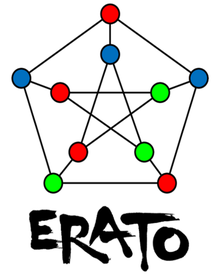
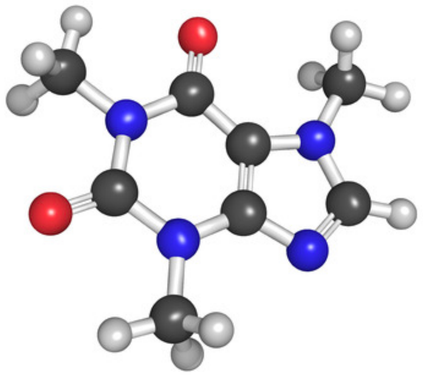


Graph Neural Networks: Generalization and Extrapolation

Keyulu Xu

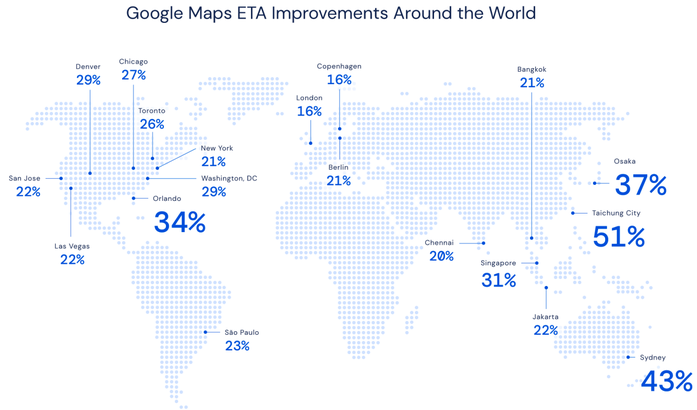
MIT

Applications



Drug discovery
(Duvenaud et al. 2015)

Recommender system
(Ying et al. 2018)



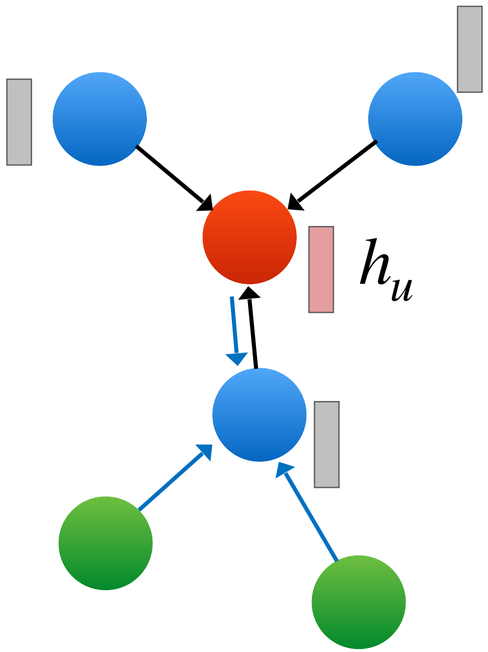
Google Map ETA
(Lange et al. 2020)

Physical reasoning
(Wu et al. 2017)

Question: `Calculate -841880142.544 + 411127.`
Answer: `-841469015.544`
Question: `Let x(g) = 9*g + 1. Let q(c) = 2*c + 1. Let f(i) = 3*i - 39. Let w(j) = q(x(j)). Calculate f(w(a)).`
Answer: `54*a - 30`
Question: `Let e(l) = l - 6. Is 2 a factor of both e(9) and 2?`
Answer: `False`

Symbolic mathematics
(Saxton et al 2019, Lample et al. 2020)

Graph Neural Networks (GNNs)



In each round:

For $u \in V$ concurrently:

Aggregate over neighbors

Representation of neighbor node v in round $k-1$

$$h_u^{(k)} = \text{AGGREGATE}^{(k)}\left(\left\{ \left(h_v^{(k-1)}, h_u^{(k-1)} \right) \right\} \middle| v \in \mathcal{N}(u) \right)$$

.....

Graph-level **readout**

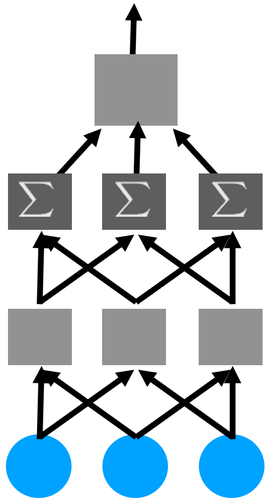
$$h_G = \text{READOUT}\left(\left\{ h_u^{(K)} \right\} \middle| u \in V \right)$$

(Gori et al. 2005, Merkwirth & Lengauer 2005, Scarselli et al 2009, Duvenaud et al., 2015, Battaglia et al., 2016, Dai et al., 2016, Defferrard et al., 2016, Kearnes et al., 2016, Li et al., 2016, Gilmer et al., 2017, Hamilton et al., 2017, Kipf & Welling, 2017, Velickovic et al., 2018, Xu et al., 2018)

Training GNNs

1. Parameterize AGGREGATE$^{(k)}$ and READOUT

$$\boldsymbol{h}_u^{(k)} = \sum_{v \in \mathcal{N}(u)} \text{MLP}^{(k)}\left(\boldsymbol{h}_u^{(k-1)}, \boldsymbol{h}_v^{(k-1)}, \boldsymbol{w}_{(v,u)}\right), \quad \boldsymbol{h}_G = \text{MLP}^{(K+1)}\left(\sum_{u \in G} \boldsymbol{h}_u^{(K)}\right)$$



Other aggregation also possible, e.g., attention

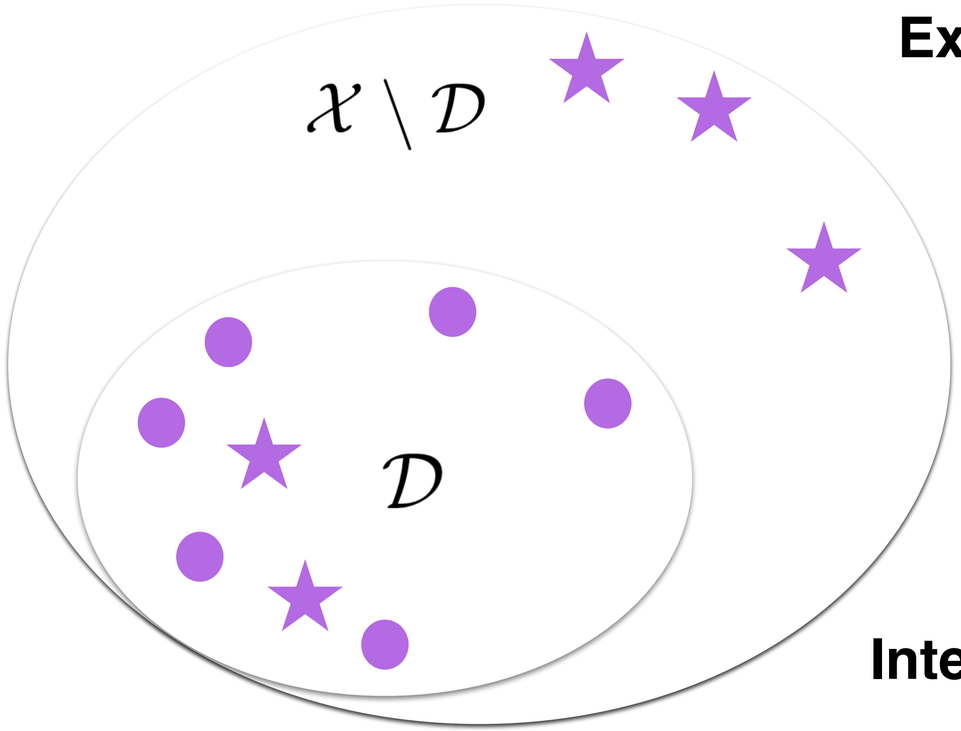
2. Specify a loss on node/graph/edge representations

3. Train on data points with SGD

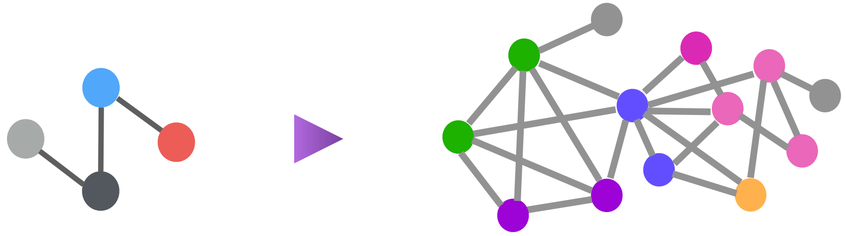
Extrapolation vs. interpolation

Train NN f to learn underlying function $g : \mathcal{X} \to \mathbb{R}$ with training set $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n \subset \mathcal{D}$

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



Extrapolation

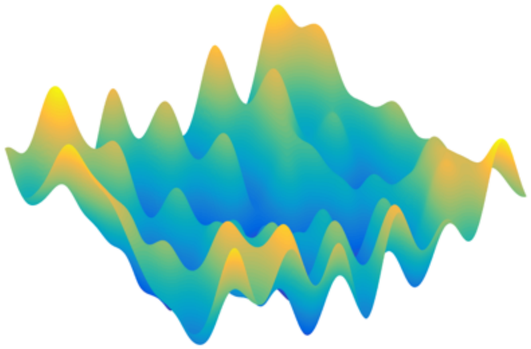


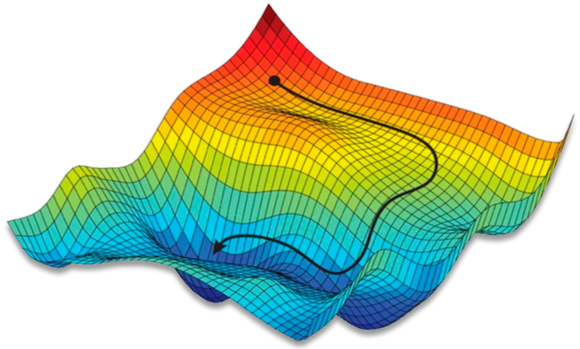
Train

Test

Interpolation $\mathcal{P}_{\text{train}} = \mathcal{P}_{\text{test}}$

Approaches of generalization analysis





Complexity

(Scarselli et al 2018, Garg et al 2020)

+ Training algorithm

*(Du, Hou, Poczos, Salakhutdinov, Wang, **X.** 2019)*

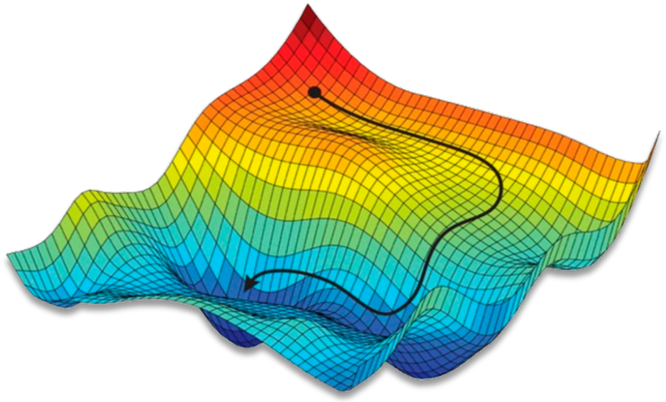
+ Network & task structure

*(**X.**, Zhang, Li, Du, Kawarabayashi, Jegelka 2020, 2021)*

more "practical"

more assumptions

Learning dynamics: Graph NTK



Parameter trajectory

$\theta_{GNN}(t)$

GNN output $f(\theta_{GNN}, G)$

DHPSWX'19

Over-parameterized GNNs trained by GD is equivalent to that of kernel regression with Graph NTK:

$$k(G, G') = \mathbb{E}_{\theta_{GNN} \sim \mathscr{W}} \left[\left\langle \frac{\partial f(\theta_{GNN}, G)}{\partial \theta_{GNN}}, \frac{\partial f(\theta_{GNN}, G')}{\partial \theta_{GNN}} \right\rangle \right]$$

Refer to paper for exact formula of Graph NTK

Assumptions: very wide, infinitesimally small learning rate, initialization with certain scaling.

(NTK theory: Jacot et al 2018, Li and Liang 2018, Allen-Zhu et al 2019, Arora et al 2019ab, Cao and Gu 2019, Du et al 2019ab…)

Generalization error

Wide GNNs trained by GD = Graph NTK

$$\frac{\sqrt{\boldsymbol{y}^\top \boldsymbol{H}^{-1} \boldsymbol{y} \cdot \operatorname{tr}(\boldsymbol{H})}}{n}$$

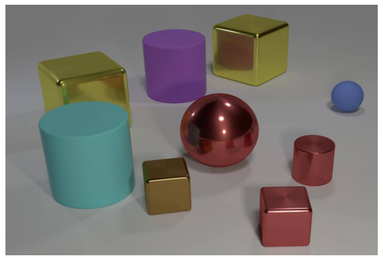
(Bartlett and Mendelson 2002)

$\boldsymbol{H}$ - *graph NTK matrix (computable based on training data)*

$\boldsymbol{y}$ - *training labels*

n - *number of training data*

Task structure in algorithmic tasks



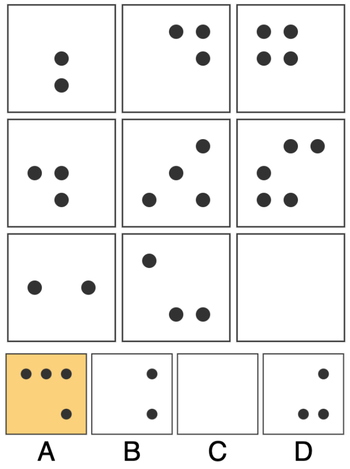
VQA

(Santoro et al 2016)

Question: `Calculate -841880142.544 + 411127.`
Answer: `-841469015.544`
Question: `Let x(g) = 9*g + 1. Let q(c) = 2*c + 1. Let f(i) = 3*i - 39. Let w(j) = q(x(j)). Calculate f(w(a)).`
Answer: `54*a - 30`
Question: `Let e(l) = l - 6. Is 2 a factor of both e(9) and 2?`
Answer: `False`

Mathematical reasoning

(Saxton et al. 2019, Lample et al 2020)



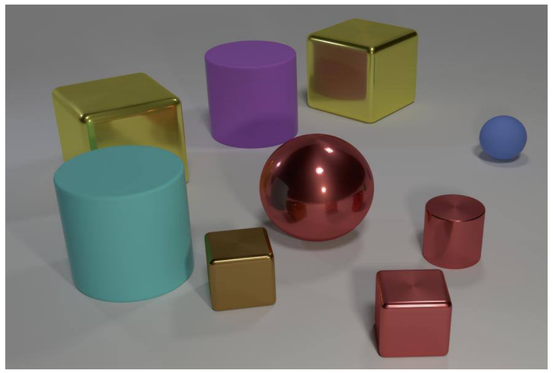
IQ tests

(Santoro et al. 2018, Zhang et al 2019)

Physical reasoning

(Wu et al. 2017, Battagalia et al 2016, Janner et al 2019)

Architecture is crucial for generalization



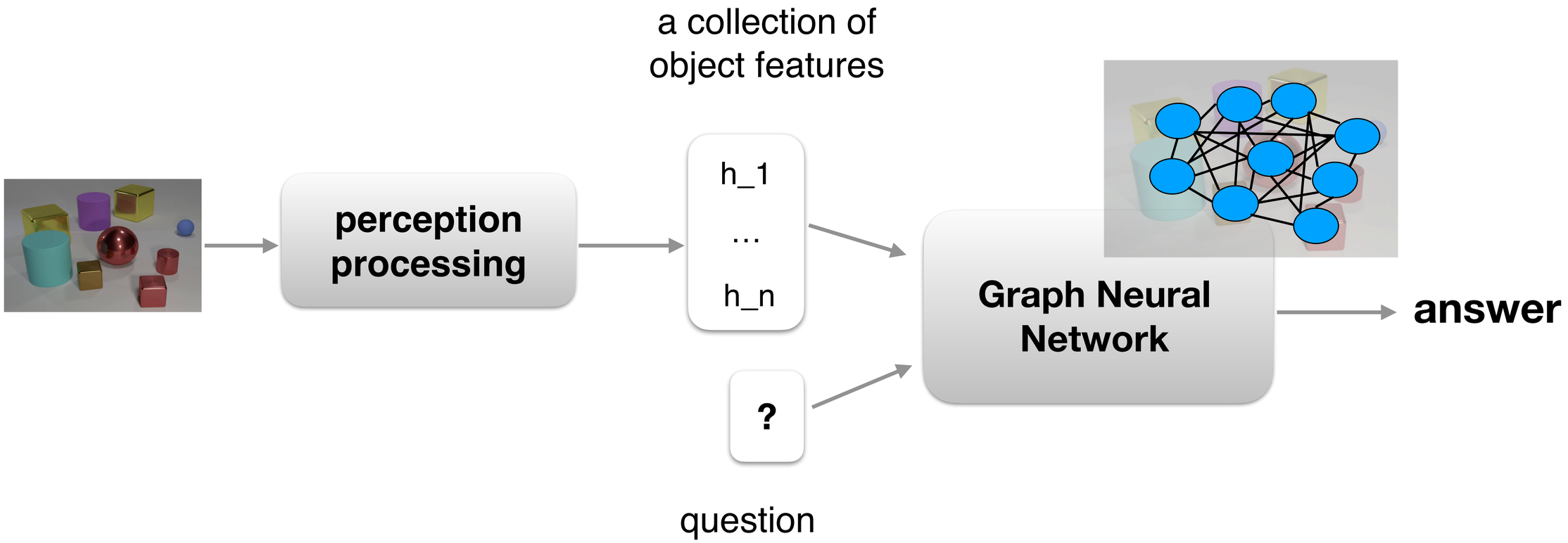
Neural Network
MLP
CNN
RNN
…

answer

? *e.g., colors of the furthest pair of objects?*

(Weston et al., 2015; Johnson et al., 2017a; Wu et al. 2017, Fleuret et al., 2011; Antol et al., 2015; Battaglia et al., 2016, 2018; Watters et al., 2017; Fragkiadaki et al., 2016; Chang et al., 2017, 2019; Saxton et al., 2019; Santoro et al., 2018…)

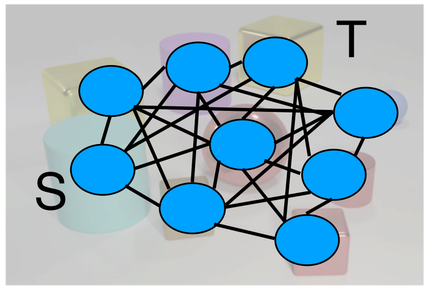
GNN for algorithmic reasoning tasks



(Weston et al., 2015; Johnson et al., 2017a; Wu et al. 2017, Fleuret et al., 2011; Antol et al., 2015; Battaglia et al., 2016, 2018; Watters et al., 2017; Fragkiadaki et al., 2016; Chang et al., 2017, 2019; Saxton et al., 2019; Santoro et al., 2018…)

How task & NN structure affect sample efficiency

Example



shortest path distance?

Graph Neural Network

for k = 1 … GNN iter:

for u in S:

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

No need to learn for-loops

Bellman-Ford algorithm

for k = 1 … |S| - 1:

for u in S:

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

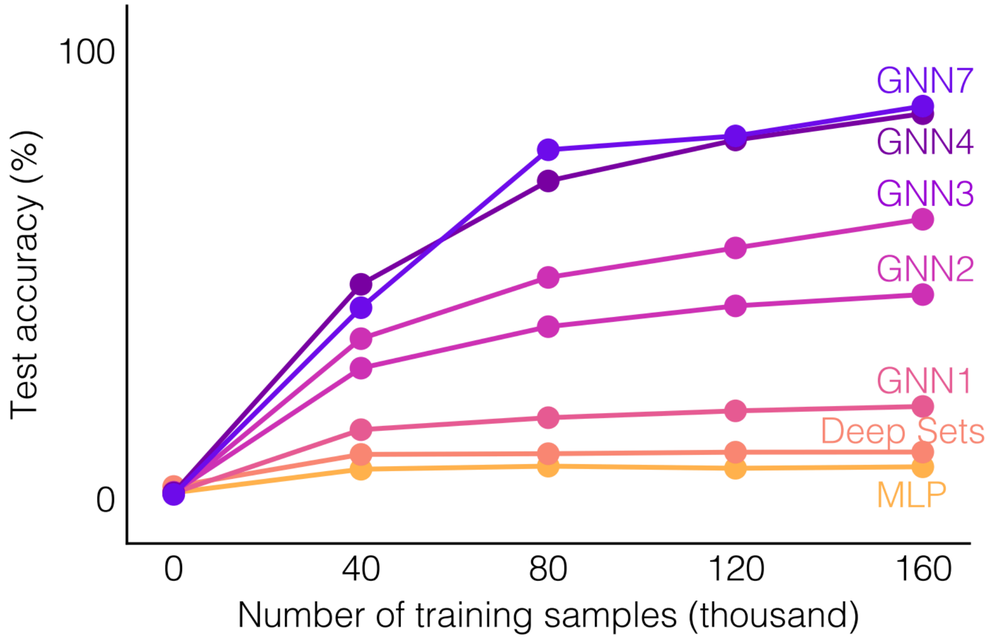
Learns a simple reasoning step

Other architectures need to learn functions with higher complexity, e.g., for-loops

Algorithmic alignment: formalizing inductive biases

Algorithmic alignment (XLZDKJ'20)
Network can simulate algorithm via *few, easy-to-learn* "modules".

Claim: Better algo alignment implies better generalization.



Better alignment implies better generalization

Algorithmic alignment (XLZDKJ'20)

A neural network (M, ϵ, δ)-aligns with an algorithm if it can simulate the algorithm via n weight-shared modules, each of which is (ϵ, δ) PAC-learnable with M/n samples.

* *Sample complexity of modules by e.g., NTK*

Theorem (XLZDKJ'20)

If a neural network and a task algorithm (M, ϵ, δ)-align, then, under assumptions*, the task is $(O(\epsilon), O(\delta))$ PAC-learnable by the network with M examples.

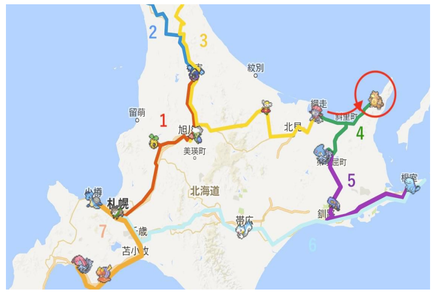
* *Lipschitznes and SGD sequential training*
* *Related work experimenting assumptions: Veličković et al 2020*

GNNs can sample-efficiently learn DP

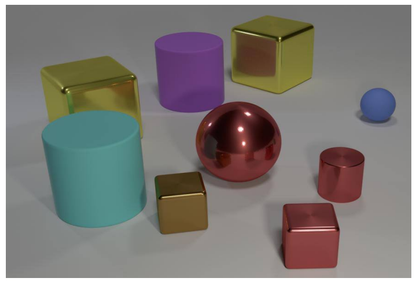
$$\text{Answer}[k][i] = \text{DP-Update}(\{\text{Answer}[k-1][j],\ j = 1 \dots n\})$$

$$h_s^{(k)} = \sum_{t \in S} \mathbf{MLP}_1^{(k)} \left(h_s^{(k-1)}, h_t^{(k-1)} \right)$$

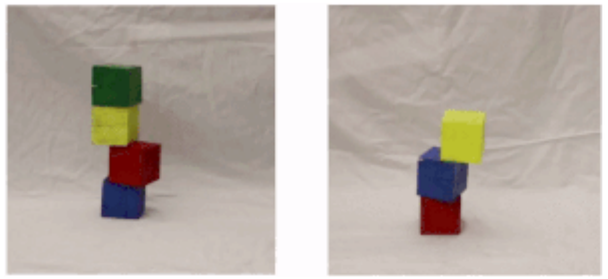
Reasoning tasks as dynamic programming (DP):



graph algorithms



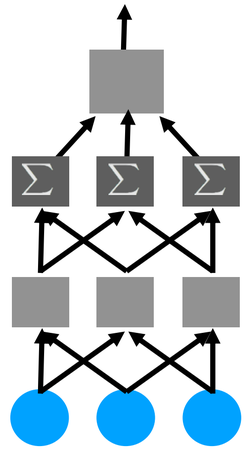
visual question answering

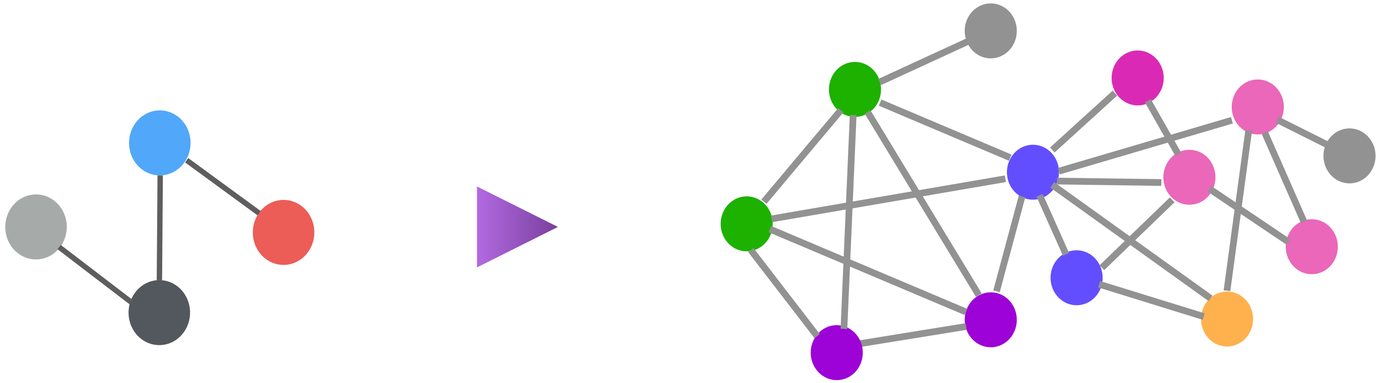


Intuitive physics

Extrapolation

What function does a GNN implement outside training distribution?



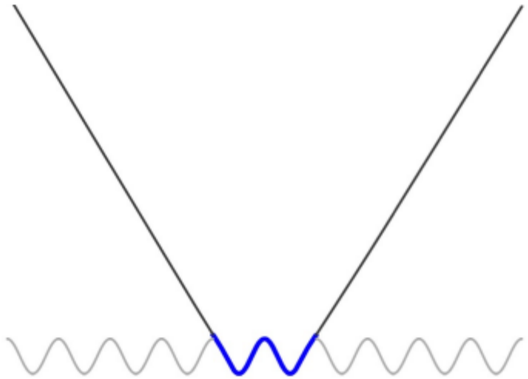


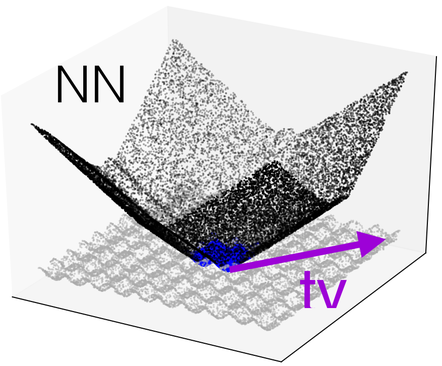
Train

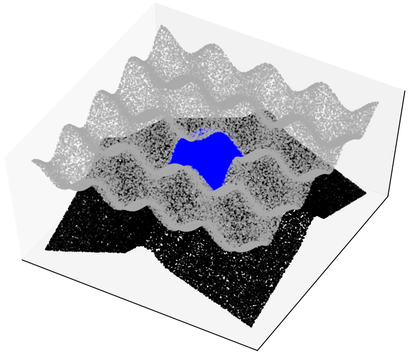
Test

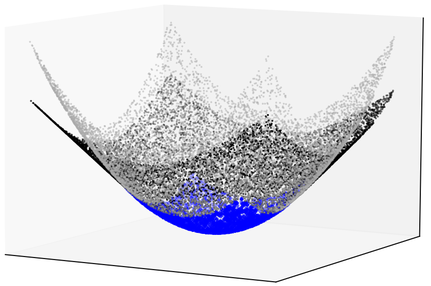
Generalize across graph structure, size, node & edge features?

Linear extrapolation behavior of ReLU MLPs







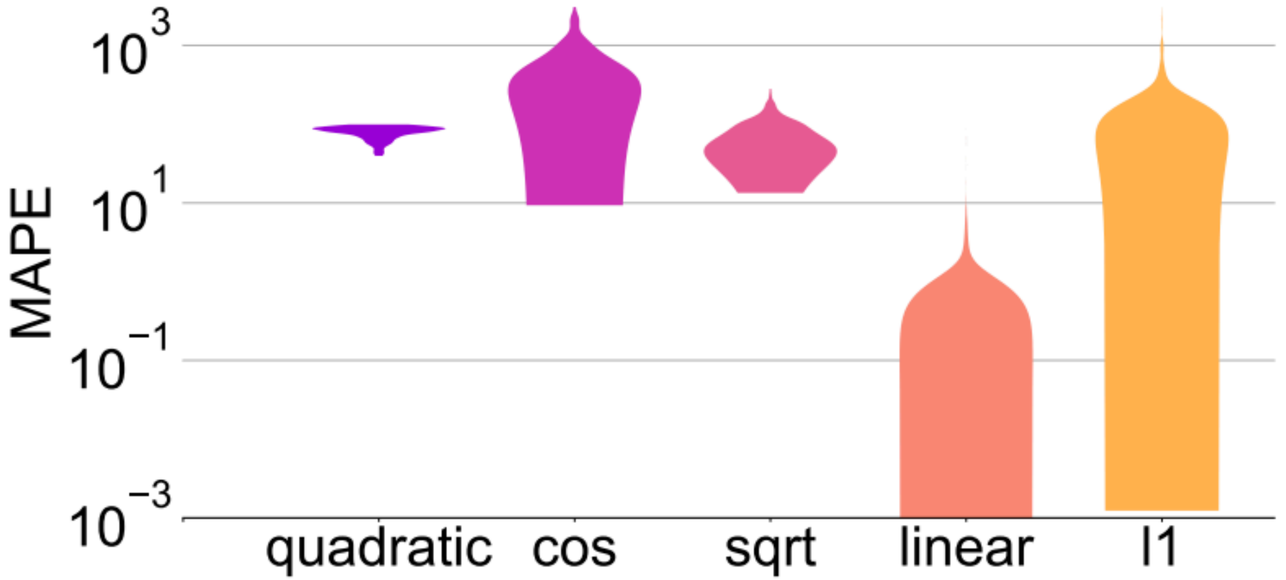


Theorem (XZLDKJ'21)

Let f be a two-layer ReLU MLP trained by GD*. For any direction $v \in \mathbb{R}^d$, let $x = tv$. For any $h > 0$, as $t \to \infty$, $f(x + hv) - f(x) \to \beta_v h$ with rate $O(1/t)$

* *Assumption: NTK regime*

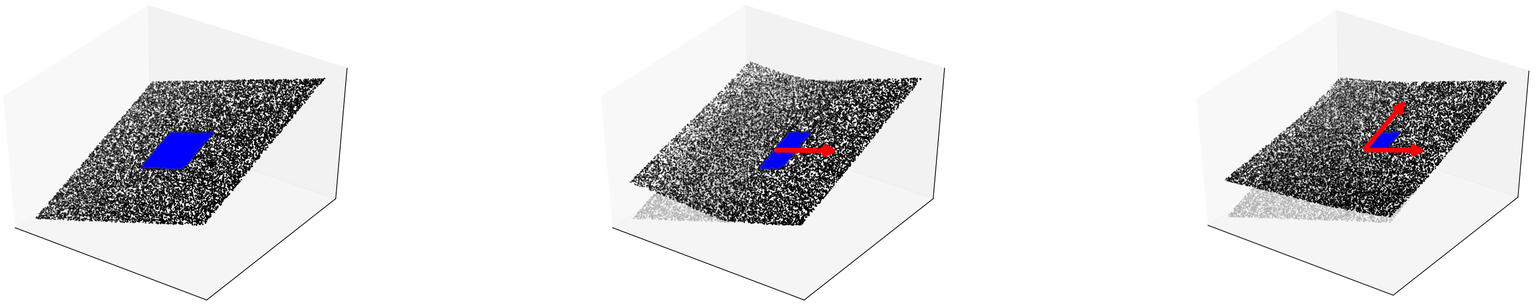
Implication of linear extrapolation



MAPE extrapolation error: lower the better

* *Note: this does not follow from ReLU networks have finitely many linear egions, which only implies asymptotic behavior*

Data geometry for learning linear functions



Theorem (XZLDKJ'21)

Let f be a two-layer ReLU MLP trained by GD*. Suppose target function is $\beta^\intercal x$ and support of training distribution covers all directions. As the number of training examples $n \to \infty, f(x) \to \beta^\intercal x$.

* *Assumption: NTK regime*

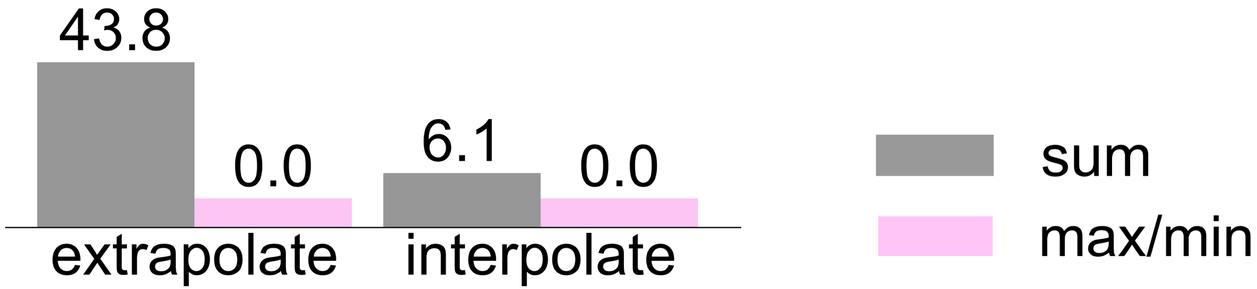
Implications for GNNs

Shortest Path: $d[k][u] = \min_{v \in \mathcal{N}(u)} d[k-1][v] + \boldsymbol{w}(v,u)$

GNN (sum): $h_u^{(k)} = \Sigma_v \ \mathbf{MLP}^{(k)}\left(h_v^{(k-1)}, h_u^{(k-1)}, w(v,u)\right)$

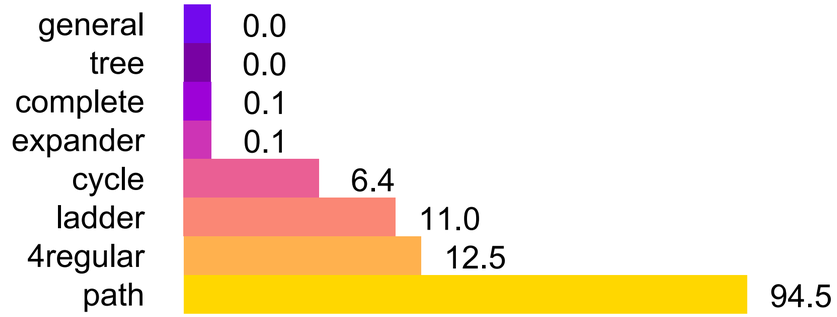
GNN that encodes the nonlinearity min

$$h_u^{(k)} = \min_v \mathbf{MLP}^{(k)}\left(h_v^{(k-1)}, h_u^{(k-1)}, w(v,u)\right)$$

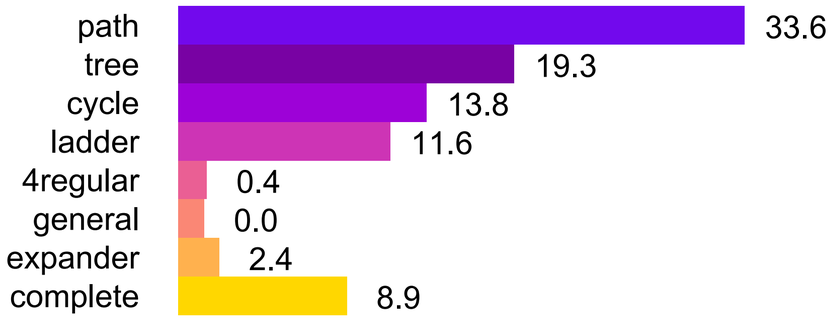


Data distribution and architecture

Data diversity: feature direction (MLP), graph structure (GNN)



Max Degree



Shortest Path

Theorem (XZLDKJ'21)

A GNN encoding max in aggregation trained by GD* learns max degree if training data $\{\deg_{\max}(G_i), \deg_{\min}(G_i), N_i^{\max} \deg_{\max}(G_i), N_i^{\min} \deg_{\min}(G_i)\}_{i=1}^n$ spans $\mathbb{R}^4$.

* *Assumption: NTK regime*

Linear algorithmic alignment

Linear algorithmic alignment (XZLDKJ'21)
Network can simulate underlying function via ~~*easy-to-learn*~~ *linear* "modules"

Hypothesis: Linear algo alignment helps *extrapolation*

Application: Encode nonlinearity in **architecture** or **input representation**.

Encoding nonlinearities in architecture

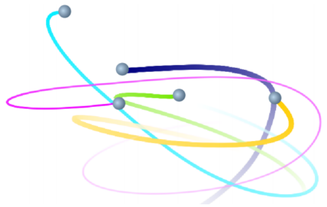
Activation, pooling, symbolic operations etc…

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

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

Encode **exp log** for learning multiplication

(Trask et al. 2018, Madsen & Johansen 2020)



$$\vec{a}_i = \frac{C}{M_i} \sum_{j \neq i} (1 - r_{ij}) \hat{r}_{ij}$$

Symbolic output *(Cranmer et al 2020)*

Q: What direction is the closest creature facing?

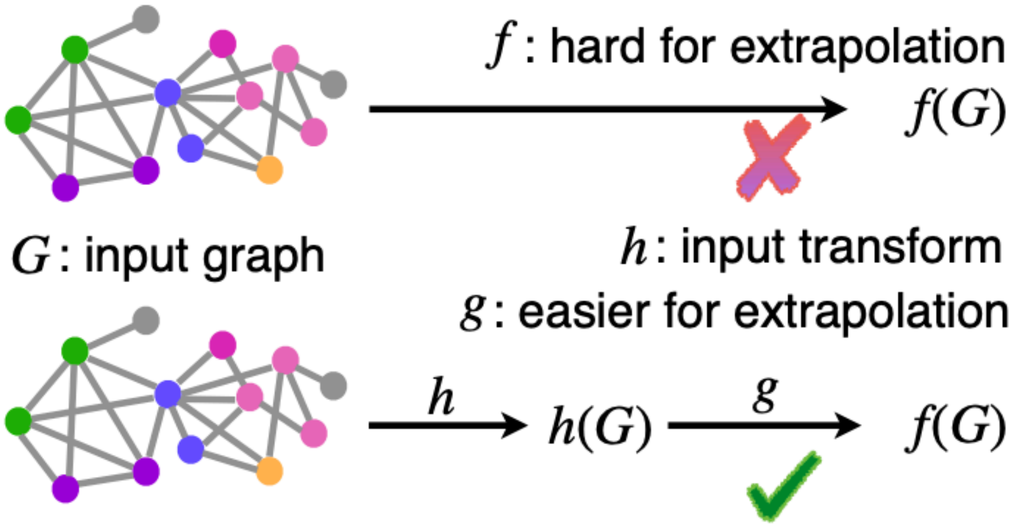
P: `scene, filter_creature, filter_closest, unique, query_direction`

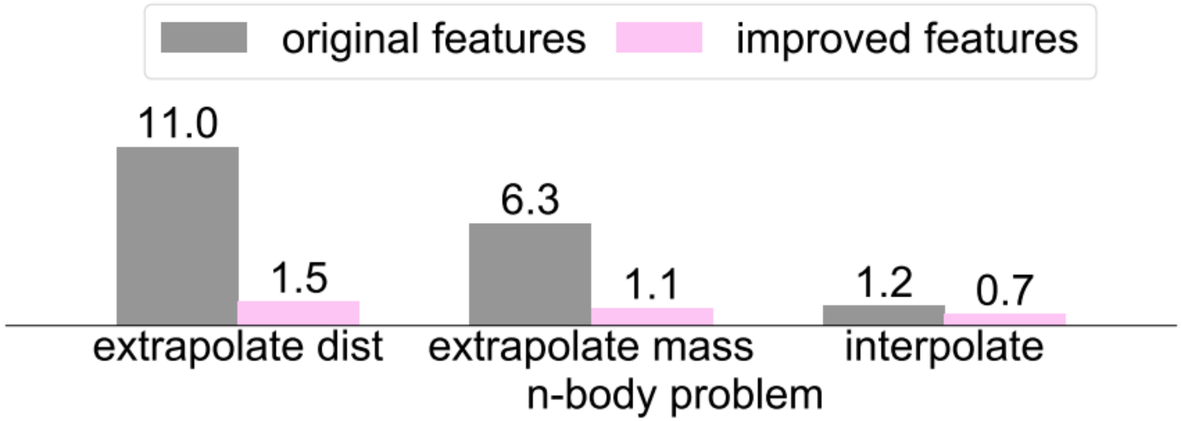
A: left

Encode **a library of programs** (~2K)

(Johnson et al 2017, Yi et al. 2018, Mao et al 2019…)

Encoding nonlinearities in input representation





Specialized features, feature transformation

Representation learning with out-of-distribution data (e.g., BERT)

Summary

1. Analysis of training algorithm, network & task structure, data distribution
2. Better alignment implies better generalization
3. Non-linearities matter for extrapolation

Graph Neural Tangent Kernel: Fusing Graph Neural Networks with Graph Kernels. S. S. Du, K. Hou, B. Poczos, R. Salakhutdinov, R. Wang, K. Xu. NeurIPS 2019.

What Can Neural Networks Reason About? K. Xu, J. Li, M. Zhang, S. S. Du, K. Kawarabayashi, S. Jegelka. ICLR 2020.

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