Decision-focused learning: integrating downstream combinatorics in ML

Bistra Dilkina
Associate Professor of Computer Science
Co-Director of USC Center on AI in Society
University of Southern California

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Workshop on Deep Learning and Combinatorial Optimization

ML ⟷ Combinatorial Optimization

- Exciting and growing research area

Infusing Discrete Optimization with Machine Learning

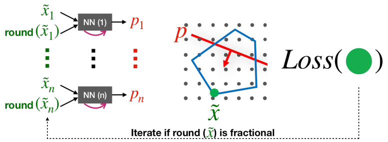
ML Paradigm

Self-Supervised Learning

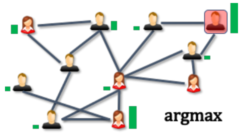
Reinforcement Learning

Supervised Learning

General IP Heuristic

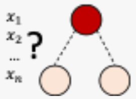


Greedy Heuristic



Exact Solving

Branching



Heuristic Selection

Graph Optimization

Integer Programming

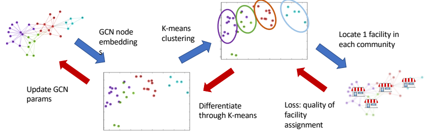
Problem Type

Elias Khalil

Augment discrete optimization algorithms with learning components

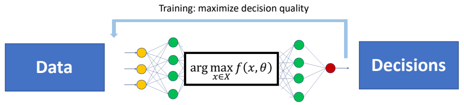
Infusing ML with Constrained Decision Making

ClusterNET: Differentiable kmeans for a class **graph optimization problems**



MIPaaL: **MIP** as a layer in Neural Networks

Decision-focused learning for **submodular optimization and LP**



Learning methods that incorporate the combinatorial decisions they inform

Bryan Wilder

The data-decisions pipeline

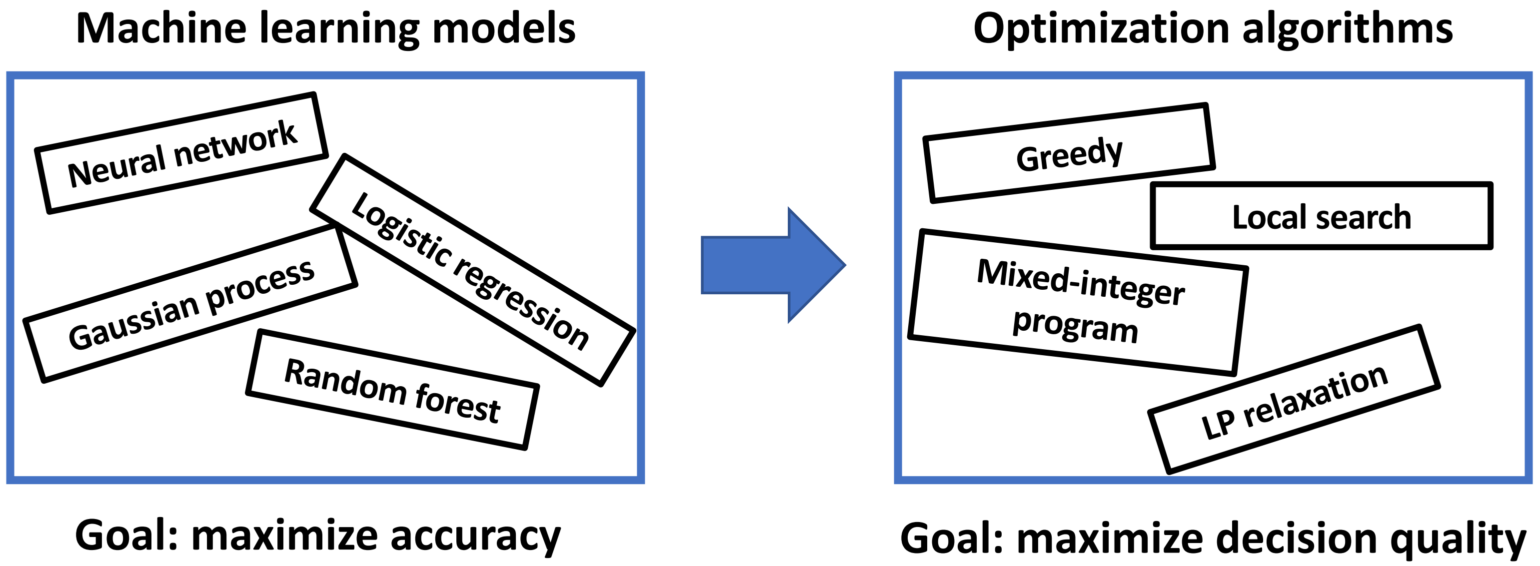
Many real-world applications of AI involve a common template:

[Horvitz and Mitchell 2010; Horvitz 2010]

Observe data ➡ Predictions ➡ Decisions

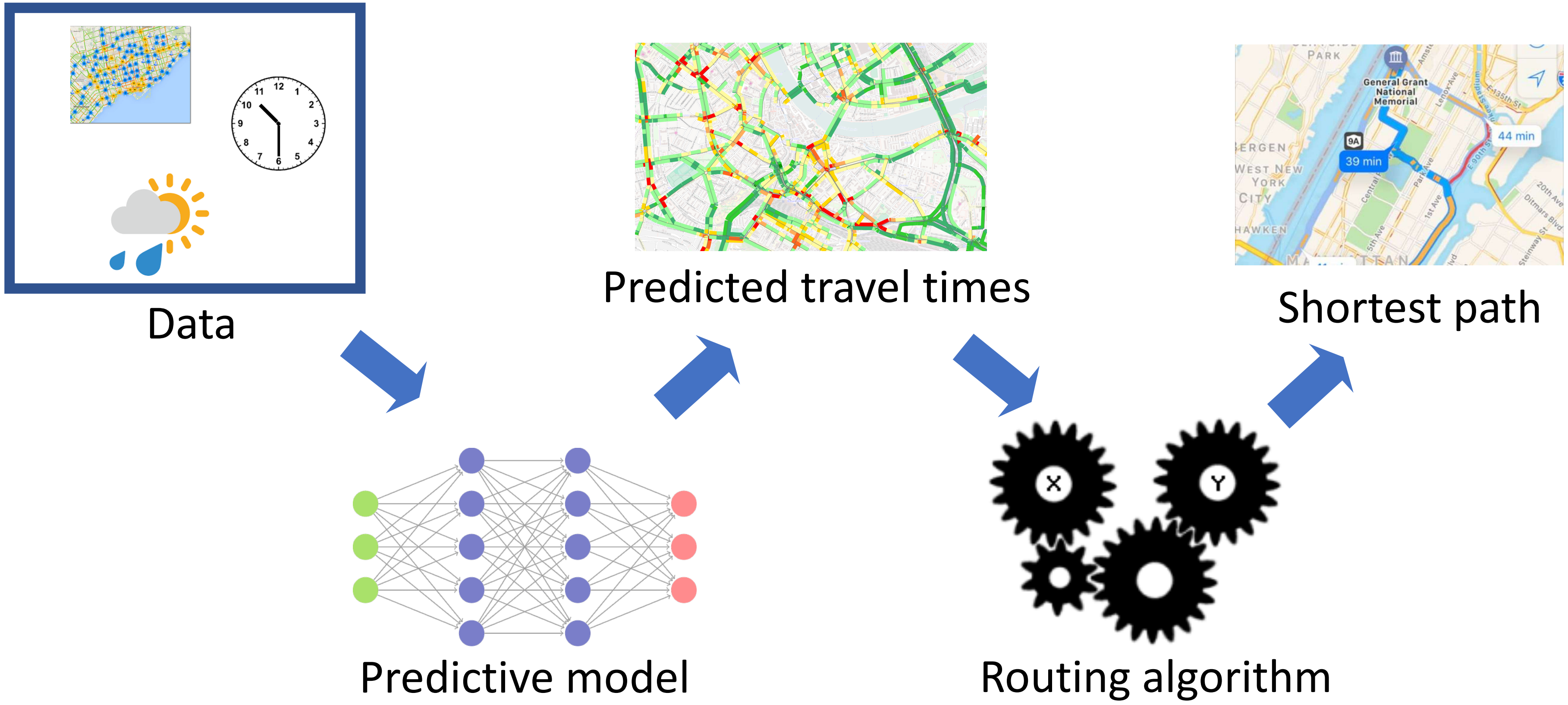
[Wilder et al., AAAI 2019]

Typical two-stage approach



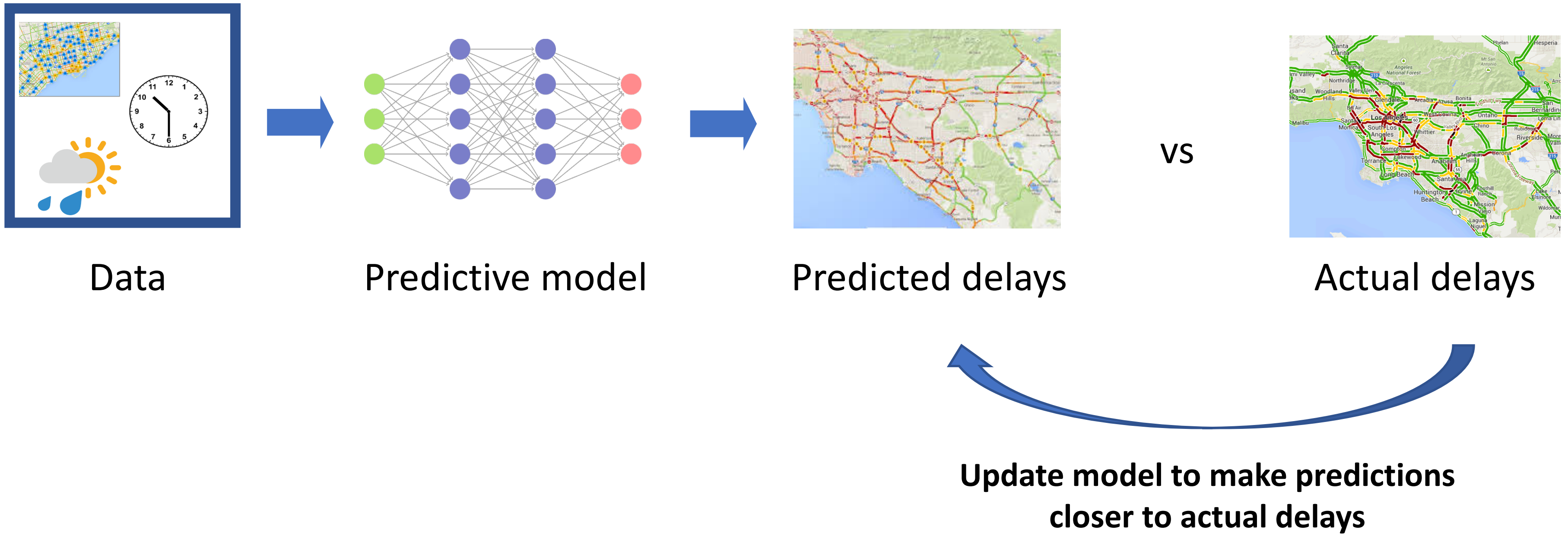
[Wilder et al., AAAI 2019]

Google maps



[Wilder et al., AAAI 2019]

Two-stage training



Challenge

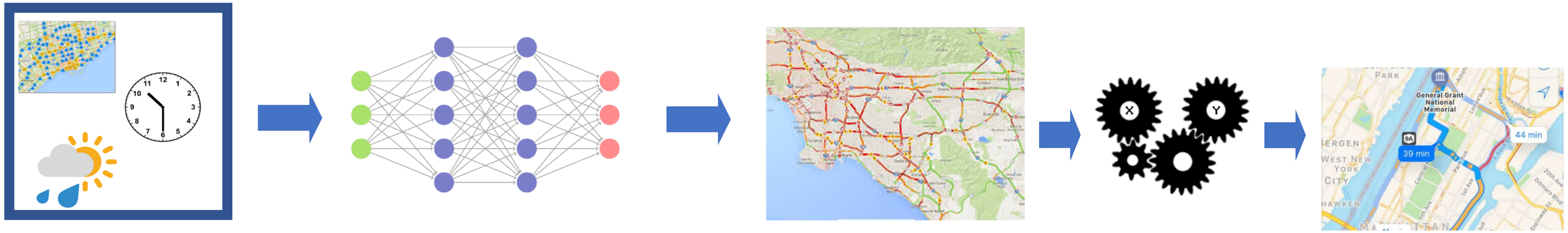
- Maximizing accuracy ≠ maximizing decision quality
- "All models are wrong, some are useful"
- Two-stage training doesn't align with end goal

[Wilder et al., AAAI 2019]

Key idea:

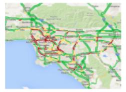
Decision-focused learning

Automatically shape the ML model’s loss by incorporating the combinatorial optimization problem into the training loop



Data | Predictive model | Predicted delays | Optimization algorithm | Shortest path

Update model to improve chosen path (**w.r.t. actual delays**)



Ferber et al (2020), Wilder et al. (2019), Donti, Amos, and Kolter (2017), …., Bengio (1997)

Wilder, Dilkina, Tambe. Melding the Data-Decisions Pipeline: Decision-Focused Learning for Combinatorial Optimization. AAAI 2019.

Decision-focused learning

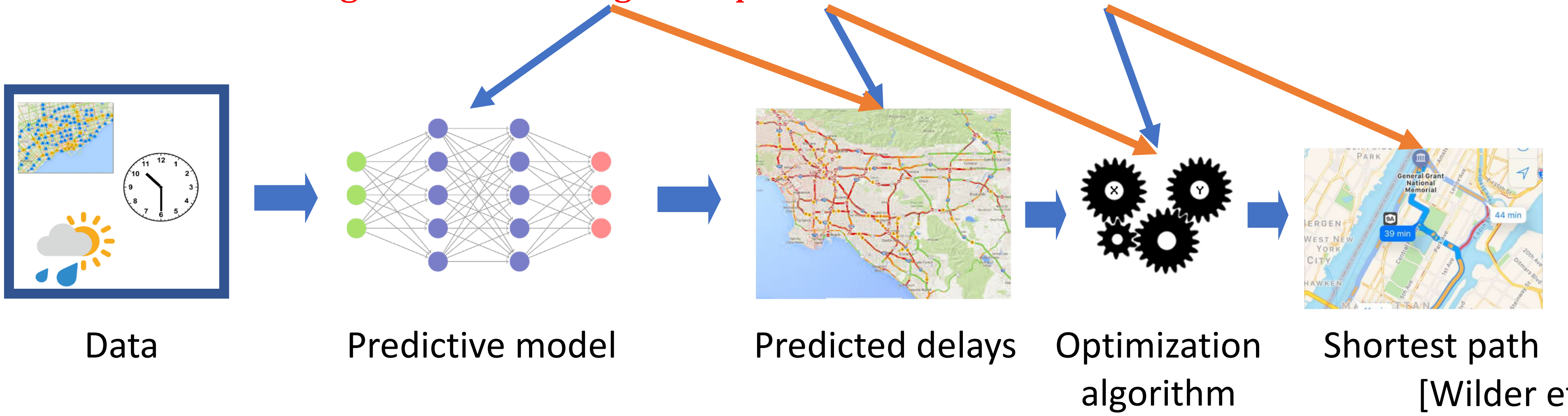
Objective function $f(x, \theta)$

$x \in \{0, 1\}^n$ are the **discrete** decision variables

θ are **unknown parameters** (i.e. the coefficients in the objective e.g., true travel times)

Idea: **Take derivative of decision objective w.r.t. ML model weights**, train model via gradient descent (e.g. *similar approach for convex opt. [Donti et al ’17]*)

$$\frac{\partial \text{obj(decision)}}{\partial \text{weights}} = \frac{\partial \text{prediction}}{\partial \text{weights}} \frac{\partial \text{decision}}{\partial \text{prediction}} \frac{\partial \text{obj(decision)}}{\partial \text{decision}}$$



[Wilder et al., AAAI 2019]

Approach

[Wilder, Dilkina, Tambe, AAAI 2019]

- **Challenge:** the optimization problem is discrete!
- **Solution: relax to continuous problem, differentiate, round**

Discrete		Continuous
$\max_{x \in X} f(x, \theta)$	➡	$\max_{x \in conv(X)} F(x, \theta)$
x = binary decision		x = fractional decision F = continuous objective

- How to compute $\frac{dx^*}{d\theta}$?
- Idea: (locally) optimal continuous solution must satisfy KKT conditions (which are sufficient for convex problems)
- The KKT conditions define a system of linear equations based on the gradients of the objective and constraints around the optimal point.
- Differentiate those equations at optimum (e.g. convex opt. [Donti, Amos, and Kolter 2017])

[Wilder et al., AAAI 2019]

Linear programs

Model exactly <u>combinatorial</u> problems like bipartite matching, shortest path, mincut, etc.

Or correspond to a relaxation of other <u>combinatorial</u> problems

Standard form:

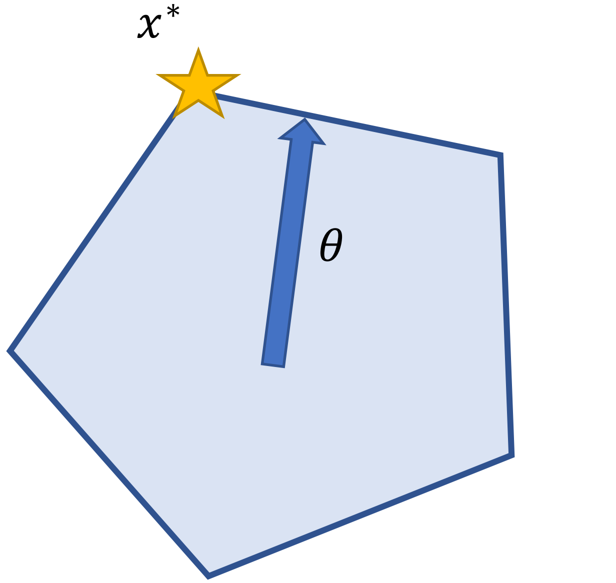
$$\max_x \theta^T x$$
$$Ax \leq b$$

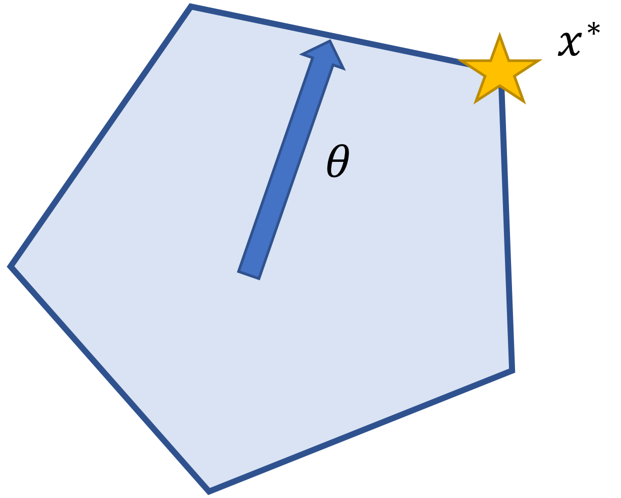
- $\frac{dx^*}{d\theta}$ doesn't exist!

- Solution: add a regularizer to smooth things out

$$\max_x \theta^T x \; - \gamma \|x\|_2^2$$
$$Ax \leq b$$

- Now, Hessian is $\nabla_x^2 f(x, \theta) = -2\gamma I \prec 0$
- Provably (a) differentiable and (b) close to original LP





[Wilder et al., AAAI 2019]

Results

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- Combinatorial problems: encoded as LP, e.g. **bipartite maximum matching**
- Combinatorial problems: submodular maximization, e.g. **influence maximization, budget allocation, diverse recommendation**

- Decision-focused has consistently better solution quality
  - **15-70% improvement in solution over 2-Stage**, across three domains

Table 1: Solution quality of each method for the full data-decisions pipeline.

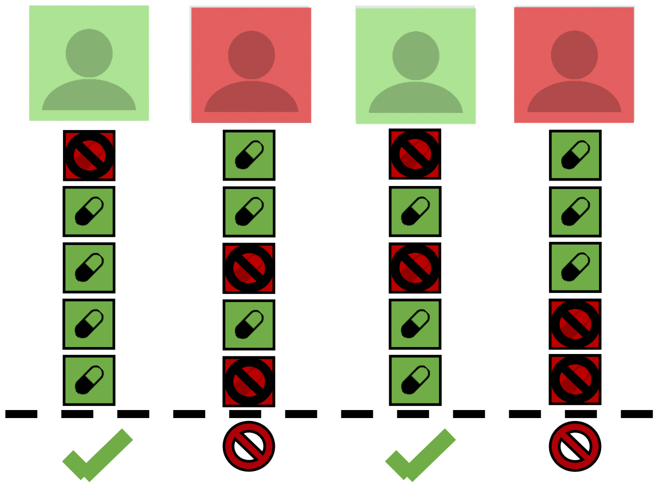
	Budget allocation			Matching	Diverse recommendation		
$k =$	5	10	20	–	5	10	20
NN1-Decision	**49.18 ± 0.24**	**72.62 ± 0.33**	**98.95 ± 0.46**	2.50 ± 0.56	**15.81 ± 0.50**	**29.81 ± 0.85**	**52.43 ± 1.23**
NN2-Decision	44.35 ± 0.56	67.64 ± 0.62	93.59 ± 0.77	**6.15 ± 0.38**	13.34 ± 0.77	26.32 ± 1.38	47.79 ± 1.96
NN1-2Stage	32.13 ± 2.47	45.63 ± 3.76	61.88 ± 4.10	2.99 ± 0.76	4.08 ± 0.16	8.42 ± 0.29	19.16 ± 0.57
NN2-2Stage	9.69 ± 0.05	18.93 ± 0.10	36.16 ± 0.18	3.49 ± 0.32	11.63 ± 0.43	22.79 ± 0.66	42.37 ± 1.02

- But typically much less accurate (wrt AUC, MSE etc.)

[Wilder et al., AAAI 2019]

Application: Tuberculosis treatment

- Follow-on work improving treatment in Indian TB system
- In collaboration with Everwell (NGO)
- **Predict** if patients will miss daily dose
- **Optimize** health worker visits subject to knapsack constraints (LP)

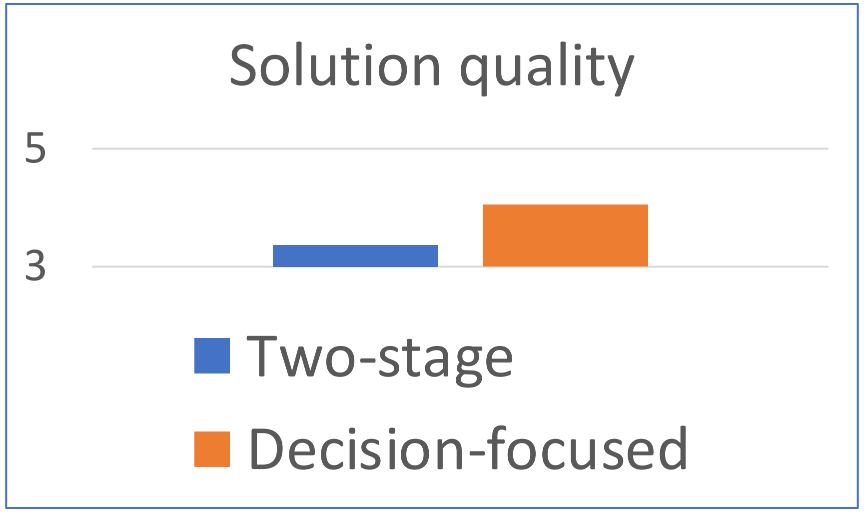


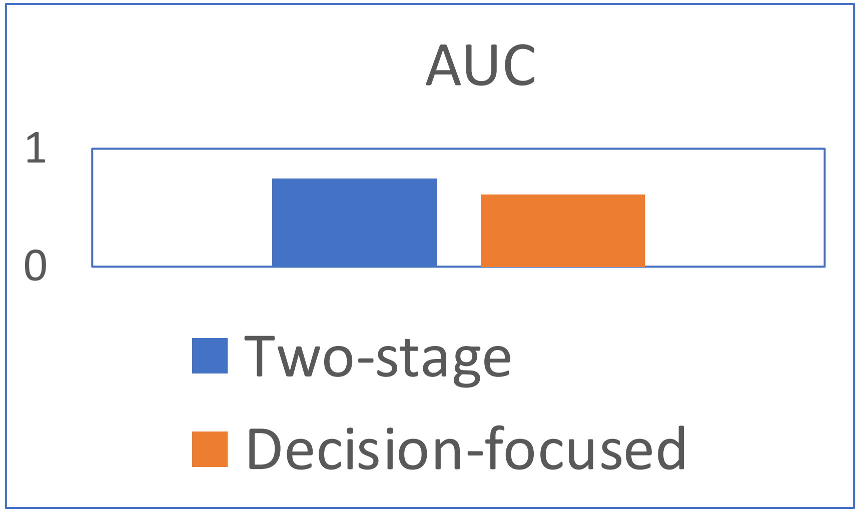
- More in our paper

Killian, Wilder, Sharma, Choudhary, Dilkina, Tambe. **Learning to Prescribe Interventions for Tuberculosis Patients using Digital Adherence Data.** KDD 2019.

[Killian et al, KDD 2019]

Application: Tuberculosis treatment





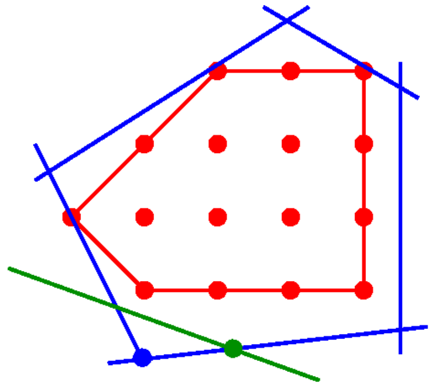
Less “accurate”, but +15% successful interventions!

[Killian et al, KDD 2019]

Decision Focused Learning for Mixed Integer Programming (MIP) problems

- MIPs capture many combinatorial problems that do not have a nice relaxation-based algorithm
- ..and we know how to differentiate through LP optimization

- Idea: cutting planes for MIP results in LP with added cuts
- Differentiate through Cutting-plane-generated LP for training



- At test time, obtain predictions and solve MIP with Branch-and-Bound

Ferber, Wilder, Dilkina, Tambe. **MIPaaL: Mixed Integer Program as a Layer.** AAAI 2020.

[Ferber et al, AAAI 2020]

Domains

- **Portfolio Optimization**
  - Predict monthly rate of return (% return)
  - Optimize monthly return for portfolio
  - Limiting risk, sector exposure, transactions…
  - Data: SP500 (USA), DAX (Germany)
- **Diverse Bipartite Matching**
  - Predict match success probability
  - Optimize total number of successful matches
  - Matching constraints: each node matched at most once
  - Ensure min % of proposed matches are different/same type
  - Data: CORA citation network, nodes = papers, edges = citations
- **Energy Production Knapsack**
  - Predict energy prices
  - Optimize total revenue
  - Limit on number of time periods we can generate energy
  - Data: ICON Energy Scheduling Challenge

[Ferber et al, AAAI 2020]

Results: decision quality at test time

Objective: monthly % increase for portfolio optimization (SP500 and DAX), number of pairs successfully matched for Matching (CORA), and value of items for Knapsack (Energy).

	SP500	DAX	Matching	Knapsack
MIPaaL	**2.79 ± 0.17**	**5.70 ± 0.68**	**4.80 ± 0.71**	**507.70 ± 0.471**
MIPaaL-Warm	1.09 ± 0.18	0.68 ± 1.01	2.14 ± 0.51	499.60 ± 0.566
MIPaaL-Hybrid	1.08 ± 0.15	0.74 ± 1.10	3.21 ± 0.73	503.36 ± 0.578
MIPaaL-1000	2.60 ± 0.16	4.39 ± 0.66	3.45 ± 0.71	506.34 ± 0.662
MIPaaL-100	1.25 ± 0.14	0.35 ± 0.63	2.57 ± 0.54	505.99 ± 0.621
RootLP (Wilder et al. 2019)	1.97 ± 0.17	-1.97 ± 0.69	3.17 ± 0.60	501.58 ± 0.662
TwoStage	1.19 ± 0.15	0.70 ± 1.46	3.42 ± 0.78	501.49 ± 0.523

- MIPaaL gives **2x monthly returns on SP500 and 8x on DAX**
- MIPaaL **improves the objective by 40.3% and 1.2% for Matching and Knapsack respectively**.
- MIPaaL outperforms all other variants considered.

[Ferber et al, AAAI 2020]

Transfer Learning

- Learn on one distribution of assets (30[a] SP assets) and test on another (30[b] other SP assets and 30 DAX assets), keeping the MIP size the same
- Learn on one size of MIPs (number of assets available, 30 SP) and **test on larger MIPs** (with more assets to choose from 50-500 SP)

		SP-30[b]	DAX	SP-50	SP-100	SP-200	SP500
Decision Quality	MIPaaL	$\mathbf{2.02 \pm 0.48}$	$\mathbf{2.77 \pm 0.40}$	$\mathbf{1.93 \pm 0.13}$	$\mathbf{2.27 \pm 0.11}$	$\mathbf{2.17 \pm 0.48}$	$\mathbf{2.26 \pm 0.37}$
	RootLP	1.81 ± 0.44	1.74 ± 0.43	1.50 ± 0.09	1.58 ± 0.08	1.82 ± 0.41	1.90 ± 0.29
	TwoStage	0.71 ± 0.04	0.82 ± 0.54	1.58 ± 0.13	1.22 ± 0.09	1.50 ± 0.58	1.11 ± 0.35
ML Loss	MIPaaL	4.81 ± 8.59	4.59 ± 8.80	5.42 ± 3.16	5.42 ± 2.37	5.25 ± 1.83	5.43 ± 1.67
	RootLP	5.14 ± 1.02	5.39 ± 1.04	4.73 ± 3.17	4.88 ± 2.58	4.81 ± 1.91	4.83 ± 1.56
	TwoStage	$\mathbf{0.08 \pm 0.05}$	$\mathbf{0.07 \pm 0.03}$	$\mathbf{0.08 \pm 0.02}$	$\mathbf{0.07 \pm 0.01}$	$\mathbf{0.08 \pm 0.01}$	$\mathbf{0.08 \pm 0.01}$

Decision-Focused Learning

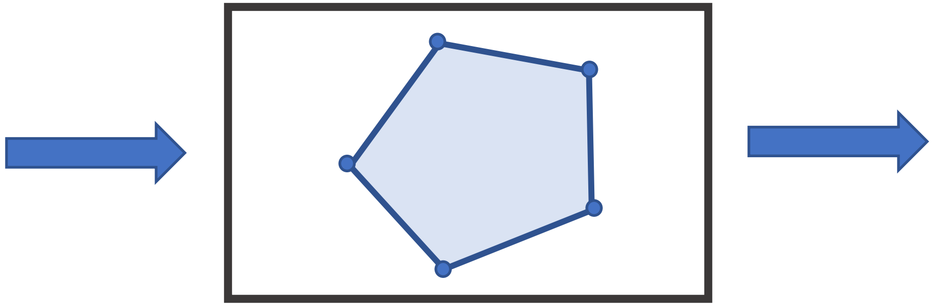
- No need to silo out ML vs Optimization tasks
- When data is scarce, we want predictions to be accurate where it matters most for decision making
- Marrying predictive and prescriptive tasks in a unified **end-to-end system**

Related Frameworks:

- Empirical decision model learning (M Lombardi, M Milano, A Bartolini, Artificial Intelligence 2017)
- "Predict-and-optimize" framework and its variants
  (Elmachtoub & Grigas, 2017; Demirovic et al., 2019; Mandi et al., AAAI 2020)
- Blackbox differentiation of combinatorial solvers
  (Vlastelica et al, ICLR 2020; Rolínek et al, ECCV 2020; Paulus et al NeurIPS 2020 LMCA Workshop)

Relax + differentiate

Forward pass: run a solver



Backward pass: sensitivity analysis via KKT conditions

Convex QPs *[Amos and Kolter 2017, Donti et al 2017]*
Linear and submodular programs *[Wilder, Dilkina, Tambe 2019]*
MAXSAT (via SDP relaxation) *[Wang, Donti, Wilder, Kolter 2019]*
MIPs *[Ferber, Wilder, Dilkina, Tambe 2020]*

Some problems don't have good relaxations
Slow to solve continuous optimization problem
Slow to backprop through – $O(n^3)$

[Wilder et al, NeurIPS 2019]

An Alternative Approach

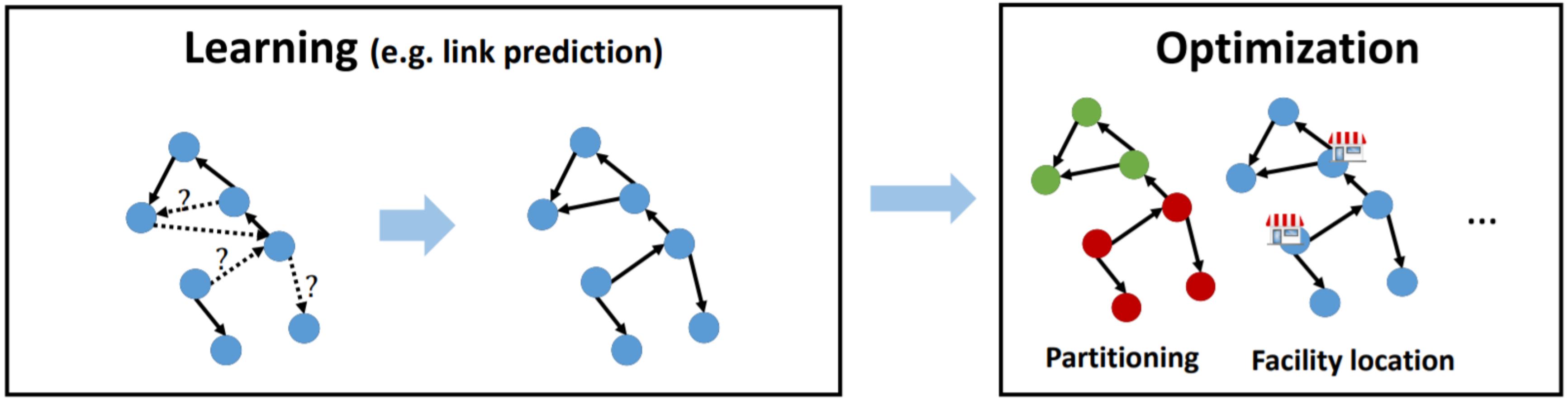
- Learn a **representation** that maps the original problem to a simpler (efficiently differentiable) **proxy problem**.

- **Instantiation for a class of graph problems**: k-means clustering in embedding space.

Wilder, Ewing, Dilkina, Tambe. **End to End Learning and Optimization on Graphs.** NeurIPS 2019.

[Wilder et al, NeurIPS 2019]

Graph learning + graph optimization



[Wilder et al, NeurIPS 2019]

Problem classes

- **Partition the nodes into K disjoint groups**
  - Community detection, maxcut, …
- **Select a subset of K nodes**
  - Facility location, influence maximization, …
- Methods of choice are often combinatorial/discrete

Approach

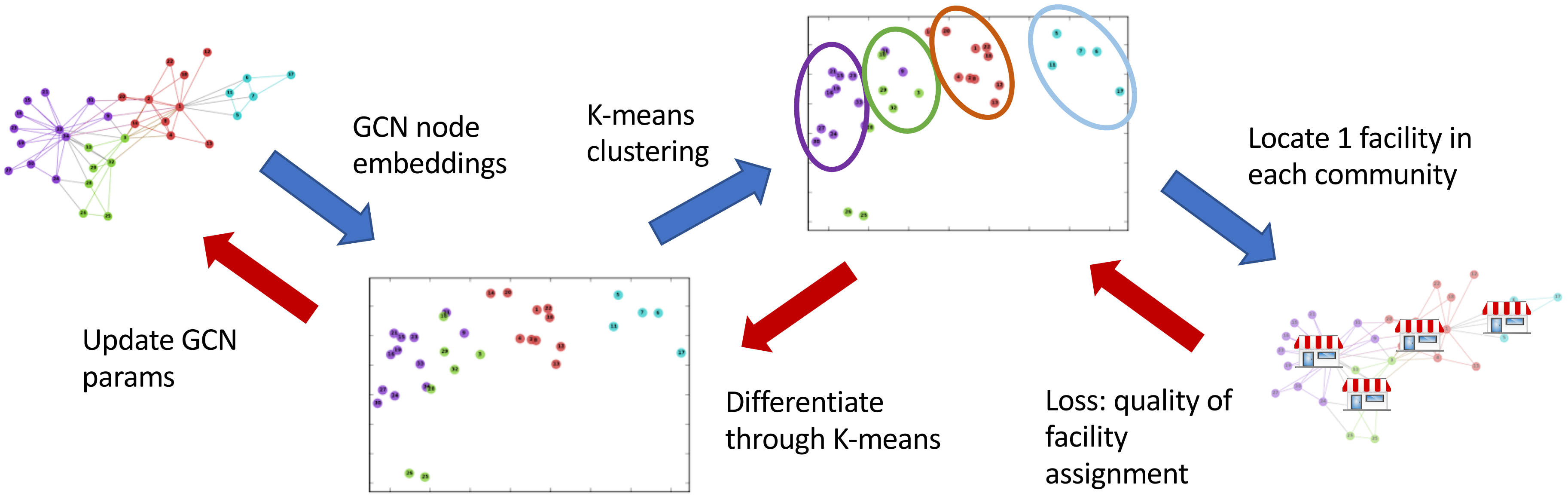
- Observation: **clustering nodes** is a good proxy
  - Partitioning: correspond to well-connected subgroups
  - Facility location: put one facility in each community
- Observation: graph learning approaches already embed into R^n

[Wilder et al, NeurIPS 2019]

ClusterNet

One architecture and training process for all problems in these classes, which automatically learns a differentiable solver for a given problem

1. Embed nodes with GCN (Goal: train GCN to produce task-specific embeddings)
2. Run soft K-means on embeddings
3. Interpret clustering as optimization solution
4. Backpropagate optimization objective value



[Wilder et al, NeurIPS 2019]

Differentiable K-means

Forward pass

$$\mu_k = \frac{\sum_j r_{jk} x_j}{\sum_j r_{jk}}$$

Update cluster centers

$$r_{jk} = \frac{\exp(-\beta||x_j - \mu_k||)}{\sum_\ell \exp(-\beta||x_j - \mu_\ell||)}$$

Softmax update to node assignments

[Wilder et al, NeurIPS 2019]

Differentiable K-means

Backward pass

- Option 1: **differentiate through the fixed-point condition**

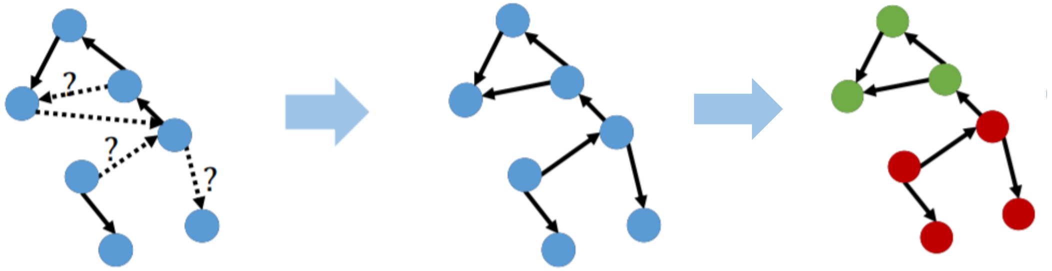
$$\mu^t = \mu^{t+1}$$

  - Prohibitively slow, memory-intensive
- Option 2: **unroll the entire series of updates**
  - Cost scales with # iterations
  - Have to stick to differentiable operations
- **Option 3: get the solution, then unroll one update**
  - Do anything to solve the forward pass
  - Linear time/memory, implemented in vanilla pytorch

Theorem [informal]: provided the clusters are sufficiently balanced and well-separated, the Option 3 approximate gradients converge exponentially quickly to the true ones.

[Wilder et al, NeurIPS 2019]

Example: community detection



Observe partial graph

Predict unseen edges

Find communities

max **modularity**

$$\max_{r} \frac{1}{2m} \sum_{u,v \in V} \sum_{k=1}^{K} \left[A_{u,v} - \frac{d_u d_v}{2m} \right] r_{uk} r_{vk}$$

$$r_{uk} \in \{0,1\} \quad \forall u \in V, k = 1 \ldots K$$

$$\sum_{k=1}^{K} r_{uk} = 1 \quad \forall u \in V$$

- **Useful in scientific discovery** (social groups, functional modules in biological networks)
- In applications, **two-stage approach is common**: [Yan & Gegory ’12, Burgess et al ‘16, Berlusconi et al ‘16, Tan et al ‘16, Bahulker et al ’18…]

[Wilder et al, NeurIPS 2019]

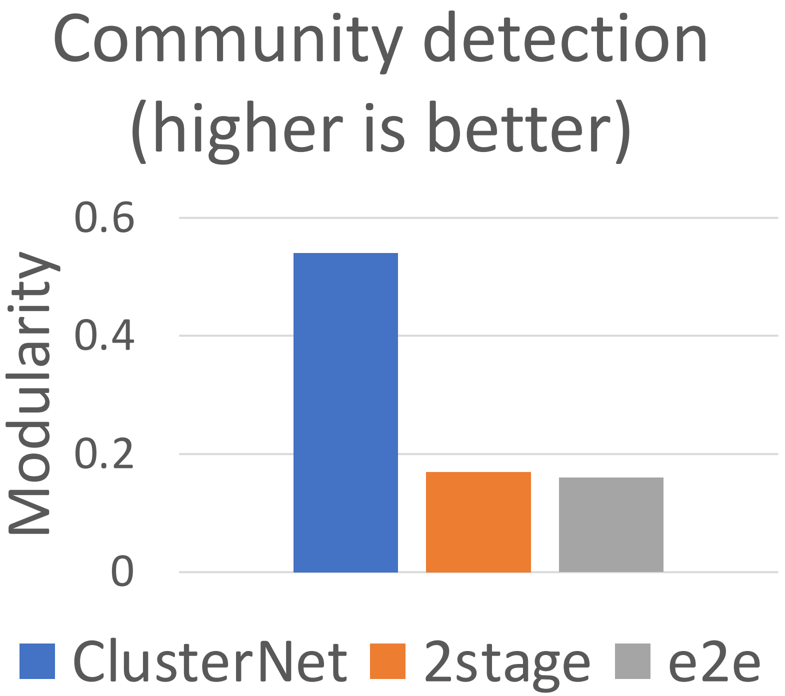
Experiments

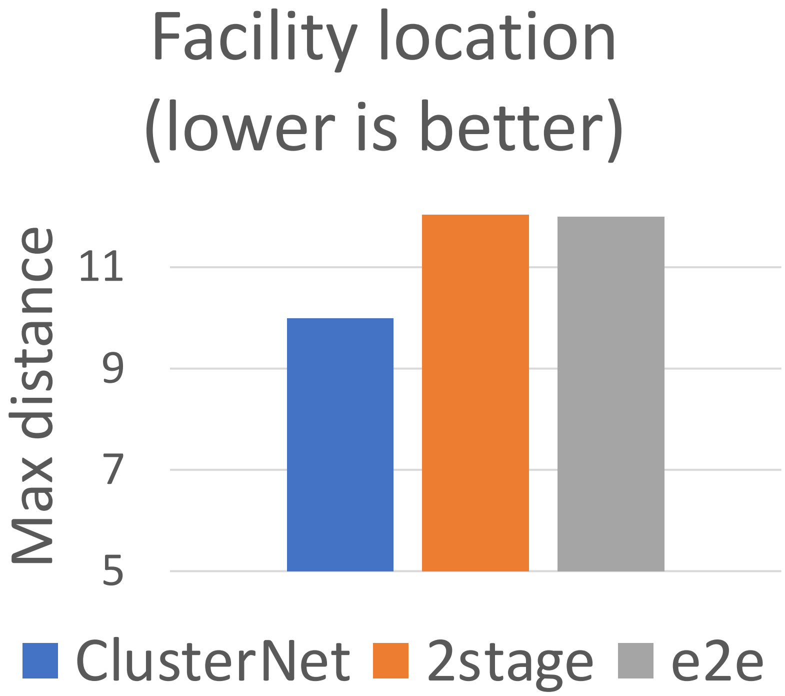
- **Learning problem**: link prediction
- **Optimization:**
  - community detection
  - facility location problems
- Train **GCNs** as predictive component

- **Comparison**
  - Two stage: GCN + expert-designed algorithm (**2Stage**)
  - Pure end to end: Deep GCN to predict optimal solution (**e2e**)
  - **ClusterNet**:
  - Community detection (use clusters as-is, measure modularity)
  - Facility location (one location in each cluster, measure max distance)

[Wilder et al, NeurIPS 2019]

Results: single-graph link prediction



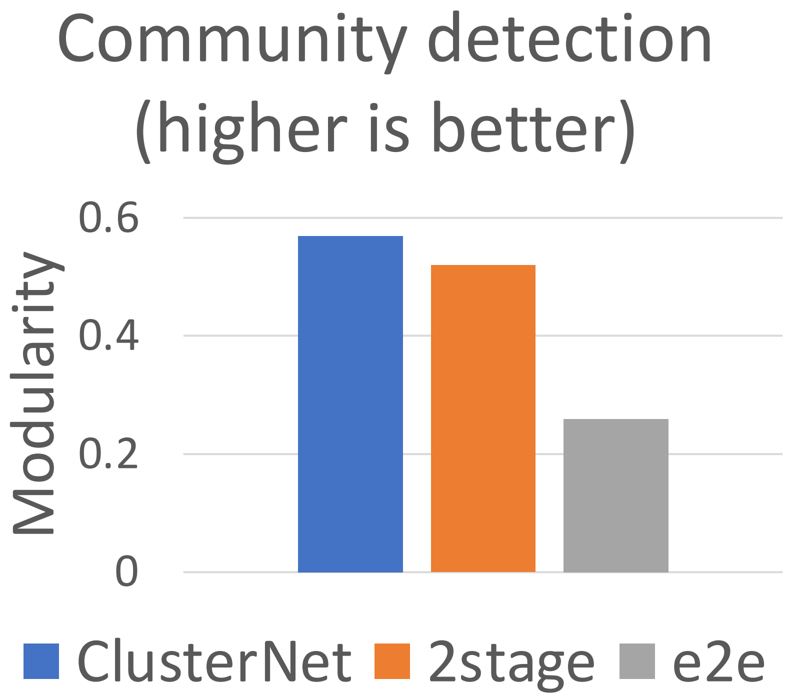


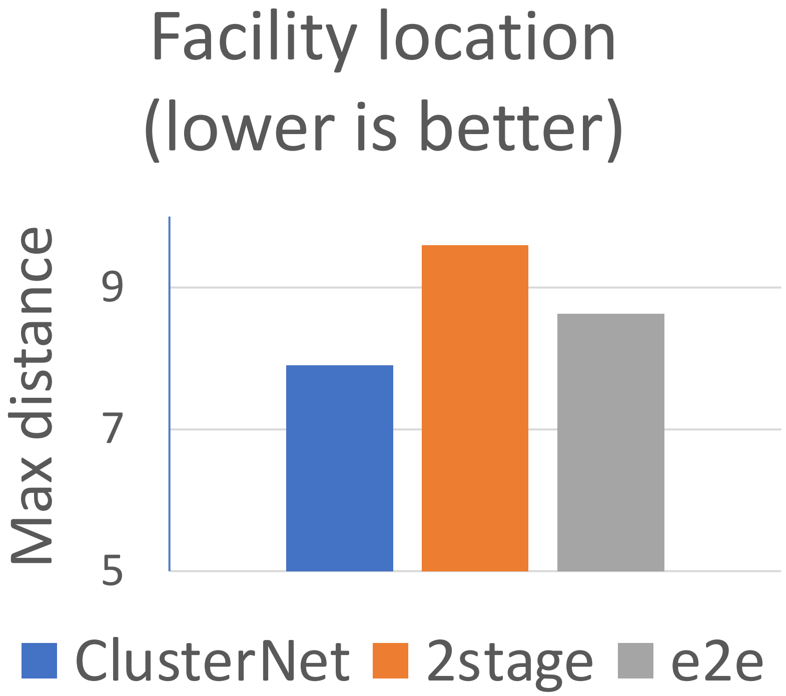
Representative example from **cora**, citeseer, protein interaction, facebook, adolescent health networks

Community algos: CNM, Newman, SpectralClustering
Facility Locations algos: greedy, gonzalez2approx

[Wilder et al, NeurIPS 2019]

Results: generalization across graphs





ClusterNet learns generalizable strategies for optimization!

[Wilder et al, NeurIPS 2019]

USC

Takeaways

- Decoupled approaches (2-stage) and pure end-to-end methods miss out on useful structure
- Good decisions require integrating learning and optimization as in decision-focused learning
- Even simple optimization primitives (e.g. clustering) provide good inductive bias