Massachusetts Institute of Technology

Machine Learning for discrete optimization: Graph Neural Networks, generalization under shifts, and loss functions

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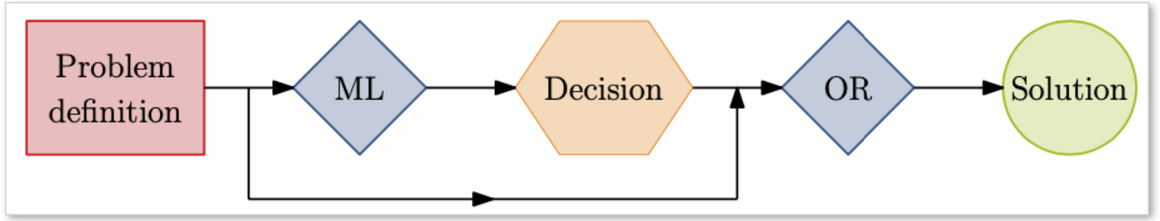
based on joint work with
Keyulu Xu, Ching-Yao Chuang, Nikolaos Karalias, Joshua Robinson, Andreas Loukas, Jingling Li, Mozhi Zhang, Simon S. Du, Ken-ichi Kawarabayashi

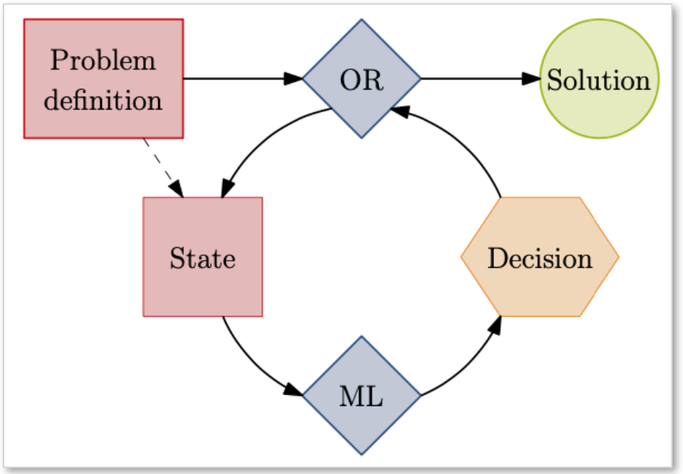
TILOS

Learning and Algorithms

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

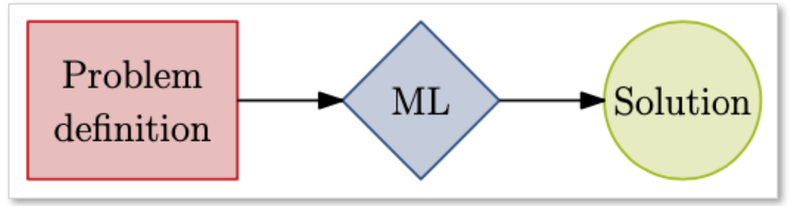


- Predicting problem parameters
  (Amos & Kolter 2017, Wilder et al 2019, Donti et al 2019, Elmachtoub & Grigas 2020, Mandi & Guns 2020, Berthet et al…)



- 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

Learning and Algorithms

- Predicting good configurations / solvers
- Predicting problem parameters
- Machine learning oracles within a fixed algorithm
  (online algorithms, branch-and-bound,…)
- Learning a full algorithm, Algorithm implemented as a neural network

Algorithms with Predictions*

Michael Mitzenmacher† Sergei Vassilvitskii‡

ML4OR-22

AAAI Workshop on Machine Learning for Operations Research

ipam institute for pure & ap

Deep Learning and Combinatorial Optimization

February 22 - 25, 2021

End-to-End Constrained Optimization Learning: A Survey

James Kotary[1] , **Ferdinando Fioretto**[1] , **Pascal Van Hentenryck**[2] and **Bryan Wilder**[3]

Combinatorial Optimization and Reasoning with Graph Neural Networks

Quentin Cappart, Didier Chételat, Elias B. Khalil, Andrea Lodi, Christopher Morris, Petar Veličković

Invited Review

Machine learning for combinatorial optimization: A methodological tour d'horizon

Yoshua Bengio [c, b] ✉, Andrea Lodi [a, b] ✉, Antoine Prouvost [a, b] ✉

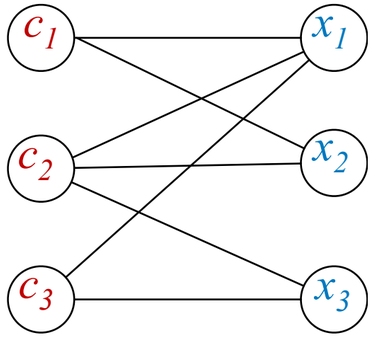
Today:
Some thoughts on learning (for) algorithms

Disclaimer

- Learning for algorithms is still a nascent field
  ("Although most of the approaches […] are still at an exploratory level of deployment […], we strongly believe that this is just the beginning of a new era for combinatorial optimization algorithms." (Bengio et al 2020))
- Not the "latest & greatest" here…
- … but some ideas to better understand ML models' behavior

How to do learning for algorithms?

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

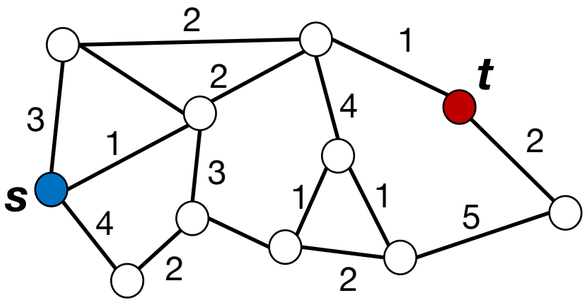


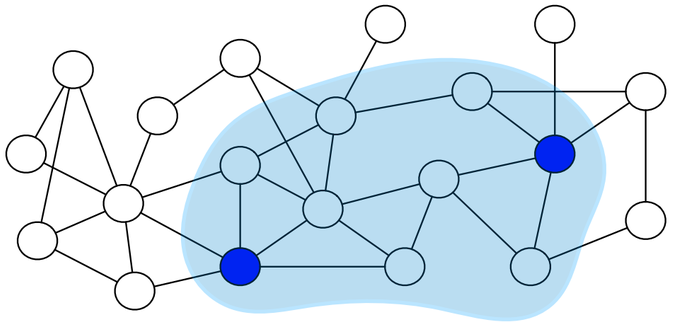
constraints — variables

clauses — variables

(Gasse et al 2019)

(Selsam et al 2018, Yau et al 2023)



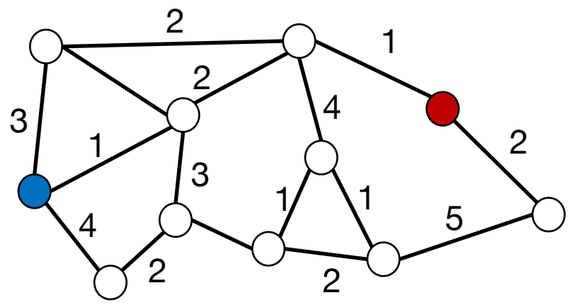


(e.g. Shafi et al 2023)

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*

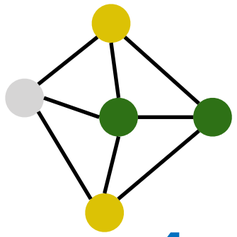
- Goal: find a function $f \in \mathcal{F}$ that *generalizes* (= low “risk”)

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

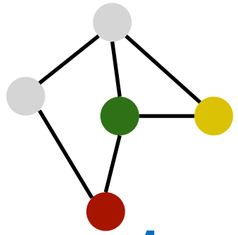
Other aspects:
- learning setting
- loss
- constraints …

Learning

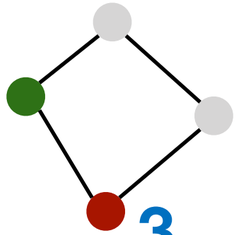
Training data:



4



1



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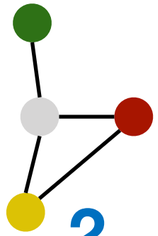
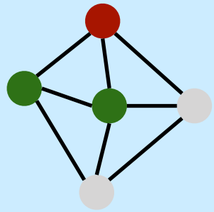


2

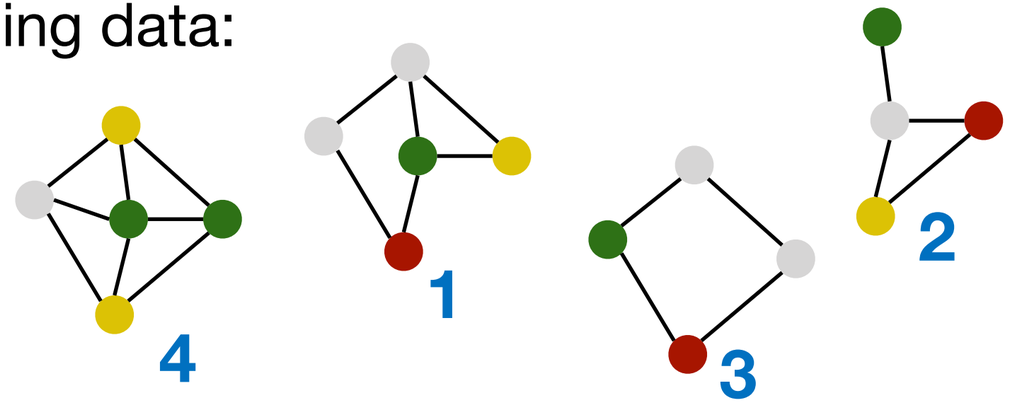
$$\min_{f \in \mathcal{F}} \frac{1}{N} \sum_{i=1}^{N} \ell\big(f(x_i), g(x_i)\big)$$

"Learn" function

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

Learning

Training data:



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

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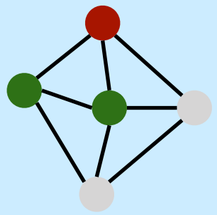
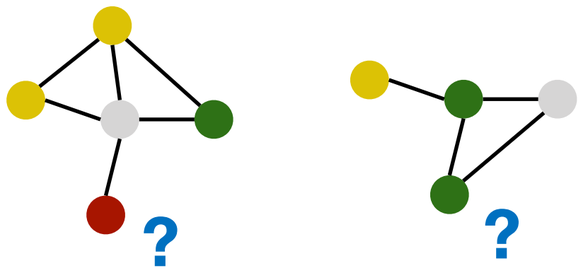
$\hat{f}($  $) =$ *predicted label*

Test data:

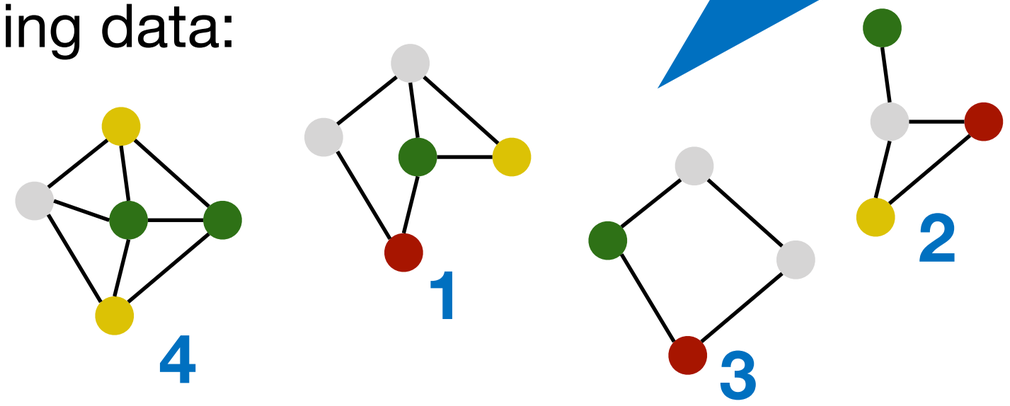


Evaluation: generalization

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

Learning questions

Training data:



2. What training data helps identify the right function?

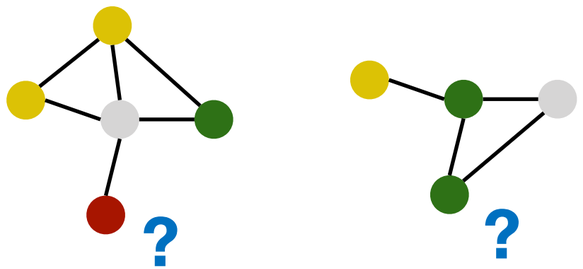
1. What functions can my ML model encode?

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

"Learn" function

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

Test data:



Evaluation: generaliza

3. How do model class and training procedure affect fitting and generalization?

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

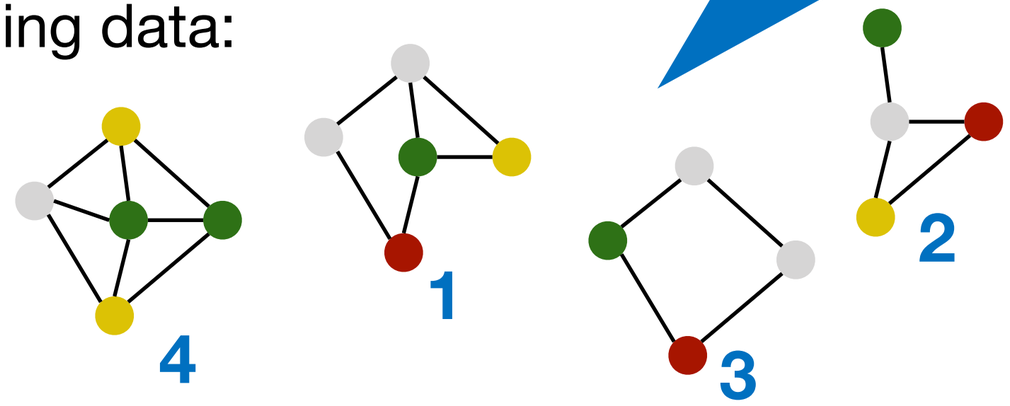
4. What will the neural network predict on different data?

Learning questions

2. What training data helps identify the right function?

1. What functions can my ML model encode?

Training data:

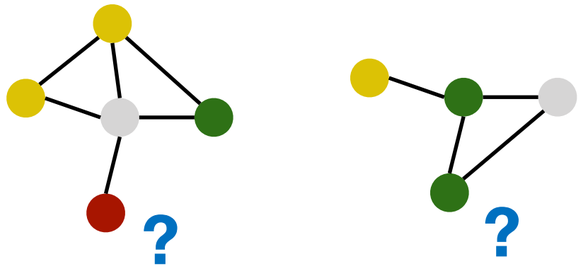


$$\min_{f \in \mathcal{F}} \frac{1}{N} \sum_{i=1} \ell(f(x_i), g(x_i))$$

"Learn" function

$$\hat{f}\left(\ \right) = \textit{predicted label}$$

Test data:



Evaluation: generaliza

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

3. How do model class and training procedure affect fitting and generalization?

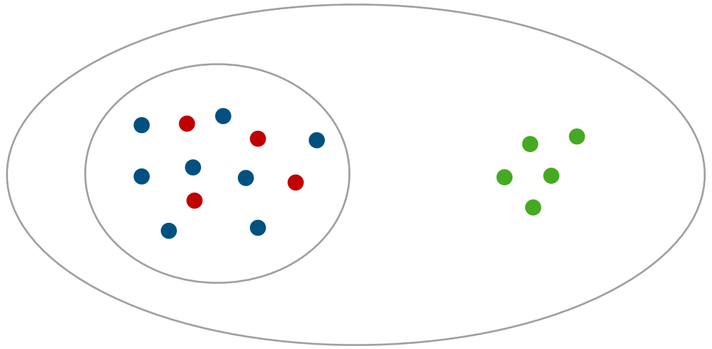
4. What will the neural network predict on different data?

Outline

- Graph Neural Networks

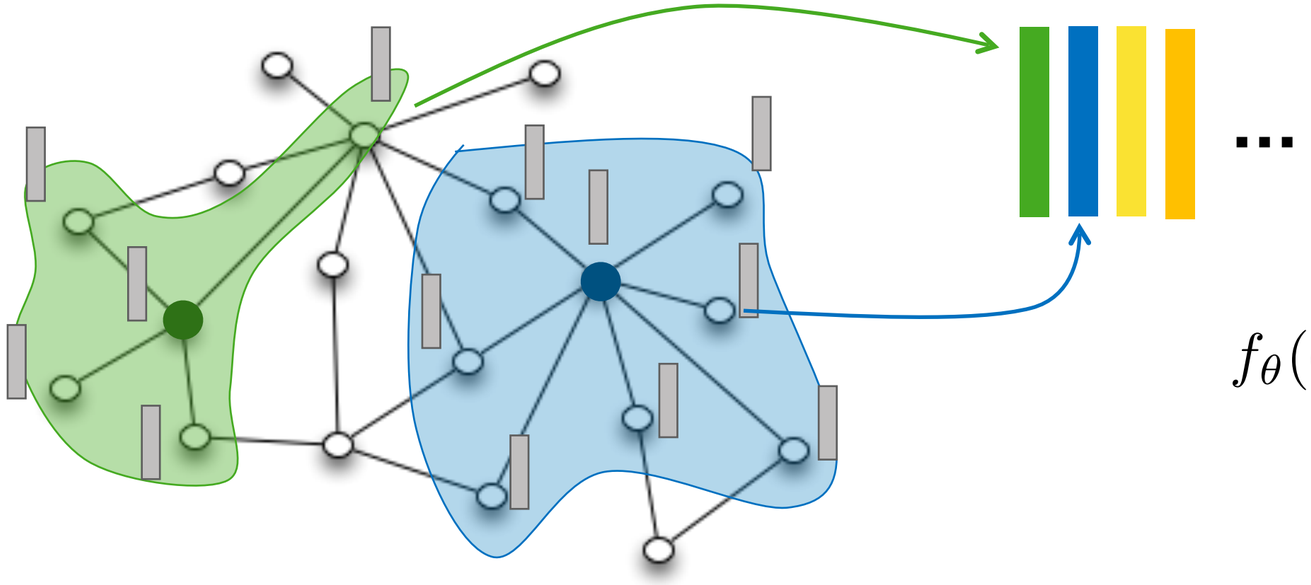
- **To what kinds of instances will my model generalize?**
  Prediction under distribution shifts
  - stability: measuring data shifts appropriately
  - large shifts: understanding model behavior by decomposition

- 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 $w(u,v) \in \mathbb{R}^{d'}$



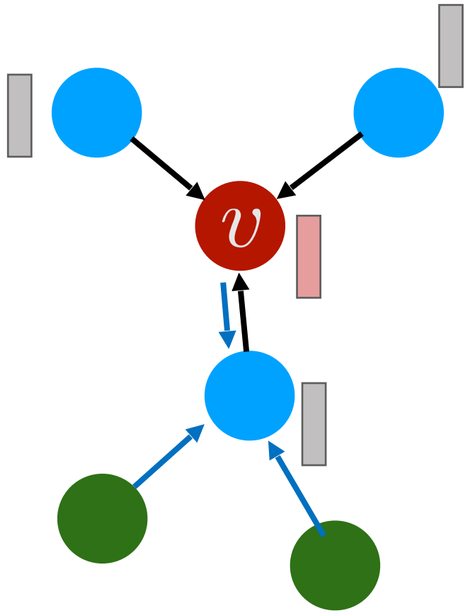
$$f_\theta(G) = f_{\text{Read}}(\{\!\{h_v \mid v \in V\}\!\})$$

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

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*:

feature description of node u in round k-1

Aggregate over neighbors

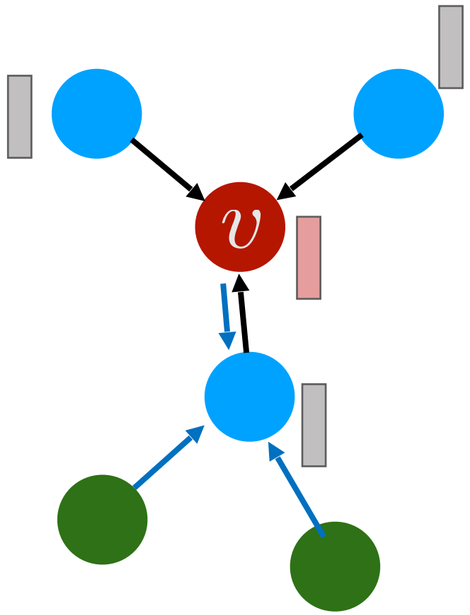
$$m_{\mathcal{N}(v)}^{(k)} = \text{AGGREGATE}^{(k)}\left(\left\{\left\{h_u^{(k-1)} : u \in \mathcal{N}(v)\right\}\right\}\right)$$

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

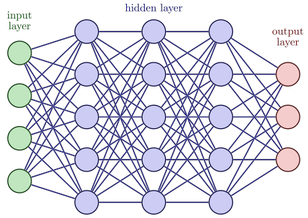


In each round k:

Aggregate over neighbors

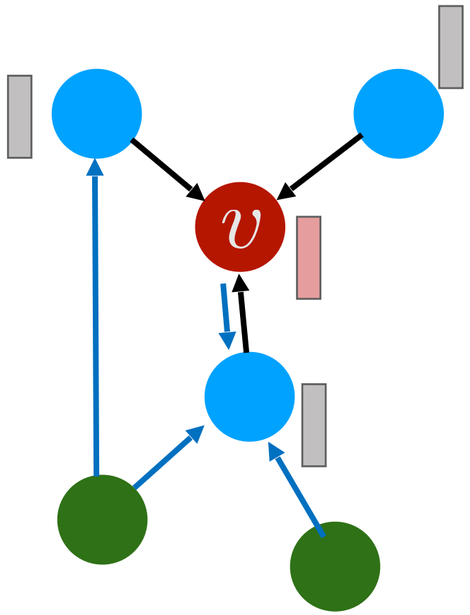
feature description of node u in round k-1

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



(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; …)

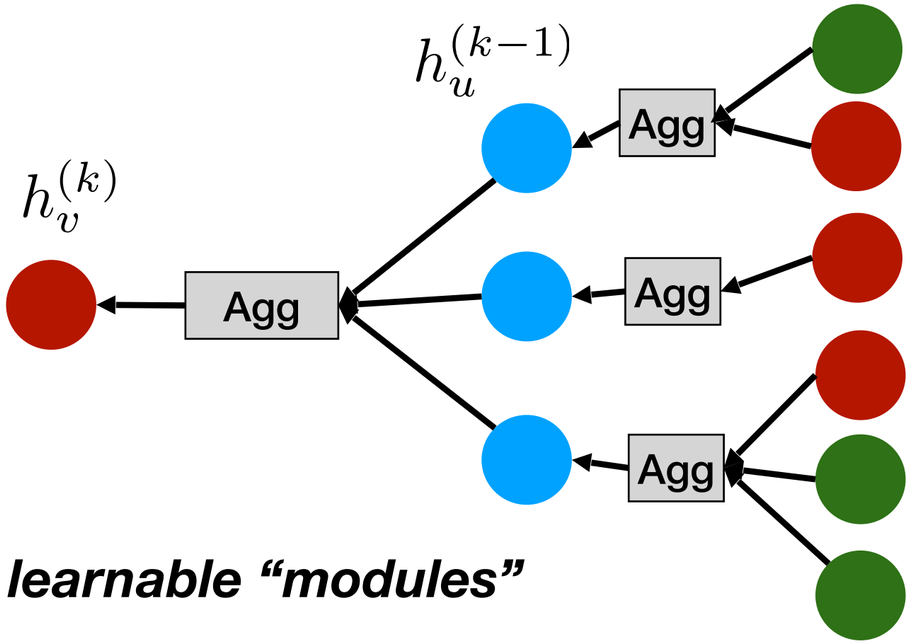
Message passing unrolled



In each round *k*:

Aggregate over neighbors and update representation

"Unrolled": **computation tree**



Structured arrangement of learnable "modules"

Outline

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  Prediction under distribution shifts
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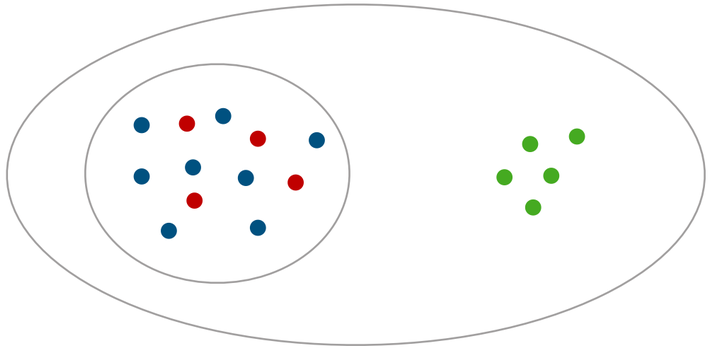
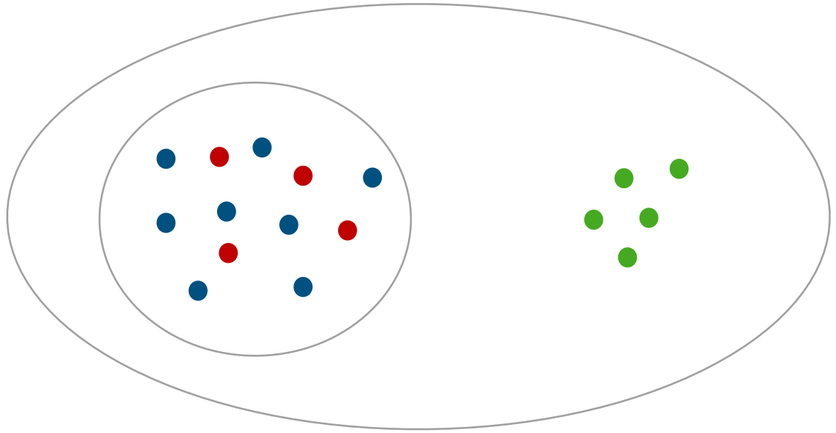
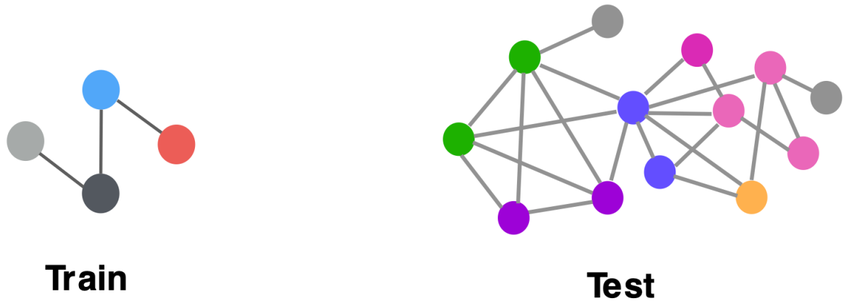


Graph predictions and distribution shifts

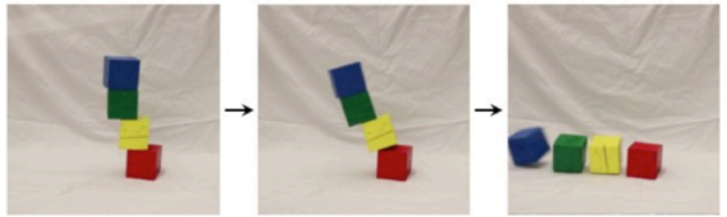


$$\mathbb{E}_{x\sim\mathcal{Q}}\left[\ell(f_\theta(x), g(x))\right]$$

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

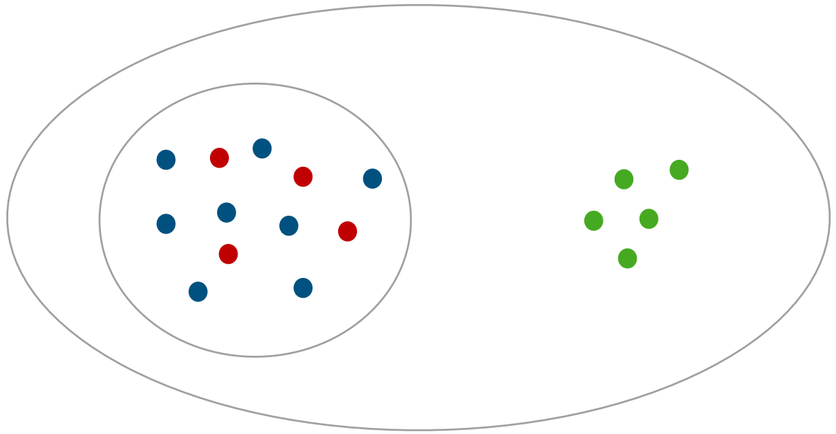


different *graph size,*
graph structure, edge weights, …
(Battagalia et al 2018, Dai et al 2018, Velickovic et al 2020)



Physical reasoning
different position, mass, number of objects

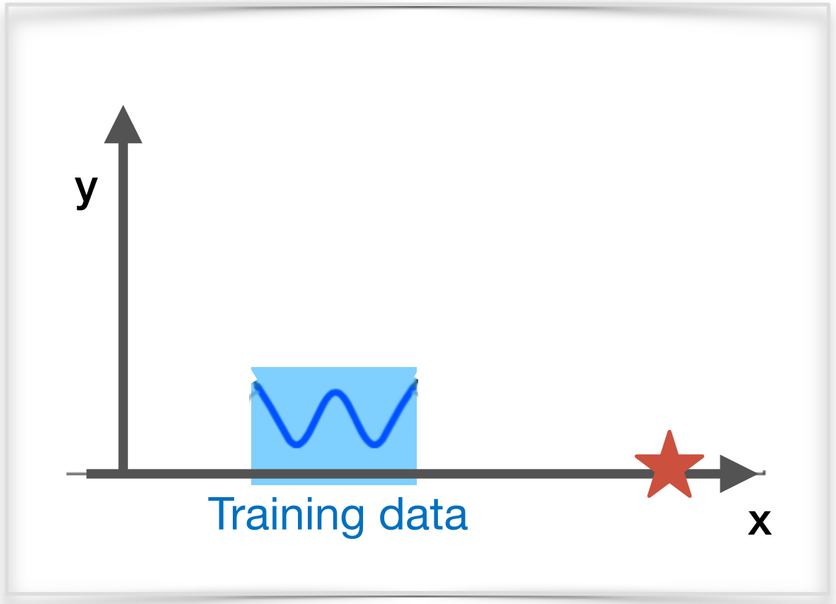
Graph predictions and distribution shifts



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

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

When may this work?



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 *(Levie-Huang-Bucci-Bronstein-Kutyniok 2019, Ruiz-Chamon-Ribeiro 2020, Keriven-Bietti-Vaiter 2020, Le & Jegelka 2023)*

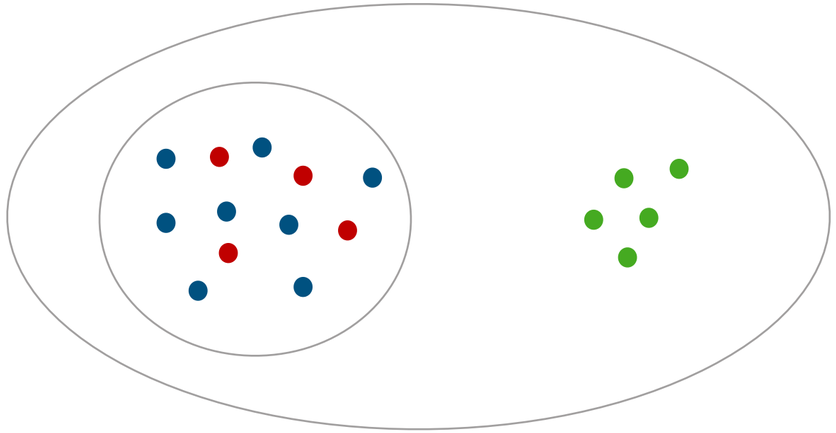
   --- or … ---

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 $\mathscr{Q}^t \setminus \mathscr{P}^t$, 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 $\mathscr{Q}$.

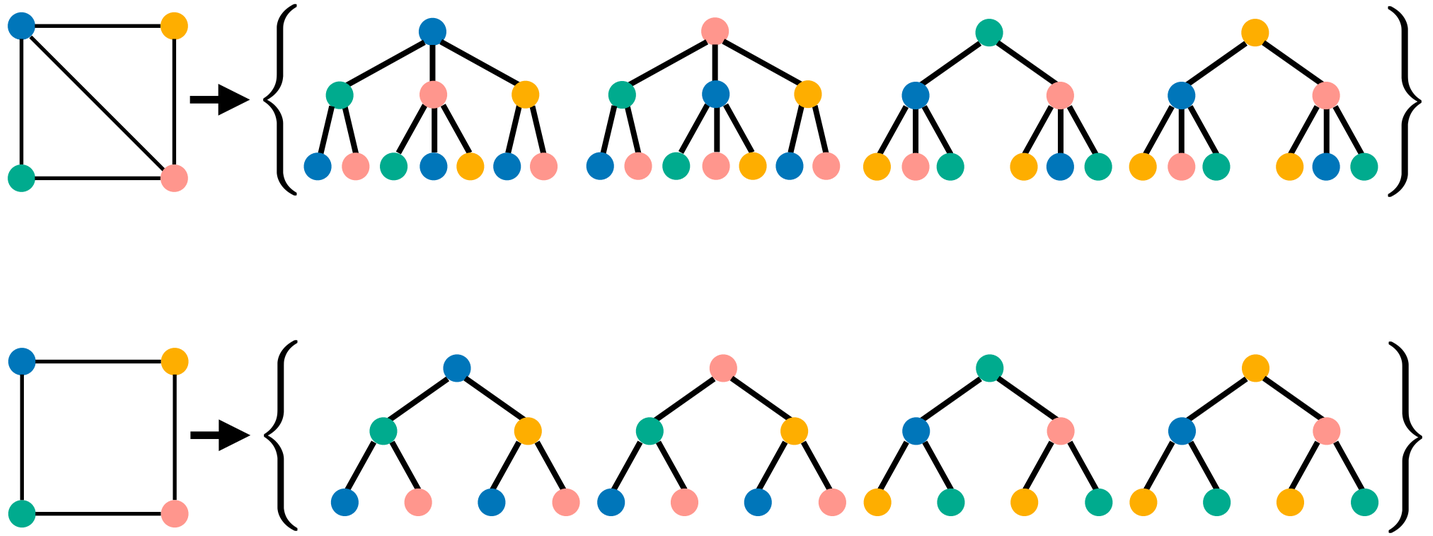
"Smoother" degrading performance for small perturbations with appropriate metric on graphs?

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:

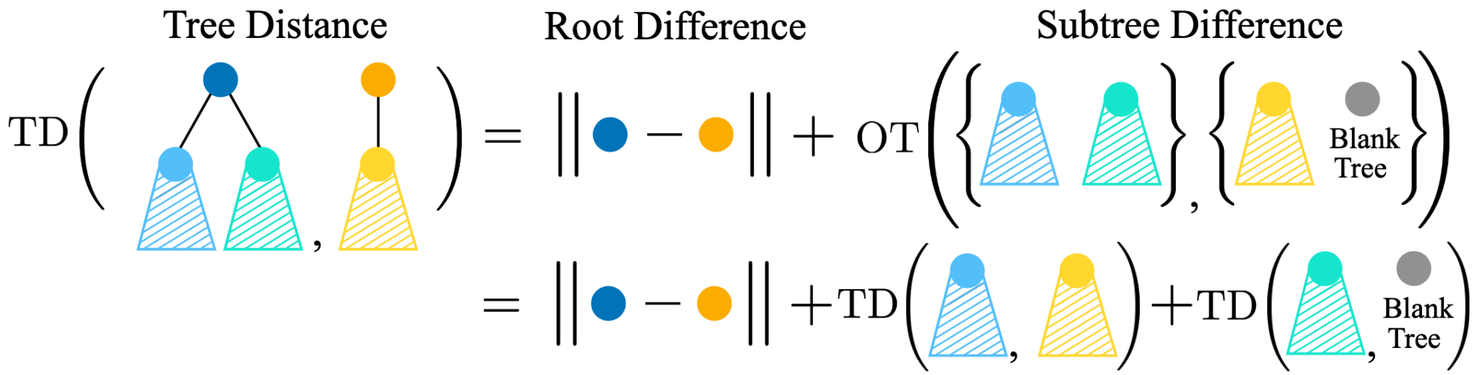
$$\min_{\gamma \in \Gamma(X,Y)} \sum_{i,j=1}^{n,m} d(x_i, y_j) \cdot \gamma_{ij}$$

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

Distance between vectors

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

Tree Distance via Hierarchical OT



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

Recursive!

where $L = \max(\mathbf{Depth}(T_a), \mathbf{Depth}(T_b))$ and $w : \mathbb{N} \to \mathbb{R}^+$ 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)

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

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

$$R_T(h) \leq R_S(h) + 2\mathrm{Lip}(h) \cdot \mathcal{W}_1(p_S, p_T) + \text{small value}$$

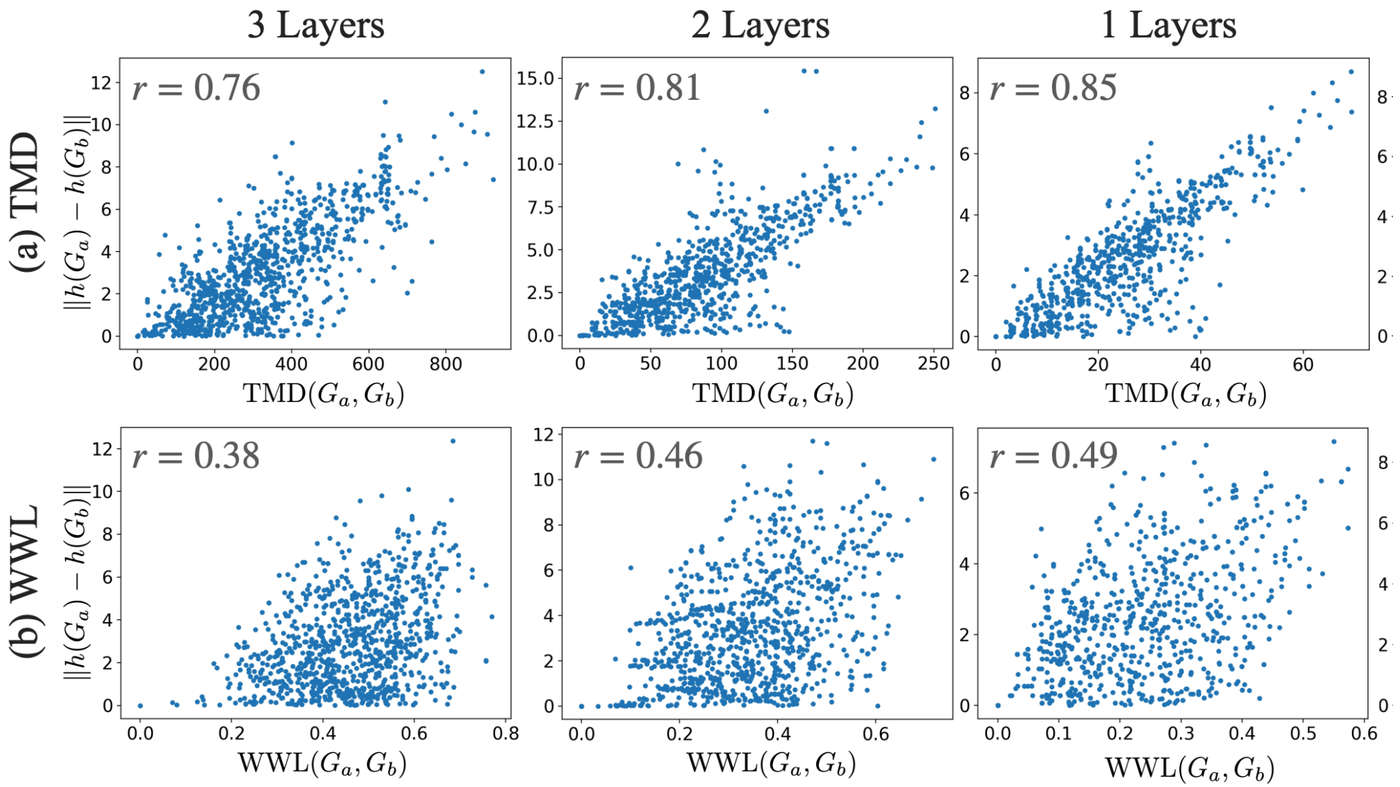
Target Risk *Source Risk* *Domain Discrepancy*

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

Empirically

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

1. **stability:**



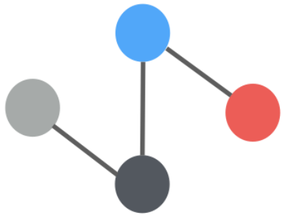
MUTAG data,
randomly sampled pairs

2. correlation with **accuracy drops under domain shifts** (PTC data): **WWL: 0.489**
TMD: 0.712

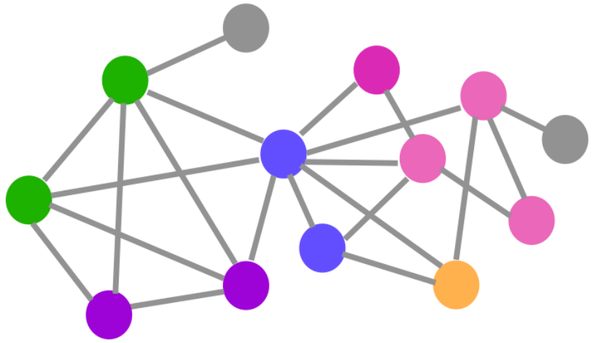
Large perturbations: inductive biases

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

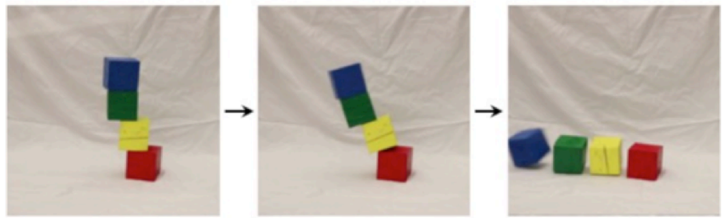


Train

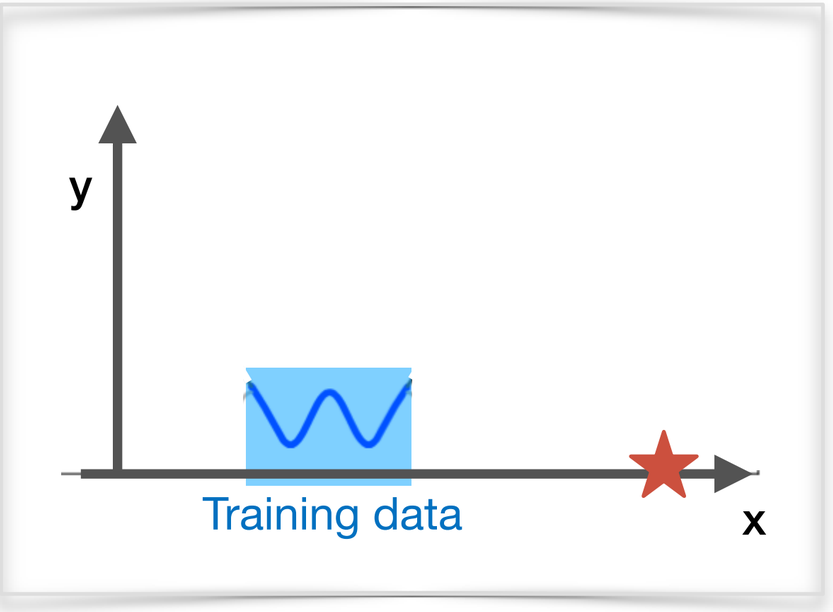


Test

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 *(Levie et al 2019, Ruiz et al 2020, Le & Jegelka 2023)*

--- or … ---

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

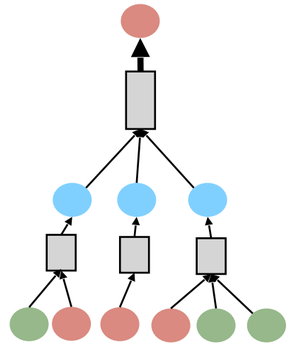
(Xu-Zhang-Li-Du-Kawarabayashi-Jegelka 21)

Neural network structure, optimization algorithm, data geometry

our strategy: understand parts -> understand full model

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) = Σ_v MLP(h_v^(k-1), h_u^(k-1))
```

Algorithmic Alignment:

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

Examples of Algorithmic Alignment

A Generalist Neural Algorithmic Learner

Borja Ibarz, Vitaly Kurin, George Papamakarios, Kyriacos Nikiforou, Mehdi Bennani, Róbert Csordás, Andrew Joseph Dudzik, Matko Bošnjak, Alex Vitvitskyi, Yulia Rubanova, Andreea Deac, Beatrice Bevilacqua, Yaroslav Ganin, Charles Blundell, Petar Veličković *Proceedings of the First Learning on Graphs Conference*, PMLR 198:2:1-2:23, 2022.

Neural Bellman-Ford Networks: A General Graph Neural Network Framework for Link Prediction

Zhaocheng Zhu[1,2], Zuobai Zhang[1,2], Louis-Pascal Xhonneux[1,2], Jian Tang[1,3,4]
Mila - Québec AI Institute[1], Université de Montréal[2]
HEC Montréal[3], CIFAR AI Chair[4]
{zhaocheng.zhu, zuobai.zhang, louis-pascal.xhonneux}@mila.quebec
jian.tang@hec.ca

Discovering Symbolic Models from Deep Learning with Inductive Biases

Miles Cranmer[1] Alvaro Sanchez-Gonzalez[2] Peter Battaglia[2] Rui Xu[1]
Kyle Cranmer[3] David Spergel[4,1] Shirley Ho[4,3,1,5]

[1] Princeton University, Princeton, USA [2] DeepMind, London, UK
[3] New York University, New York City, USA [4] Flatiron Institute, New York City, USA
[5] Carnegie Mellon University, Pittsburgh, USA

Computer Science > Machine Learning

[Submitted on 3 Jul 2023]

PlanE: Representation Learning over Planar Graphs

Radoslav Dimitrov, Zeyang Zhao, Ralph Abboud, İsmail İlkan Ceylan

Learning to Configure Computer Networks with Neural Algorithmic Reasoning

Luca Beurer-Kellner[1,*] Martin Vechev[1] Laurent Vanbever[1] Petar Veličković[2]

[1]ETH Zurich, Switzerland [2]DeepMind

Article | Open Access | Published: 01 December 2021

Advancing mathematics by guiding human intuition with AI

Alex Davies, Petar Veličković, Lars Buesing, Sam Blackwell, Daniel Zheng, Nenad Tomašev, Richard Tanburn, Peter Battaglia, Charles Blundell, András Juhász, Marc Lackenby, Geordie Williamson, Demis Hassabis & Pushmeet Kohli

Computer Science > Machine Learning

[Submitted on 8 Jul 2023]

Parallel Algorithms Align with Neural Execution

Valerie Engelmayer, Dobrik Georgiev, Petar Veličković

Published as a conference paper at ICLR 2020

NEURAL EXECUTION OF GRAPH ALGORITHMS

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NN-Baker: A Neural-network Infused Algorithmic Framework for Optimization Problems on Geometric Intersection Graphs

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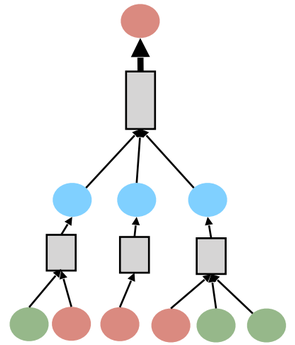
From understanding parts to understanding the model

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



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```

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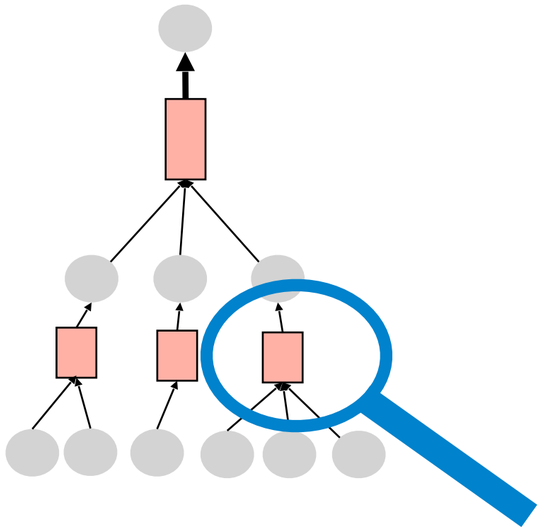
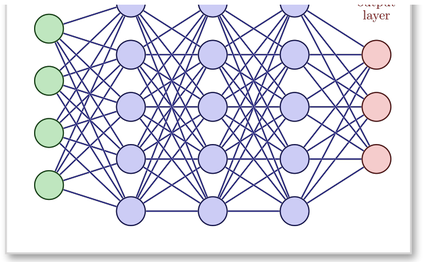
Neural Network can mimic algorithm via ***few, easy-to-learn*** “modules”

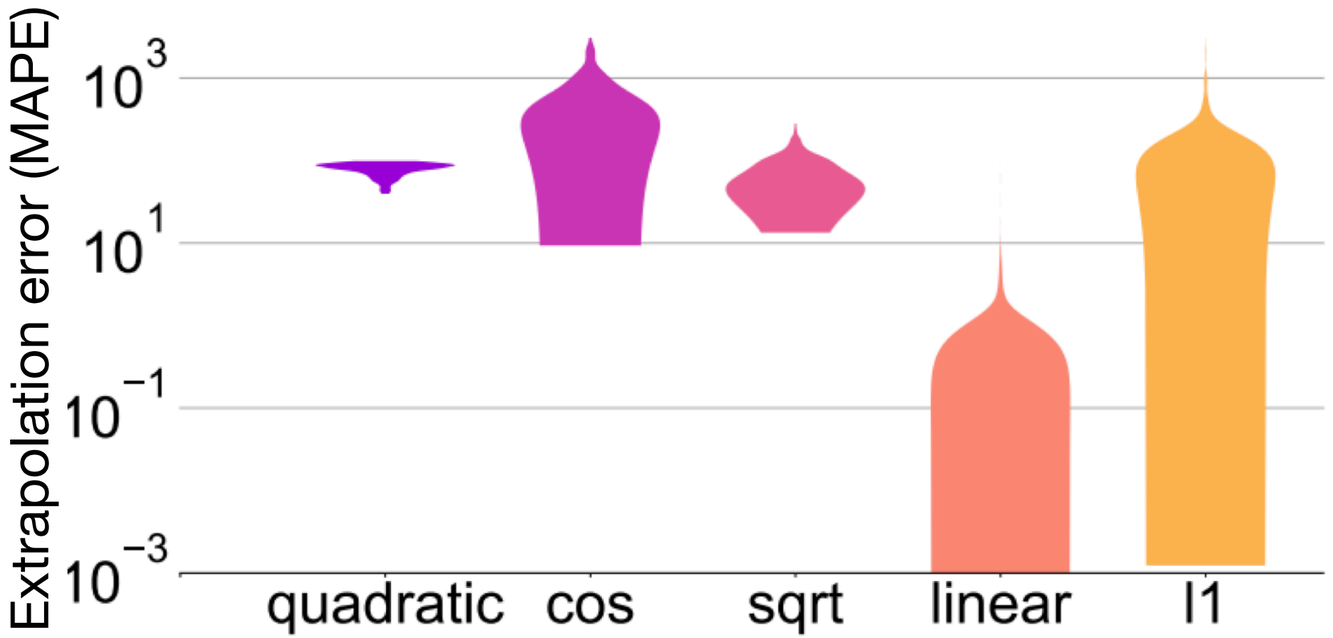
Empirically: MLP with ReLU activations

$$\mathrm{ReLU}(a) = \max\{0, a\}$$

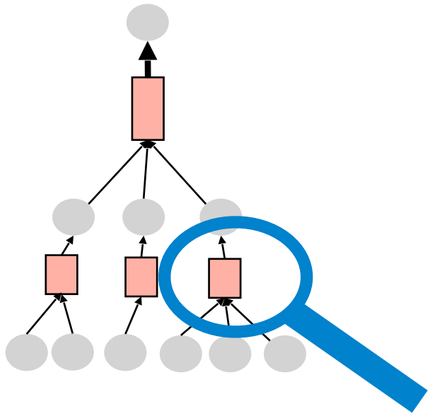


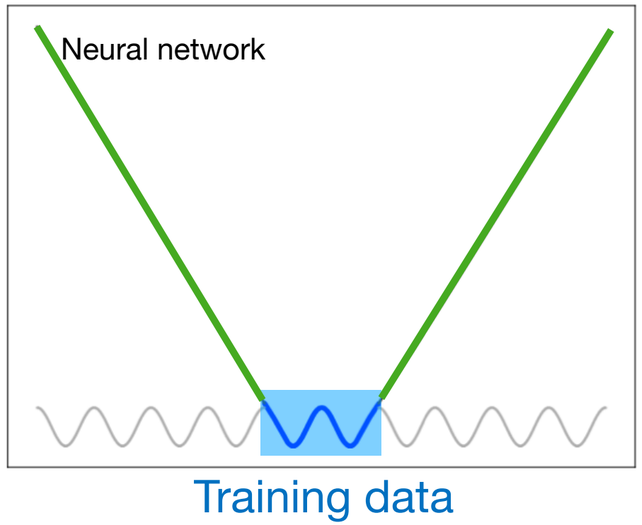
$$h_{v_i}^{(k)} = \sum_{v_j \in \mathcal{N}(i)} \mathrm{MLP}^{(k)}\left(h_{v_i}^{(k-1)}, h_{v_j}^{(k-1)}\right)$$

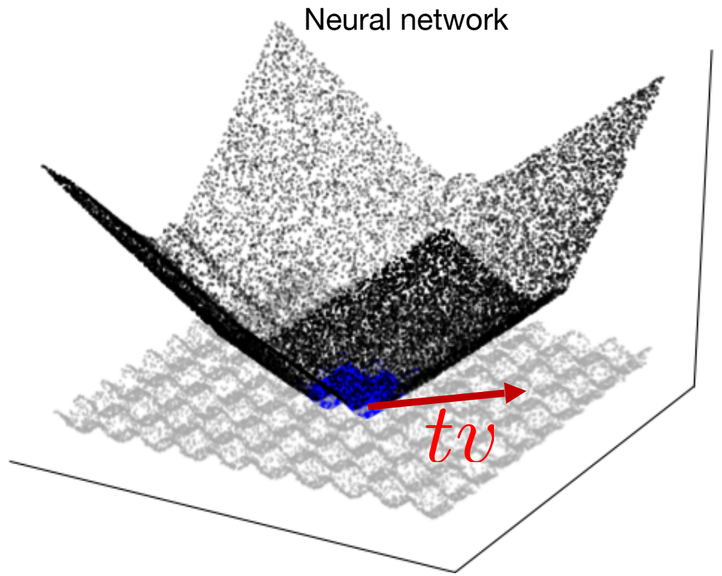




Extrapolation in fully connected ReLU networks



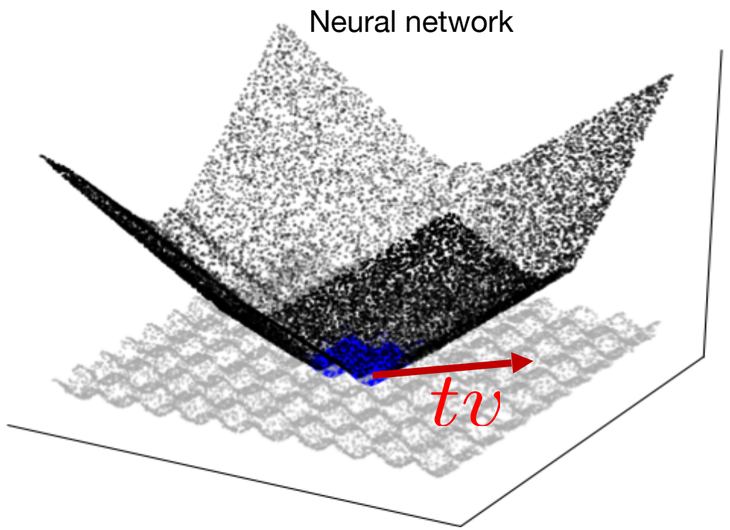




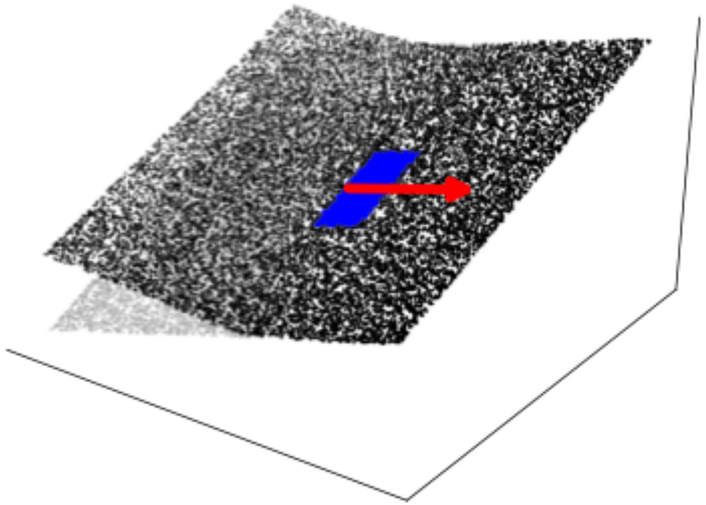
Theorem *(Xu-Zhang-Li-Du-Kawarabayashi-J 21)*
Let f be a 2-layer ReLU MLP trained with Gradient Descent. Along any direction $v \in \mathbb{R}^d$ f approaches a linear function: let $x = tv$. As $t \to \infty$: $f(x + hv) - f(x) \to \beta_v h$ with rate $O(1/t)$.

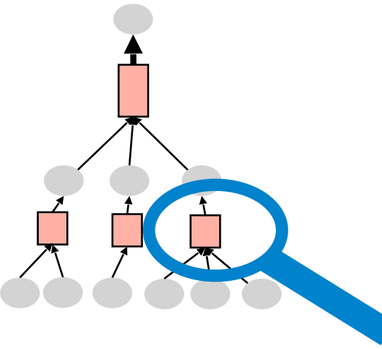
(Linear regions: Montufar et al 2014, Arora et al 2018, Hanin & Rolnick, 2019; Hein et al., 2019, XZDKJ20)

Implications



1. Can only extrapolate linear functions





2. Training Data geometry

Implications for the full GNN

Shortest Path: (target)

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

Need MLP to be nonlinear!

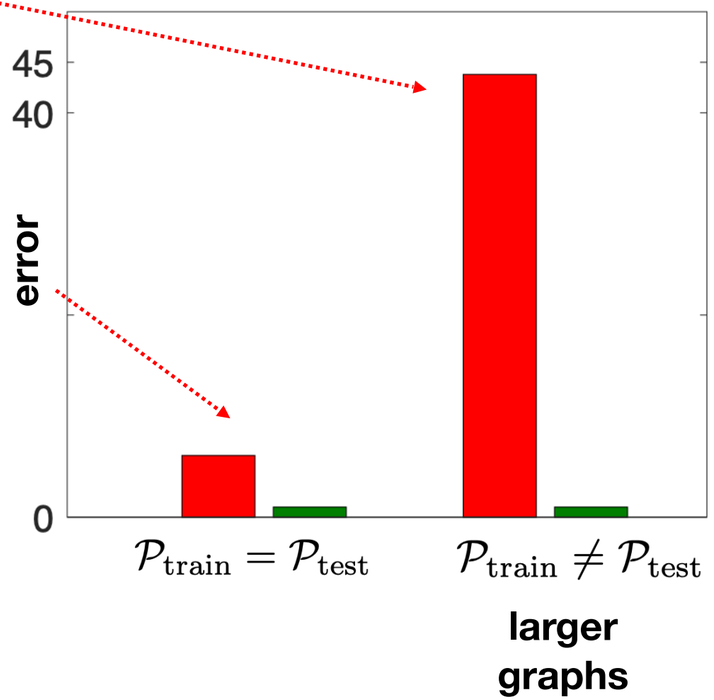
GNN:

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

GNN II:

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

(Veličkovic et al 2020)



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

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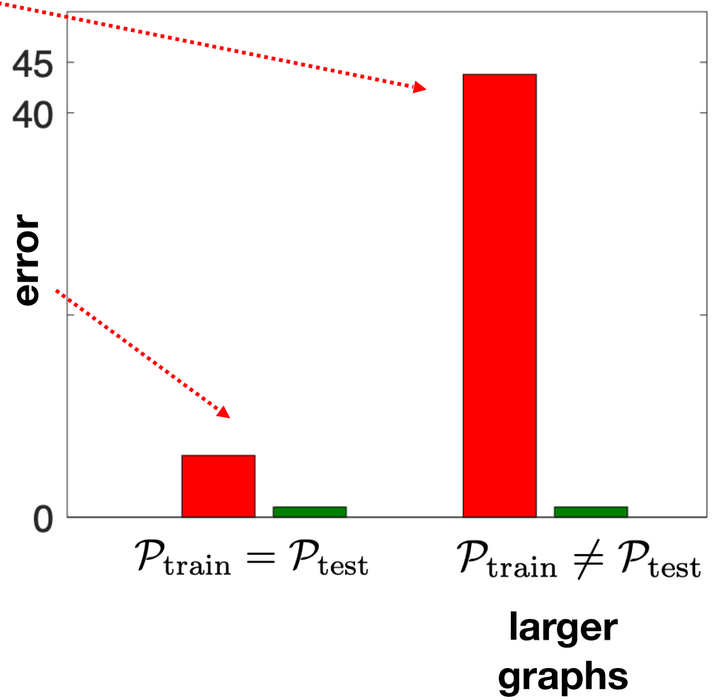
GNN II:

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

(Veličkovic et al 2020)

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

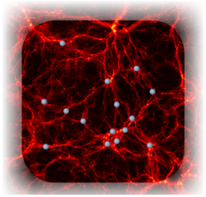
NALU: $\mathbf{y} = \mathbf{g} \odot \mathbf{a} + (1 - \mathbf{g}) \odot \mathbf{m}$

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

Exp log for learning multiplication
(Trask et al 2018)

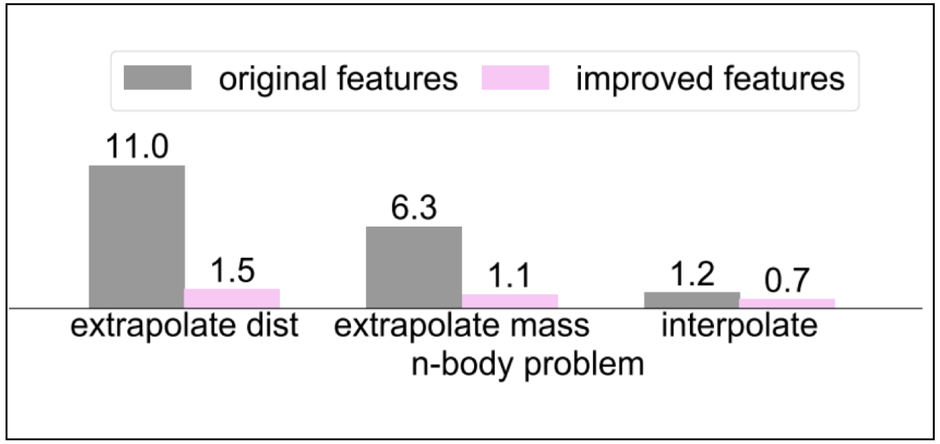
Q: What direction is the closest creature facing?
P: `scene, filter_creature, filter_closest, unique, query_direction`
A: left

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

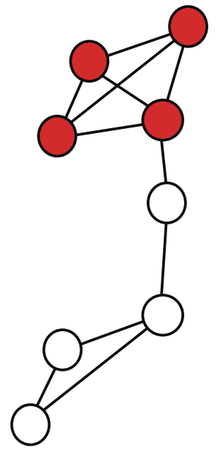
(figure of n-body system: Battaglia et al 2018)

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

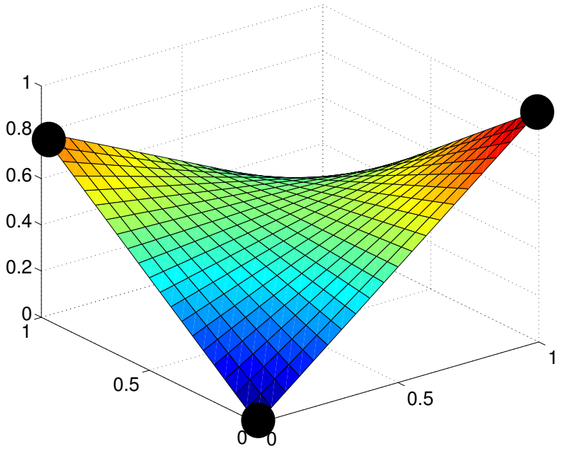
Setup

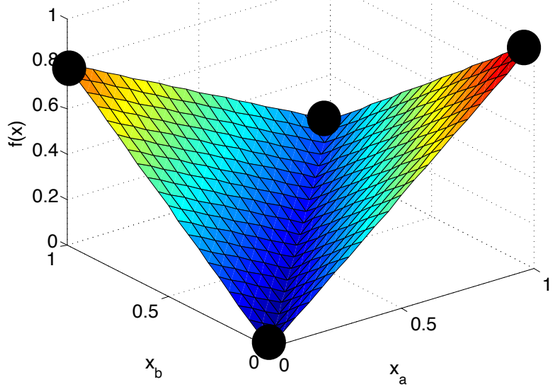
- use NN as “solver”, and objective function of the optimization problem as a loss
- What if the objective is a set function? $F(S), S \subseteq [n]$



- Continuous extension:

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





- 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

Guarantees

Proposition

If $f(x) = \sum_{S \subseteq [n]} p_x(S) F(S)$ with $\mathbb{E}_{S \sim p_x}[1_s] = x$ then:

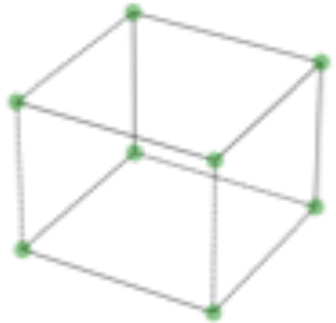
$$\min_x f(x) = \min_{S \subseteq [n]} F(S)$$

$$\arg\min_x f(x) \subseteq \operatorname{conv}\Big(\arg \min_{1_S : S \subseteq [n]} f(S) \Big)$$

Extensions

NN outputs…

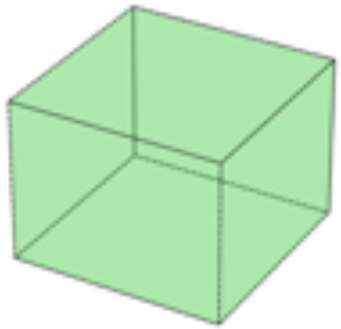
$S \in \{0,1\}^n$



$F(S)$

We want:

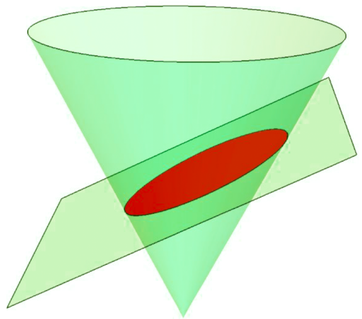
$x \in [0,1]^n$



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

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

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



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

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

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

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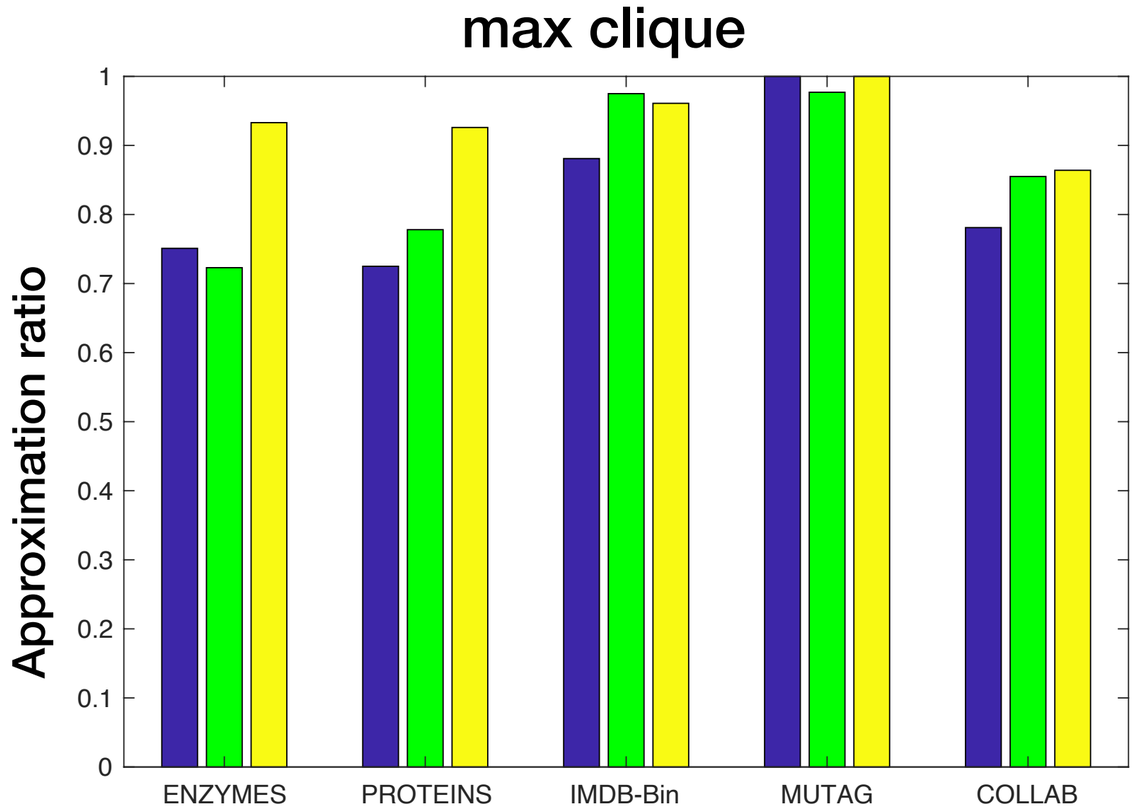
- use SDP version of this

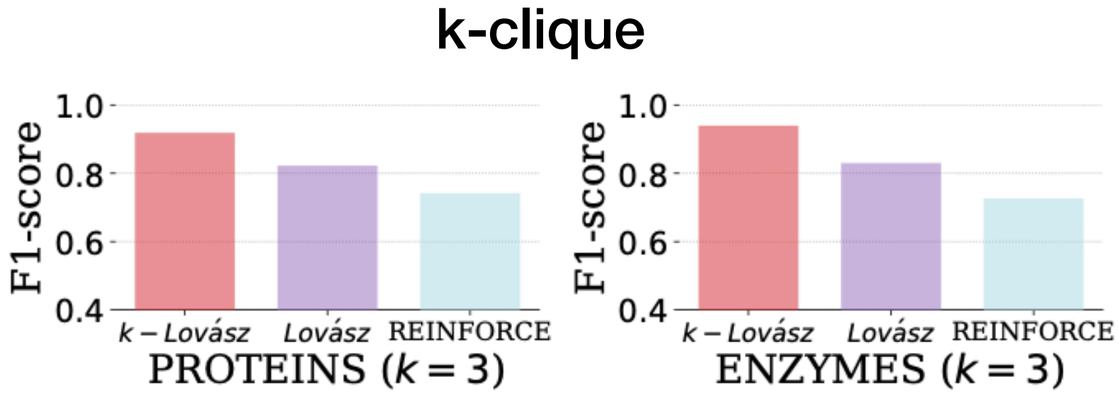
- any valid vector extension leads to a valid matrix extension: Let $X = \sum_i \lambda_i v_i v_i^\top$

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

Empirical results



REINFORCE
LOVASZ EXT
MATRIX LOVASZ

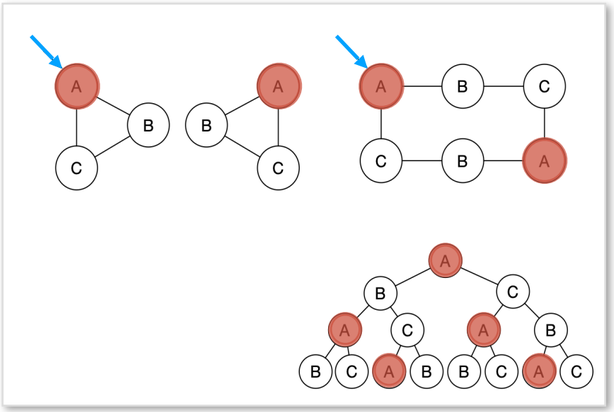


$$\mathbf{S}\, p_x = x$$

Other considerations: expressive power

- Distinguish most graphs, but not all
  (upper bounded by 1-dim. Weisfeiler-Leman algorithm / color refinement)
  (Xu-Hu-Leskovec-J 2019, Morris-Ritzert-Fey-Hamilton-Lenssen-Rattan-Grohe 2019)

- Without node identification: cannot compute structural properties like
  graph diameter, k-clique, conjoint cycle, subgraph counting, …
  (Garg-J-Jaakkola 2020, Chen-Chen-Villar-Bruna 2020)



...

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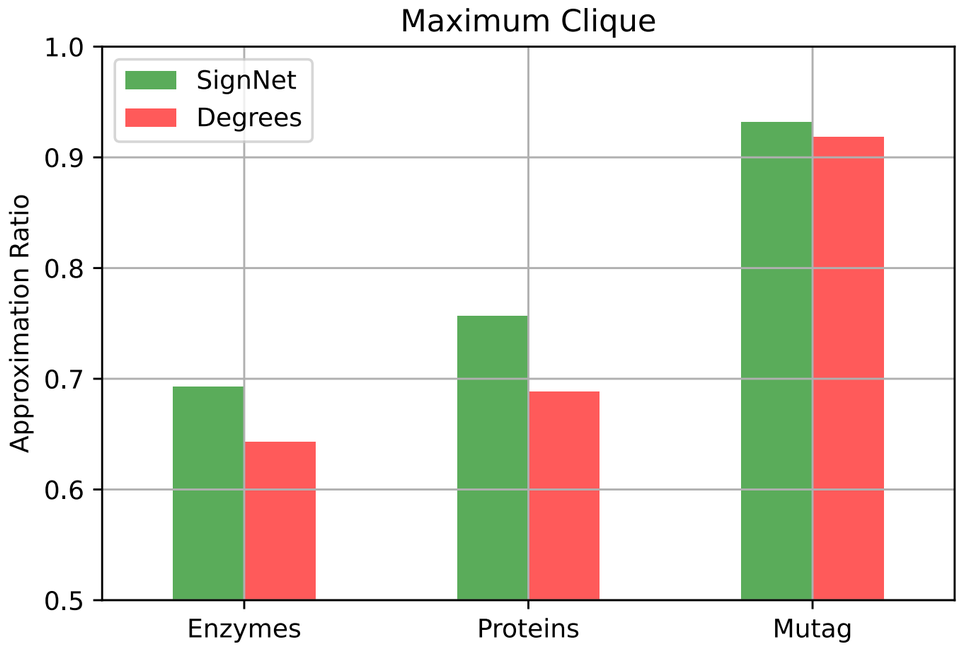
- Unique node IDs: equivalent to LOCAL model, Turing complete (if “large enough”)
  (Loukas 2020) or random node IDs *(Abboud-Ceylan-Grohe-Lukasiewicz 2019)*

Other considerations: expressive power

- Message passing GNNs can, in general, not recognize structural motifs (cycles, etc) *(Xu-Hu-Leskovec-J 2019, Morris-Ritzert-Fey-Hamilton-Lenssen-Rattan-Grohe 2019, Garg-J-Jaakkola 2020, Chen-Chen-Villar-Bruna 2020)*
- One solution: add "positional encodings" of nodes from Laplacian eigenvectors - provably increases expressive power *(e.g., Lim-Robinson-Zhao-Smidt-Sra-Maron-J 2023)*



NN: Graph Attention Network

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

- Other aspects: expressive power, data, “shortcuts”,…