Massachusetts
Institute of
Technology

Two aspects of learning algorithms: generalization under shifts and loss functions

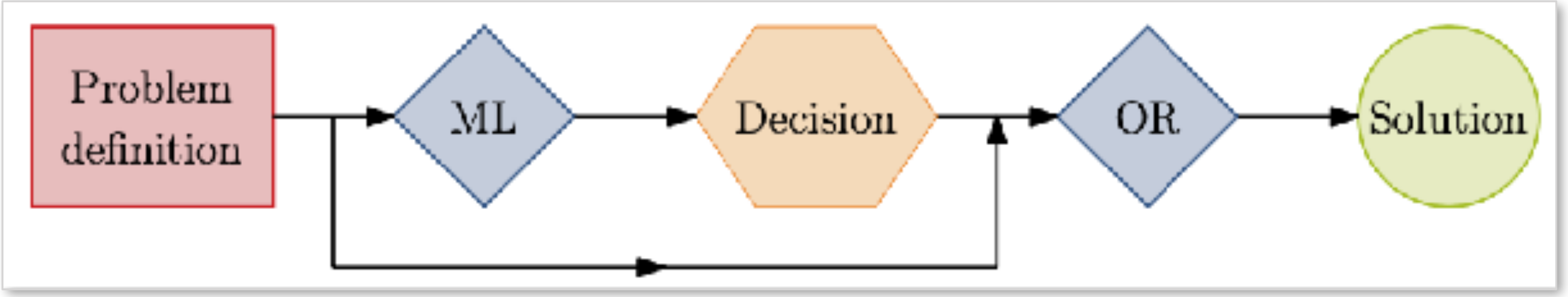
Stefanie Jegelka
MIT

based on joint work with
Keyulu Xu, Ching-Yao Chuang, Nikolaos Karalias, Joshua Robinson, Andreas Loukas, Jingling Li, Mozhi Zhang, Simon S. Du, Ken-ichi Kawarabayashi

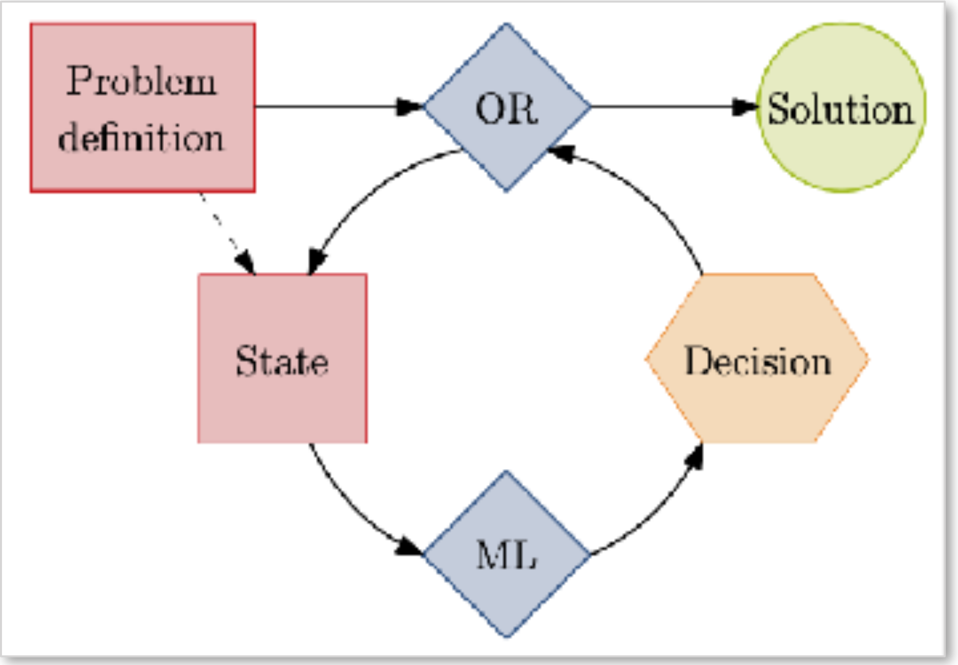
TILOS

Learning and Algorithms

- Predicting good configurations / solvers
  (Leyton-Brown et al 2002, Hutter et al 2011, Gupta et al 2015, Balcan et al 2017..)

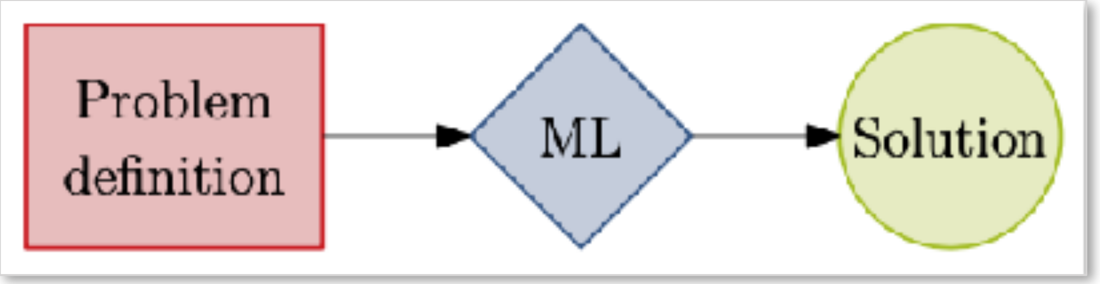


- Predicting problem parameters
  (Amos & Kolter 2017, Wilder et al 2019, Donti et al 2019, Elmachtoub & Grigas 2020, Mandi & Guns 2020, Berthet et a…)



- Machine learning oracles within a fixed algorithm (online algorithms, branch-and-bound,…)
  (Kraska et 2018, Balcan et al 2018, Hsu et al 2019, Gasse et al 2019, Dong et al 2020..)

- Learning a full algorithm, Algorithm implemented as a neural network
  (Graves et al 2014, Kaiser & Sutskever 2015, Kurach et al 2015, Kool & Welling 2018, Veličković et al 2020, Karalias & Loukas 2020, Kotary et al 2021, Schuetz et al 2022,…)



Figures: Bengio, Lodi, Provoust 2020

Today:

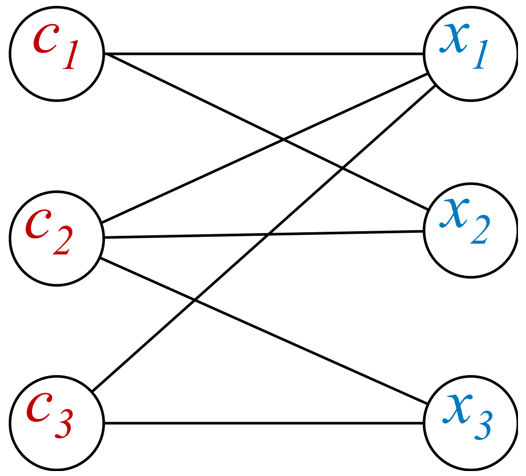
Some thoughts on learning (for) algorithms

Disclaimer

- Not the “latest & greatest” here in terms of experiments…
- … but some ideas to better understand ML models’ behavior

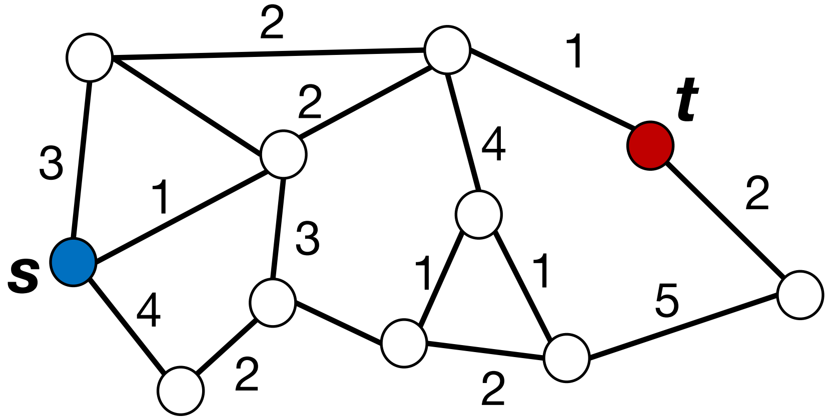
How to do learning for algorithms?

$$\min_x \; c^\top x$$
$$Ax \leq b$$
$$l \leq x \leq u$$
$$x \in \mathbb{Z}^p \times \mathbb{R}^{n-p}$$



constraints variables *(Gasse et al 2019)*

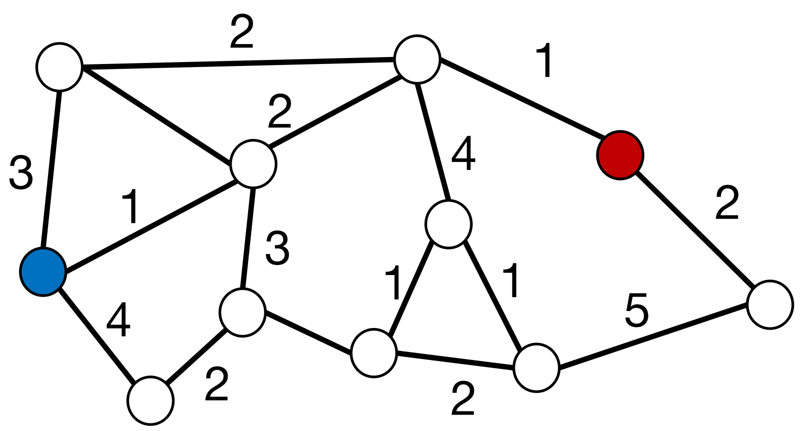
clauses variables *(Selsam et al 2018)*



Focus here:
Input is a graph
with attributes

Setup: learning task

"graph regression"



$g(x) = 4$

- Input x: graph (or set) with attributes (optimization instance)
- Desired output $g(x)$: optimal value

- Training data: $\{(x^{(i)}, g(x^{(i)}))\}_{i=1}^{N}$ with $x^{(i)} \sim P$ ← *P unknown*

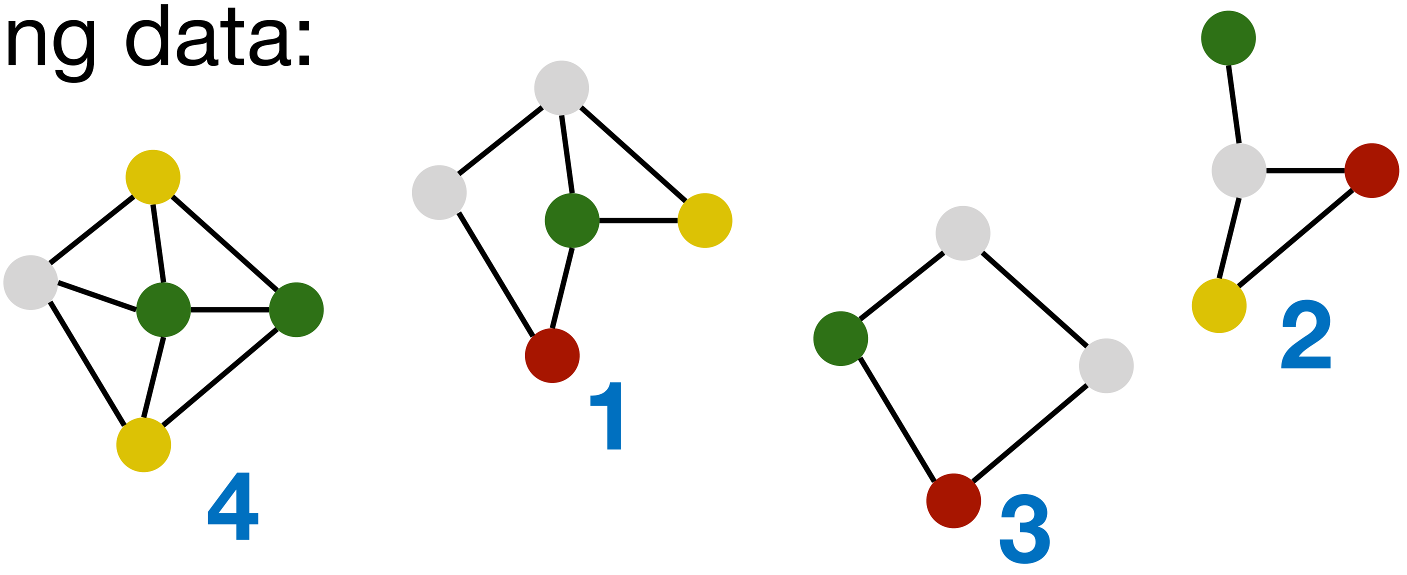
- Goal: find a function $f \in \mathcal{F}$ that *generalizes* (= low "risk")

$$\mathbb{E}_{x \sim P}[\,\ell(f(x), g(x))\,]$$

Other aspects:
- learning setting
- loss
- constraints

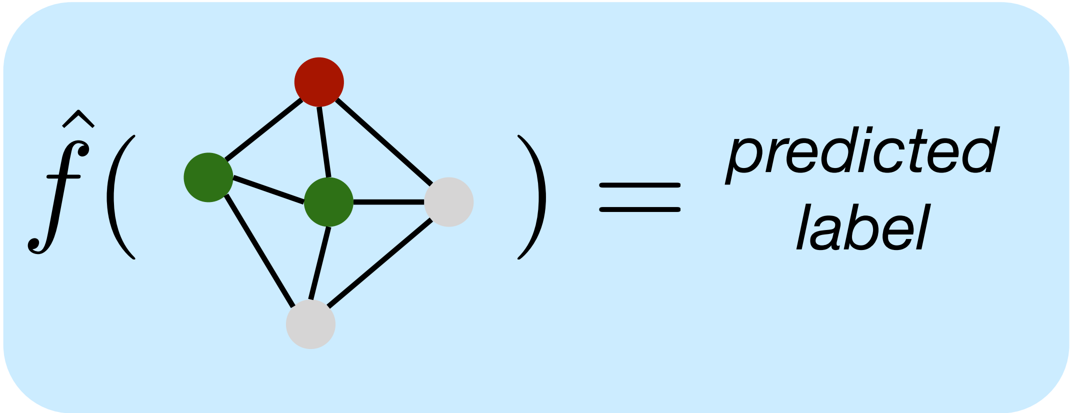
Learning

Training data:



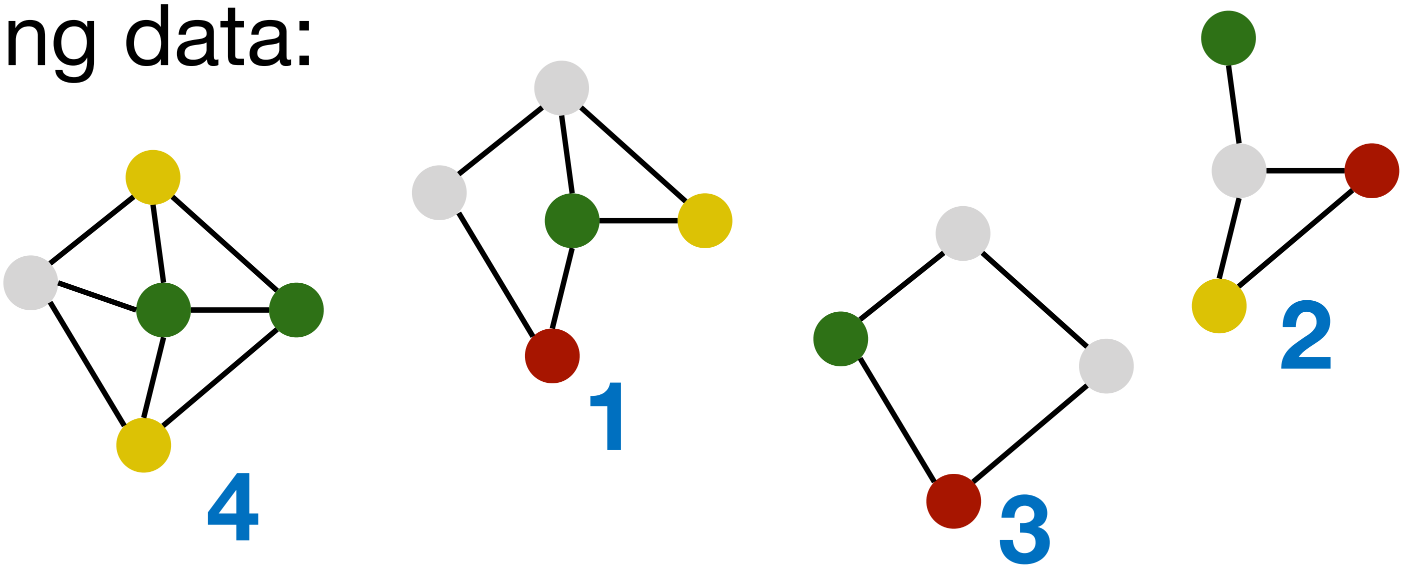
$$\min_{f \in \mathcal{F}} \frac{1}{N} \sum_{i=1}^{N} \ell(f(x_i), g(x_i))$$

"Learn" function



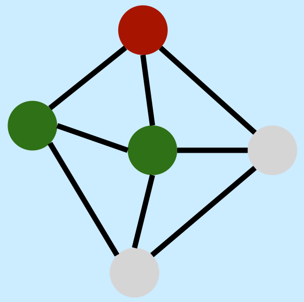
Learning

Training data:

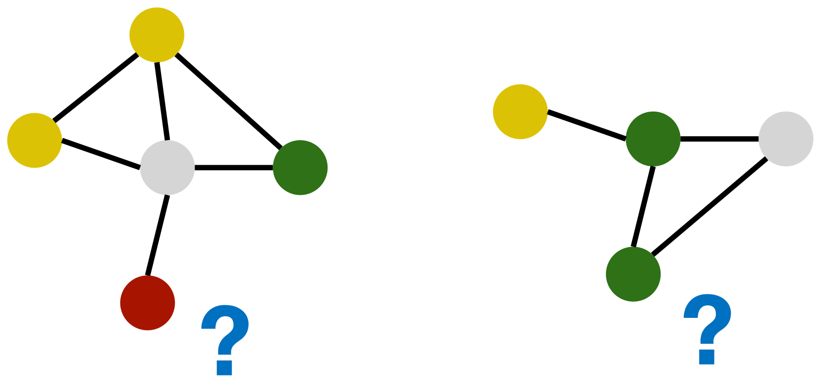


$$\min_{f \in \mathcal{F}} \frac{1}{N} \sum_{i=1}^{N} \ell(f(x_i), g(x_i))$$

"Learn" function

$\hat{f}($  $) =$ *predicted label*

Test data:



Evaluation: generalization

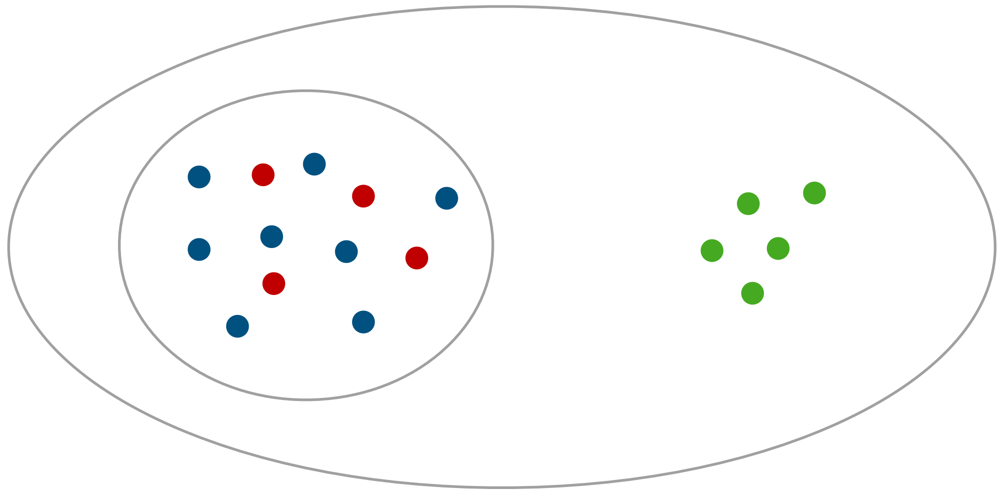
$$\mathbb{E}_{x \sim P}[\,\ell(f(x), g(x))\,]$$

Outline

- Graph Neural Networks

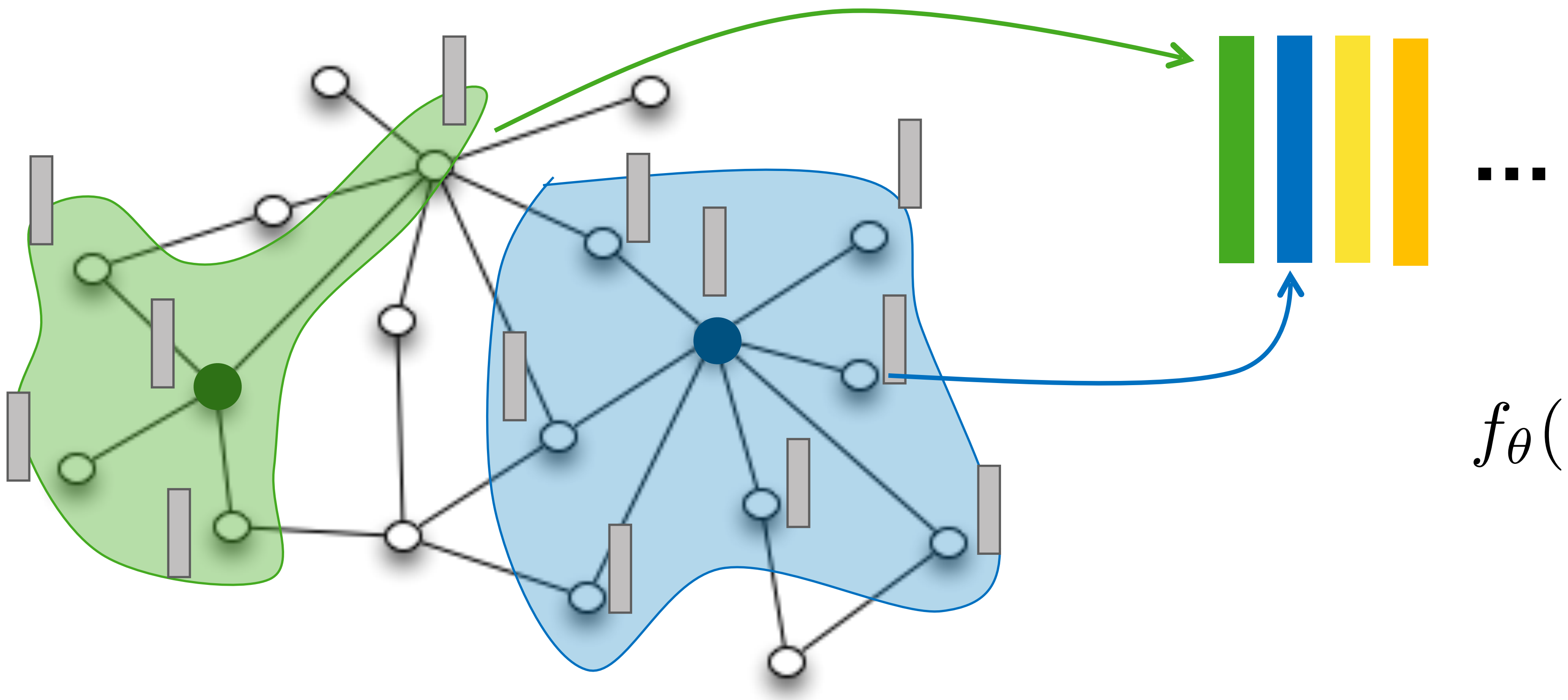
- **To what kinds of instances will my model generalize?**
  Prediction under distribution shifts
  - stability: measuring data shifts appropriately
  - large shifts: understanding model behavior by decomposition

- Beyond regression: extending set functions as loss functions for neural networks



(Message passing) Graph neural networks

Input: graph G with node attributes $x_v \in \mathbb{R}^{d_0}$, edge attributes $w(u, v) \in \mathbb{R}^{d'}$



$$f_\theta(G) = f_{\mathrm{Read}}(\{\!\{h_v \mid v \in V\}\!\})$$

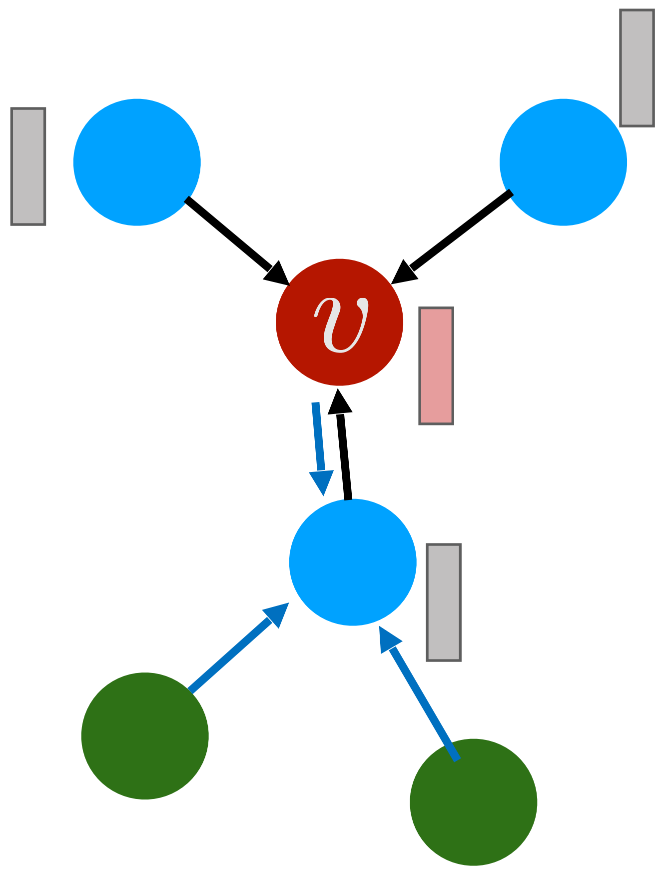
$$\in \mathbb{R}^{d_{\mathrm{out}}}$$

Idea:

1. Encode each node (node's neighborhood): *node embedding*
2. Aggregate *set* of node embeddings into a *graph embedding*

Node embedding: message passing

$$h_v^{(0)} = x_v, \ \forall v \in V \qquad h_v^{(t)} \in \mathbb{R}^{d_t}$$



In each round *k*:

Aggregate over neighbors

feature description of node u in round k-1

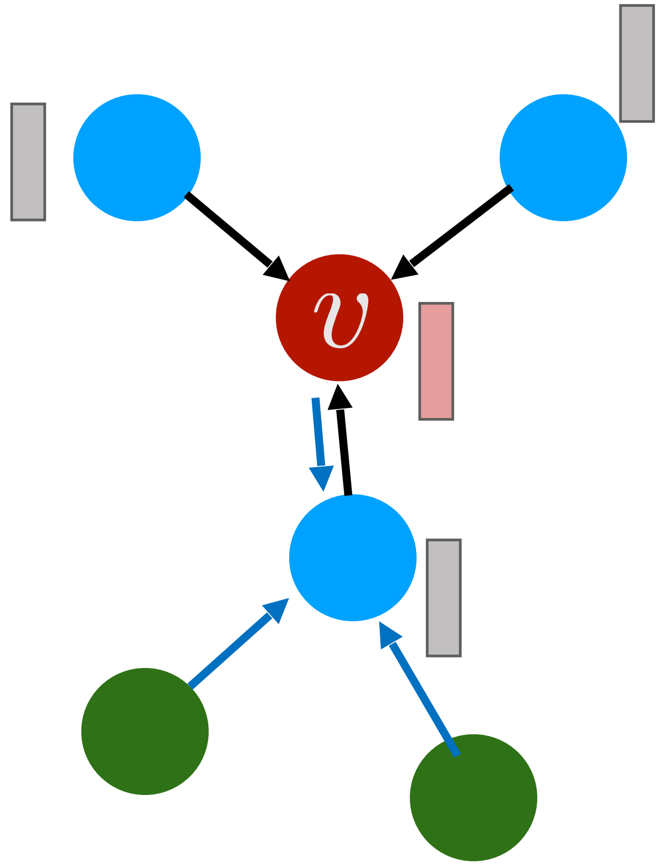
$$m_{\mathcal{N}(v)}^{(k)} = \text{AGGREGATE}^{(k)}\left(\{\!\{h_u^{(k-1)} : u \in \mathcal{N}(v)\}\!\}\right)$$

Update: Combine with current node

$$h_v^{(k)} = \text{COMBINE}^{(k)}\left(h_v^{(k-1)}, m_{\mathcal{N}(v)}^{(k)}\right)$$

(Merkwirth & Lengauer 2005; Scarselli et al 2009; Bruna et al 2014; Dai et al 2016; Battaglia et al., 2016; Defferrard et al., 2016; Duvenaud et al., 2015; Hamilton et al., 2017; Kearnes et al., 2016; Kipf & Welling, 2017; Li et al., 2016; Velickovic et al., 2018; Verma & Zhang, 2018; Ying et al., 2018; Zhang et al., 2018; …)

Node embedding: message passing

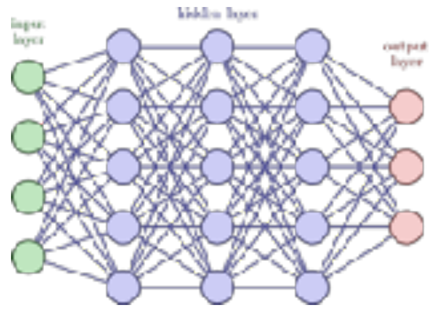


In each round *k*:

Aggregate over neighbors

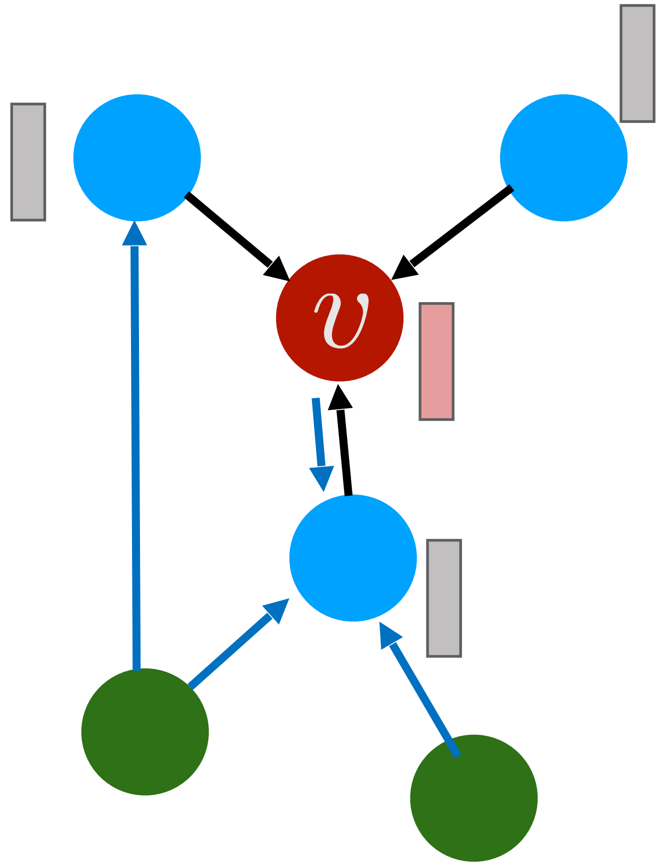
feature description of node u in round k-1

$$m^{(k)}_{\mathcal{N}(v)} = \sum_{v \in \mathcal{N}(u)} \boxed{\mathrm{MLP}^{(k)}}\left(\boldsymbol{h}_u^{(k-1)}, \boldsymbol{h}_v^{(k-1)}, \boldsymbol{w}_{(v,u)}\right)$$



(Merkwirth & Lengauer 2005; Scarselli et al 2009; Bruna et al 2014; Dai et al 2016; Battaglia et al., 2016; Defferrard et al., 2016; Duvenaud et al., 2015; Hamilton et al., 2017; Gilmer et al 2017; Kearnes et al., 2016; Kipf & Welling, 2017; Li et al., 2016; Velickovic et al., 2018; Verma & Zhang, 2018; Ying et al., 2018; Zhang et al., 2018; …)

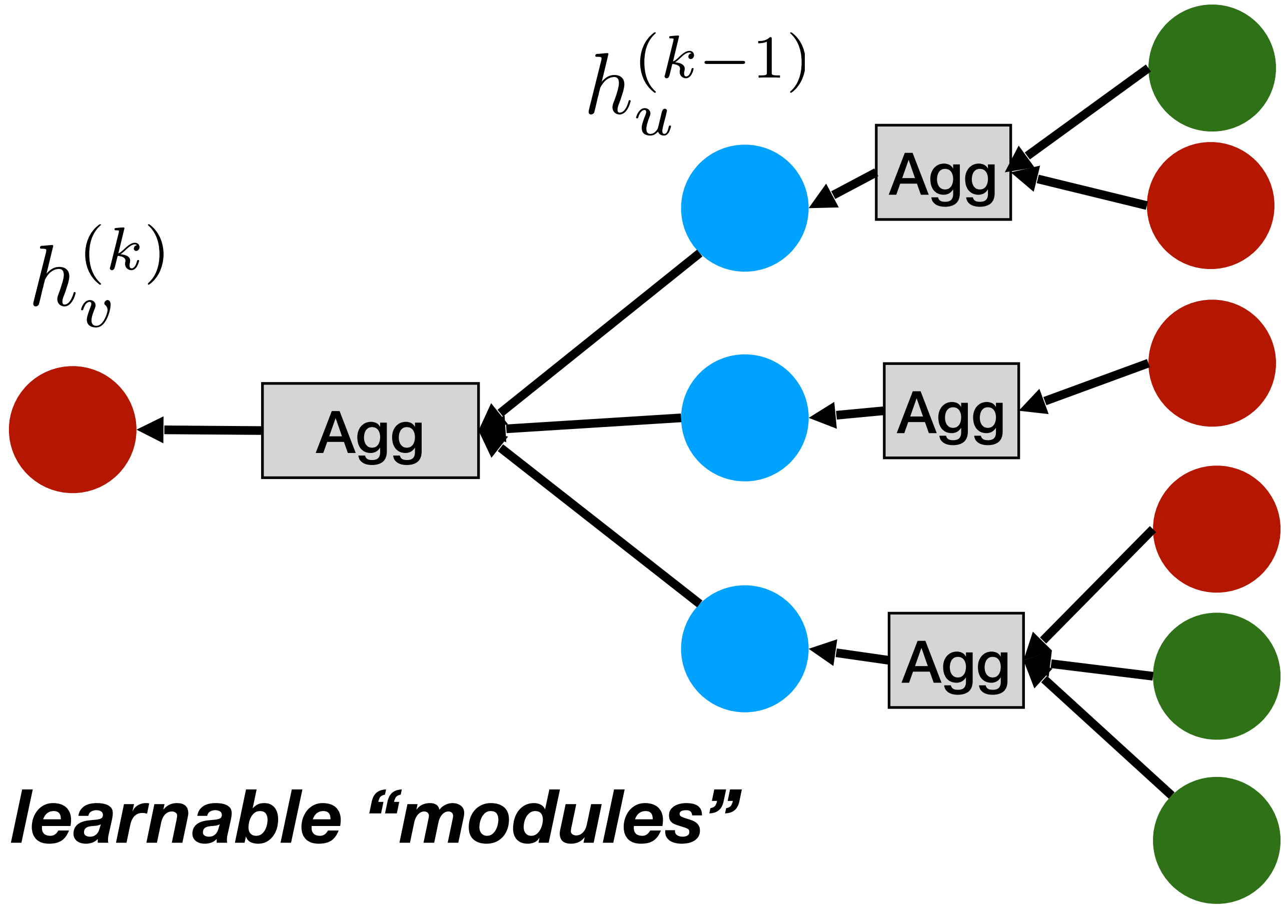
Message passing unrolled



In each round *k*:

Aggregate over neighbors and update representation

"Unrolled": **computation tree**



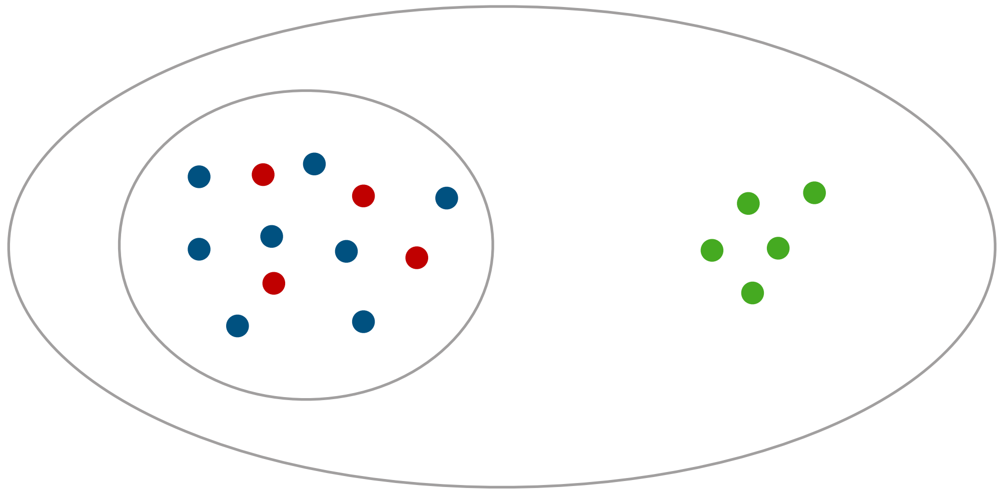
Structured arrangement of learnable "modules"

Outline

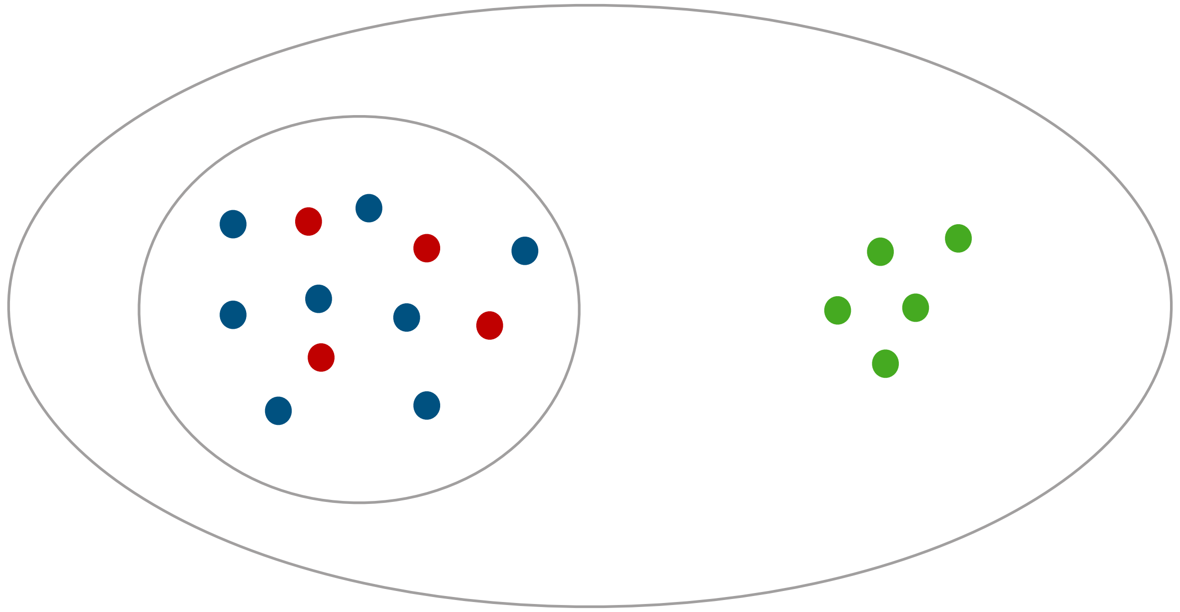
- Graph Neural Networks

- To what kinds of instances will my model generalize?
  Prediction under distribution shifts
  - stability: measuring data shifts appropriately
  - large shifts: understanding model behavior by decomposition

- Beyond regression: extending set functions as loss functions for neural networks

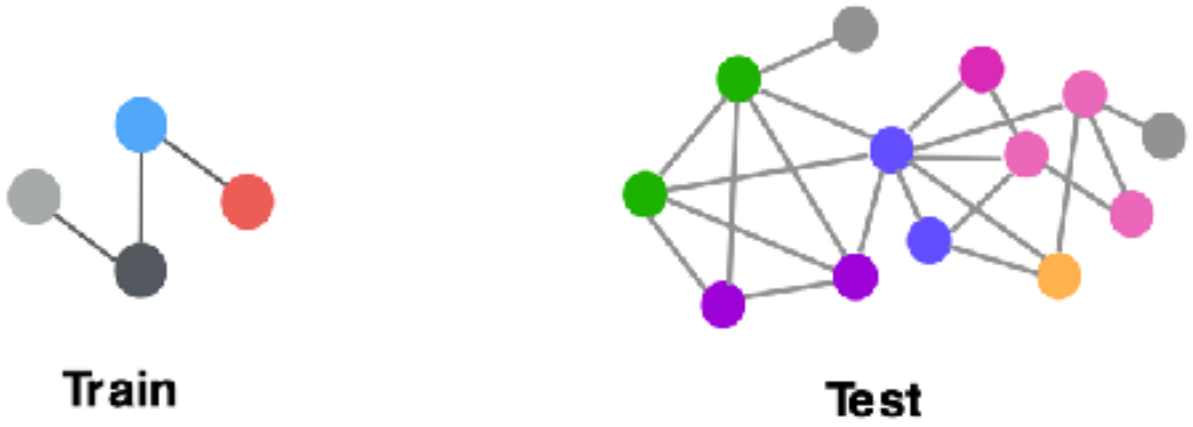


Graph predictions and distribution shifts

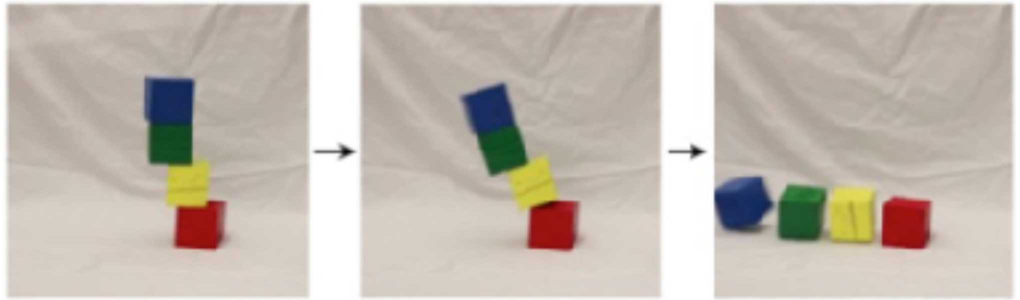


$$\mathbb{E}_{x\sim\mathcal{Q}}\left[\ell(f_\theta(x), g(x))\right]$$

$$\text{support}(Q) \supset \text{support}(\text{training dist})$$



different *graph size,*
graph structure, edge weights, …
(Battagalia et al 2018, Dai et al 2018, Velickovic et al 2020)



Physical reasoning
different position, mass, number of objects

Big picture: when may extrapolation "work"?

1) **Data distributions in training and test are sufficiently similar**

    same distribution of computation trees (message passing GNNs) *(Yehudai-Fetaya-Meirom-Chechik-Maron 21)*

    shared underlying structure (spectral GNNs) *(Levie et al 2019, Ruiz et al 2020)*

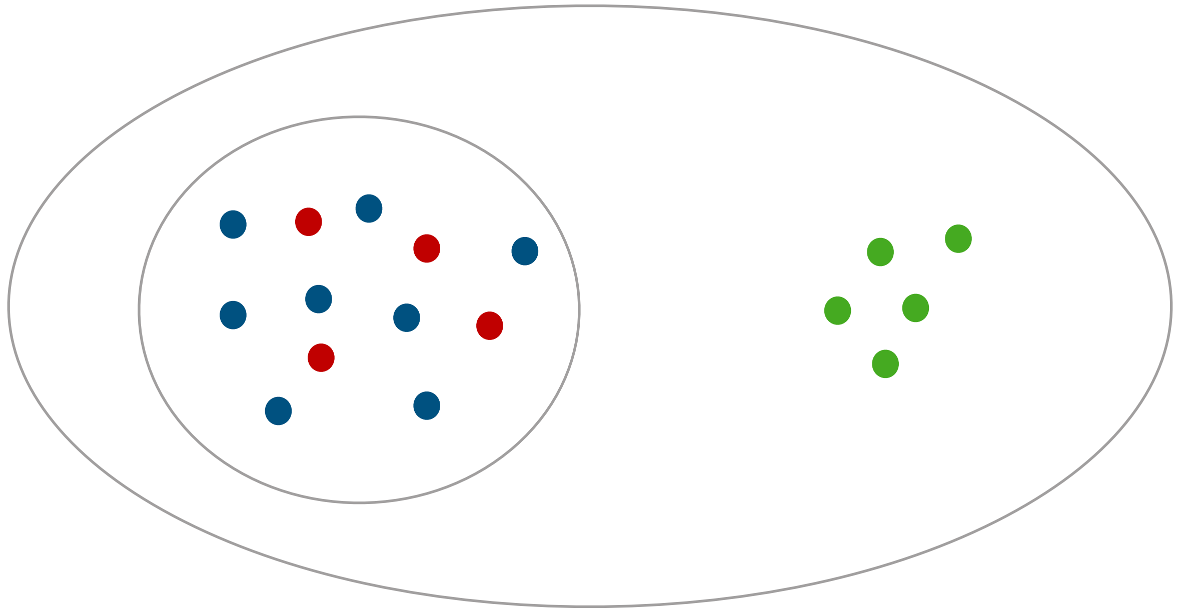
--- or … ---

2) **Understand what the model "learns", and work around that: restrict the model via prior knowledge**

    (Xu-Zhang-Li-Du-Kawarabayashi-Jegelka 21)

Neural network structure, optimization algorithm, data geometry

Graph predictions and distribution shifts



$$\mathbb{E}_{x\sim\mathcal{Q}}\left[\ell(f_\theta(x), g(x))\right]$$

$$\text{support}(Q) \supset \text{support}(\text{training dist})$$

- **Worst-case scenario**: arbitrary predictions on unseen computation trees

Theorem *(Yehudai et al 2021)*: Let $\mathscr{P}$ and $\mathscr{Q}$ be finitely supported distributions on graphs, and $\mathscr{P}^t$, $\mathscr{Q}^t$ the distribution of computation trees at depth t. If any graph in $\mathscr{Q}$ contains a tree in $\mathscr{Q}^t \backslash \mathscr{P}^t$, then there is a GNN with depth at most $t+3$ that perfectly solves the task on $\mathscr{P}$ but has arbitrarily large error on all graphs from $\mathscr{Q}$.

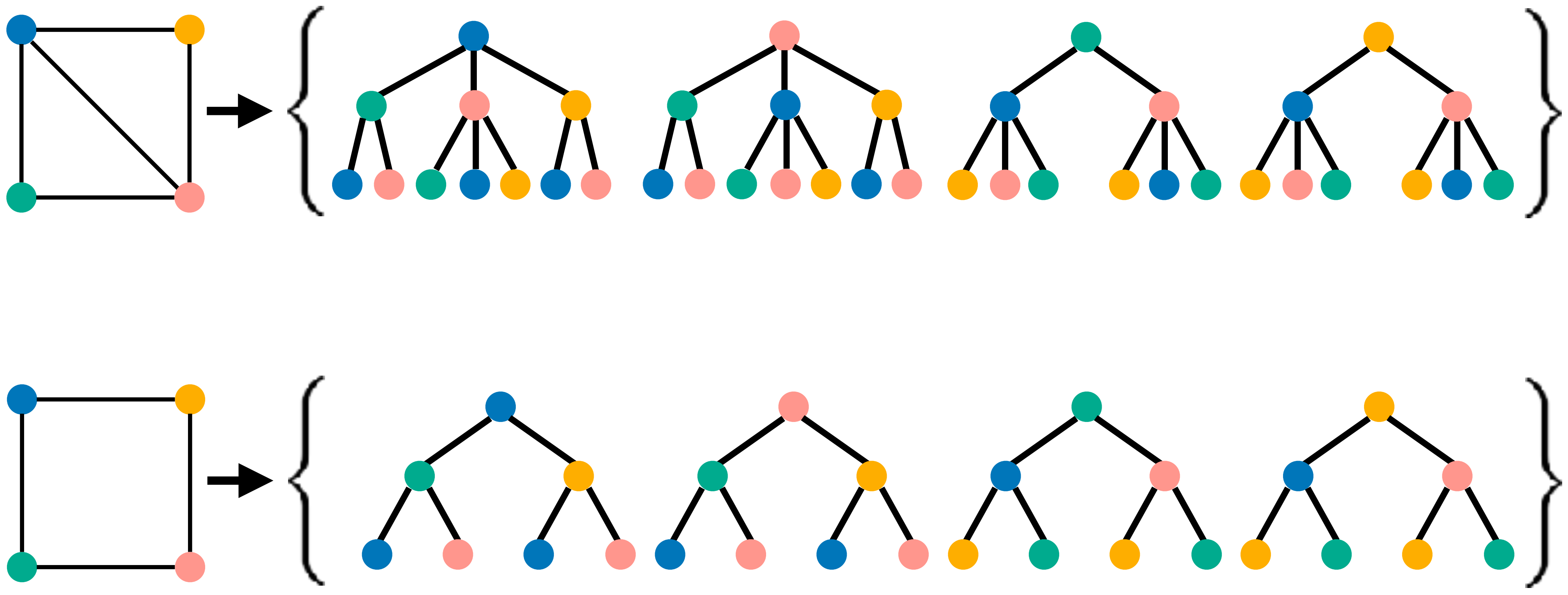
Smoother degrading performance with appropriate metric on graphs?

Stability and measuring perturbations: Tree mover's distance

C. Chuang, S. Jegelka. Tree Mover's Distance: Bridging Graph Metrics and Stability of Graph Neural Networks. NeurIPS, 2022

An appropriate metric?

- Metric should capture Lipschitz/stability properties of GNNs, including invariances



- Message passing GNN compares sets of computation trees (subtree patterns)
- Idea: Optimal transport distance

Tree mover's distance

- Earth mover's distance between sets in Euclidean space:

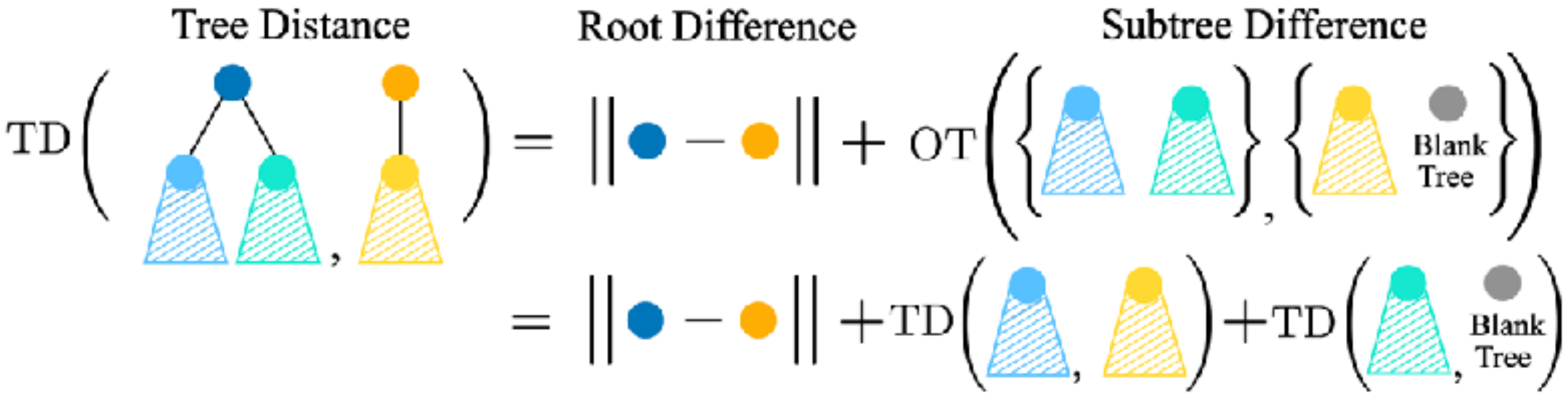
$$\min_{\gamma \in \Gamma(X,Y)} \sum_{i,j=1}^{n,m} \boxed{d(x_i, y_j)} \cdot \gamma_{ij}$$

$$\Gamma(X,Y) = \{\gamma \in \mathbb{R}_+^{n\times m} \mid \gamma \mathbf{1}_m = \mathbf{1}_n;\ \gamma^\top \mathbf{1}_n = \mathbf{1}_m\}$$

Distance between vectors

- Tree mover's distance: x_i, x_j are trees.
  Distance between trees?

Tree Distance via Hierarchical OT



$$\mathbf{TD}_w(T_a, T_b) := \begin{cases} \|x_{r_a} - x_{r_b}\| + w(L) \cdot \mathbf{OT}_{\mathrm{TD}_w}(\rho(\mathcal{T}_{r_a}, \mathcal{T}_{r_b})) & \textit{if } L > 1 \\ \|x_{r_a} - x_{r_b}\| & \textit{otherwise}, \end{cases}$$

Recursive!

where $L = \max(\mathrm{Depth}(T_a), \mathrm{Depth}(T_b))$ and $w : \mathbb{N} \rightarrow \mathbb{R}^+$ is a depth-dependent weighting function.

Properties & implications of Tree mover's distance

- pseudo-metric: distinguishes the same graphs as the color refinement / Weisfeiler-Leman algorithm and GNNs, but graded: same "invariances"!

- relation to stability of GNNs: Lipschitz constant of GNN (GIN)

$$\|h(G_a) - h(G_b)\| \leq \prod_{l=1}^{L+1} K_\phi^{(l)} \cdot \mathrm{TMD}_w^{L+1}(G_a, G_b)$$

- use TMD in cross-domain generalization bound *(Shen et al, 2018)*:

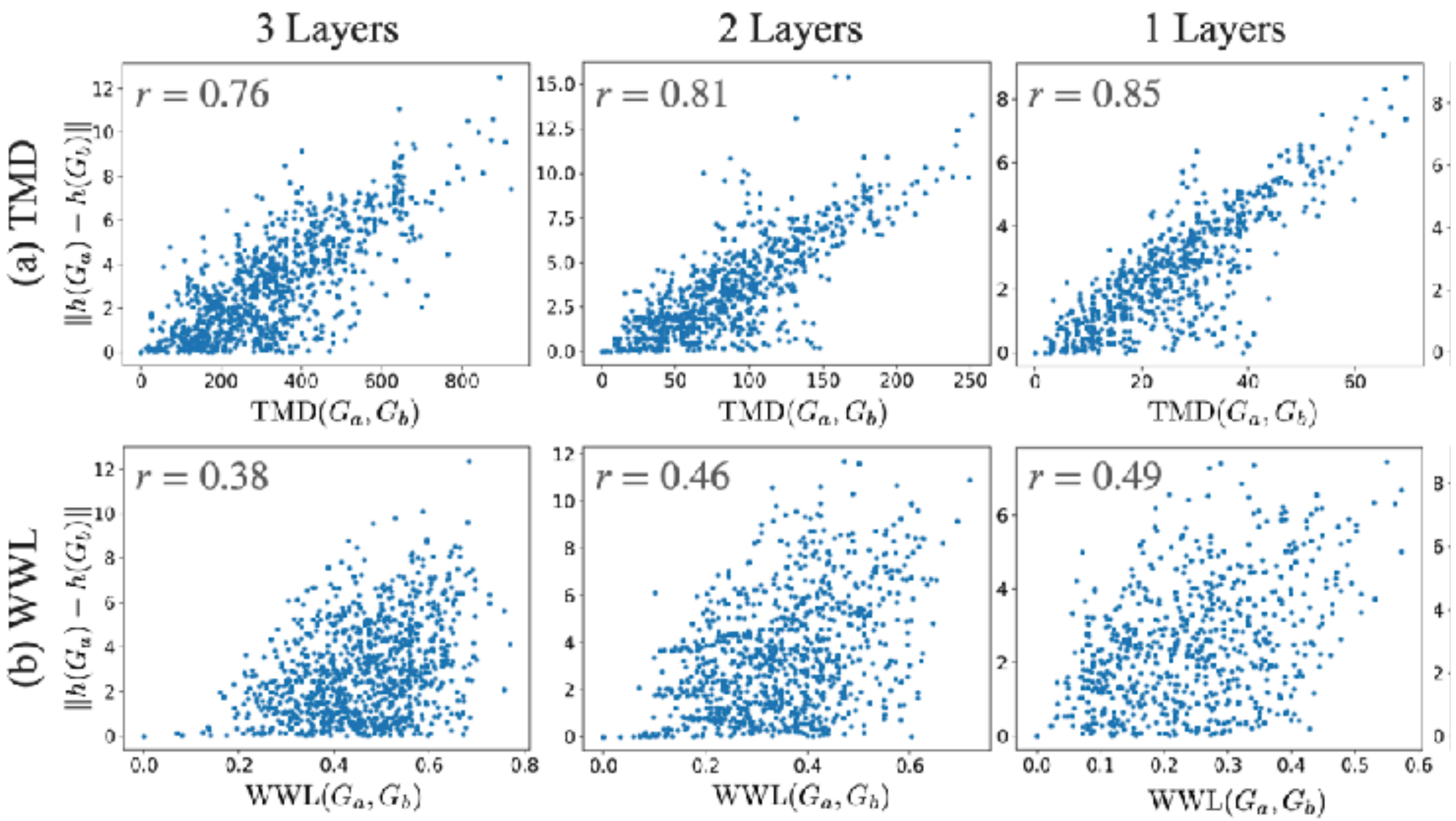
$$\underbrace{R_T(h)}_{\text{Target Risk}} \leq \underbrace{R_S(h)}_{\text{Source Risk}} + 2\mathrm{Lip}(h) \cdot \underbrace{\mathcal{W}_1(p_S, p_T)}_{\text{Domain Discrepancy}} + \text{small value}$$

$$\inf_{\pi \in \Pi(p_S, p_T)} \int \mathrm{TMD}_w^{L+1}(G_a, G_b) d\pi(G_a, G_b)$$

Empirically

- comparison with Wasserstein Weisfeiler-Leman metric *(Togninalli et al 2019)*

1. **stability:**



MUTAG data,
randomly sampled pairs

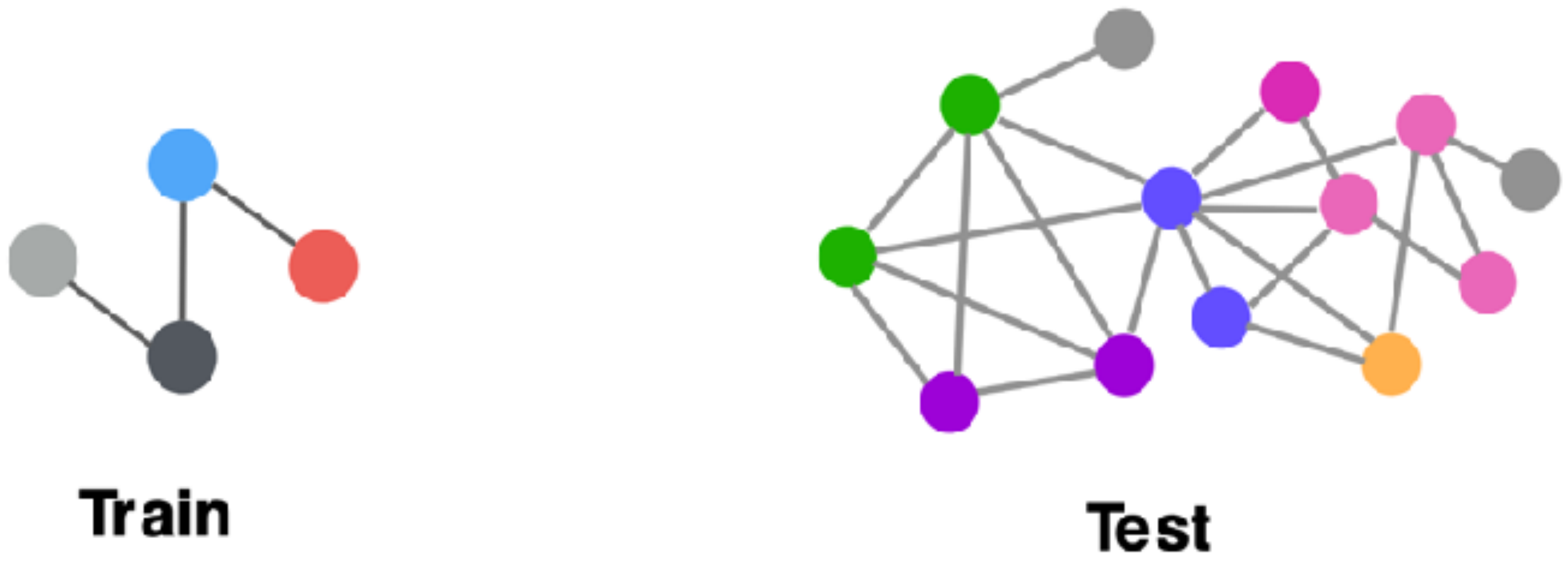
2. correlation with **accuracy drops under domain shifts** (PTC data):

WWL: 0.489
TMD: 0.712

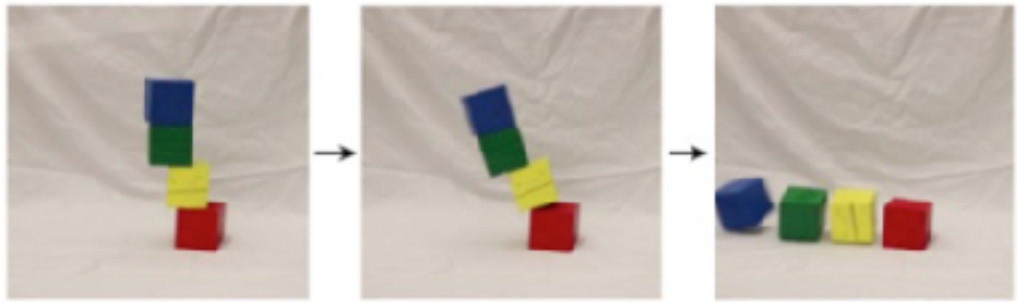
Large perturbations: inductive biases

K. Xu, J. Li, M. Zhang, S. Du, K. Kawarabayashi, S. Jegelka. How Neural Networks Extrapolate: From Feedforward to Graph Neural Networks. ICLR, 2021.

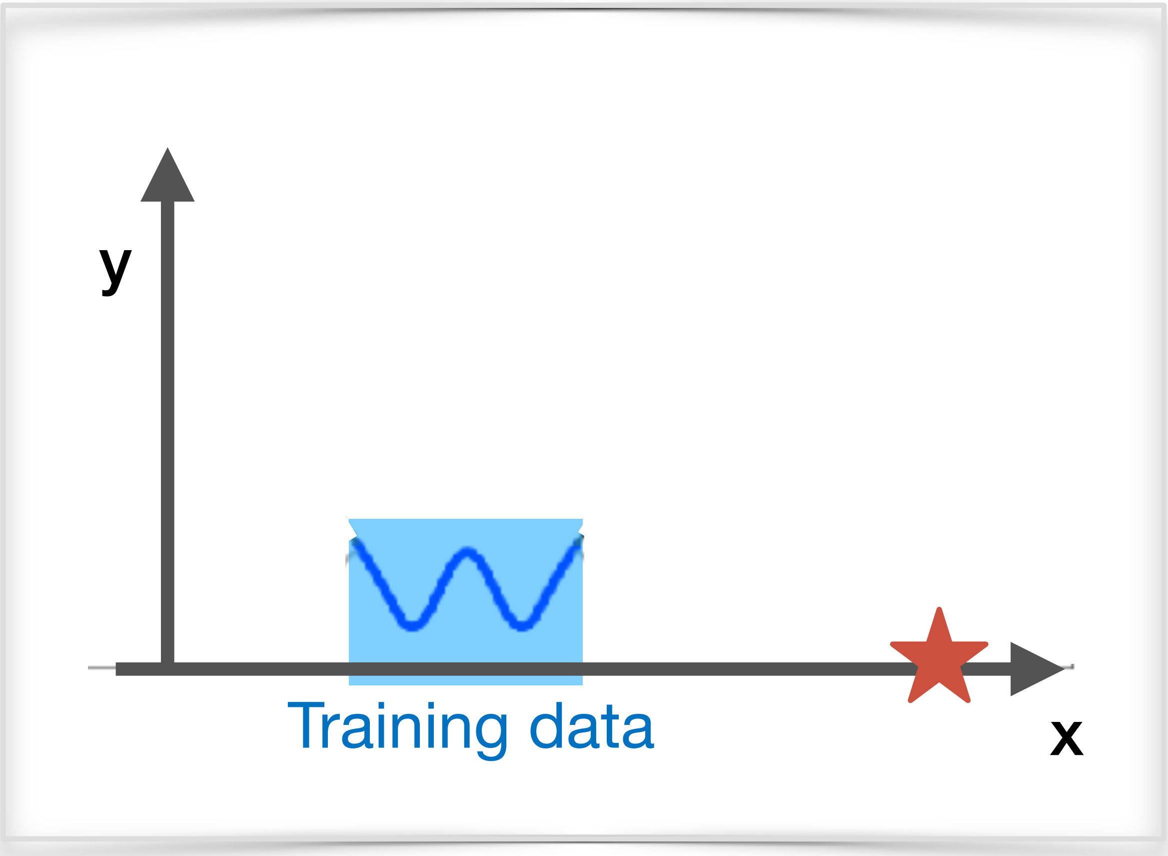
Generalization to very different data



different *graph size,*
graph structure, edge weights, …
(Battagalia et al 2018, Dai et al 2018, Velickovic et al 2020)



Physical reasoning
different position, mass, number of objects



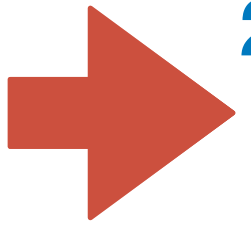
Big picture: when may extrapolation “work”?

1) **Data distributions in training and test are sufficiently similar**

same distribution of computation trees (message passing GNNs) *(Yehudai-Fetaya-Meirom-Chechik-Maron 21)*

shared underlying structure (spectral GNNs) *(Levie et al 2019, Ruiz et al 2020)*

--- or … ---

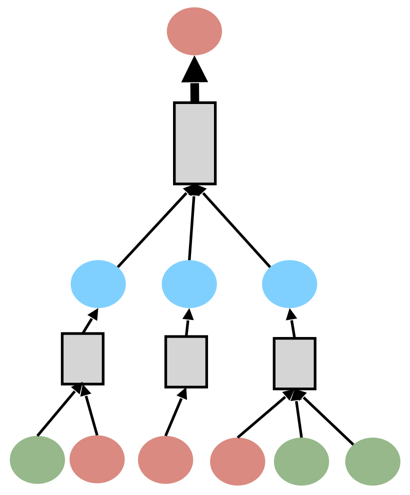


2) **Understand what the model “learns”, and work around that: restrict the model via prior knowledge**
(Xu-Zhang-Li-Du-Kawarabayashi-Jegelka 21)

Neural network structure, optimization algorithm, data geometry

Neural network architecture and algorithms

- Algorithm = structured arrangement of subroutines
- (Graph) Neural network = structured arrangement of learnable "modules"



Bellman-Ford

for k = 1 ... |S| - 1:

for u in S:

$d[k][u] = \min_v d[k-1][v] + cost(v, u)$

GNN

for k = 1 ... GNN iter:

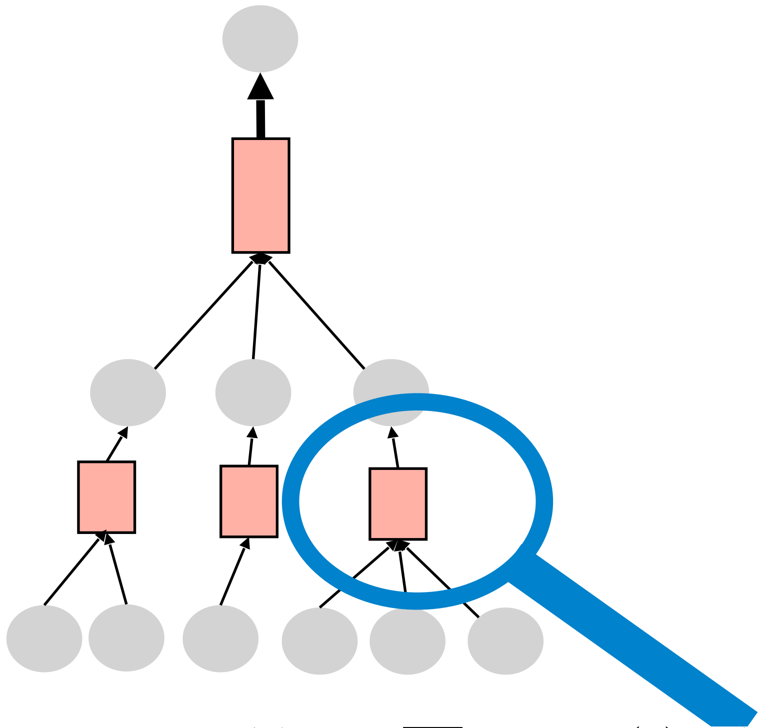
for u in S:

$h_u^{(k)} = \Sigma_v MLP(h_v^{(k-1)}, h_u^{(k-1)})$

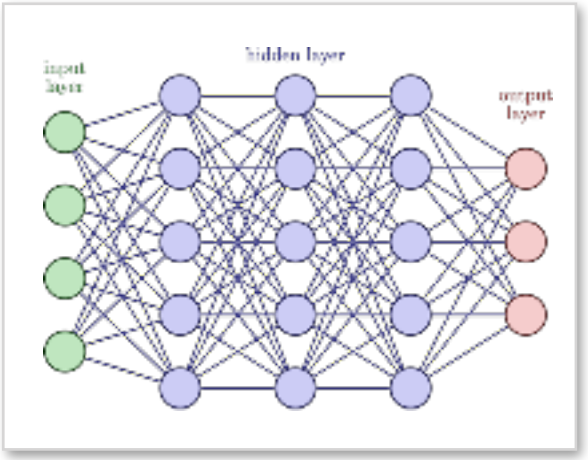
Algorithmic Alignment:

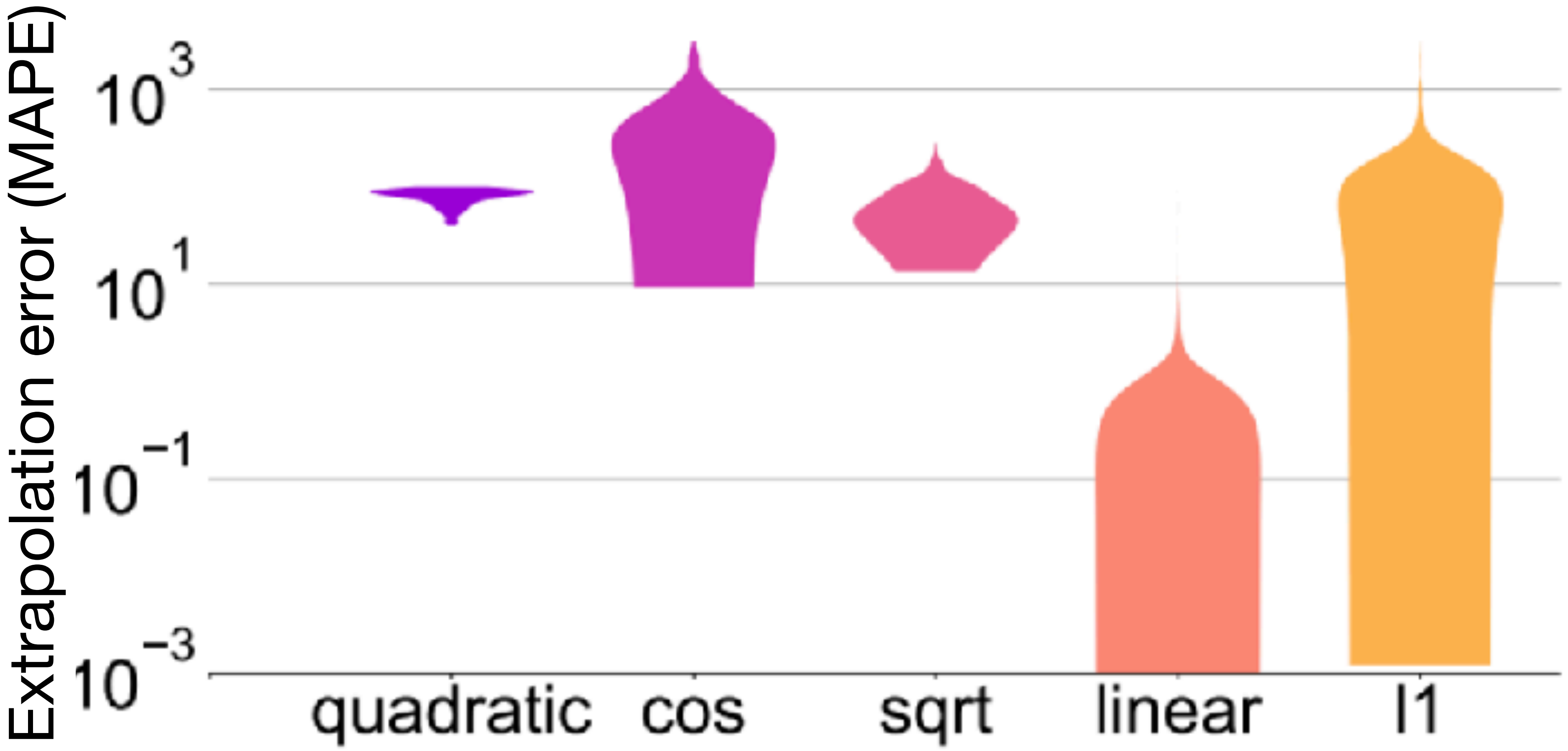
Neural Network can mimic algorithm via *few, easy-to-learn* "modules"

Empirically: MLP with ReLU activations

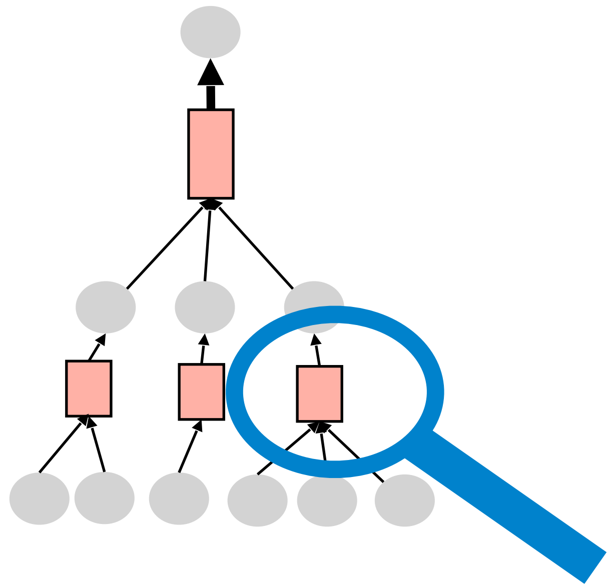


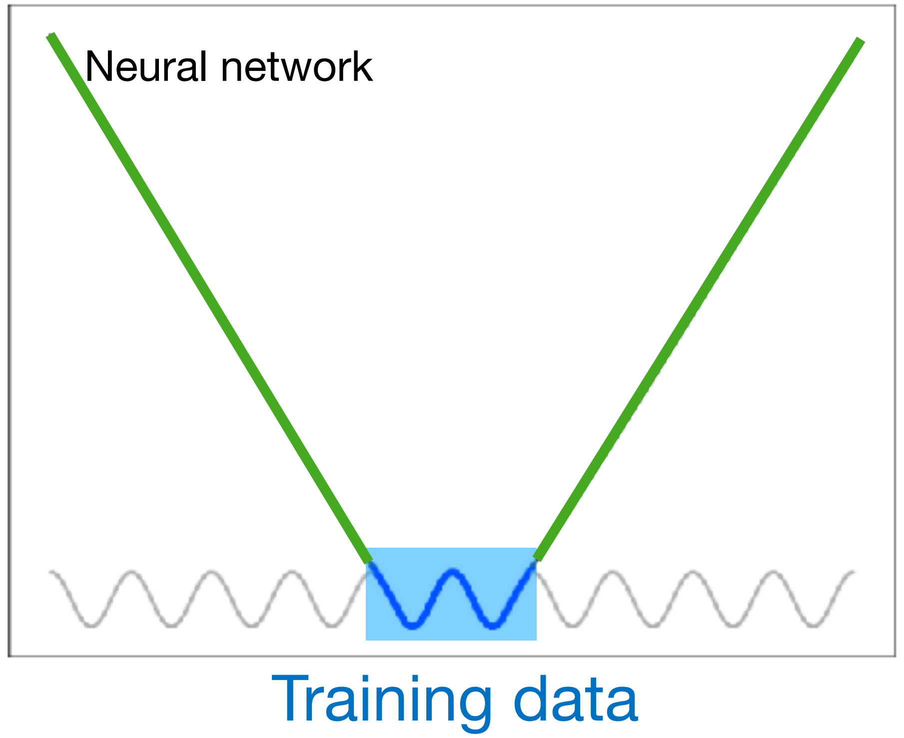
$$h_{v_i}^{(k)} = \sum_{v_j \in \mathcal{N}(i)} \mathrm{MLP}^{(k)}\left(h_{v_i}^{(k-1)}, h_{v_j}^{(k-1)}\right)$$

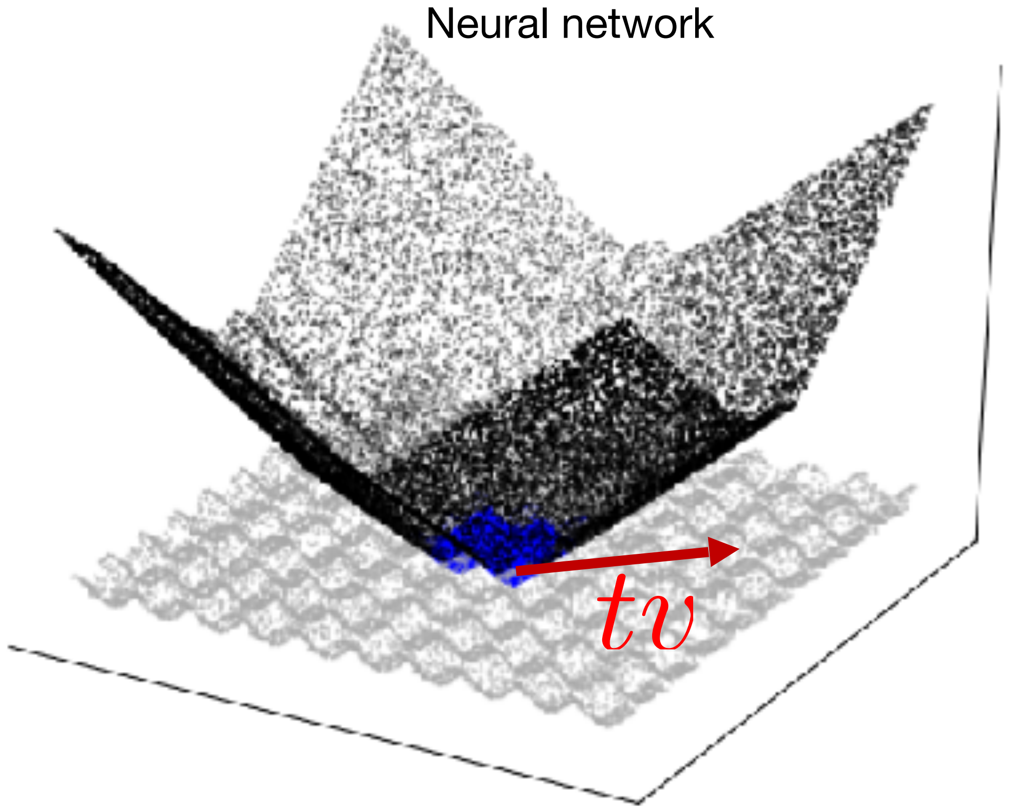




Extrapolation in fully connected ReLU networks



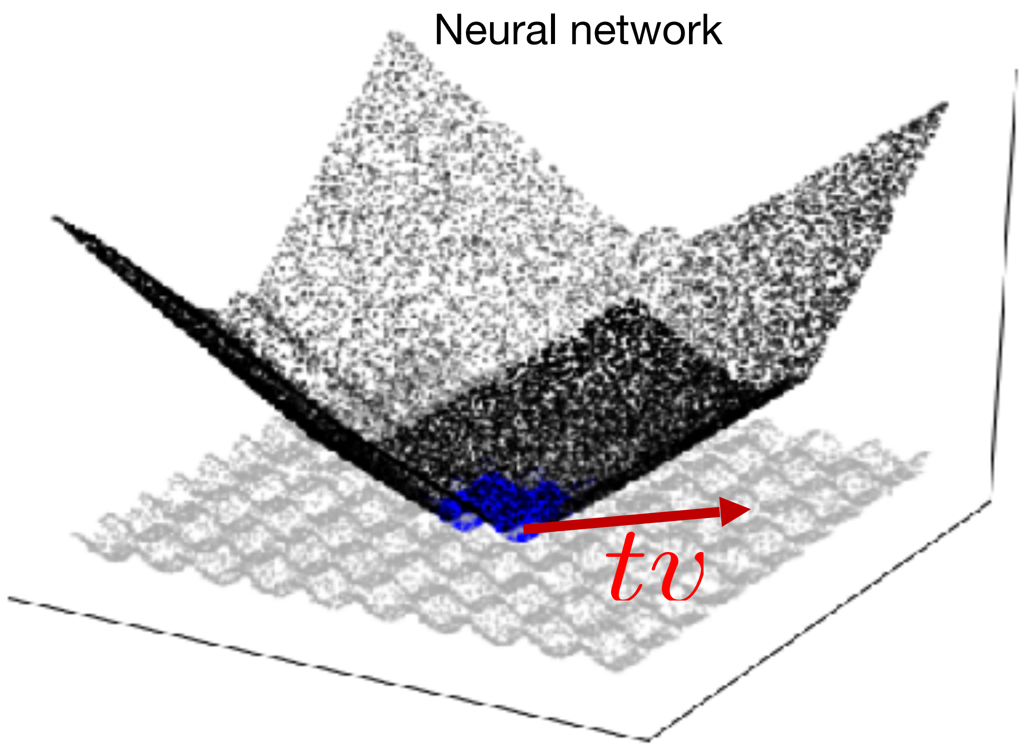




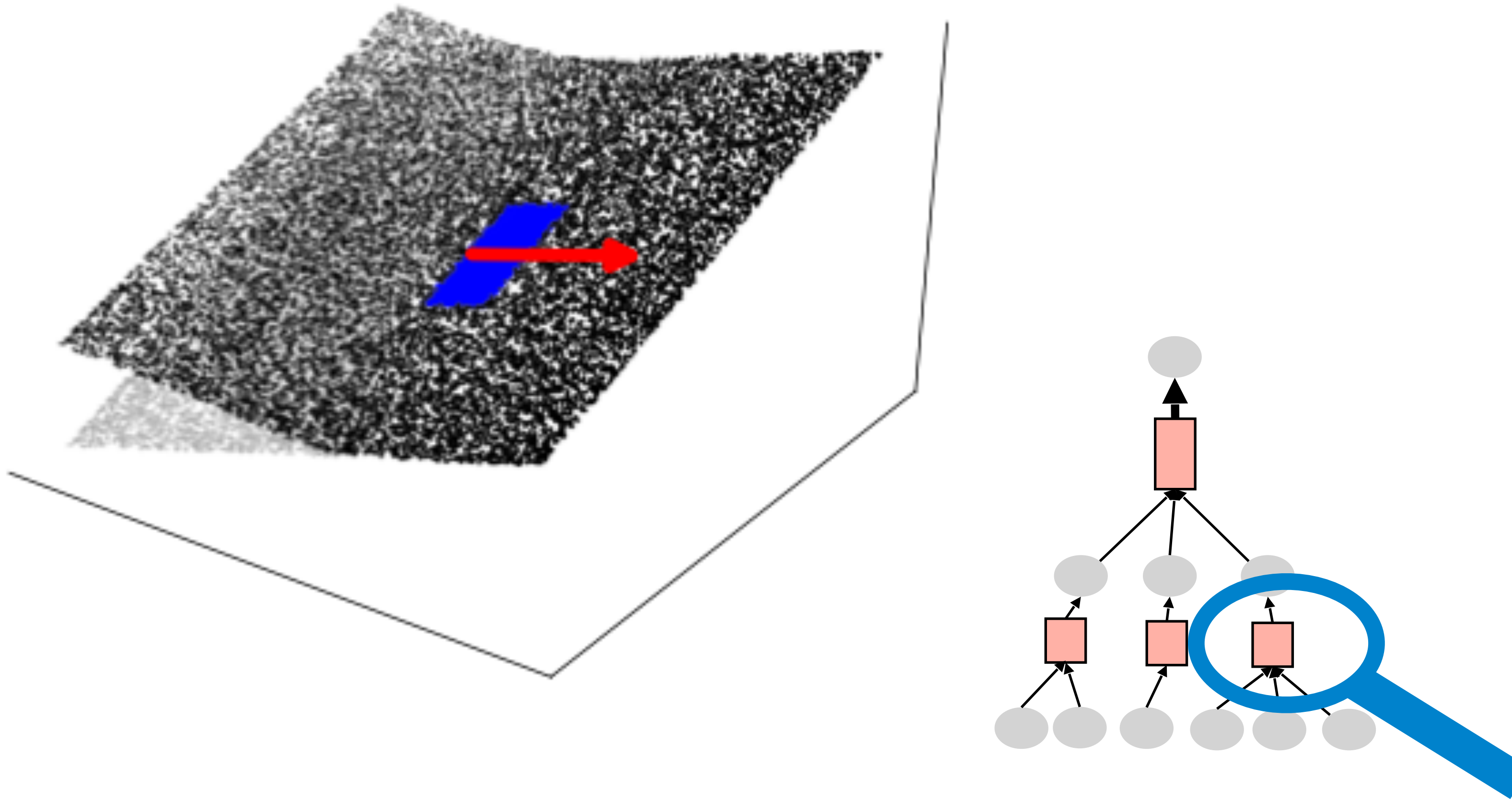
Theorem *(Xu-Zhang-Li-Du-Kawarabayashi-J 21)*
Let f be a 2-layer ReLU MLP trained with Gradient Descent. Along any direction $v \in \mathbb{R}^d$ f approaches a linear function: let $x = tv$. As $t \to \infty$: $f(x + hv) - f(x) \to \beta_v h$ with rate $O(1/t)$.

(Linear regions: Montufar et al 2014, Arora et al 2018, Hanin & Rolnick, 2019; Hein et al., 2019, XZDKJ20)

Implications



1. Can only extrapolate linear functions



2. Training Data geometry

Implications for the full GNN

Shortest Path: (target)

$$\text{dist}[k][v] = \boxed{\min_{u \in \mathcal{N}(v)}} \text{dist}[k-1][u] + w(u,v)$$

Need MLP to be nonlinear!

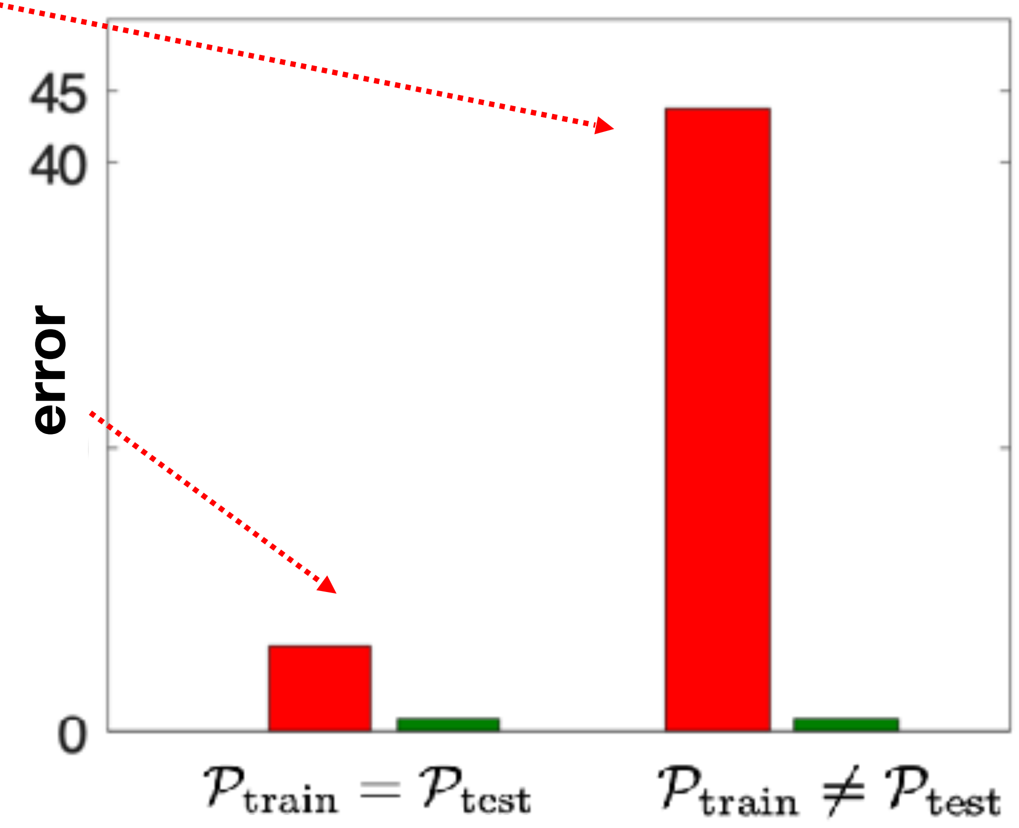
GNN:

$$h_v^{(k)} = \boxed{\sum_{u \in \mathcal{N}(v)}} \text{MLP}\left(h_u^{(k-1)}, h_v^{(k-1)}, w(u,v)\right)$$

GNN II:

(Veličkovic et al 2020)

$$h_v^{(k)} = \boxed{\max_{u \in \mathcal{N}(v)}} \text{MLP}\left(h_u^{(k-1)}, h_v^{(k-1)}, w\right.$$



larger graphs

Implications for the full GNN

Shortest Path: (target)

$$\text{dist}[k][v] = \boxed{\min_{u \in \mathcal{N}(v)}} \text{dist}[k-1][u] + w(u,v)$$

Need MLP to be nonlinear!

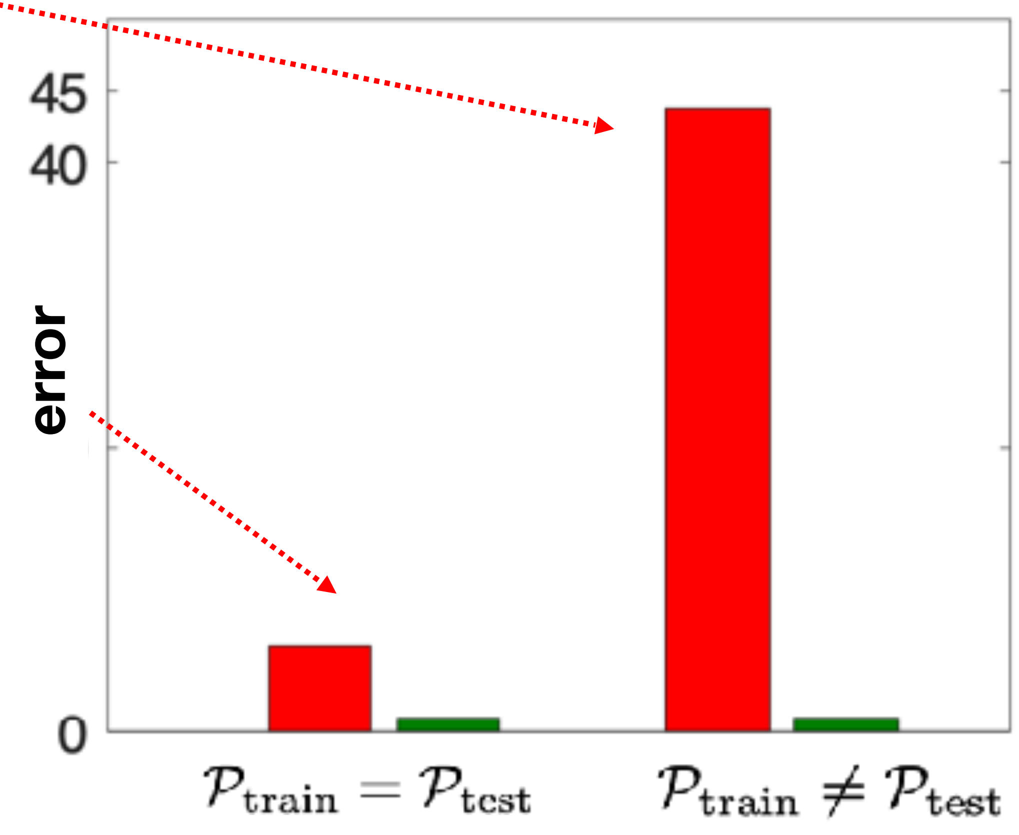
GNN:

$$h_v^{(k)} = \boxed{\sum_{u \in \mathcal{N}(v)}} \text{MLP}(h_u^{(k-1)}, h_v^{(k-1)}, w(u,v))$$

GNN II:

$$h_v^{(k)} = \boxed{\max_{u \in \mathcal{N}(v)}} \text{MLP}(h_u^{(k-1)}, h_v^{(k-1)}, w$$

(Veličkovic et al 2020)



larger graphs

Task-specific nonlinearities help extrapolation.
Empirically reflected in many works
(Trask et al 2018, Johnson et al 2017, Yi et al 2018, Mao et al 2019,Cranmer et al 2019,2020, Veličkovic et al 2020 …)

Encode nonlinearities in the …

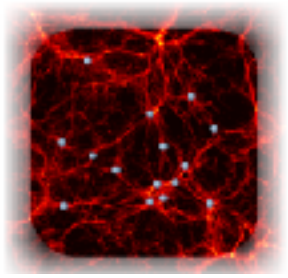
… architecture

NALU: $\mathbf{y} = \mathbf{g} \odot \mathbf{a} + (1 - \mathbf{g}) \odot \mathbf{m}$

$$\mathbf{m} = \exp \mathbf{W}(\log(|\mathbf{x}| + \epsilon)), \ \mathbf{g} = \sigma(\mathbf{G}\mathbf{x})$$

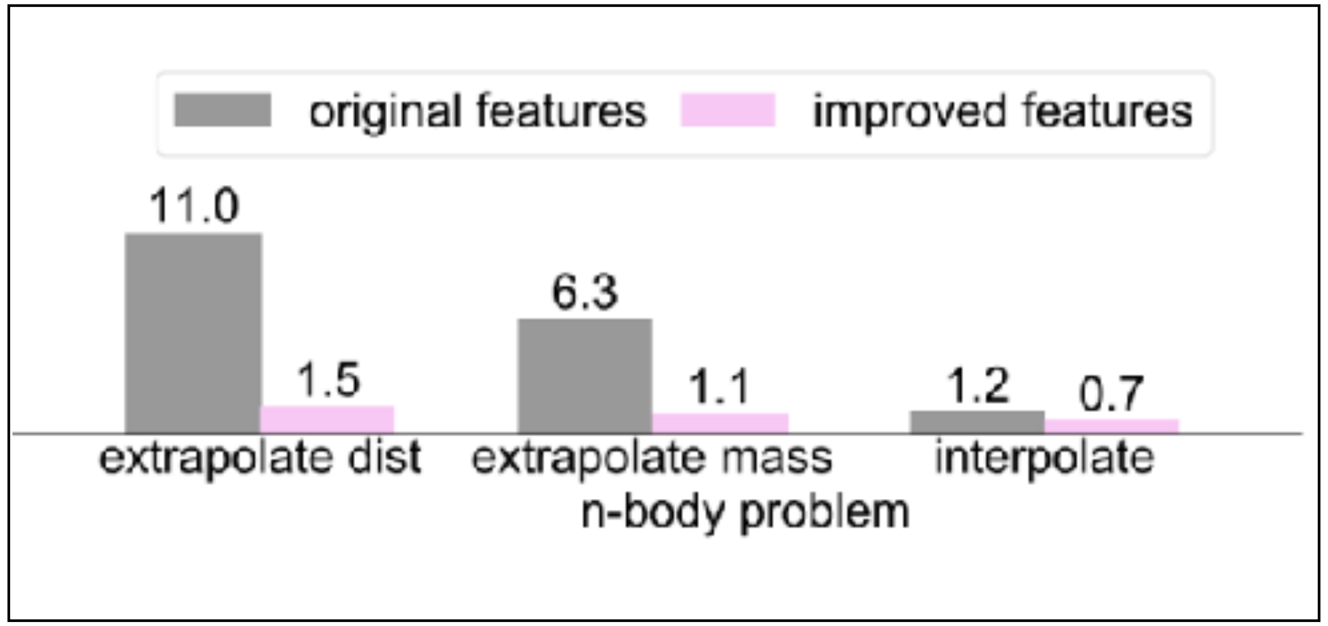
Exp log for learning multiplication
(Trask et al 2018)

Library of programs
(Johnson et al 2017, Yi et al 2018, Mao et al 2019, …)



Learning physics laws
(Cranmer et al 2019,2020)

… input representation



Prior knowledge or representation learning

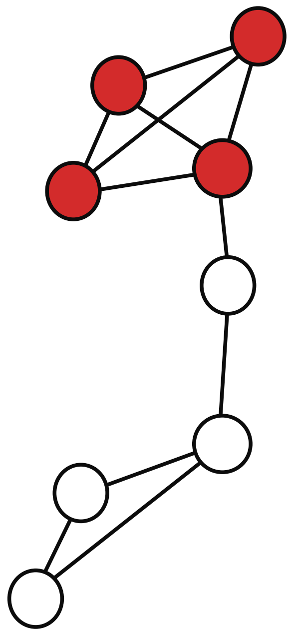
(figure of n-body system: Battaglia et al 2018)

Neural Network Losses from Set Function Extensions

N. Karalias, J. Robinson, A. Loukas, S. Jegelka. Neural set function extensions: learning with discrete functions in high dimensions. NeurIPS, 2022

Setup

- use NN as "solver", and objective function of the optimization problem as a loss
- What if the objective is a set function? $F(S), S \subseteq [n]$



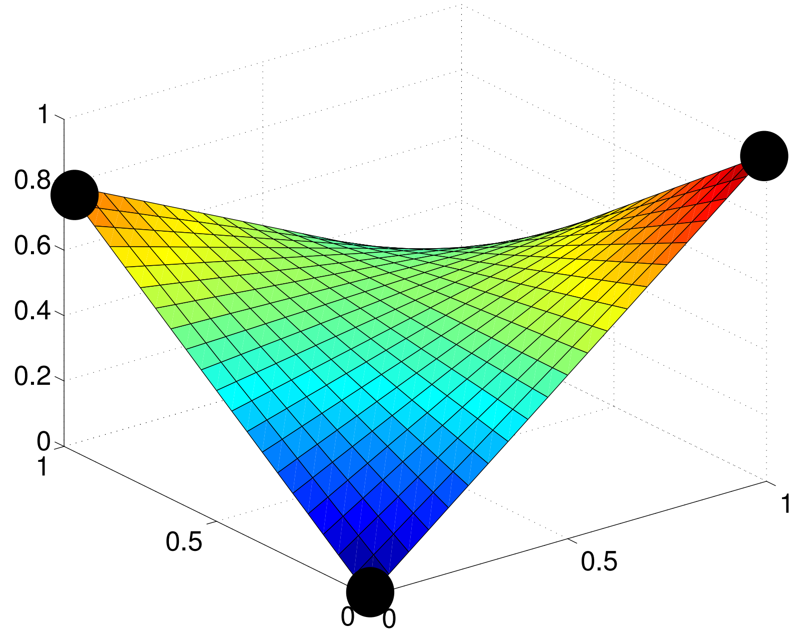
- Continuous extension:

$$F : \{0,1\}^n \to \mathbb{R} \qquad \longrightarrow \qquad f : [0,1]^n \to \mathbb{R}$$

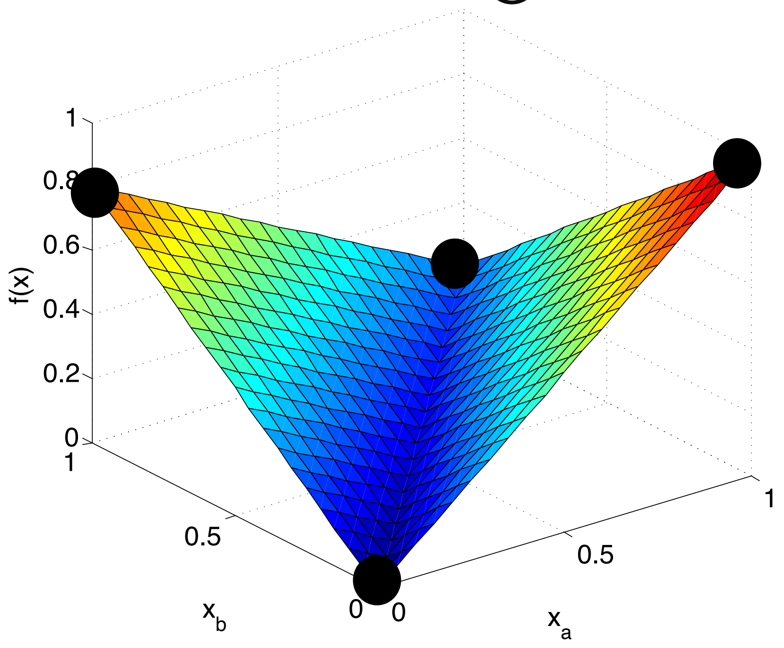
- Want that:
  - f is continuous
  - $f(\mathbf{1}_S) = F(S)$

- Strategy:

$$f(x) = \sum_{S \subseteq [n]} p_x(S) F(S)$$



marginals:
$p_x(i \in S) = x_i$

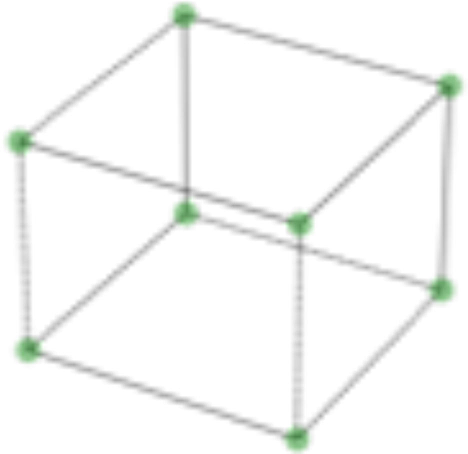


Example: Lovász extension of submodular set function

Extensions: higher-dimensional

NN outputs…

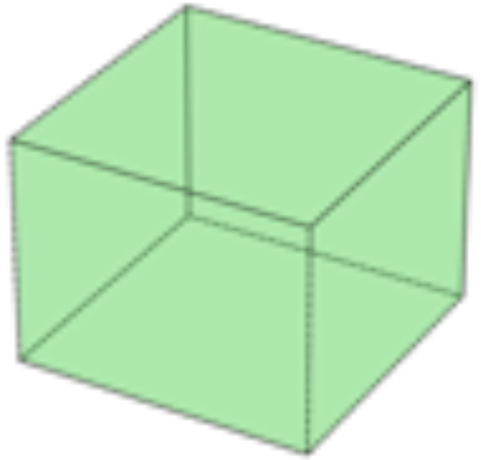
$S \in \{0,1\}^n$



$F(S)$

We want:

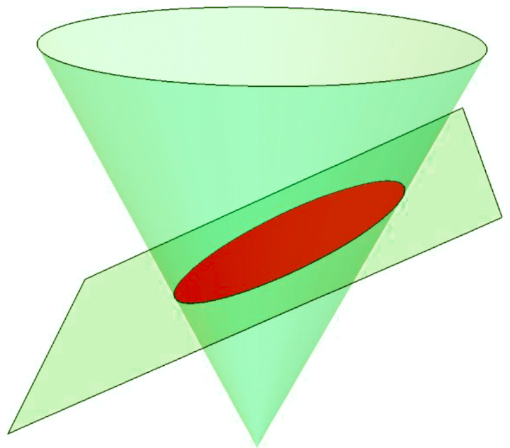
$x \in [0,1]^n$



$$f(x) = \sum_{S \subseteq [n]} p_x(S) F(S)$$

$$f(\mathbf{1}_S) = F(S)$$

$X \in \mathbb{S}_+$



$$f(X) = \sum_{S,T \subseteq [n]} p_X(S,T) F(S \cap T)$$

$$f(\mathbf{1}_S \mathbf{1}_S^\top) = F(S)$$

Derivation in a nutshell

- vector extension for $x \in [0,1]^n$: $p_x(S)$ solution to dual of "f is a convex envelope of F":

$$\min_{\{y_S \geq 0\}_{S \subseteq [n]}} \sum_{S \subseteq [n]} y_S F(S) \qquad \text{s.t.} \qquad \sum_{S \subseteq [n]} y_S \mathbf{1}_S = x, \quad \sum_{S \subseteq [n]} y_S = 1$$

=> **marginals**

$$p_x(i \in S) = x_i$$

Derivation in a nutshell

- vector extension for $x \in [0,1]^n$: $p_x(S)$ solution to dual of "f is a convex envelope of F":

$$\min_{\{y_S \geq 0\}_{S \subseteq [n]}} \sum_{S \subseteq [n]} y_S F(S) \qquad \text{s.t.} \qquad \sum_{S \subseteq [n]} y_S \mathbf{1}_S = x, \quad \sum_{S \subseteq [n]} y_S = 1$$

- use SDP version of this

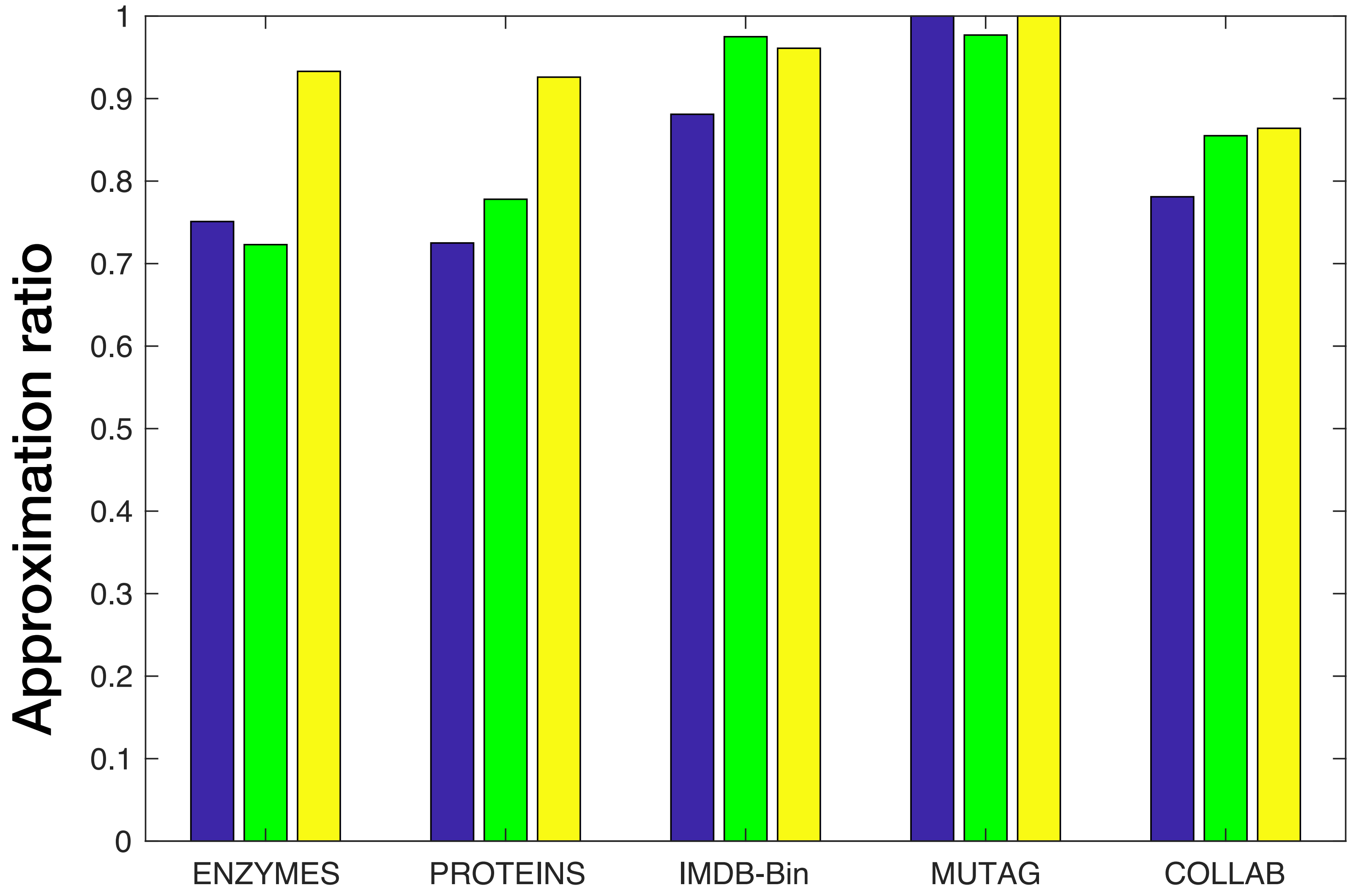
- any valid vector extension leads to a valid matrix extension: Let $X = \sum_i \lambda_i v_i v_i^\top$

$$\sum_{S,T \subseteq [n]} p_X(S,T) F(S \cap T) \qquad \text{with} \qquad p_X(S,T) = \sum_i \lambda_i p_{v_i}(S) p_{v_i}(T)$$

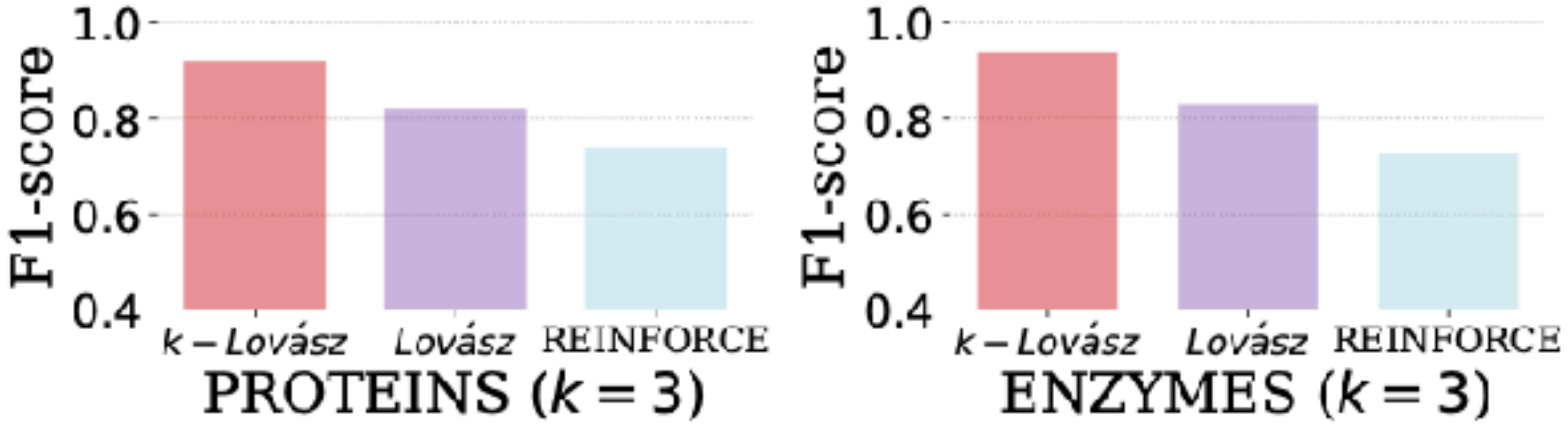
Empirical results

REINFORCE
LOVASZ EXT
MATRIX LOVASZ

max clique



k-clique



GNNs for Learning for Combinatorial Optimization

- Active, recent area, but need to understand learned functions

- To what examples will my models generalize? - understanding the data space.
  metric from the GNN perspective
- What are important architectural choices? - understanding the model.
  nonlinearities and alignment with algorithms

- How to train the model? - choice of loss function.
  higher-dimensional extensions of set functions tend to work better

chat more? stefje@mit.edu