l)$$

$$o_n = g_w(x_n, l_n) \qquad o = G_w(x, l_N)$$

equilibrium configuration!

Non-positional graphs

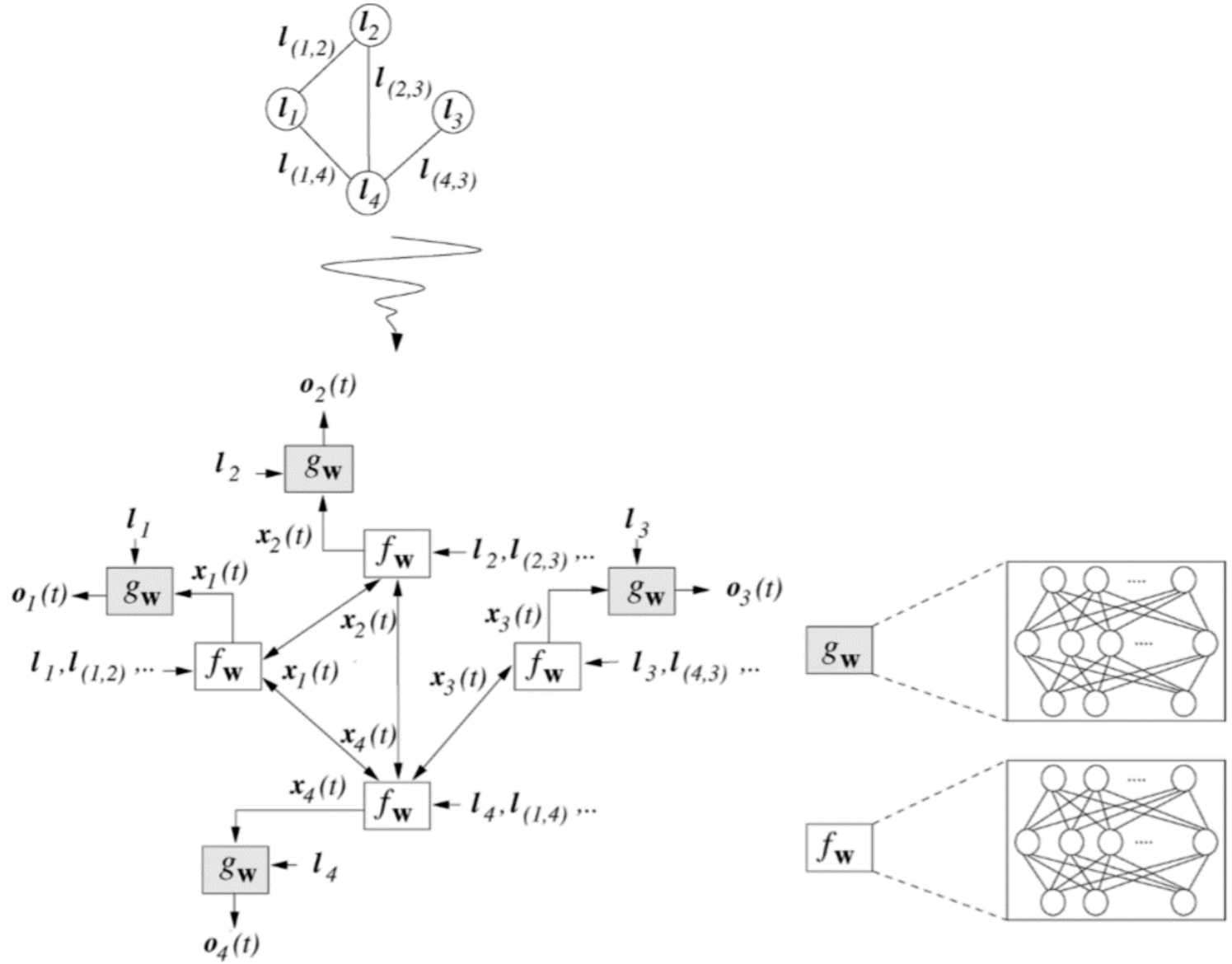


$$x_n^{(t)} = \sum_{(n,v)\in E} f_w(l_n, l_{(n,v)}, x_v^{(t-1)}, l_v)$$

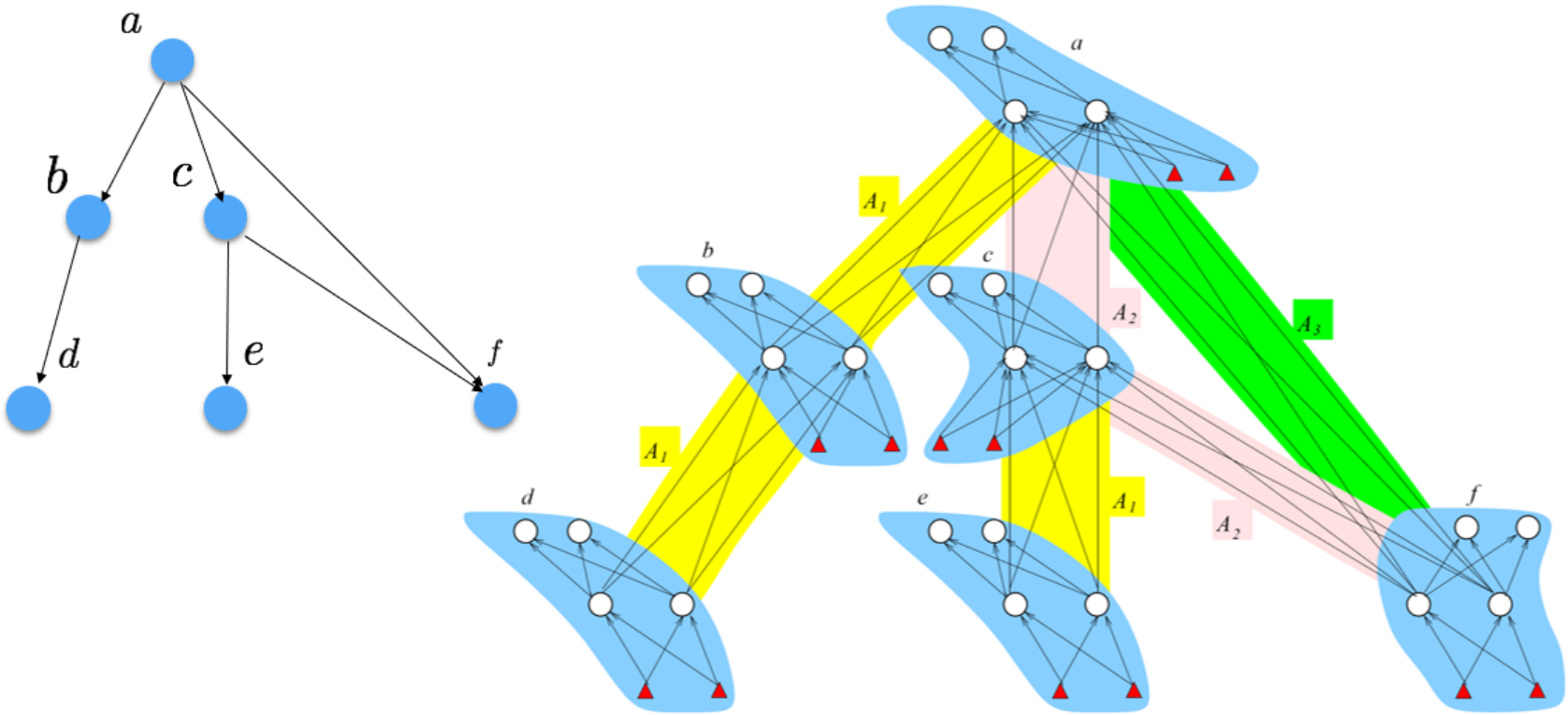
permutation-independent

$$o_n = g_w(x_n^{(T)}, l_n)$$

Graph Encoding



Graph Encoding



From the encoding network to the encoding neural network ...

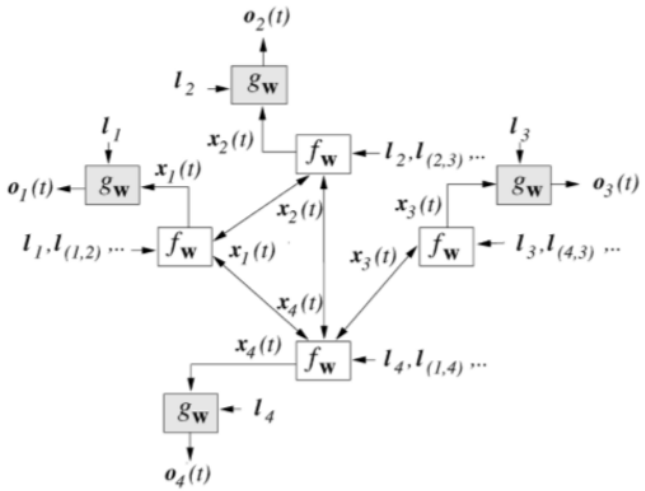
Convergence procedure

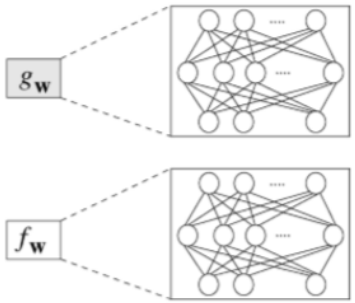
- The recursive application of the state transition function $f_w()$ on the graph nodes yields a diffusion mechanism, whose range depends on T
- In the original GNN model [Scarselli et al. 2009] the convergence procedure is executed until convergence of the state representation, i.e. until $x_n^{(t)} \simeq x_n^{(t-1)}, v \in V$.
- This scheme corresponds to the computation of the *fixed point* of the state transition function $f_w()$ on the input graph. In order to guarantee the convergence of this phase, the transition function is required to be a *contraction map*.
  Banach Fixed Point Theorem

Reaching Equilibrium

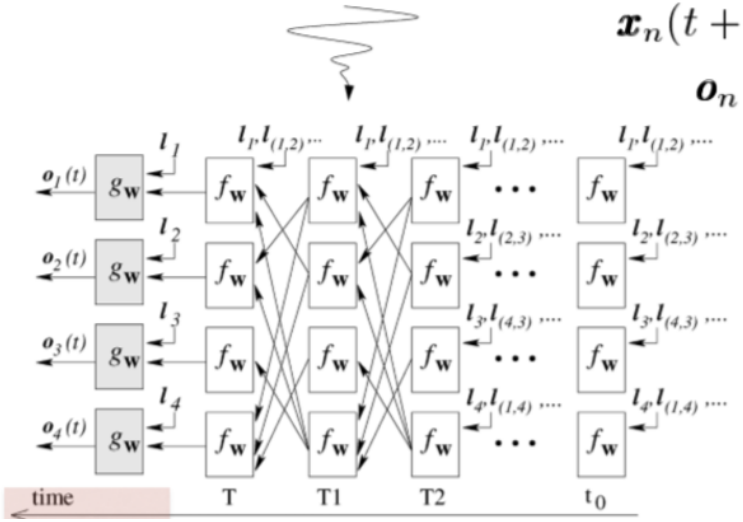
How we get the equilibrium points?

Relaxation to an equilibrium





$$\boldsymbol{x}_n(t+1) = f_{\boldsymbol{w}}(\boldsymbol{l}_n, \boldsymbol{l}_{\mathrm{co}[n]}, \boldsymbol{x}_{\mathrm{ne}[n]}(t), \boldsymbol{l}_{\mathrm{ne}[n]})$$
$$\boldsymbol{o}_n(t) = g_{\boldsymbol{w}}(\boldsymbol{x}_n(t), \boldsymbol{l}_n), \qquad n \in \boldsymbol{N}.$$



$$\boldsymbol{x}(t+1) = F_{\boldsymbol{w}}(\boldsymbol{x}(t), \boldsymbol{l})$$

Lagrangian GNN

GNN: a Constraint formulation

- Basically, the encoding phase, through the iteration of $f_w()$, finds a solution to the fixed point problem defined by the constraint

$$\forall n \in V, x_n = \sum_{(n,v)\in E} f_w(l_n, l_{(n,v)}, x_v, l_v) \tag{1}$$

  In this case, the states encode the information contained in the whole graph.
- This diffusion mechanism is more general than executing only a fixed number of iterations (i.e. stacking a fixed number of layers).
- However, it can be computationally heavy and, hence, many recent GNN architectures apply only a fixed number of iterations for all nodes [Scarselli et al. 2009].

Lagrangian Propagation GNN

- With an approach related to [Carreira-Perpinan et al., 2014] [Taylor et al. 2016], we consider a Lagrangian formulation of the problem by adding free variables corresponding to the node states x_n
- With $L(g_w(x_v), y_v)$ as the loss function (target fitting approximation for node $v \in S$), the formulation of the learning task is

$$\begin{aligned} \text{minimize} \quad & \sum_{v \in S} L(g_w(x_v), y_v) \\ \text{subject to} \quad & \mathcal{G}(x_v - \sum_{(n,v) \in E} f_w(l_v, l_{(v,n)}, x_n, l_n)) = 0, \quad \forall\, v \in V \end{aligned} \tag{2}$$

  and $\mathcal{G}(x)$ is a function characterized by $\mathcal{G}(0) = 0$.
- Apart from classical choices, like $\mathcal{G}(x) = x$ or $\mathcal{G}(x) = x^2$, we can design different function shape with desired properties.

	lin	*lin-*ϵ	*abs*	*abs-*ϵ	*squared*
$\mathcal{G}(x)$	x	$\max(x, \epsilon) - \max(-x, \epsilon)$	$\lvert x \rvert$	$\max(\lvert x \rvert - \epsilon, 0)$	x^2
Unilateral	$\times$	$\times$	✓	✓	✓
ϵ-insensitive	$\times$	✓	$\times$	✓	$\times$

Optimization procedure: search for saddle points

- The constrained optimization problem can be solved in the Lagrangian framework by introducing for each constraint a Lagrange multiplier λ_v, to define the Lagrangian function $\mathcal{L}(\theta_{f_w}, \theta_{g_w}, X, \Lambda)$ where Λ is the set of the $|V|$ Lagrangian multipliers.
- We can define the unconstrained optimization problem as the search for saddle points in the adjoint space $(\theta_{f_w}, \theta_{g_w}, X, \Lambda)$ as:

$$\min_{\theta_{f_w}, \theta_{g_w}, X} \max_{\Lambda} \mathcal{L}(\theta_{f_w}, \theta_{g_w}, X, \Lambda)$$

  where θ_{f_w} and θ_{g_w} are the weights of the MLPs implementing the state transition function and the output function,
- The problem can be solved by gradient *descent* with respect to the variables $\theta_{f_w}, \theta_{g_w}, X$ and gradient *ascent* with respect to the Lagrange multipliers Λ.

Optimization procedure: search for saddle points

- The diffusion mechanism of the state computation is enforced by means of the constraints.
- The learning algorithm is based on a mixed strategy where :
  - Backpropagation is used to efficiently update the weights of the neural networks that implement the state transition and output functions
  - The diffusion mechanism evolves gradually by enforcing the convergence of the state transition function to a fixed point by means of the constraints.

Reaching Equilibrium

$$\mathcal{L}(\theta_{f_a}, \theta_{f_r}, X, \Lambda) = \sum_{v \in S} [L(f_r(x_v|\theta_{f_r}), y_v) + \\ + \lambda_v \mathcal{G}\left(x_v - f_a(x_{\text{ne}[v]}, l_{\text{ne}[v]}, l_{(v,\text{ch}[v])}, l_{(\text{pa}[v],v)}, x_v, l_v|\theta_{f_a})\right)]$$

$$\min_{\theta_{f_a}, \theta_{f_r}, X} \max_{\Lambda} \mathcal{L}(\theta_{f_a}, \theta_{f_r}, X, \Lambda)$$

$$\frac{\partial \mathcal{L}}{\partial x_v} = L' f'_{r,v} + \lambda_v \mathcal{G}'_v (1 - f'_{a,v}) - \sum_{w: v \in ne[w]} \lambda_w \mathcal{G}'_w f'_{a,w}$$

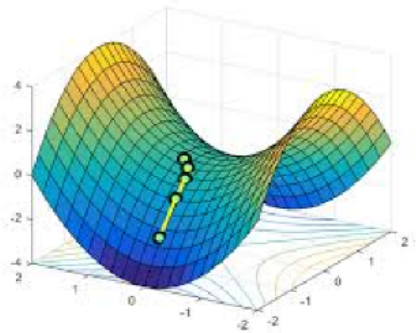
$$\frac{\partial \mathcal{L}}{\partial \theta_{f_a}} = -\sum_{v \in S} \lambda_v \mathcal{G}'_v f'_{a,v}$$

$$\frac{\partial \mathcal{L}}{\partial \theta_{f_r}} = \sum_{v \in S} L' f'_{r,v}$$

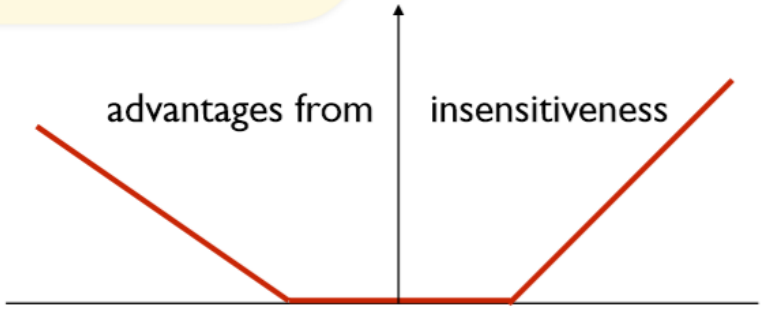
gradient descent

$$\frac{\partial \mathcal{L}}{\partial \lambda_v} = \mathcal{G}_v$$

gradient ascent



better suited for generalization



Experiments

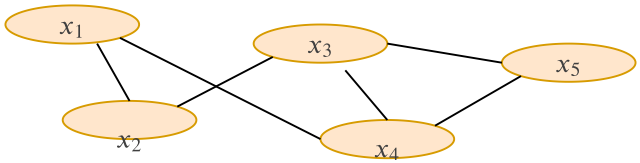
Experiments: node classification benchmarks

Table: Accuracies on the artificial datasets, for the proposed model (Lagrangian Propagation GNN - LP-GNN) and the standard GNN model for different settings.

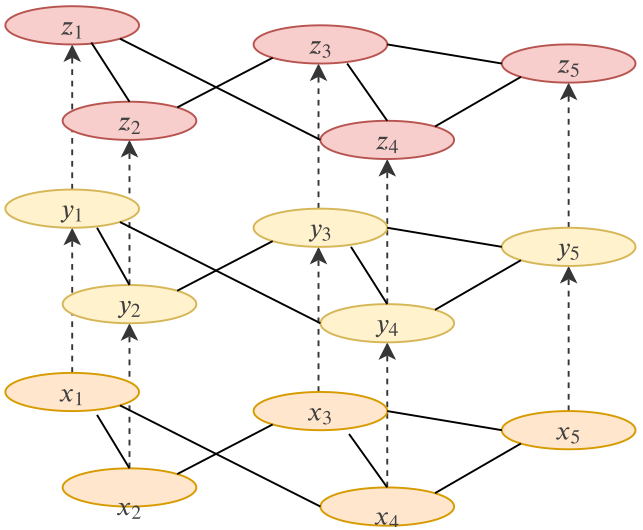
Model			Subgraph		Clique	
	$\mathcal{G}$	ϵ	*Acc(avg)*	*Acc(std)*	*Acc(avg)*	*Acc(std)*
LP-GNN	*abs*	0.00	96.25	0.96	88.80	4.82
		0.01	**96.30**	0.87	88.75	5.03
		0.10	95.80	0.85	85.88	4.13
	lin	0.00	95.94	0.91	84.61	2.49
		0.01	95.94	0.91	85.21	0.54
		0.10	95.80	0.85	85.14	2.17
	squared	-	96.17	1.01	**93.07**	2.18
Scarselli et al. 2009	-	-	95.86	0.64	91.86	1.12

Evolutions: MultiLayer Lagrangian GNNs

- Even though the state transition function can be implemented by Deep Neural Networks, the GNN is still shallow.
- A multilayer version of our algorithm can be easily introduced by simply adding the corresponding constraints
- Label of hidden nodes are simply the states of the nodes of the layer below.
- The new constraints add new variables (e.g. y_i, z_i, etc.)



(a) A shallow GNN.



(b) A deep GNN.

- The optimization problem is easily updated into:

$$\begin{aligned}
\text{minimize} \quad & \sum_{v \in S} L(g_w(z_v), t_v) \\
\text{subject to} \quad & \mathcal{G}(x_v - \sum_{(v,n)\in E} f_w^0(x_n, l_v, l_n)) = 0, \quad \forall\, v \in V \qquad (3) \\
& \mathcal{G}(y_v - \sum_{(v,n)\in E} f_w^1(y_n, x_n, x_v)) = 0, \quad \forall\, v \in V \qquad (4) \\
& \mathcal{G}(z_v - \sum_{(v,n)\in E} f_w^2(z_n, y_n, y_v)) = 0, \quad \forall\, v \in V \qquad (5)
\end{aligned}$$

Experiments: graph classification benchmarks

Table: Test set classification average accuracies and standard deviations for the graph classification benchmarks.

Datasets	IMDB-B	IMDB-M	MUTAG	PROT.	PTC	NCI1
# graphs	1000	1500	188	1113	344	4110
# classes	2	3	2	2	2	2
Avg # nodes	19.8	13.0	17.9	39.1	25.5	29.8
DCNN	49.1	33.5	67.0	61.3	56.6	62.6
PatchySan	71.0 $\pm$ 2.2	45.2 $\pm$ 2.8	92.6 $\pm$ 4.2	75.9 $\pm$ 2.8	60.0 $\pm$ 4.8	78.6 $\pm$ 1.9
DGCNN	70.0	47.8	85.8	75.5	58.6	74.4
AWL	74.5 $\pm$ 5.9	51.5 $\pm$ 3.6	87.9 $\pm$ 9.8	–	–	–
GIN	75.1 $\pm$ 5.1	52.3 $\pm$ 2.8	89.4 $\pm$ 5.6	76.2 $\pm$ 2.8	64.6 $\pm$ 7.0	82.7 $\pm$ 1.7
GNN	60.9 $\pm$ 5.7	41.1 $\pm$ 3.8	88.8 $\pm$ 11.5	76.4 $\pm$ 4.4	61.2 $\pm$ 8.5	51.5 $\pm$ 2.6
LP-GNN	71.2 $\pm$ 4.7	46.6 $\pm$ 3.7	87.7 $\pm$ 6.5	75.7 $\pm$ 4.5	61.7 $\pm$ 6.8	64.5 $\pm$ 2.2
LP-GNN-Multi*	76.2 $\pm$ 3.2	50.8 $\pm$ 2.0	89.4 $\pm$ 7.2	77.2 $\pm$ 3.9	67.9 $\pm$ 7.2	69.0 $\pm$ 1.7

Semisupervised Learning in Graph Domains

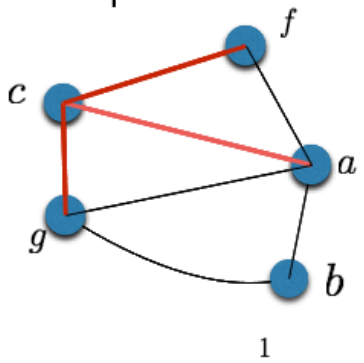
- In supervised node classification tasks, all the nodes in the training data needs to be labeled.
- Simple extension to tackle the Semisupervised tasks. In particular, by splitting the nodes into supervised and unsupervised, we can:
  - On **supervised** nodes, enforce state transition constraints and the objective function
  - On **unsupervised** nodes, enforce state transition constraints only
- This will allow to exploit the topological patterns of unsupervised data to make state transition function converge also for unsupervised nodes.

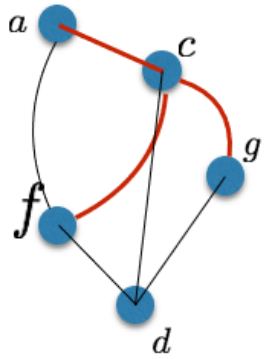
When new graphs come ...

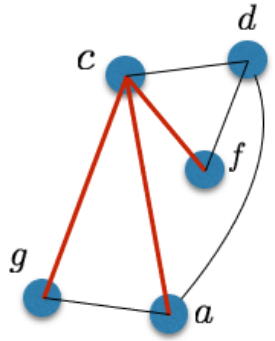
semi-supervised learning

constraints on state propagation

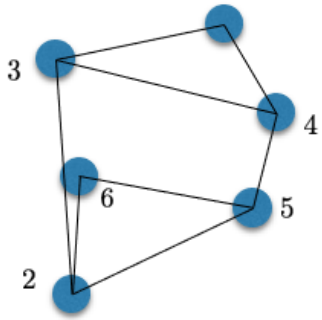
constraints on supervision







constraints on state propagation



you can always enforce state propagation

$$\forall n \in V, x_n = \sum_{(n,v)\in E} f_w(l_n, l_{(n,v)}, x_v, l_v)$$

Conclusions

- GNN learning task casted as a constrained optimization problem allows us to avoid the explicit computation of the fixed point needed to encode the graph.
- Jointly optimize the model weights and the state representation without the need of separate phases.
- Simplify the computational scheme of GNNs and allows us to incorporate alternative strategies in the fixed point optimization by the choice of the constraint function
- The constraint-based scheme can be extended to all the other methods proposed in the literature that exploit more sophisticated architectures.