Machine learning for algorithm design: Theoretical guarantees and applied frontiers

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How to integrate **machine learning** into **algorithm design**?

- **Algorithm configuration**
  How to tune an algorithm's parameters?
- **Algorithm selection**
  Given a variety of algorithms, which to use?
- **Algorithm design**
  Can machine learning guide algorithm discovery?

How to integrate **machine learning** into **algorithm design**?

Algorithm configuration

How to tune an algorithm's parameters?

Algorithm selection

Given a variety of algorithms, which to use?

Algorithm design

Can machine learning guide algorithm discovery?

Algorithm configuration

Example: **Integer programming solvers**

Most popular tool for solving combinatorial (& nonconvex) problems

Routing

Manufacturing

Scheduling

Planning

Finance

Algorithm configuration

IP solvers (CPLEX, Gurobi) have a **ton** parameters

- CPLEX has **170-page** manual describing **172** parameters
- Tuning by hand is notoriously **slow**, **tedious**, and **error-prone**

Algorithm configuration

IP solvers (CPLEX, Gurobi) have a **ton** parameters

- CPLEX has **170-page** manual describing **172** parameters
- Tuning by hand is notoriously **slow**, **tedious**, and **error-prone**

What's the best **configuration** for the application at hand?

Best configuration for **routing** problems likely not suited for **scheduling**

How to integrate **machine learning** into **algorithm design**?

Algorithm configuration

How to tune an algorithm's parameters?

Algorithm selection

Given a variety of algorithms, which to use?

Algorithm design

Can machine learning guide algorithm discovery?

Algorithm selection in theory

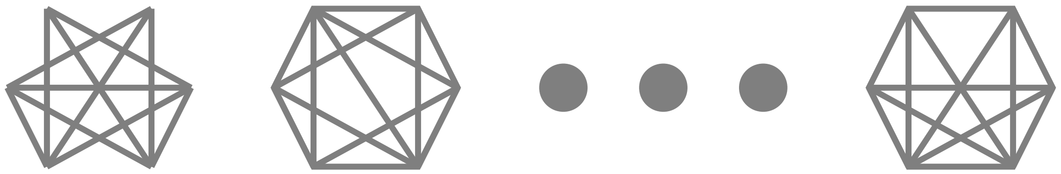
Worst-case analysis has been the main framework for decades

Has led to beautiful, practical algorithms

Worst-case instances **rarely occur in practice**

In practice:

Instances solved in **past** are similar to **future** instances…



In practice, we have data about the application domain

Routing problems a shipping company solves

In practice, we have data about the application domain

Clustering problems a biology lab solves

In practice, we have data about the application domain

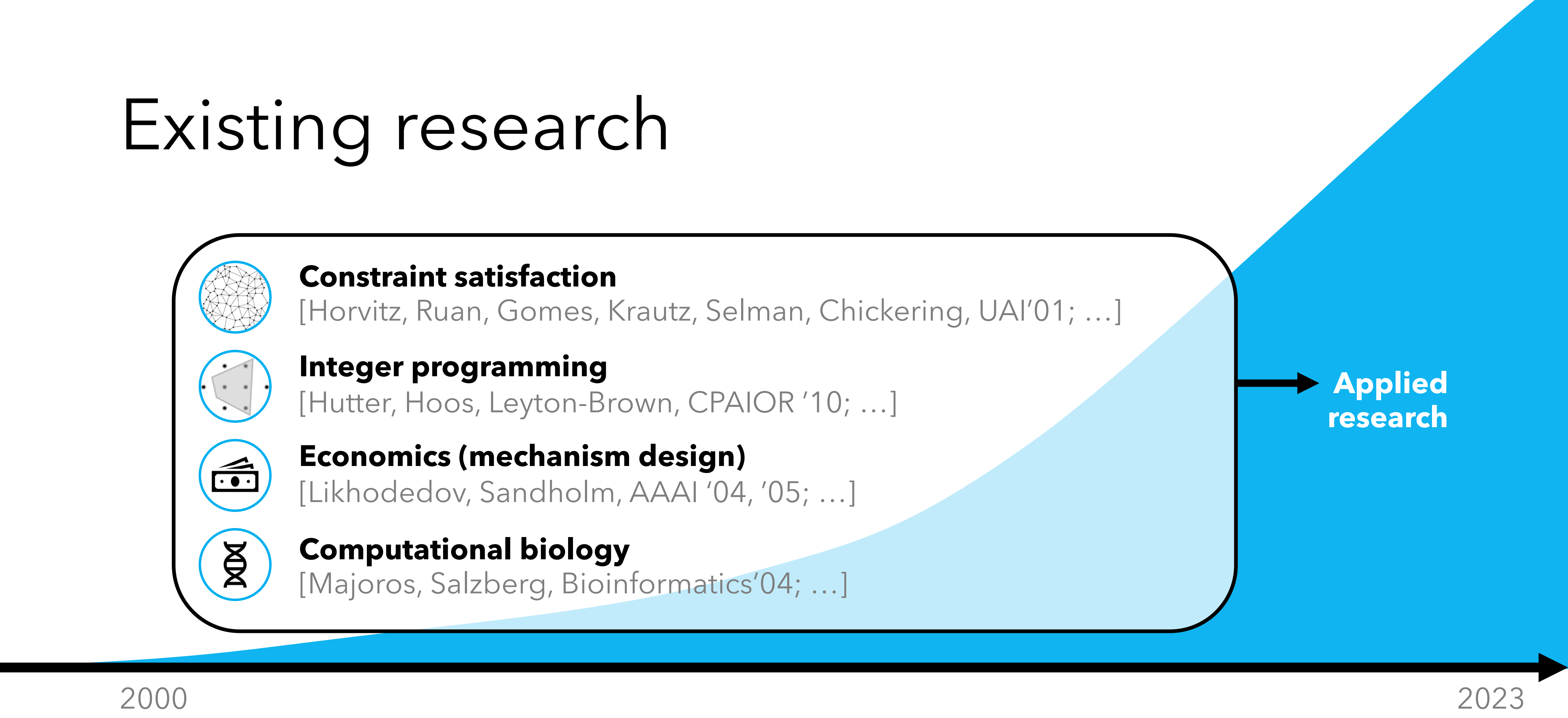
Existing research

Constraint satisfaction
[Horvitz, Ruan, Gomes, Krautz, Selman, Chickering, UAI'01; ...]

Integer programming
[Hutter, Hoos, Leyton-Brown, CPAIOR '10; ...]

Economics (mechanism design)
[Likhodedov, Sandholm, AAAI '04, '05; ...]

Computational biology
[Majoros, Salzberg, Bioinformatics'04; ...]

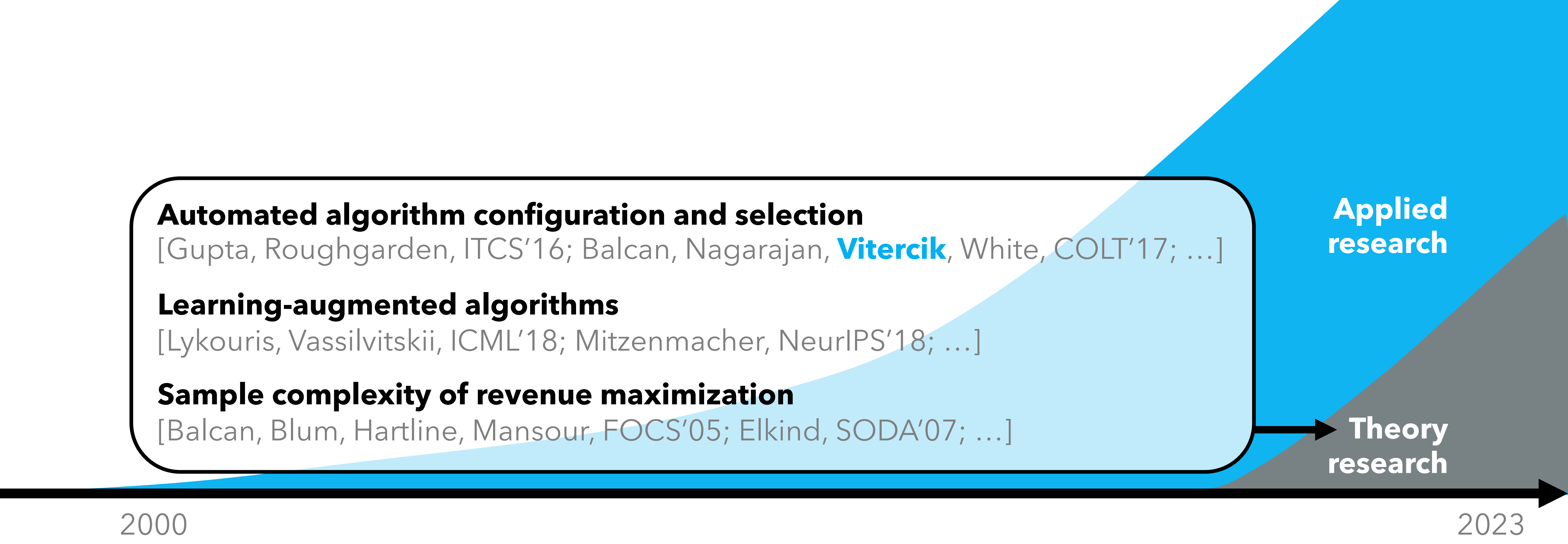


Existing research

Automated algorithm configuration and selection
[Gupta, Roughgarden, ITCS'16; Balcan, Nagarajan, **Vitercik**, White, COLT'17; …]

Learning-augmented algorithms
[Lykouris, Vassilvitskii, ICML'18; Mitzenmacher, NeurIPS'18; …]

Sample complexity of revenue maximization
[Balcan, Blum, Hartline, Mansour, FOCS'05; Elkind, SODA'07; …]



ML + algorithm design: Potential impact

Example: integer programming

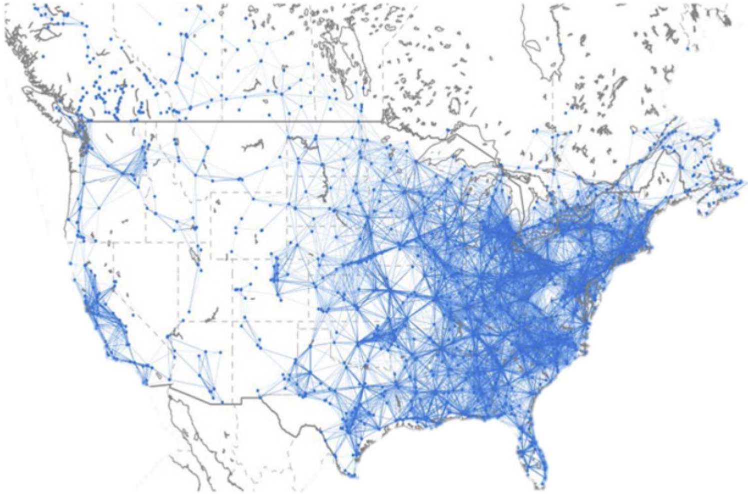
- Used heavily throughout industry and science
- **Many** different ways to incorporate **learning** into solving
- Solving is very difficult, so ML can make a huge difference

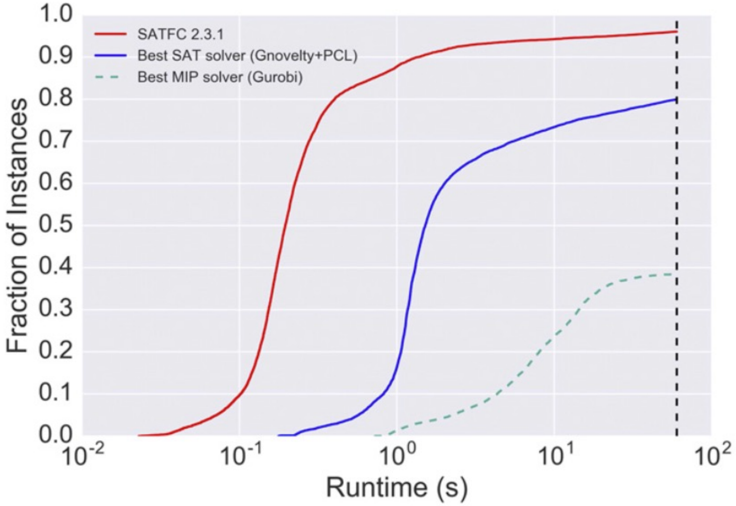




Example: Spectrum auctions

- In '16–'17, FCC held a $19.8 billion radio spectrum auction
  - Involves solving huge graph-coloring problems





- SATFC uses algorithm configuration + selection
- Simulations indicate SATFC saved the government billions

Leyton-Brown et al., PNAS'17; Leyton-Brown and Hutter, ICML'19 tutorial

Plan for tutorial

1. **Theoretical guarantees**
   a. Statistical guarantees for algorithm configuration
   b. Online algorithm configuration

2. **Applied techniques**
   a. Graph neural networks
   b. Reinforcement learning

Plan for tutorial

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   b. Online algorithm configuration

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   a. Graph neural networks
   b. Reinforcement learning

Gupta, Roughgarden, ITCS'16
Balcan, DeBlasio, Dick, Kingsford, Sandholm, **Vitercik**, STOC'21
Balcan, Prasad, Sandholm, **Vitercik**, NeurIPS'21
Balcan, Prasad, Sandholm, **Vitercik**, NeurIPS'22

Running example: Sequence alignment

Goal: Line up pairs of strings

Applications: Biology, natural language processing, etc.

vitterchik

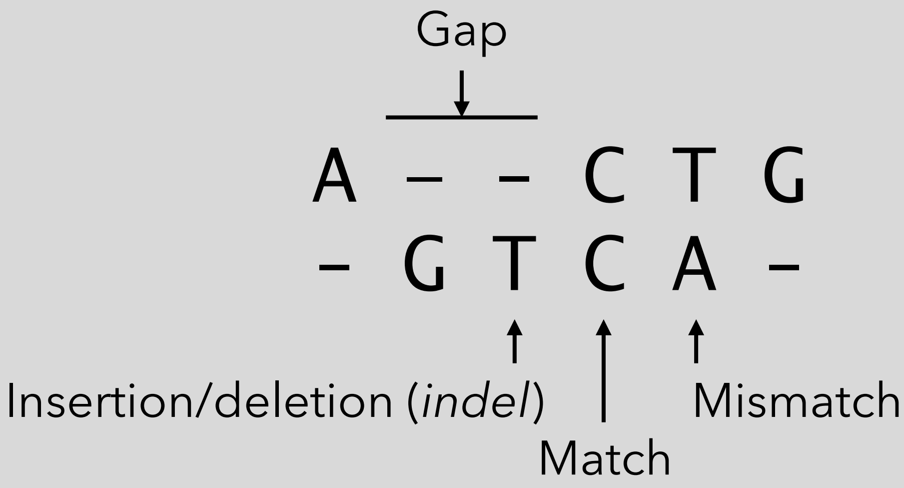
Did you mean: **vitercik**

Sequence alignment algorithms

Input: Two sequences S and S'

$$S = \text{A C T G}$$
$$S' = \text{G T C A}$$

Output: Alignment of S and S'



Sequence alignment algorithms

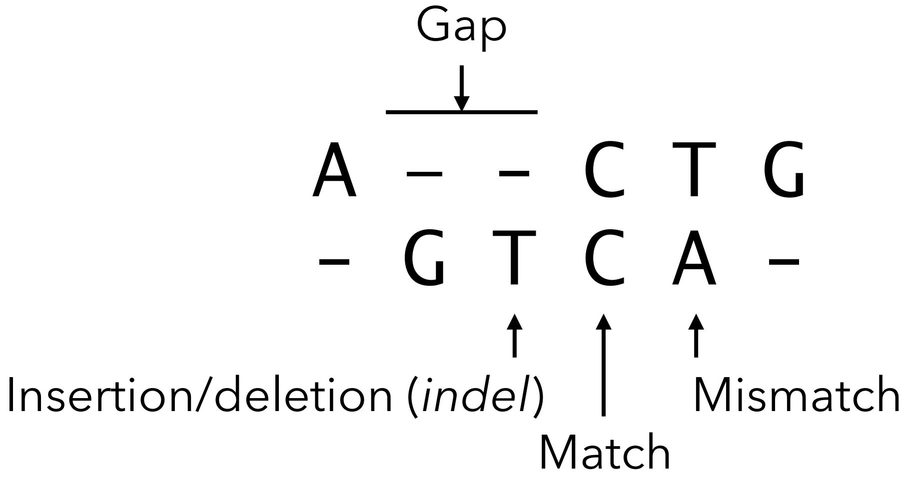
Standard algorithm with parameters $\rho_1, \rho_2, \rho_3 \geq 0$:

Return alignment maximizing:

$$(\text{\# matches}) - \rho_1 \cdot (\text{\# mismatches}) - \rho_2 \cdot (\text{\# indels}) - \rho_3 \cdot (\text{\# gaps})$$

S = A C T G

S' = G T C A



Sequence alignment algorithms

Can sometimes access **ground-truth, reference** alignment

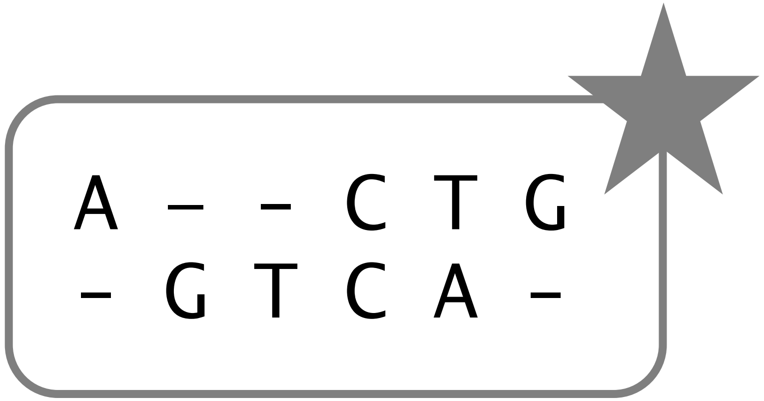
E.g., in computational biology: Bahr et al., Nucleic Acids Res.'01; Raghava et al., BMC Bioinformatics '03; Edgar, Nucleic Acids Res.'04; Walle et al., Bioinformatics'04

Requires extensive manual alignments

…rather just run parameterized algorithm

How to tune algorithm's parameters?

*"There is **considerable disagreement** among molecular biologists about the **correct choice**"* [Gusfield et al. '94]



Sequence alignment algorithms

```
-GRTCPKPDDLPFSTVVP-LKTFYEPGEEITYSCKPGYVSRGGMRKFICPLTGLWPINTLKCTP
E-VKCPFPSRPDNGFVNYPAKPTLYYKDKATFGCHDGYSLDGP-EEIECTKLGNWSAMPSC-KA
```

Ground-truth alignment of protein sequences

Sequence alignment algorithms

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Alignment by algorithm with **poorly-tuned** parameters

Sequence alignment algorithms

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Alignment by algorithm with **poorly-tuned** parameters

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```

Alignment by algorithm with **well-tuned** parameters

Automated parameter tuning procedure

1. Fix parameterized algorithm
2. Receive training set T of "typical" inputs

Sequence S_1 Sequence S_1' Reference alignment A_1	Sequence S_2 Sequence S_2' Reference alignment A_2	...

3. Find parameter setting w/ good avg performance over T

Runtime, solution quality, etc.

Automated parameter tuning procedure

1. Fix parameterized algorithm
2. Receive training set T of "typical" inputs

Sequence S_1 Sequence S_1' Reference alignment A_1	Sequence S_2 Sequence S_2' Reference alignment A_2	…

3. Find parameter setting w/ good avg performance over T

On average, output alignment is close to reference alignment

Automated parameter tuning procedure

1. Fix parameterized algorithm
2. Receive training set T of "typical" inputs

Sequence S_1
Sequence S_1'
Reference alignment A_1

Sequence S_2
Sequence S_2'
Reference alignment A_2

…

3. Find parameter setting w/ good avg performance over T

Key question:

How to find parameter setting with good avg performance?

Automated parameter tuning procedure

Key question:
How to find parameter setting with good avg performance?

E.g., for sequence alignment:
algorithm by Gusfield et al. ['94]

Many other generic search strategies
E.g., Hutter et al. [JAIR'09, LION'11], Ansótegui et al. [CP'09], …

Automated parameter tuning procedure

1. Fix parameterized algorithm
2. Receive training set T of "typical" inputs

Sequence S_1
Sequence S_1'
Reference alignment A_1

Sequence S_2
Sequence S_2'
Reference alignment A_2

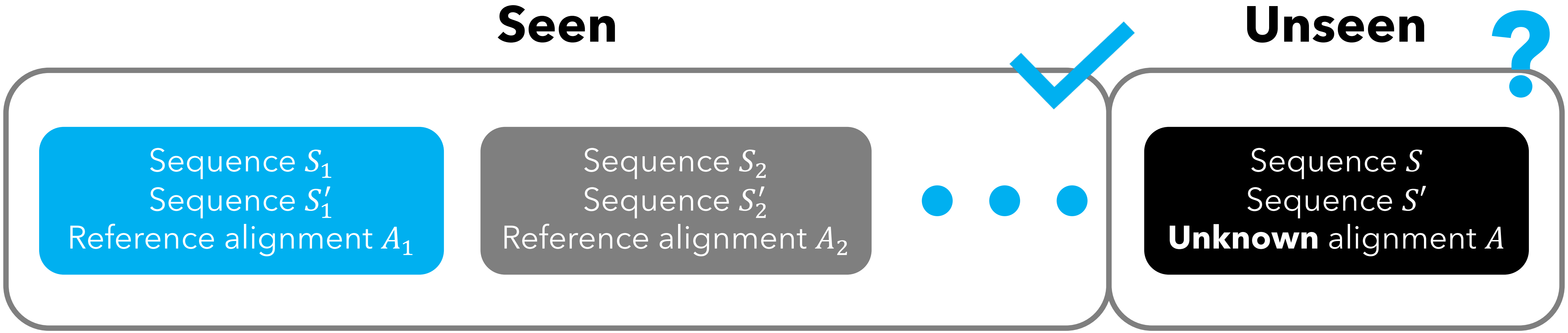
…

3. Find parameter setting w/ good avg performance over T

Key question (focus of this section):

Will that parameter setting have good **future** performance?

Automated parameter tuning procedure



Key question (focus of this section):

Will that parameter setting have good **future** performance?

Generalization

Key question **(focus of this section):**

Good performance on **average** over **training set** implies good **future** performance?

Greedy algorithms

Gupta, Roughgarden, ITCS'16 ← First to ask question for algorithm configuration

Clustering

Balcan, Nagarajan, **V**, White, COLT'17
Garg, Kalai, NeurIPS'18
Balcan, Dick, White, NeurIPS'18
Balcan, Dick, Lang, ICLR'20

Search

Sakaue, Oki, NeurIPS'22

Numerical linear algebra

Bartlett et al., COLT'22

And many other areas…

This section: Main result

Key question (focus of this section):

Good performance on **average** over **training set** implies good **future** performance?

Answer this question for any parameterized algorithm where:

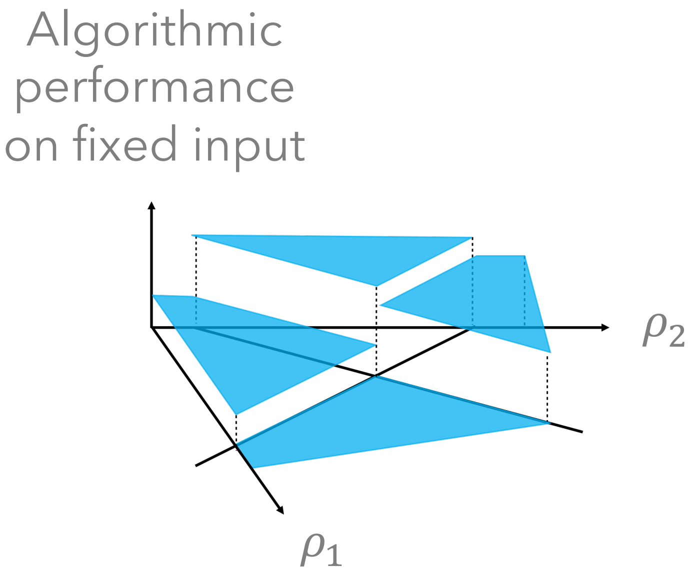
Performance is **piecewise-structured** function of parameters

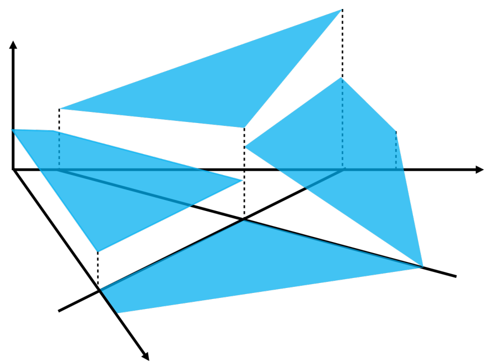
Piecewise constant, linear, quadratic, …

This section: Main result

Performance is **piecewise-structured** function of parameters

Piecewise constant, linear, quadratic, …



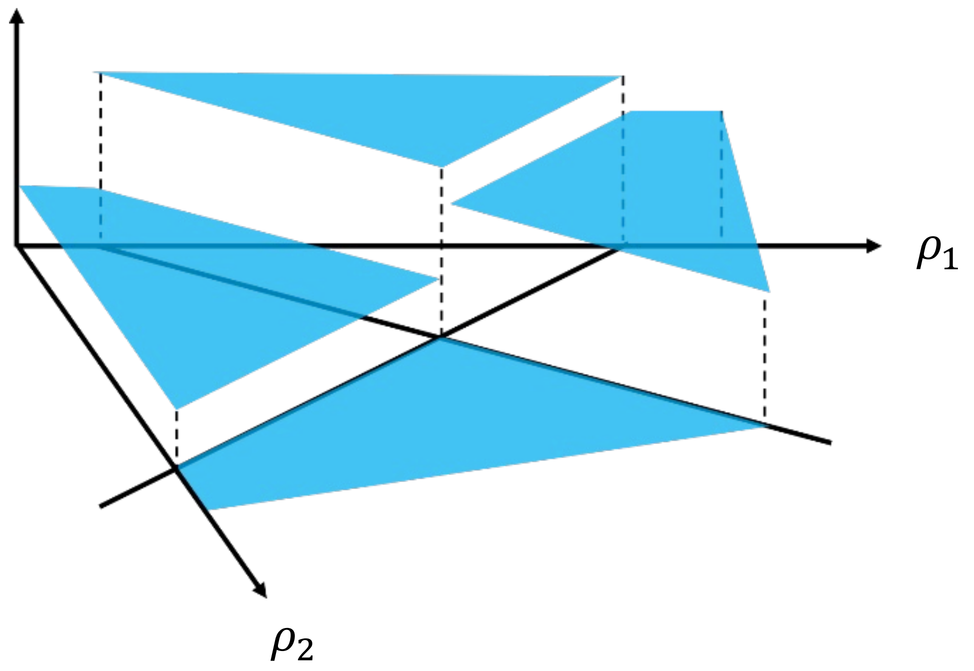


Piecewise constant **Piecewise linear** **Piecewise …**

Balcan, DeBlasio, Dick, Kingsford, Sandholm, **Vitercik**, STOC'21

Example: Sequence alignment

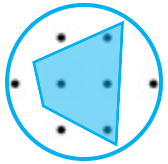
Distance between **algorithm's output** given S, S'
and **ground-truth** alignment is p-wise constant



Balcan, DeBlasio, Dick, Kingsford, Sandholm, **Vitercik**, STOC'21

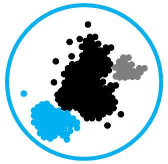
Piecewise structure

Piecewise structure unifies **seemingly disparate** problems:



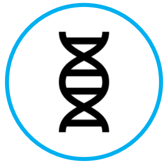
Integer programming

Balcan, Dick, Sandholm, **V**, ICML'18
Balcan, Prasad, Sandholm, **V**, NeurIPS'21
Balcan, Prasad, Sandholm, **V**, NeurIPS'22



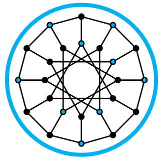
Clustering

Balcan, Nagarajan, **V**, White, COLT'17
Balcan, Dick, White, NeurIPS'18
Balcan, Dick, Lang, ICLR'20



Computational biology

Balcan, DeBlasio, Dick, Kingsford, Sandholm, **V**, STOC'21



Greedy algorithms

Gupta, Roughgarden, ITCS'16

Mechanism configuration

Balcan, Sandholm, **V**, EC'18

Ties to a long line of research on machine learning for **revenue maximization**
Likhodedov, Sandholm, AAAI'04, '05; Balcan, Blum, Hartline, Mansour, FOCS'05; Elkind, SODA'07; Cole, Roughgarden, STOC'14; Mohri, Medina, ICML'14; Devanur, Huang, Psomas, STOC'16; …

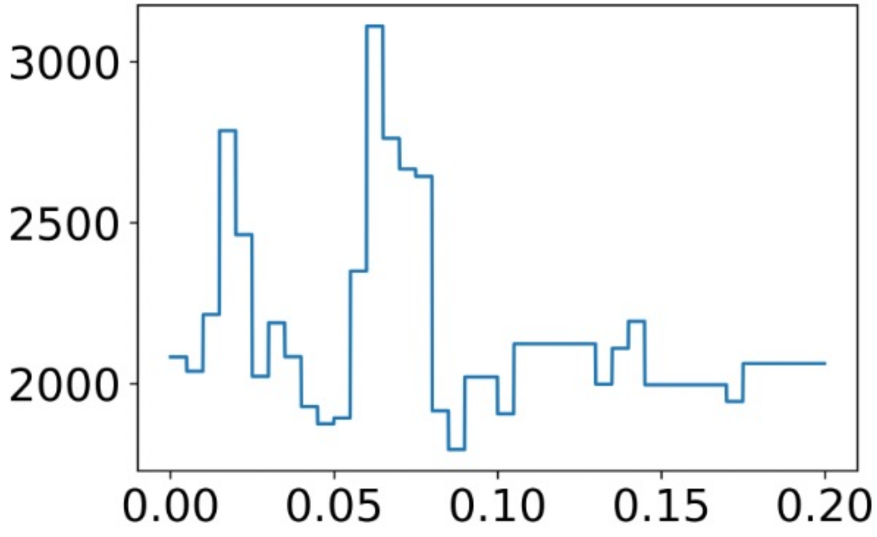
Balcan, DeBlasio, Dick, Kingsford, Sandholm, **Vitercik**, STOC'21

Primary challenge

Algorithmic performance is a **volatile** function of parameters

Complex connection between parameters and performance

Solver search tree size



Integer programming solver parameter

Balcan, Prasad, Sandholm, **Vitercik**, NeurIPS'21

Outline (theoretical guarantees)

1. Statistical guarantees for algorithm configuration
   i. **Model**
   ii. Piecewise-structured algorithmic performance
   iii. Main result
   iv. Applications
2. Online algorithm configuration

Model

$\mathbb{R}^d$: Set of all parameters

$\mathcal{X}$: Set of all inputs

Example: Sequence alignment

$\mathbb{R}^3$: Set of alignment algorithm parameters

$\mathcal{X}$: Set of sequence pairs

$$S = \text{A C T G}$$
$$S' = \text{G T C A}$$

One sequence pair $x = (S, S') \in \mathcal{X}$

Algorithmic performance

$u_{\boldsymbol{\rho}}(x)$ = utility of algorithm parameterized by $\boldsymbol{\rho} \in \mathbb{R}^d$ on input x

E.g., runtime, solution quality, distance to ground truth, …

Assume $u_{\boldsymbol{\rho}}(x) \in [-1,1]$

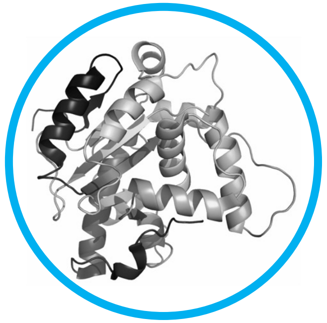
Can be generalized to $u_{\boldsymbol{\rho}}(x) \in [-H, H]$

Model

Standard assumption: Unknown distribution $\mathcal{D}$ over inputs

Distribution models specific application domain at hand

E.g., distribution over pairs of DNA strands



E.g., distribution over pairs of protein sequences

Generalization bounds

Key question: For any parameter setting $\boldsymbol{\rho}$,
is **average** utility on training set close to **expected** utility?

Formally: Given samples $x_1, \ldots, x_N \sim \mathcal{D}$, for any $\boldsymbol{\rho}$,

$$\left| \underbrace{\frac{1}{N} \sum_{i=1}^{N} u_{\boldsymbol{\rho}}(x_i)}_{\text{Empirical average utility}} - \underbrace{\mathbb{E}_{x \sim \mathcal{D}}\left[u_{\boldsymbol{\rho}}(x)\right]}_{\text{Expected utility}} \right| \leq \textbf{?}$$

Good **average empirical** utility ➡ Good **expected** utility

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      b. Dual function definition
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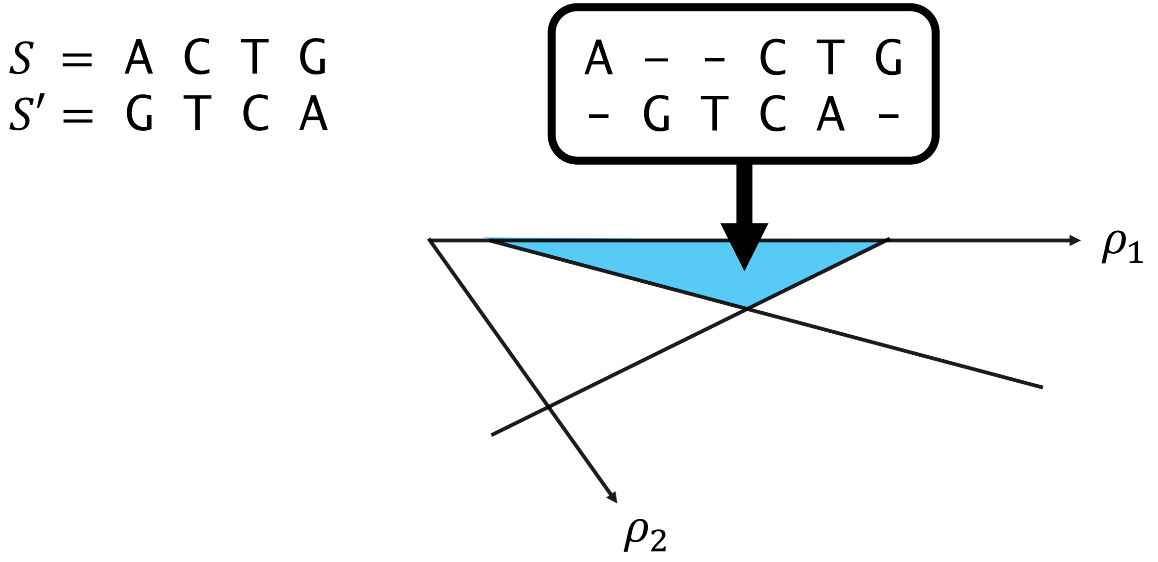
Sequence alignment algorithms

Lemma:

For any pair S, S'

algorithm's output is fixed across all parameters in region



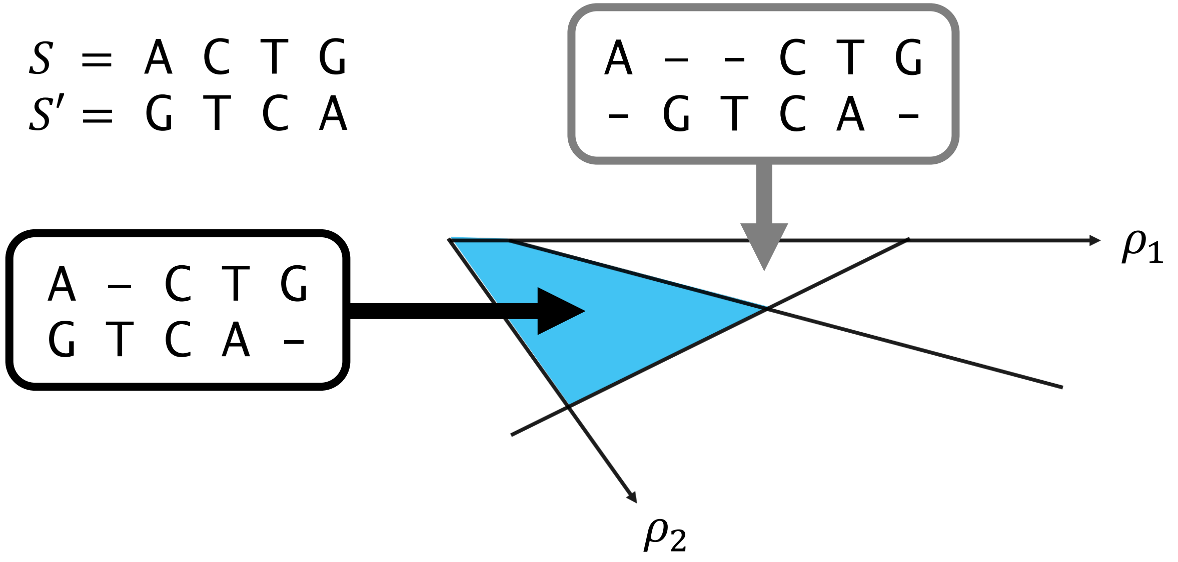
Gusfield et al., Algorithmica '94; Fernández-Baca et al., J. of Discrete Alg. '04

Sequence alignment algorithms

Lemma:

Defined by $(\max\{|S|, |S'|\})^3$ hyperplanes

For any pair S, S', there's a partition of $\mathbb{R}^3$ s.t. in any region, algorithm's output is fixed across all parameters in region



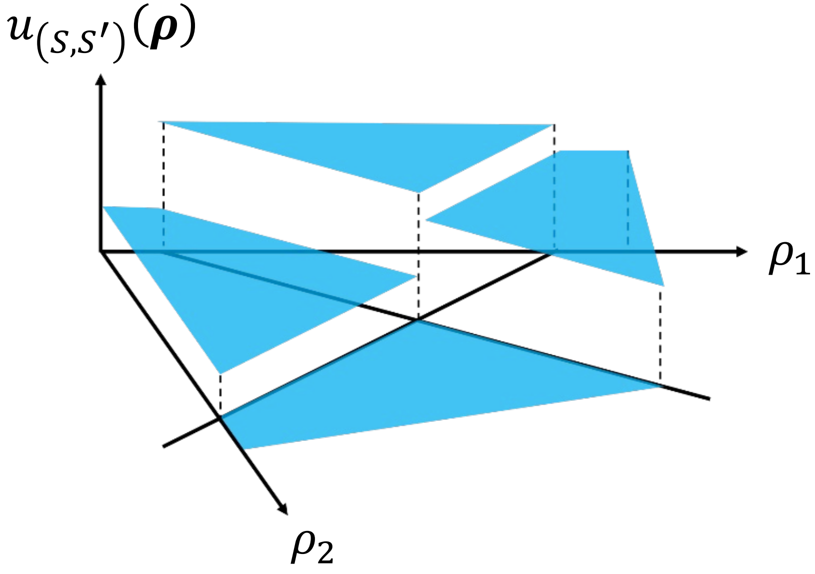
Gusfield et al., Algorithmica '94; Fernández-Baca et al., J. of Discrete Alg. '04

Piecewise-constant utility function

Corollary:

Utility is piecewise constant function of parameters

Distance between algorithm's output and ground-truth alignment



Balcan, DeBlasio, Dick, Kingsford, Sandholm, **Vitercik**, STOC'21

Outline (theoretical guarantees)

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Primal & dual classes

$u_{\boldsymbol{\rho}}(x)$ = utility of algorithm parameterized by $\boldsymbol{\rho} \in \mathbb{R}^d$ on input x
$\mathcal{U} = \{u_{\boldsymbol{\rho}}: \mathcal{X} \to \mathbb{R} \mid \boldsymbol{\rho} \in \mathbb{R}^d\}$ "Primal" function class

Typically, prove guarantees by bounding ***complexity*** of $\mathcal{U}$

Challenge: $\mathcal{U}$ is gnarly

E.g., in sequence alignment:

- Each domain element is a pair of sequences
- Unclear how to plot or visualize functions $u_{\boldsymbol{\rho}}$
- No obvious notions of Lipschitz continuity or smoothness to rely on

Balcan, DeBlasio, Dick, Kingsford, Sandholm, **Vitercik**, STOC'21

Primal & dual classes

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$\mathcal{U} = \left\{u_{\boldsymbol{\rho}} : \mathcal{X} \to \mathbb{R} \,\middle|\, \boldsymbol{\rho} \in \mathbb{R}^d\right\}$ "Primal" function class

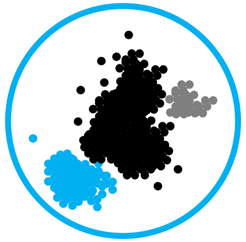
$u_x^*(\boldsymbol{\rho})$ = utility as function of parameters
$u_x^*(\boldsymbol{\rho}) = u_{\boldsymbol{\rho}}(x)$
$\mathcal{U}^* = \left\{u_x^* : \mathbb{R}^d \to \mathbb{R} \,\middle|\, x \in \mathcal{X}\right\}$ "Dual" function class

- Dual functions have simple, Euclidean domain
- Often have ample structure can use to bound complexity of $\mathcal{U}$

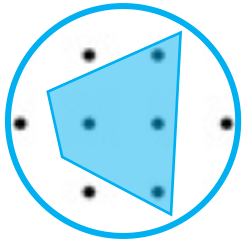
Balcan, DeBlasio, Dick, Kingsford, Sandholm, **Vitercik**, STOC'21

Piecewise-structured functions

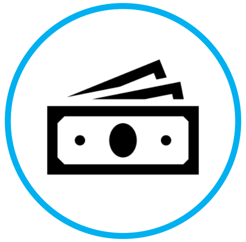
Dual functions $u_x^*: \mathbb{R}^d \to \mathbb{R}$ are **piecewise-structured**



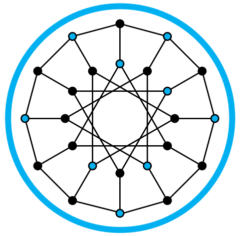
Clustering algorithm configuration



Integer programming algorithm configuration



Selling mechanism configuration



Greedy algorithm configuration

Computational biology algorithm configuration

Voting mechanism configuration

Balcan, DeBlasio, Dick, Kingsford, Sandholm, **Vitercik**, STOC'21

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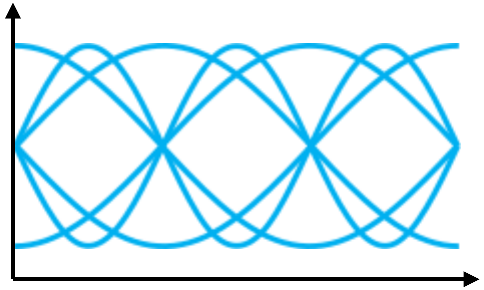
Intrinsic complexity

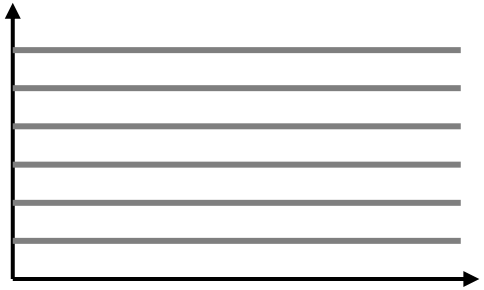
"Intrinsic complexity" of function class $\mathcal{G}$

- Measures how well functions in $\mathcal{G}$ fit complex patterns
- Specific ways to quantify "intrinsic complexity":
  - VC dimension
  - Pseudo-dimension



More complex

Less complex

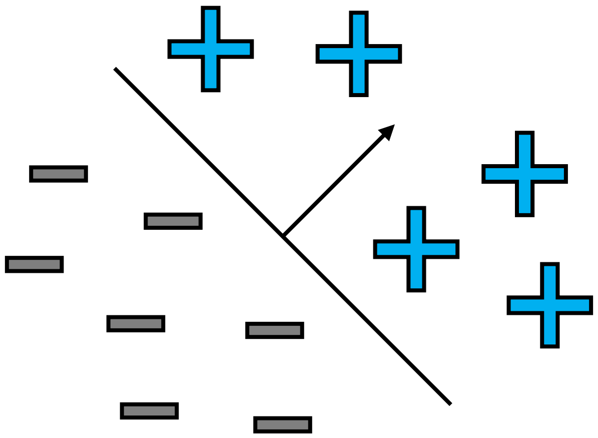


VC dimension

Complexity measure for binary-valued function classes $\mathcal{F}$

(Classes of functions $f: \mathcal{Y} \to \{-1,1\}$)

E.g., linear separators

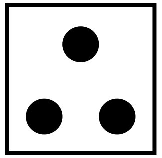


VC dimension

Size of the largest set $\mathcal{S} \subseteq \mathcal{Y}$
that can be labeled in all $2^{|\mathcal{S}|}$ ways by functions in $\mathcal{F}$

Example: $\mathcal{F}$ = Linear separators in $\mathbb{R}^2$

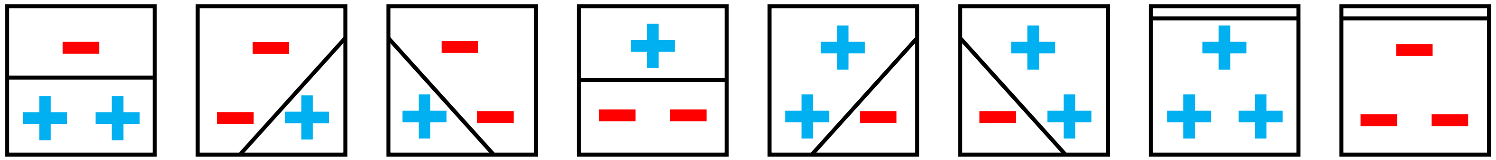
$\text{VCdim}(\mathcal{F}) \geq 3$



VC dimension

Size of the largest set $\mathcal{S} \subseteq \mathcal{Y}$
that can be labeled in all $2^{|\mathcal{S}|}$ ways by functions in $\mathcal{F}$

Example: $\mathcal{F}$ = Linear separators in $\mathbb{R}^2$ VCdim($\mathcal{F}$) ≥ 3



VCdim($\mathcal{F}$) ≤ 3

VCdim({Linear separators in $\mathbb{R}^d$}) $= d + 1$

VC dimension

Size of the largest set $\mathcal{S} \subseteq \mathcal{Y}$
that can be labeled in all $2^{|\mathcal{S}|}$ ways by functions in $\mathcal{F}$

Mathematically, for $\mathcal{S} = \{y_1, \ldots, y_N\}$,

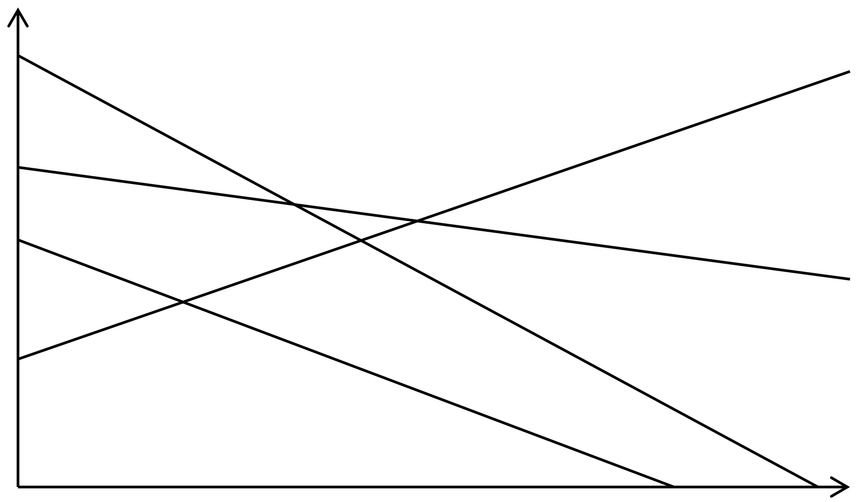
$$\left|\left\{\begin{pmatrix} f(y_1) \\ \vdots \\ f(y_N) \end{pmatrix} : f \in \mathcal{F}\right\}\right| = 2^N$$

Pseudo-dimension

Complexity measure for real-valued function classes $\mathcal{G}$

(Classes of functions $g: \mathcal{Y} \to [-1,1]$)

E.g., affine functions



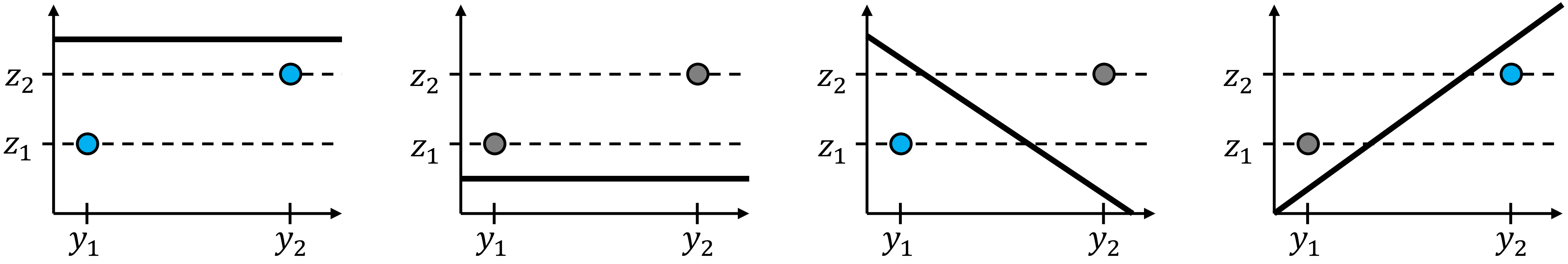
Pseudo-dimension of $\mathcal{G}$

Size of the largest set $\{y_1, \ldots, y_N\} \subseteq \mathcal{Y}$ s.t.:

for some *targets* $z_1, \ldots, z_N \in \mathbb{R}$,

all 2^N above/below patterns achieved by functions in $\mathcal{G}$

Example: $\mathcal{G}$ = Affine functions in $\mathbb{R}$ $\quad$ $\mathrm{Pdim}(\mathcal{G}) \geq 2$



Can also show that $\mathrm{Pdim}(\mathcal{G}) \leq 2$

Pseudo-dimension of $\mathcal{G}$

Size of the largest set $\{y_1, \dots, y_N\} \subseteq \mathcal{Y}$ s.t.:

for some *targets* $z_1, \dots, z_N \in \mathbb{R}$,

all 2^N above/below patterns achieved by functions in $\mathcal{G}$

Mathematically,

$$\left|\left\{\begin{pmatrix} \mathbf{1}_{\{g(y_1) \geq z_1\}} \\ \vdots \\ \mathbf{1}_{\{g(y_N) \geq z_N\}} \end{pmatrix} : g \in \mathcal{G}\right\}\right| = 2^N$$

Sample complexity using pseudo-dim

In the context of **algorithm configuration**:

- $\mathcal{U} = \{u_{\boldsymbol{\rho}} : \boldsymbol{\rho} \in \mathbb{R}^d\}$ measure algorithm **performance**
- For $\epsilon, \delta \in (0,1)$, let $N = O\left(\frac{\text{Pdim}(\mathcal{U})}{\epsilon^2} \log \frac{1}{\delta}\right)$
- With probability at least $1 - \delta$ over $x_1, \ldots, x_N \sim \mathcal{D}, \forall \boldsymbol{\rho} \in \mathbb{R}^d$,

$$\left| \underbrace{\frac{1}{N} \sum_{i=1}^{N} u_{\boldsymbol{\rho}}(x_i)}_{\text{Empirical average utility}} - \underbrace{\mathbb{E}_{x \sim \mathcal{D}}\left[u_{\boldsymbol{\rho}}(x)\right]}_{\text{Expected utility}} \right| \leq \epsilon$$

Empirical average utility **Expected utility**

Main result (informal)

Boundary functions $f_1, \ldots, f_k \in \mathcal{F}$ partition $\mathbb{R}^d$ s.t. in each region,
$u_x^*(\boldsymbol{\rho}) = g(\boldsymbol{\rho})$ for some $g \in \mathcal{G}$.

Training set of size $\tilde{O}\left(\frac{\text{Pdim}(\mathcal{G}^*)+\text{VCdim}(\mathcal{F}^*)\log k}{\epsilon^2}\right)$ implies
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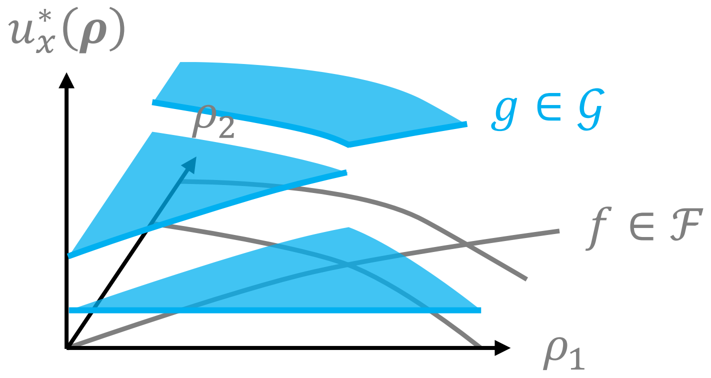

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Primal function class $\mathcal{U} = \{u_{\boldsymbol{\rho}} \mid \boldsymbol{\rho} \in \mathbb{R}^d\}$

Balcan, DeBlasio, Dick, Kingsford, Sandholm, **Vitercik**, STOC'21

Next time

1. **Theoretical guarantees**
    a. Statistical guarantees for algorithm configuration
        i. Proof of main theorem
        ii. Lots of applications
    b. Online algorithm configuration

2. **Applied techniques**
    a. Graph neural networks overview

Machine learning for algorithm design:
Theoretical guarantees and applied frontiers

Part 2

Ellen Vitercik
Stanford University

How to integrate **machine learning** into **algorithm design**?

Algorithm configuration
How to tune an algorithm's parameters?

Algorithm selection
Given a variety of algorithms, which to use?

Algorithm design
Can machine learning guide algorithm discovery?

Automated parameter tuning procedure

1. Fix parameterized algorithm
2. Receive training set T of "typical" inputs

Sequence S_1
Sequence S_1'
Reference alignment A_1

Sequence S_2
Sequence S_2'
Reference alignment A_2

• • •

3. Find parameter setting w/ good avg performance over T

Key question (focus of this section):

Will that parameter setting have good **future** performance?

Primal & dual classes

$u_{\boldsymbol{\rho}}(x) =$ **utility** of algorithm parameterized by $\boldsymbol{\rho} \in \mathbb{R}^d$ on input x

E.g., runtime, solution quality, etc.

$\mathcal{U} = \left\{u_{\boldsymbol{\rho}} : \mathcal{X} \to \mathbb{R} \,\middle|\, \boldsymbol{\rho} \in \mathbb{R}^d\right\}$ "Primal" function class

Set of problem instances, e.g., integer programs

$u_x^*(\boldsymbol{\rho}) =$ utility as function of parameters

$u_x^*(\boldsymbol{\rho}) = u_{\boldsymbol{\rho}}(x)$

$\mathcal{U}^* = \left\{u_x^* : \mathbb{R}^d \to \mathbb{R} \,\middle|\, x \in \mathcal{X}\right\}$ "Dual" function class

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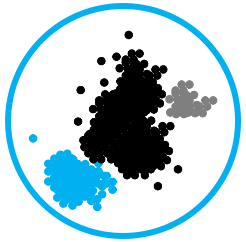
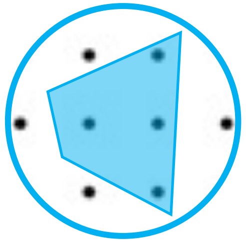
Piecewise-structured functions

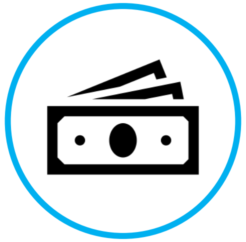
Dual functions $u_x^*: \mathbb{R}^d \to \mathbb{R}$ are **piecewise-structured**



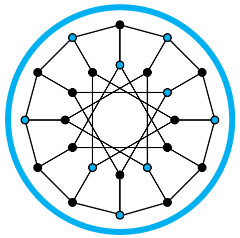
Clustering algorithm configuration



Integer programming algorithm configuration



Selling mechanism configuration



Greedy algorithm configuration

Computational biology algorithm configuration

Voting mechanism configuration

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Sample complexity

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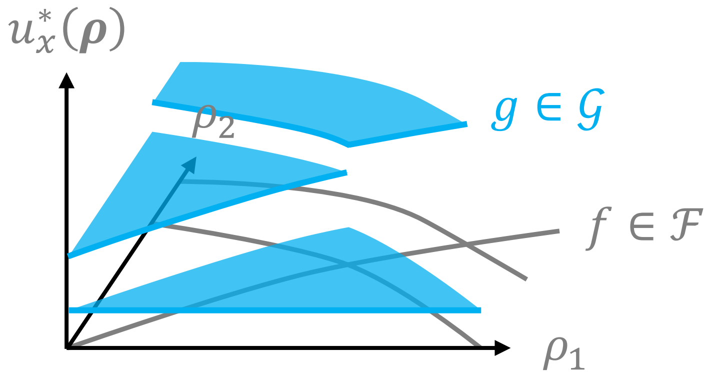

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Primal function class $\mathcal{U} = \{u_{\boldsymbol{\rho}} \mid \boldsymbol{\rho} \in \mathbb{R}^d\}$

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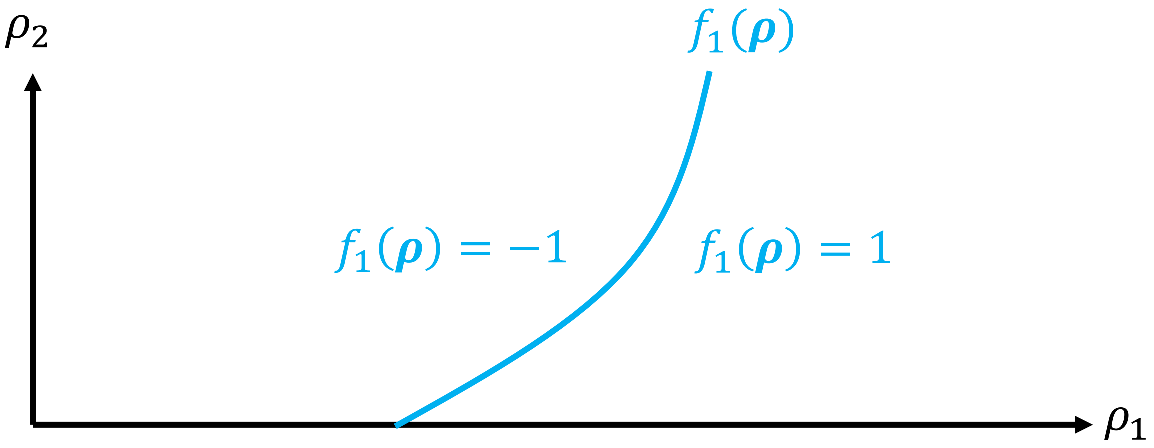
Key lemma

Each boundary function $f: \mathbb{R}^d \rightarrow \{-1,1\}$ splits $\mathbb{R}^d$ into 2 regions



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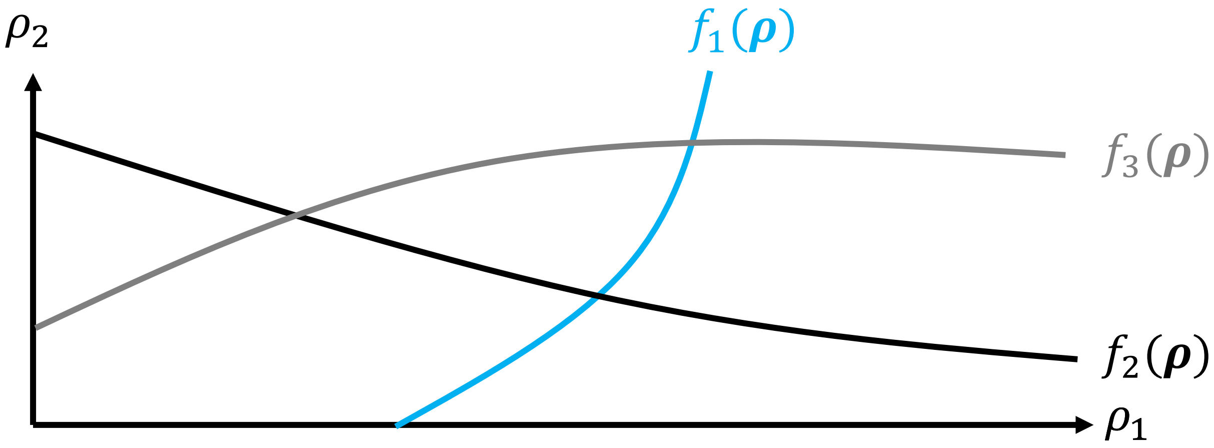
Key lemma

Given D boundaries, how many sign patterns do they make?

$$\left|\left\{\begin{pmatrix} f_1(\boldsymbol{\rho}) \\ \vdots \\ f_D(\boldsymbol{\rho}) \end{pmatrix} : \boldsymbol{\rho} \in \mathbb{R}^d\right\}\right| \leq \textbf{?}$$



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Given D boundaries, how many sign patterns do they make?

$$\left|\left\{\begin{pmatrix} f_1(\boldsymbol{\rho}) \\ \vdots \\ f_D(\boldsymbol{\rho}) \end{pmatrix} : \boldsymbol{\rho} \in \mathbb{R}^d \right\}\right| \leq \text{?}$$

Note: Sauer's lemma tells us that for any D points $\boldsymbol{\rho}_1, \ldots, \boldsymbol{\rho}_D \in \mathbb{R}^d$

$$\left|\left\{\begin{pmatrix} f(\boldsymbol{\rho}_1) \\ \vdots \\ f(\boldsymbol{\rho}_D) \end{pmatrix} : f \in \mathcal{F} \right\}\right| \leq (eD)^{\mathrm{VCdim}(\mathcal{F})}$$

This is where transitioning to the dual comes in handy!

Proof ideas

For any problem instances $x_1, \dots, x_N$ and *targets* $z_1, \dots, z_N \in \mathbb{R}$,

$$\left|\left\{\begin{pmatrix}\operatorname{sgn}\left(u_{\boldsymbol{\rho}}(x_1) - z_1\right)\\ \vdots \\ \operatorname{sgn}\left(u_{\boldsymbol{\rho}}(x_N) - z_N\right)\end{pmatrix} : \boldsymbol{\rho} \in \mathbb{R}^d\right\}\right| \leq \textbf{?}$$

Switching to the dual functions,

$$\left|\left\{\begin{pmatrix}\operatorname{sgn}\left(u^*_{x_1}(\boldsymbol{\rho}) - z_1\right)\\ \vdots \\ \operatorname{sgn}\left(u^*_{x_N}(\boldsymbol{\rho}) - z_N\right)\end{pmatrix} : \boldsymbol{\rho} \in \mathbb{R}^d\right\}\right| \leq \textbf{?}$$

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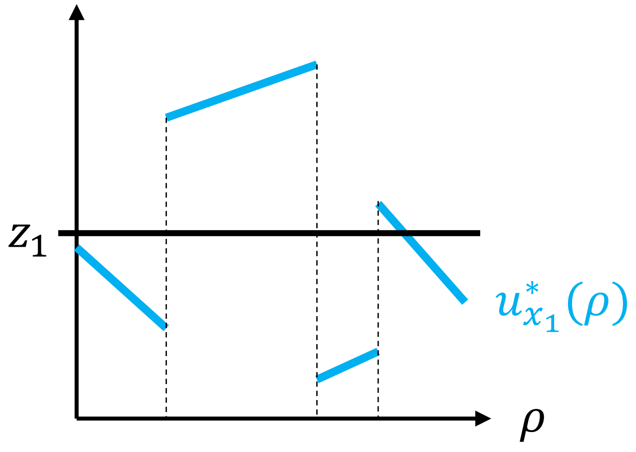
Proof ideas

$$\left|\left\{\begin{pmatrix} \operatorname{sgn}\left(u^*_{x_1}(\boldsymbol{\rho}) - z_1\right) \\ \vdots \\ \operatorname{sgn}\left(u^*_{x_N}(\boldsymbol{\rho}) - z_N\right) \end{pmatrix} : \boldsymbol{\rho} \in \mathbb{R}^d \right\}\right| \leq \text{?}$$

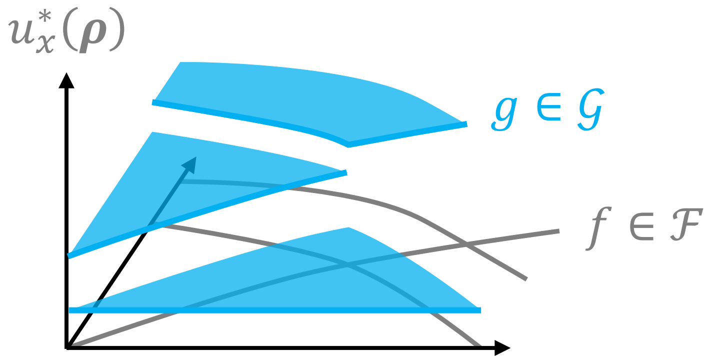


Proof ideas

$$\left|\left\{\begin{pmatrix}\operatorname{sgn}\left(u^*_{x_1}(\boldsymbol{\rho}) - z_1\right)\\ \vdots \\ \operatorname{sgn}\left(u^*_{x_N}(\boldsymbol{\rho}) - z_N\right)\end{pmatrix} : \boldsymbol{\rho} \in \mathbb{R}^d\right\}\right| \leq \ ?$$

The duals $u^*_{x_1}, \ldots, u^*_{x_N}$ correspond to Nk boundary functions in $\mathcal{F}$

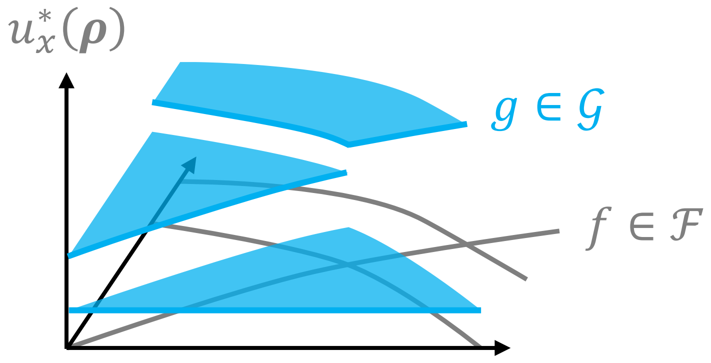
How many regions $R_1, \ldots, R_M$ in $\mathbb{R}^d$? $M \leq (eNk)^{\text{VCdim}(\mathcal{F}^*)}$



Proof ideas

$$\left|\left\{\begin{pmatrix}\mathrm{sgn}\left(u^*_{x_1}(\boldsymbol{\rho}) - z_1\right)\\ \vdots \\ \mathrm{sgn}\left(u^*_{x_N}(\boldsymbol{\rho}) - z_N\right)\end{pmatrix} : \boldsymbol{\rho} \in \boldsymbol{R_j}\right\}\right| \leq \ \mathbf{?}$$

$\forall \boldsymbol{\rho} \in R_j$, duals are simultaneously structured: $u^*_{x_i}(\boldsymbol{\rho}) = g_i(\boldsymbol{\rho}), \forall i$



Proof ideas

$$\left|\left\{\begin{pmatrix}\operatorname{sgn}\left(u^*_{x_1}(\boldsymbol{\rho}) - z_1\right)\\ \vdots \\ \operatorname{sgn}\left(u^*_{x_N}(\boldsymbol{\rho}) - z_N\right)\end{pmatrix} : \boldsymbol{\rho} \in \boldsymbol{R_j}\right\}\right| \leq \ ?$$

$\forall \boldsymbol{\rho} \in R_j$, duals are simultaneously structured: $u^*_{x_i}(\boldsymbol{\rho}) = g_i(\boldsymbol{\rho}), \forall i$

$$\left|\left\{\begin{pmatrix}\operatorname{sgn}(g_1(\boldsymbol{\rho}) - z_1)\\ \vdots \\ \operatorname{sgn}(g_N(\boldsymbol{\rho}) - z_N)\end{pmatrix} : \boldsymbol{\rho} \in R_j\right\}\right| \leq ?$$

Proof ideas

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Follows from key lemma

Proof ideas

$$\left|\left\{\begin{pmatrix}\operatorname{sgn}\left(u^*_{x_1}(\boldsymbol{\rho}) - z_1\right)\\ \vdots \\ \operatorname{sgn}\left(u^*_{x_N}(\boldsymbol{\rho}) - z_N\right)\end{pmatrix} : \boldsymbol{\rho} \in \mathbb{R}^d\right\}\right|$$

$$\leq \underbrace{(eNk)^{\text{VCdim}(\mathcal{F}^*)}}_{\text{Number of regions}} \underbrace{(eN)^{\text{Pdim}(\mathcal{G}^*)}}_{\text{Number of sign patterns within each region}}$$

Pdim($\mathcal{U}$) equals largest N s.t. $2^{\text{N}} \leq (eNk)^{\text{VCdim}(\mathcal{F}^*)}(eN)^{\text{Pdim}(\mathcal{G}^*)}$,

so Pdim($\mathcal{U}$) $= \tilde{O}\left((\text{VCdim}(\mathcal{F}^*) + \text{Pdim}(\mathcal{G}^*)) \log k\right)$

Balcan, DeBlasio, Dick, Kingsford, Sandholm, **Vitercik**, STOC'21

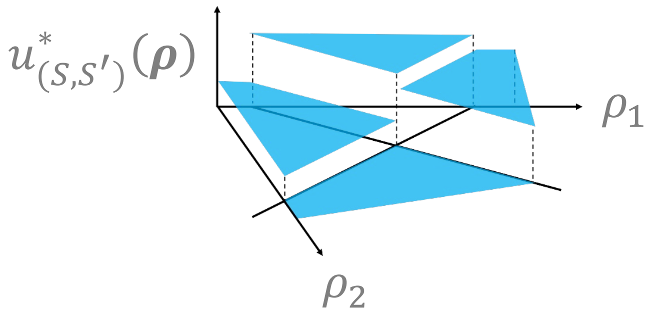
Outline (theoretical guarantees)

1. Statistical guarantees for algorithm configuration
   i. Model
   ii. Piecewise-structured algorithmic performance
   iii. Main result
   iv. Applications
      a. Sequence alignment
      b. Greedy algorithms
      c. Cutting planes
2. Online algorithm configuration

Piecewise constant dual functions

Lemma:

Utility is piecewise constant function of parameters



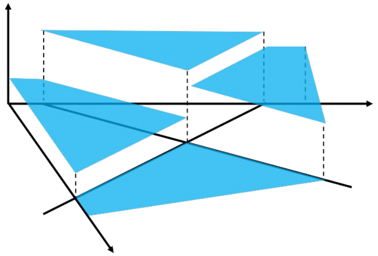
Balcan, DeBlasio, Dick, Kingsford, Sandholm, **Vitercik**, STOC'21

Sequence alignment guarantees

Theorem: Training set of size

$$\tilde{O}\left(\frac{\text{Pdim}(\mathcal{G}^*) + \text{VCdim}(\mathcal{F}^*)\log k}{\epsilon^2}\right) = \tilde{O}\left(\frac{\log(\text{max seq. length})}{\epsilon^2}\right)$$

implies WHP $\forall \boldsymbol{\rho}$, |**avg** utility over training set – **exp** utility| $\leq \epsilon$



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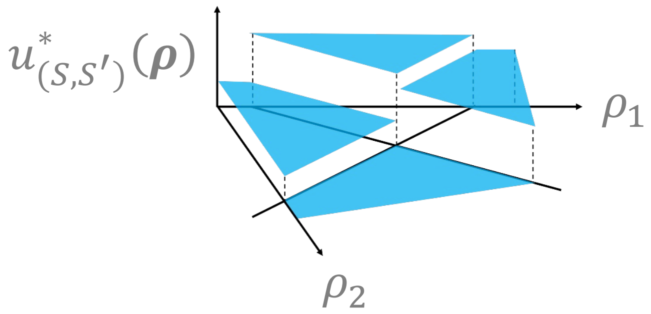
$\mathcal{G}$ = constant functions in $\mathbb{R}^3$
$\text{Pdim}(\mathcal{G}^*) = O(1)$

$\mathcal{F}$ = hyperplanes in $\mathbb{R}^3$
$\text{VCdim}(\mathcal{F}^*) = O(1)$

$(\text{max sequence length})^3$

implies WHP $\forall \boldsymbol{\rho}$, |**avg** utility over training set – **exp** utility| $\leq \epsilon$



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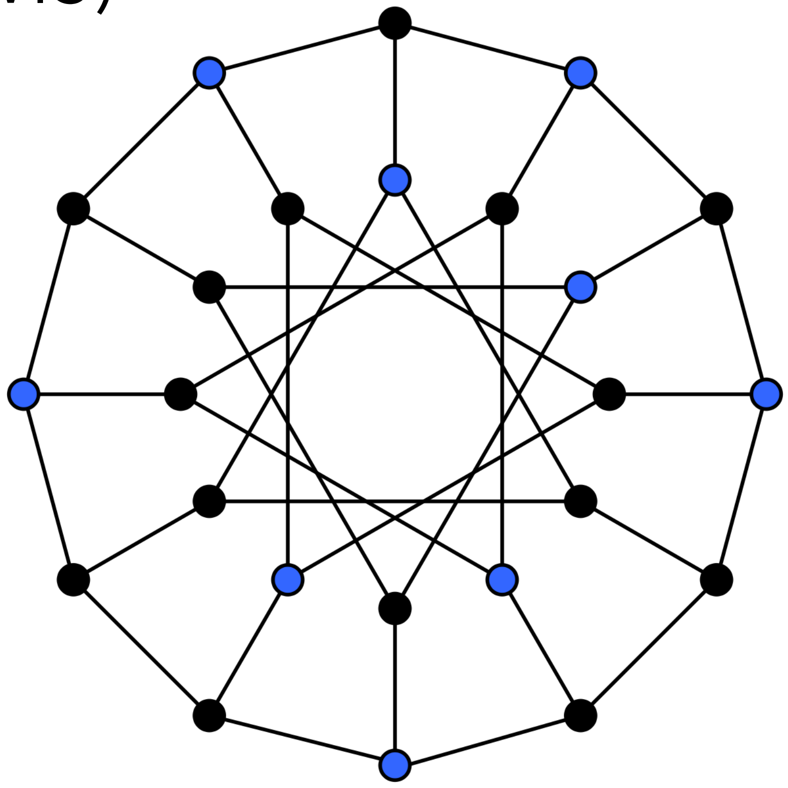
Example: MWIS

Maximum weight independent set (MWIS)



Problem instance:

- Graph $G = (V, E)$
- n vertices with weights $w_1, \ldots, w_n \geq 0$

Goal: find subset $S \subseteq [n]$

- Maximizing $\sum_{i \in S} w_i$
- No nodes $i, j \in S$ are connected: $(i, j) \notin E$

Example: MWIS

Greedy heuristic:

Greedily add vertices v in decreasing order of $\frac{w_v}{(1+\deg(v))}$

Maintaining independence

Parameterized heuristic [Gupta, Roughgarden, ITCS'16]**:**

Greedily add nodes in decreasing order of $\frac{w_v}{(1+\deg(v))^\rho}$, $\rho \geq 0$

[Inspired by knapsack heuristic by Lehmann et al., JACM'02]

Example: MWIS

Given a MWIS instance x, $u_x^*(\rho)$ = weight of IS algorithm returns

Theorem [Gupta, Roughgarden, ITCS'16]**:**
$u_x^*(\rho)$ is piecewise-constant with at most n^2 pieces

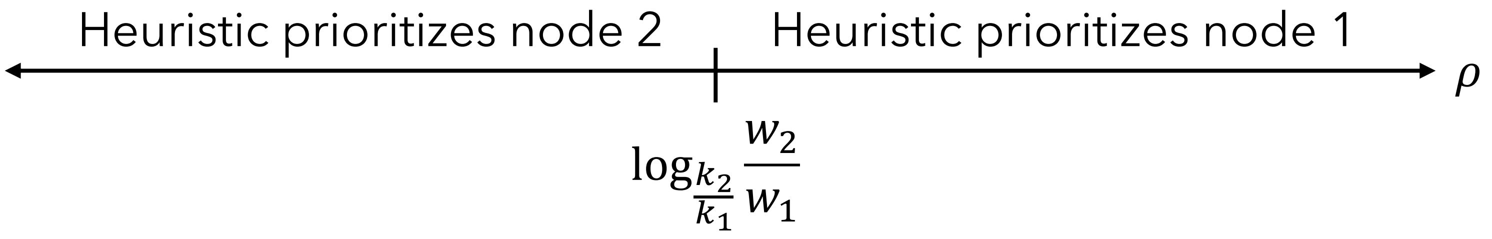
Example: MWIS

Given a MWIS instance x, $u_x^*(\rho)$ = weight of IS algorithm returns

- Weights $w_1, \dots, w_n \geq 0$
- $\deg(i) + 1 = k_i$

Algorithm parameterized by ρ would add **node 1** before **2** if:

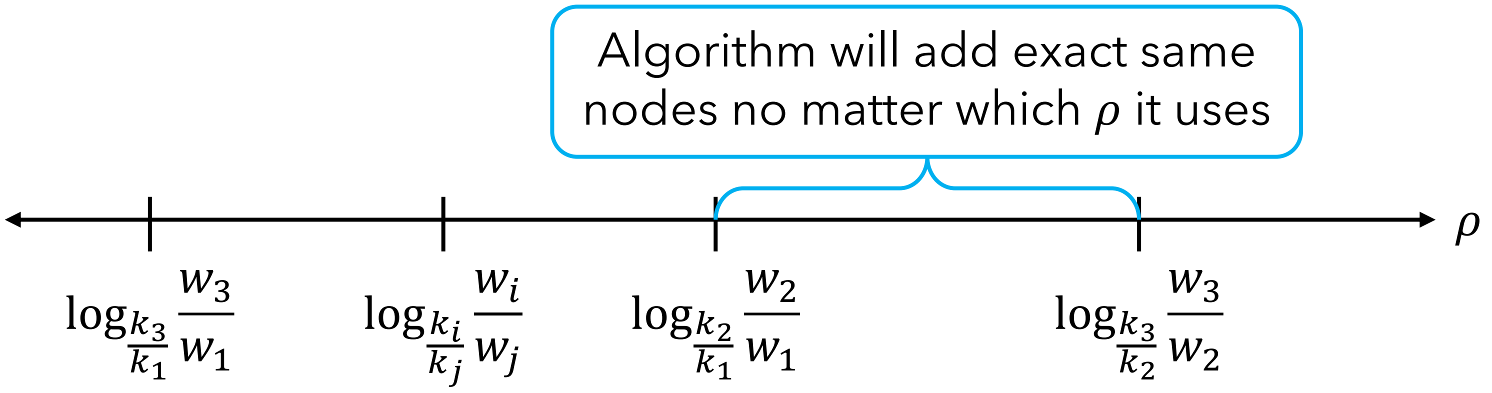
$$\frac{w_1}{k_1^\rho} \geq \frac{w_2}{k_2^\rho} \quad \Longleftrightarrow \quad \rho \geq \log_{\frac{k_2}{k_1}} \frac{w_2}{w_1}$$



Gupta, Roughgarden, ITCS'16

Example: MWIS

- $\binom{n}{2}$ thresholds per instance
- Partition $\mathbb{R}$ into regions where algorithm's output is fixed



Gupta, Roughgarden, ITCS'16

Example: MWIS

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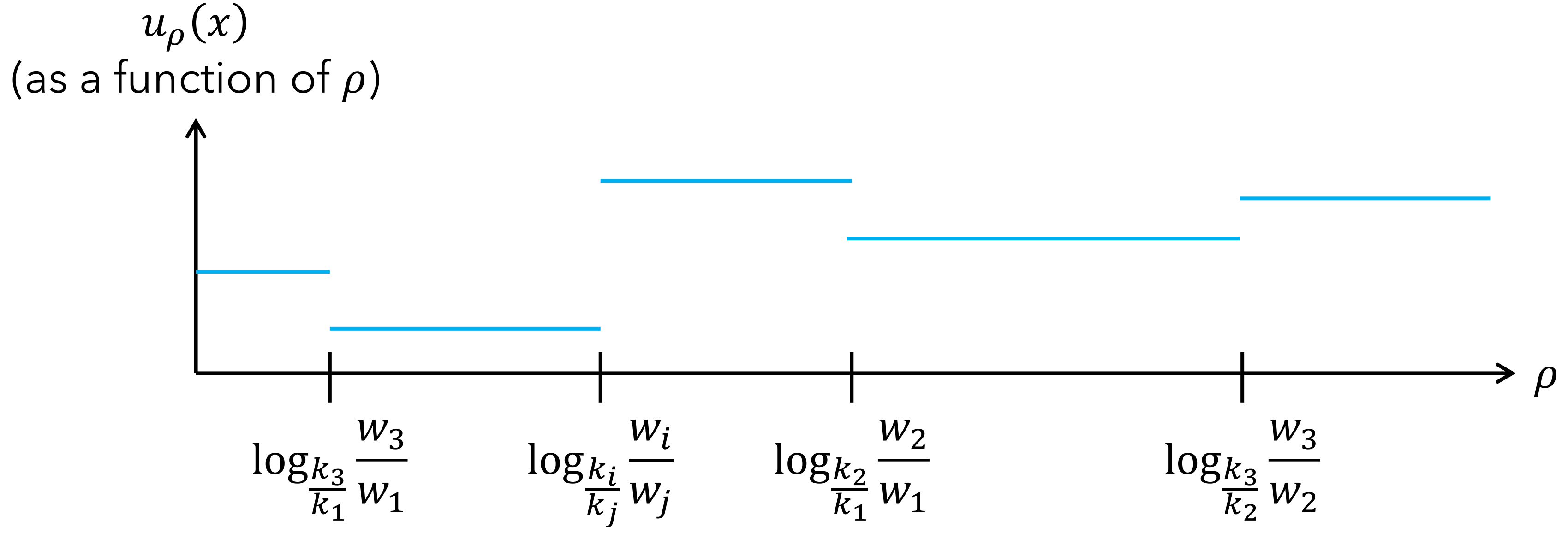
$\Rightarrow u_\rho(x)$ is constant



Gupta, Roughgarden, ITCS'16

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implies WHP $\forall \rho$, |**avg** utility over training set – **exp** utility| $\leq \epsilon$

Gupta, Roughgarden, ITCS'16; Balcan, DeBlasio, Dick, Kingsford, Sandholm, **Vitercik**, STOC'21

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$\mathcal{G}$ = constant functions, $\text{Pdim}(\mathcal{G}^*) = O(1)$

$\mathcal{F}$ = thresholds, $\text{VCdim}(\mathcal{F}^*) = O(1)$

k: n^2

implies WHP $\forall \rho$, |**avg** utility over training set – **exp** utility| $\leq \epsilon$

Gupta, Roughgarden, ITCS'16; Balcan, DeBlasio, Dick, Kingsford, Sandholm, **Vitercik**, STOC'21

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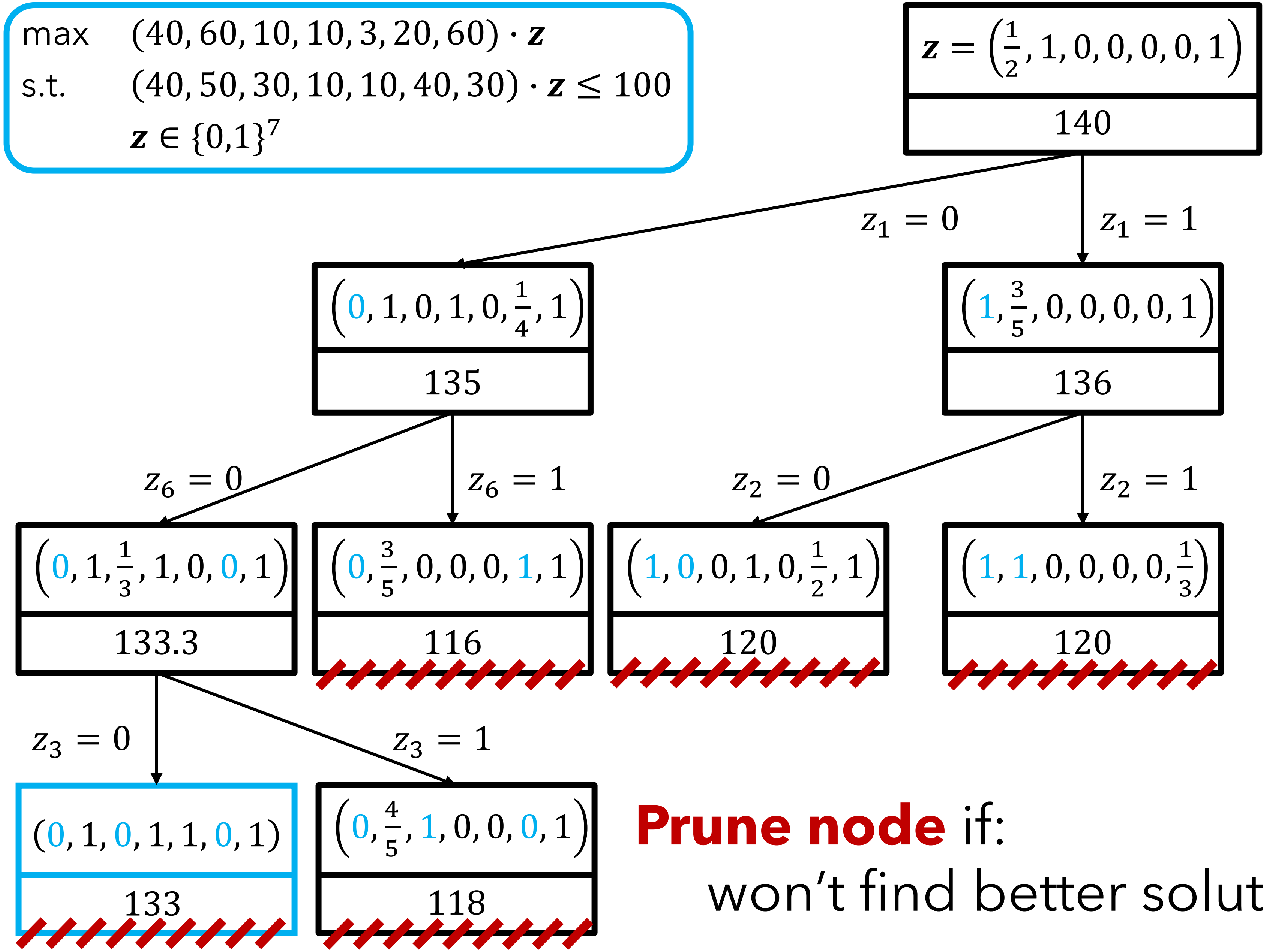
      c. **Cutting planes**
2. Online algorithm configuration

$$\begin{aligned} \max \quad & (40,60,10,10,3,20,60)\cdot \boldsymbol{z} \\ \text{s.t.} \quad & (40,50,30,10,10,40,30)\cdot \boldsymbol{z} \le 100 \\ & \boldsymbol{z} \in \{0,1\}^7 \end{aligned}$$



Branch and bound (B&B)

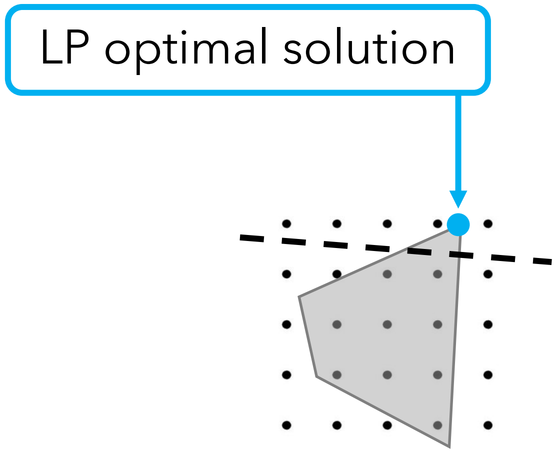
Prune node if:

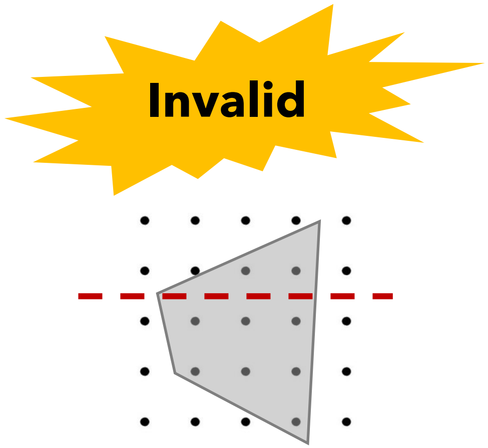
won't find better solution along branch

Cutting planes

Additional constraints that:

- Separate the LP optimal solution
  - Tightens LP relaxation to prune nodes sooner
- Don't separate any integer point





Cutting planes

Modern IP solvers add cutting planes through the B&B tree

"Branch-and-cut"

Responsible for breakthrough speedups of IP solvers

Cornuéjols, Annals of OR '07

Challenges:

- Many different types of cutting planes
  - Chvátal-Gomory cuts, cover cuts, clique cuts, …
- How to choose which cuts to apply?

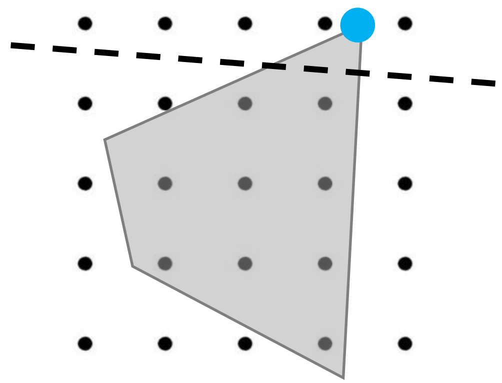
Chvátal-Gomory cuts

We study the canonical family of *Chvátal-Gomory (CG)* cuts

CG cut parameterized by $\boldsymbol{\rho} \in [0,1)^m$ is $\lfloor \boldsymbol{\rho}^T A \rfloor \boldsymbol{z} \leq \lfloor \boldsymbol{\rho}^T \boldsymbol{b} \rfloor$

Important properties:

- CG cuts are valid
- Can be chosen so it separates the LP opt



Balcan, Prasad, Sandholm, **Vitercik**, NeurIPS'21

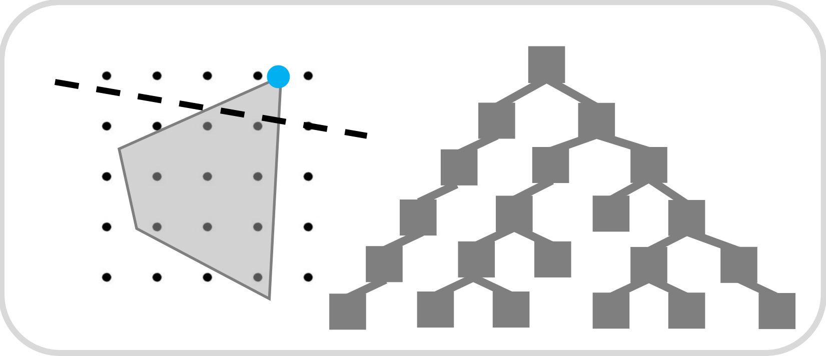
Key challenge

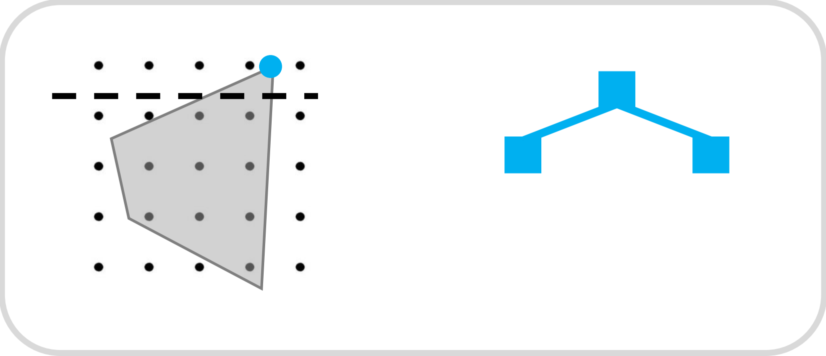
Cut (typically) remains in LPs throughout **entire** tree search

Every aspect of tree search depends on LP guidance

Node selection, variable selection, pruning, …

Tiny change in cut can cause **major changes to tree**



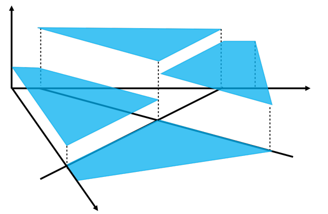


Balcan, Prasad, Sandholm, **Vitercik**, NeurIPS'21

Key lemma

Lemma: $O(\|A\|_{1,1} + \|\boldsymbol{b}\|_1 + n)$ hyperplanes partition $[0,1)^m$ into regions s.t. in any one region, B&C tree is fixed

Tree size is a piecewise-constant function of $\boldsymbol{\rho} \in [0,1)^m$



Balcan, Sandholm, Prasad, **Vitercik**, NeurIPS'21

Key lemma

Lemma: $O(\|A\|_{1,1} + \|\boldsymbol{b}\|_1 + n)$ hyperplanes partition $[0,1)^m$ into regions s.t. in any one region, B&C tree is fixed

Proof idea:

- CG cut parameterized by $\boldsymbol{\rho} \in [0,1)^m$ is $\lfloor \boldsymbol{\rho}^T A \rfloor \boldsymbol{z} \leq \lfloor \boldsymbol{\rho}^T \boldsymbol{b} \rfloor$
- For any $\boldsymbol{\rho}$ and column $\boldsymbol{a}_i$, $\lfloor \boldsymbol{\rho}^T \boldsymbol{a}_i \rfloor \in [-\|\boldsymbol{a}_i\|_1, \|\boldsymbol{a}_i\|_1]$
- For each integer $k_i \in [-\|\boldsymbol{a}_i\|_1, \|\boldsymbol{a}_i\|_1]$:

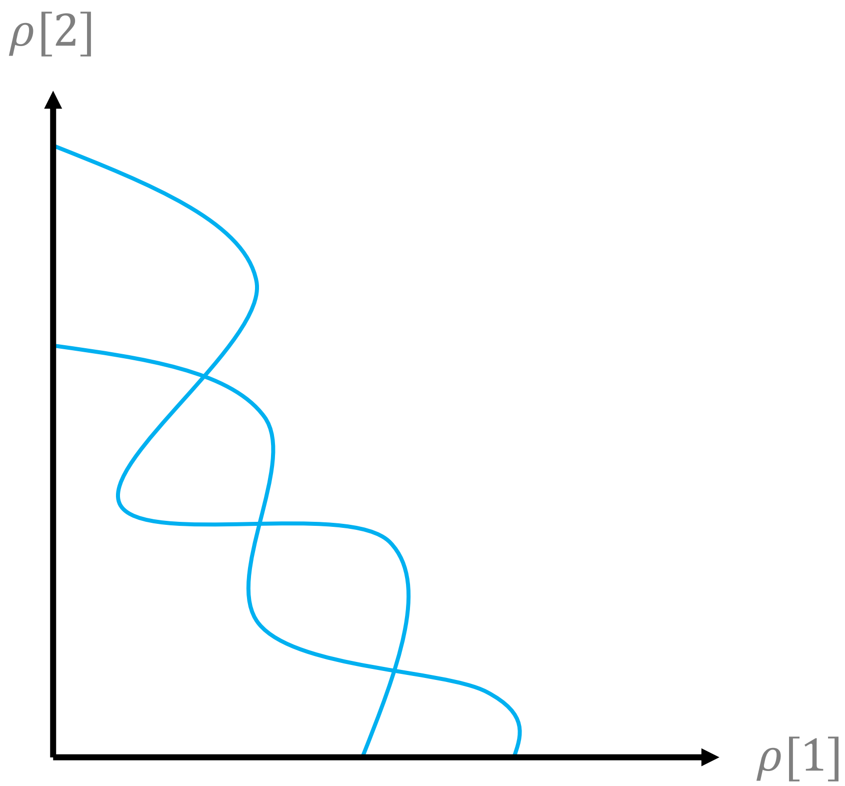
$$\lfloor \boldsymbol{\rho}^T \boldsymbol{a}_i \rfloor = k_i \text{ iff } k_i \leq \boldsymbol{\rho}^T \boldsymbol{a}_i < k_i + 1$$

$O(\|A\|_{1,1} + n)$ halfspaces

- In any region defined by intersection of halfspaces: $(\lfloor \boldsymbol{\rho}^T \boldsymbol{a}_1 \rfloor, \ldots, \lfloor \boldsymbol{\rho}^T \boldsymbol{a}_m \rfloor)$ is constant

Beyond Chvátal-Gomory cuts

For more complex families, boundaries can be more complex



Balcan, Sandholm, Prasad, **Vitercik**, NeurIPS'22

Cutting plane guarantees

Theorem: Training set of size

$$\tilde{O}\left(\frac{\mathrm{Pdim}(\mathcal{G}^*) + \mathrm{VCdim}(\mathcal{F}^*)\log k}{\epsilon^2}\right) = \tilde{O}\left(\frac{m\log\left(\|A\|_{1,1} + \|\boldsymbol{b}\|_1 + n\right)}{\epsilon^2}\right)$$

implies WHP $\forall \boldsymbol{\rho}$, |**avg** utility over training set – **exp** utility| $\leq \epsilon$

Balcan, Prasad, Sandholm, **Vitercik**, NeurIPS'21; Balcan, DeBlasio, Dick, Kingsford, Sandholm, **Vitercik**, STOC'21

Cutting plane guarantees

Theorem: Training set of size

$$\tilde{O}\left(\frac{\text{Pdim}(\mathcal{G}^*) + \text{VCdim}(\mathcal{F}^*)\log k}{\epsilon^2}\right) = \tilde{O}\left(\frac{m\log\left(\|A\|_{1,1} + \|\boldsymbol{b}\|_1 + n\right)}{\epsilon^2}\right)$$

$\|A\|_{1,1} + \|\boldsymbol{b}\|_1 + n$

$\mathcal{F}$ = hyperplanes in $\mathbb{R}^m$
$\text{VCdim}(\mathcal{F}^*) = O(m)$

$\mathcal{G}$ = constant functions in $\mathbb{R}^m$
$\text{Pdim}(\mathcal{G}^*) = O(m)$

implies WHP $\forall \boldsymbol{\rho}$, |**avg** utility over training set – **exp** utility| $\leq \epsilon$

Balcan, Prasad, Sandholm, **Vitercik**, NeurIPS'21; Balcan, DeBlasio, Dick, Kingsford, Sandholm, **Vitercik**, STOC'21

Outline (theoretical guarantees)

1. Statistical guarantees for algorithm configuration
2. **Online algorithm configuration**

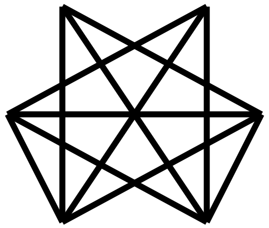
Gupta, Roughgarden, ITCS'16
Balcan, Dick, **Vitercik**, FOCS'18
Balcan, Dick, Pegden, UAI'20

Online algorithm configuration

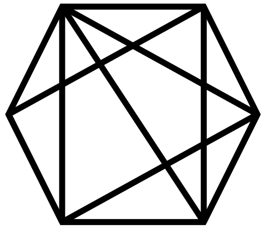
What if inputs are not i.i.d., but even adversarial?

E.g., MWIS:

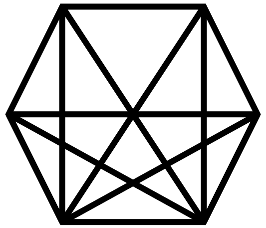
Day 1: ρ_1



Day 2: ρ_2



Day 3: ρ_3



Goal: Compete with best parameter setting in hindsight

- Impossible in the worst case
- Under what conditions is online configuration possible?

Online model

Over T timesteps $t = 1, \dots, T$:

1. Learner chooses **parameter setting $\boldsymbol{\rho}_t$**
2. Nature (or adversary 😈) chooses **problem instance** x_t
3. Learner obtains **reward** $u_{\boldsymbol{\rho}_t}(x_t) = u^*_{x_t}(\boldsymbol{\rho}_t)$
4. Learner **observes function** $u^*_{x_t}$ (full information feedback)
   - Simplest setting so we'll start here
   - Will look at other feedback models later (e.g., bandit)

Online model

Over T timesteps $t = 1, \dots, T$:

1. Learner chooses **parameter setting** $\boldsymbol{\rho}_t$
2. Nature (or adversary 😈) chooses **problem instance** x_t
3. Learner obtains **reward** $u_{\boldsymbol{\rho}_t}(x_t) = u^*_{x_t}(\boldsymbol{\rho}_t)$
4. Learner **observes function** $u^*_{x_t}$ (full information feedback)

Goal: Minimize ***regret*** $\max_{\boldsymbol{\rho}} \sum_{t=1}^{T} u_{\boldsymbol{\rho}}(x_t) - \sum_{t=1}^{T} u_{\boldsymbol{\rho}_t}(x_t)$

Ideally, $\frac{1}{T} \cdot (\text{Regret}) \to 0$ as $T \to \infty$

On average, competing with best algorithm in hindsight

Outline (theoretical guarantees)

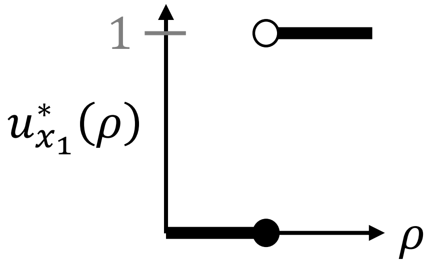
1. Statistical guarantees for algorithm configuration
2. Online algorithm configuration
   i. **Worst-case instance**
   ii. Dispersion
   iii. Semi-bandit model

Worst-case MWIS instance

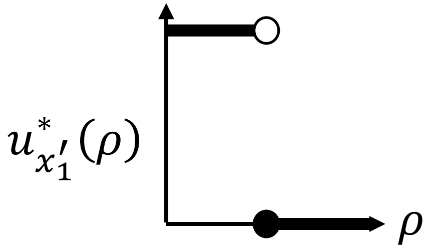
Exists adversary choosing MWIS instances s.t.:

Every full information online algorithm has **linear regret**

Round 1:



Dual function: Utility on instance x_1 as function of ρ



Dual function: Utility on instance x_1' as function of ρ

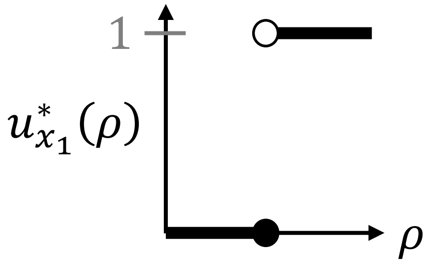
Gupta and Roughgarden, ITCS'16

Worst-case MWIS instance

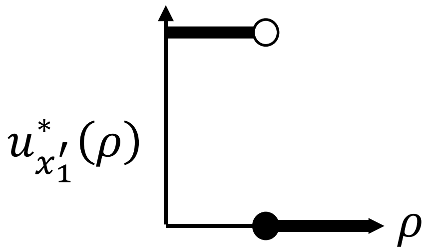
Exists adversary choosing MWIS instances s.t.:

Every full information online algorithm has **linear regret**

Round 1:



Adversary chooses x_1 or x_1' with equal probability



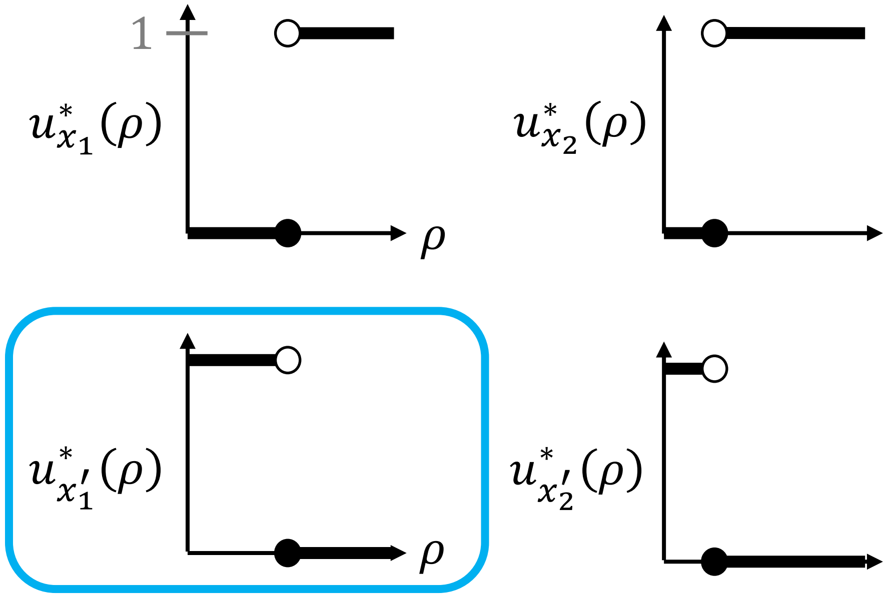
Gupta and Roughgarden, ITCS'16

Worst-case MWIS instance

Exists adversary choosing MWIS instances s.t.:

Every full information online algorithm has **linear regret**

Round 1: Round 2:



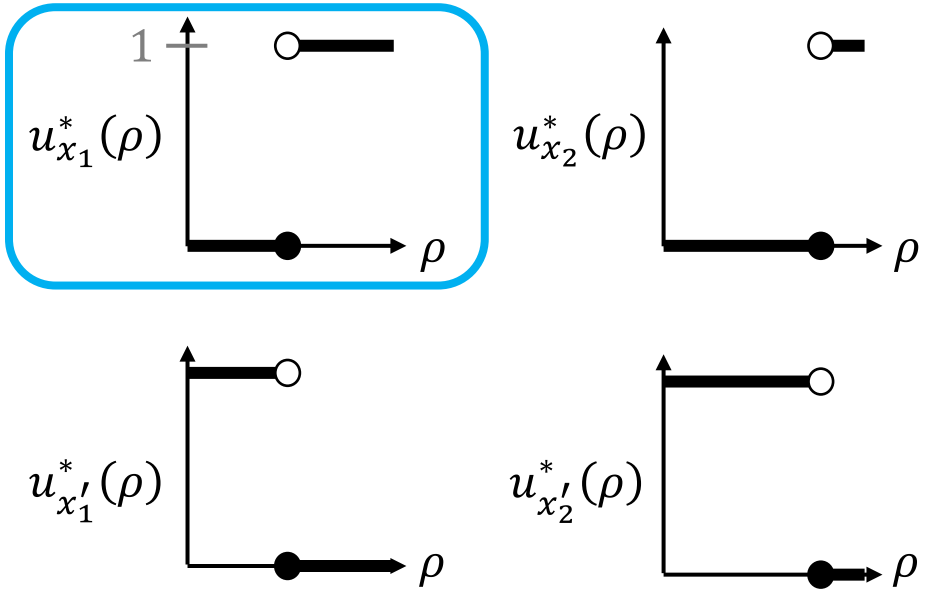
Gupta and Roughgarden, ITCS'16

Worst-case MWIS instance

Exists adversary choosing MWIS instances s.t.:

Every full information online algorithm has **linear regret**

Round 1: Round 2:



Repeatedly halves optimal region

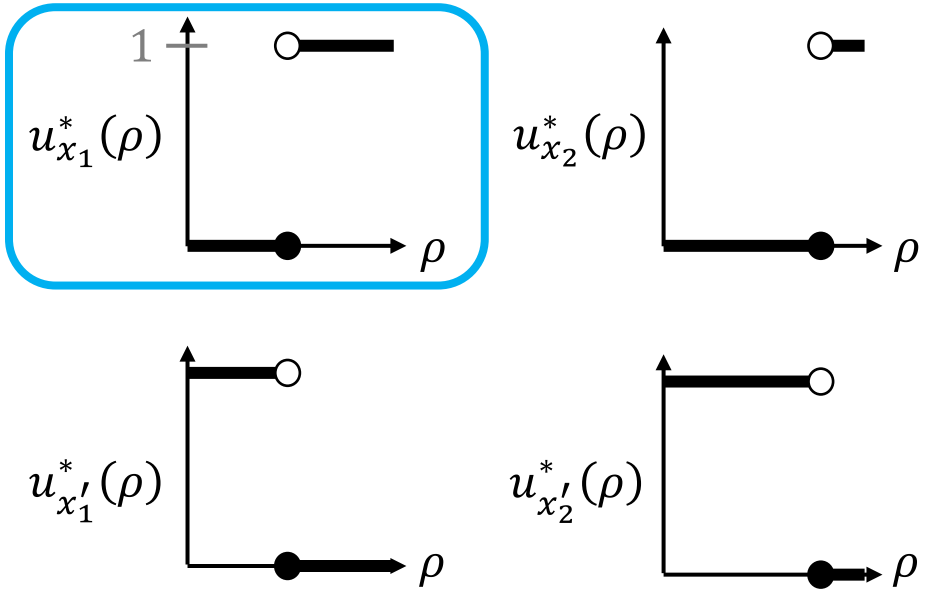
Gupta and Roughgarden, ITCS'16

Worst-case MWIS instance

Exists adversary choosing MWIS instances s.t.:

Every full information online algorithm has **linear regret**

Round 1: Round 2:



Repeatedly halves optimal region

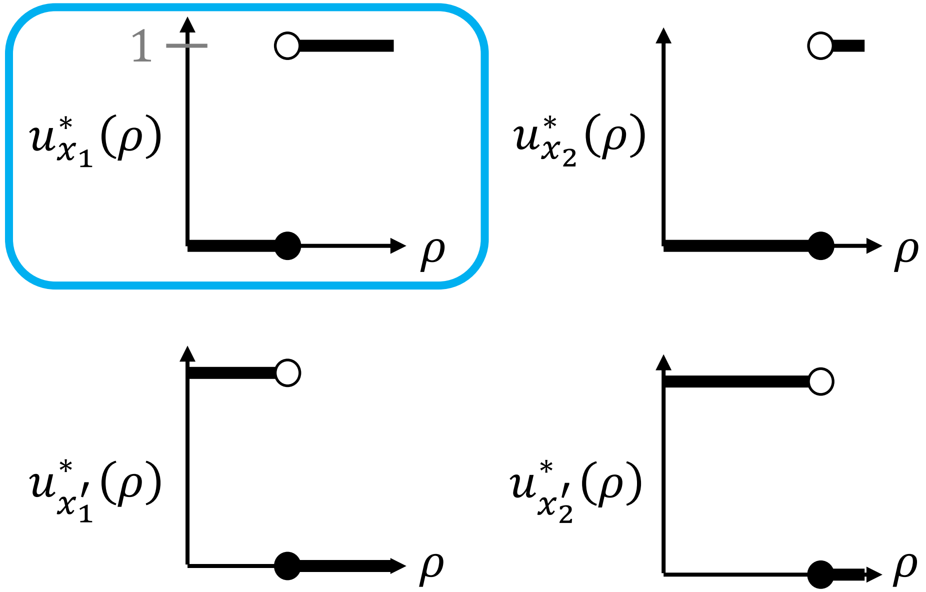
Gupta and Roughgarden, ITCS'16

Worst-case MWIS instance

Exists adversary choosing MWIS instances s.t.:

Every full information online algorithm has **linear regret**

Round 1: Round 2:



Repeatedly halves optimal region

Learner's expected reward: $\frac{T}{2}$

Reward of best ρ in hindsight: T

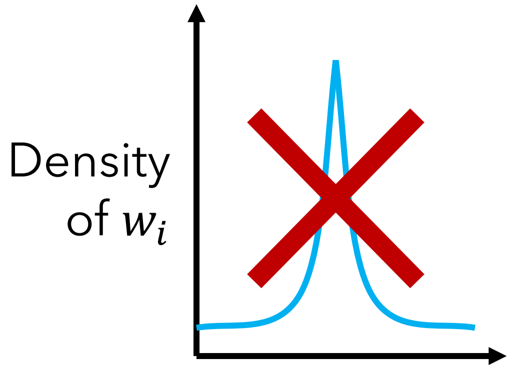
Expected regret = $\frac{T}{2}$

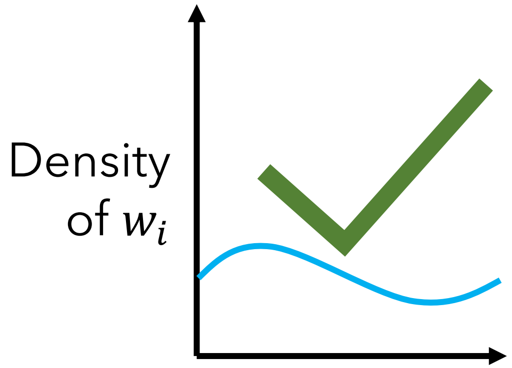
Gupta and Roughgarden, ITCS'16

Smoothed adversary: MWIS

Sub-linear regret is possible if adversary has a "shaky hand":

- Node weights $w_1, \dots, w_n$ and degrees $k_1, \dots, k_n$ are stochastic
- Joint density of (w_i, w_j, k_i, k_j) is bounded





Later generalized by Cohen-Addad, Kanade [AISTATS, '17]; Balcan, Dick, Vitercik [FOCS'18]; Balcan et al. [UAI'20]; …

Gupta and Roughgarden, ITCS'16

Outline (theoretical guarantees)

1. Statistical guarantees for algorithm configuration
2. Online algorithm configuration
    i. Worst-case instance
    ii. Dispersion
    iii. Semi-bandit model

Dispersion

Mean adversary concentrates discontinuities near maximizer ρ^*

Even points very close to ρ^* have low utility!

$u^*_{x_1}, \dots, u^*_{x_T}: B(\mathbf{0}, 1) \to [-1,1]$ are (w, k)***-dispersed at point*** ρ if:

Can be generalized to any bounded subset

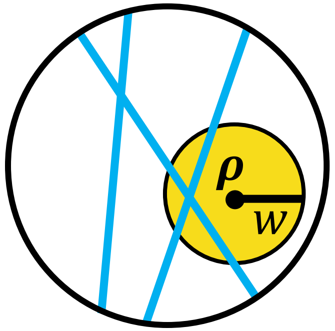
Dispersion

Mean adversary concentrates discontinuities near maximizer ρ^*

Even points very close to ρ^* have low utility!

$u_{x_1}^*, \ldots, u_{x_T}^*: B(\mathbf{0}, 1) \to [-1,1]$ are ***(w, k)-dispersed at point ρ*** if:

ℓ_2-ball $B(\boldsymbol{\rho}, w)$ contains discontinuities for $\leq k$ of $u_{x_1}^*, \ldots, u_{x_T}^*$



Ball of radius w about $\boldsymbol{\rho}$ contains 2 discontinuities

$\Rightarrow (w, 2)$-dispersed at $\boldsymbol{\rho}$

Balcan, Dick, **Vitercik**, FOCS'18

Outline (theoretical guarantees)

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      b. Regret bound
      c. Bandit feedback
      d. Proving dispersion holds
   iii. Semi-bandit model

Exponentially weighted forecaster

[Freund, Schapire, JCSS'97, Cesa-Bianchi & Lugosi '06, ...]

input: Learning rate $\eta > 0$

initialization: $U_0(\boldsymbol{\rho}) = 0$ is the constant function

for $t = 1, \ldots, T$:

choose distribution $\boldsymbol{q}_t$ over $\mathbb{R}^d$ such that $\boldsymbol{q}_t(\boldsymbol{\rho}) \propto \exp\big(\eta U_{t-1}(\boldsymbol{\rho})\big)$

Exponentially upweight high-performance parameter settings

choose parameter setting $\boldsymbol{\rho}_t \sim \boldsymbol{q}_t$, receive reward $u^*_{x_t}(\boldsymbol{\rho}_t)$

observe utility function $u^*_{x_t}: \mathcal{P} \to [0,1]$

update $U_t = U_{t-1} + u^*_{x_t}$

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Regret

Regret $= \sum_{t=1}^{T} u_{x_t}^*(\boldsymbol{\rho}^*) - \sum_{t=1}^{T} u_{x_t}^*(\boldsymbol{\rho}_t)$

Theorem: Suppse $u_{x_1}^*, \dots, u_{x_T}^*: B(\mathbf{0}, 1) \to [0,1]$ are:

1. Piecewise L-Lipschitz
2. (w, k)-dispersed at $\boldsymbol{\rho}^*$

EWF has regret $O\left(\sqrt{Td \log \frac{1}{w}} + TLw + k\right)$

When is this a good bound?

For $w = \frac{1}{L\sqrt{T}}$ and $k = \tilde{O}(\sqrt{T})$, regret is $\tilde{O}(\sqrt{Td})$

Regret upper bound: Proof sketch

$$W_t = \int_{B(\mathbf{0},1)} \exp(\eta U_t(\boldsymbol{\rho}))d\boldsymbol{\rho} \qquad \left(U_t(\boldsymbol{\rho}) = \sum_{\tau=1}^{t} u_\tau^*(\boldsymbol{\rho})\right)$$

Goal: Something in terms of OPT $= \sum_{t=1}^T u_t^*(\boldsymbol{\rho}^*)$ $\leq \frac{W_T}{W_0} \leq$ Something in terms of ALG $= \sum_{t=1}^T u_t^*(\boldsymbol{\rho}_t)$

Learner's performance (ALG) is sufficiently large compared to OPT

Regret upper bound: Proof sketch

$$W_t = \int_{B(\mathbf{0},1)} \exp(\eta U_t(\boldsymbol{\rho}))d\boldsymbol{\rho}$$

$$\left(U_t(\boldsymbol{\rho}) = \sum_{\tau=1}^{t} u_\tau^*(\boldsymbol{\rho})\right)$$

Goal: Something in terms of OPT $= \sum_{t=1}^{T} u_t^*(\boldsymbol{\rho}^*)$ $\leq \frac{W_T}{W_0} \leq \exp(\text{ALG}(e^\eta - 1))$

Standard EWF analysis

Balcan, Dick, **Vitercik**, FOCS'18

Regret upper bound: Proof sketch

$$W_t = \int_{B(\mathbf{0},1)} \exp(\eta U_t(\boldsymbol{\rho}))d\boldsymbol{\rho} \qquad \left(U_t(\boldsymbol{\rho}) = \sum_{\tau=1}^{t} u_\tau^*(\boldsymbol{\rho})\right)$$

Goal: Something in terms of $\text{OPT} = \sum_{t=1}^{T} u_t^*(\boldsymbol{\rho}^*)$ $\leq \frac{W_T}{W_0} \leq \exp\left(\text{ALG}(e^\eta - 1)\right)$

$$W_T = \int_{B(\mathbf{0},1)} \exp\left(\eta \sum_{t=1}^{T} u_t^*(\boldsymbol{\rho})\right) d\boldsymbol{\rho} \geq \int_{B(\boldsymbol{\rho}^*,w)} \exp\left(\eta \sum_{t=1}^{T} u_t^*(\boldsymbol{\rho})\right) d\boldsymbol{\rho}$$

Regret upper bound: Proof sketch

Goal: Something in terms of $\mathrm{OPT} = \sum_{t=1}^{T} u_t^*(\boldsymbol{\rho}^*)$ $\leq \frac{W_T}{W_0} \leq \exp\left(\mathrm{ALG}(e^\eta - 1)\right)$

$$W_T = \int_{B(\mathbf{0},1)} \exp\left(\eta \sum_{t=1}^{T} u_t^*(\boldsymbol{\rho})\right) d\boldsymbol{\rho} \geq \int_{B(\boldsymbol{\rho}^*,w)} \exp\left(\eta \sum_{t=1}^{T} u_t^*(\boldsymbol{\rho})\right) d\boldsymbol{\rho}$$

$$\geq \int_{B(\boldsymbol{\rho}^*,w)} \exp\left(\eta(\mathrm{OPT} - k - TLw)\right) d\boldsymbol{\rho}$$

$$= \mathrm{Vol}\left(B(\boldsymbol{\rho}^*, w)\right) \exp\left(\eta(\mathrm{OPT} - k - TLw)\right)$$

Regret upper bound: Proof sketch

$$\frac{\mathrm{Vol}\left(B(\boldsymbol{\rho}^*, w)\right)\exp\left(\eta(\mathrm{OPT} - k - TLw)\right)}{\mathrm{Vol}\left(B(\mathbf{0}, 1)\right)} \leq \frac{W_T}{W_0} \leq \exp\left(\mathrm{ALG}(e^\eta - 1)\right)$$

Rearranging and setting $\eta = \sqrt{\frac{d}{T}\log\frac{1}{w}}$:

$$\text{Regret} = \mathrm{OPT} - \mathrm{ALG} = O\left(\sqrt{Td\log\frac{1}{w}} + TLw + k\right)$$

Matching lower bound

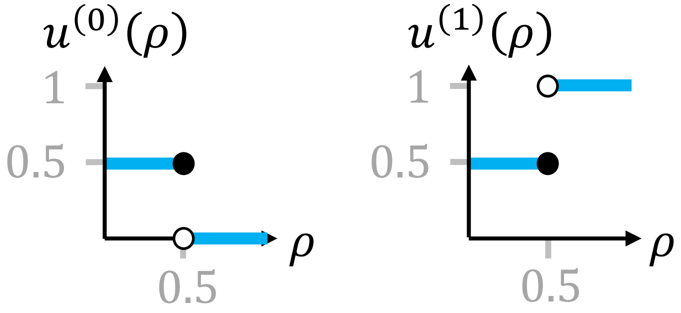
Theorem: For any algorithm, exist PW-constant $u_1^*, \ldots, u_T^*$ s.t.:

Algorithm's regret is $\Omega\left(\inf_{(w,k)} \sqrt{Td \log \frac{1}{w}} + k\right)$

Inf over all (w, k)-dispersion parameters that $u_1^*, \ldots, u_T^*$ satisfy at $\boldsymbol{\rho}^*$

Upper bound = $O\left(\inf_{(w,k)} \sqrt{Td \log \frac{1}{w}} + k\right)$

Regret lower bound: Proof sketch



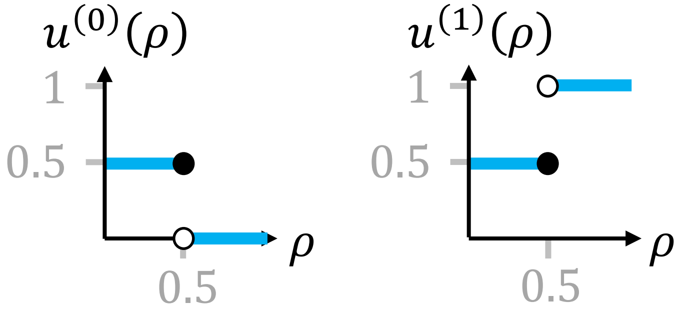
Lemma [Weed et al., COLT'16]**:**

Exist distributions μ_U, μ_L over $\{u^{(0)}, u^{(1)}\}$ s.t. for any algorithm,

$$\max_{\mu_U, \mu_L} \max_{\rho \in [0,1]} \mathbb{E}\left[\sum_{t=1}^{T} u_t^*(\rho) - \sum_{t=1}^{T} u_t^*(\rho_t)\right] \geq \frac{\sqrt{T}}{32}$$

$u_1^*, \ldots, u_T^*$ drawn from worse of μ_U, μ_L

Regret lower bound: Proof sketch



Lemma [Weed et al., COLT'16]**:**

Exist distributions μ_U, μ_L over $\{u^{(0)}, u^{(1)}\}$ s.t. for any algorithm,

$$\max_{\mu_U,\mu_L} \max_{\rho\in[0,1]} \mathbb{E}\left[\sum_{t=1}^{T} u_t^*(\rho) - \sum_{t=1}^{T} u_t^*(\rho_t)\right] \geq \frac{\sqrt{T}}{32}$$

Any $\rho > 0.5$ is optimal under μ_U, any $\rho \leq 0.5$ is optimal under μ_L

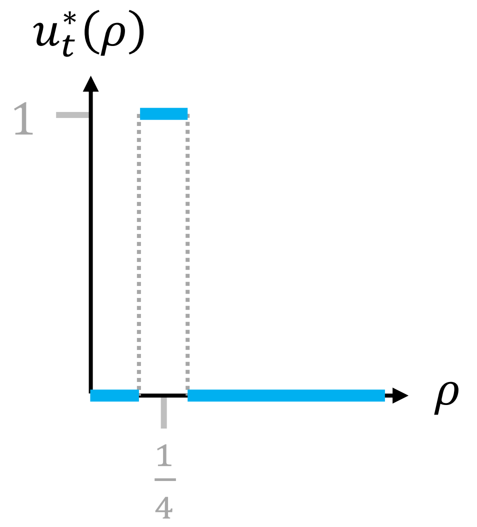
Regret lower bound: Proof sketch

Worst case instance:

1. Draw $u_1^*, \ldots, u_{T-\sqrt{T}}^*$ from worse of μ_U, μ_L and define:

$$\rho^* = \underset{\rho \in \left\{\frac{1}{4}, \frac{3}{4}\right\}}{\operatorname{argmax}} \sum_{t=1}^{T-\sqrt{T}} u_t^*(\rho)$$

2. Define $u_t^*(\rho) = \mathbf{1}_{\left\{|\rho - \rho^*| \leq \frac{1}{10}\right\}}$ for $t > T - \sqrt{T}$



Note: $\rho^* \in \operatorname{argmax} \sum_{t=1}^{T} u_t^*(\rho)$

Regret lower bound: Proof sketch

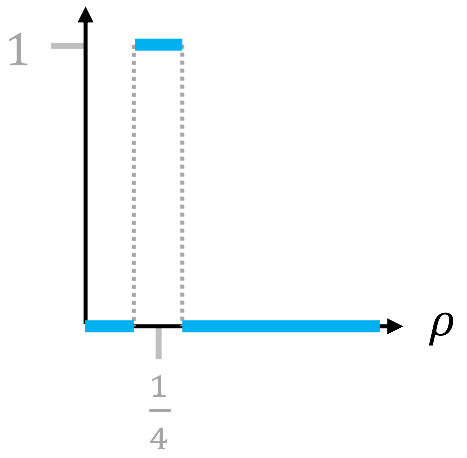
Analysis:

- Regret $\geq \frac{\sqrt{T}}{64}$ (follows from lemma by Weed et al., [COLT'16])
- Lower bound follows from fact that $\frac{\sqrt{T}}{64} = \Omega\left(\inf_{(w,k)} \sqrt{T \log \frac{1}{w}} + k\right)$

  Only last $k = \sqrt{T}$ functions have discontinuities in

  $$\left[\rho^* - \frac{1}{8}, \rho^* + \frac{1}{8}\right]$$

  $\Rightarrow u_1^*, \ldots, u_T^*$ are $\left(w = \frac{1}{8}, k = \sqrt{T}\right)$-dispersed around ρ^*



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    iii. Semi-bandit model

Bandit feedback

Over T timesteps $t = 1, \ldots, T$:

1. Learner chooses **parameter setting** $\boldsymbol{\rho}_t$
2. Nature (or adversary 😈) chooses **problem instance** x_t
3. Learner obtains **reward** $u_{\boldsymbol{\rho}_t}(x_t) = u^*_{x_t}(\boldsymbol{\rho}_t)$
4. Learner **only** observes $u^*_{x_t}(\boldsymbol{\rho}_t)$ (not entire function)

Bandit feedback

Theorem: If $u_1^*, \ldots, u_T^*: B(\mathbf{0}, 1) \to [0,1]$ are:

1. Piecewise L-Lipschitz
2. (w, k)-dispersed at $\boldsymbol{\rho}^*$

The UCB algorithm has regret $\tilde{O}\left(\sqrt{Td\left(\frac{1}{w}\right)^d} + TLw + k\right)$

- If $d = 1$, $w = \frac{1}{\sqrt[3]{T}}$, and $k = \tilde{O}\left(T^{2/3}\right)$, regret is $\tilde{O}\left(LT^{2/3}\right)$
- If $w = T^{\frac{d+1}{d+2}-1}$, $k = \tilde{O}\left(T^{\frac{d+1}{d+2}}\right)$, then regret is $\tilde{O}\left(T^{\frac{d+1}{d+2}}\left(\sqrt{d3^d} + L\right)\right)$

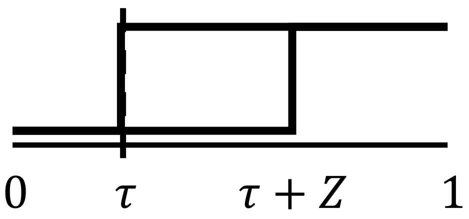
Outline (theoretical guarantees)

1. Statistical guarantees for algorithm configuration
2. Online algorithm configuration
   i. Worst-case instance
   ii. Dispersion
      a. Algorithm
      b. Regret bound
      c. Bandit feedback
      d. **Proving dispersion holds**
   iii. Semi-bandit model

Smooth adversaries and dispersion

Adversary chooses thresholds $u_t^*: [0,1] \to \{0,1\}$

Discontinuity τ "smoothed" by adding $Z \sim N(0, \sigma^2)$



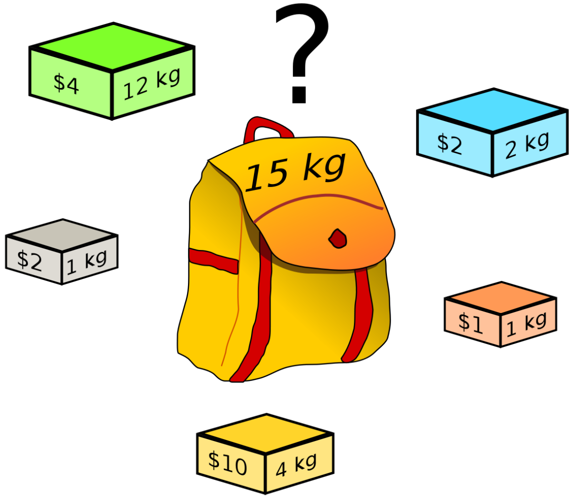
Lemma: WHP, $\forall w, u_1^*, \ldots, u_T^*$ are $\left(w, \tilde{O}\left(\frac{Tw}{\sigma} + \sqrt{T}\right)\right)$-dispersed

Corollary: $w = \frac{\sigma}{\sqrt{T}} \Rightarrow$ **Full information regret =** $\boldsymbol{O\left(\sqrt{T \log \frac{T}{\sigma}}\right)}$

Balcan, Dick, **Vitercik**, FOCS'18

Simple example: knapsack

Problem instance:
- n items, item i has value v_i and size s_i
- Knapsack with capacity K



Goal: find most valuable items that fit

Algorithm (parameterized by $\rho \geq 0$)**:**

Add items in decreasing order of $\frac{v_i}{s_i^\rho}$

[Gupta and Roughgarden, ITCS'16]

Dispersion for knapsack

Theorem: If instances randomly distributed s.t. on each round:

1. Each v_i independent from s_i
2. All (v_i, v_j) have κ-bounded joint density,

W.h.p., for any $\alpha \geq \frac{1}{2}$, $u_1^*, \ldots, u_T^*$ are

$\left(\tilde{O}\left(\frac{T^{1-\alpha}}{\kappa}\right), \tilde{O}\left((\#\text{ items})^2 T^{\alpha}\right)\right)$-dispersed

Corollary: Full information regret = $\tilde{O}\left((\#\text{ items})^2\sqrt{T}\right)$

Balcan, Dick, **Vitercik**, FOCS'18

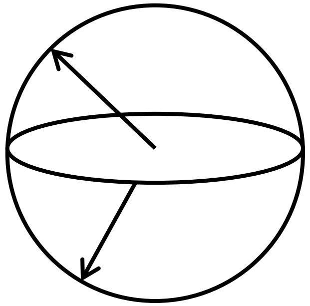
More results for algorithm configuration

Under **no assumptions**, we show dispersion for
Integer quadratic programming approximation algs

Based on semi-definite programming relaxations

- s-linear rounding [Feige & Langberg '06]
- Outward rotations [Zwick '99]
  - Both generalizations of Goemans-Williamson max-cut alg ['95]

Leverage algorithm's randomness to prove dispersion



Balcan, Dick, **Vitercik**, FOCS'18

Outline (theoretical guarantees)

1. Statistical guarantees for algorithm configuration
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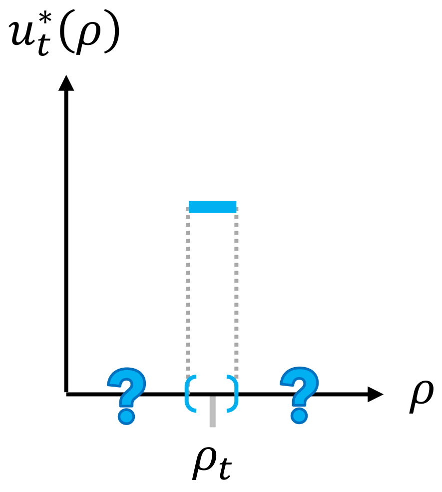
   ii. Dispersion
   iii. Semi-bandit model

Semi-bandit model

- Computing the entire function $u_t^*(\rho)$ can be challenging
- Often, it's easy to compute interval in which $u_t^*(\rho_t)$ is constant
  - E.g., in IP, simple bookkeeping with CPLEX callbacks
- **Semi-bandit model:** learner learns $u_t^*(\rho_t)$ *and* interval

Balcan, Dick, Pegden [UAI'20]**:**

- Regret bounds that are nearly as good as full info
- Introduce a more general definition of dispersion



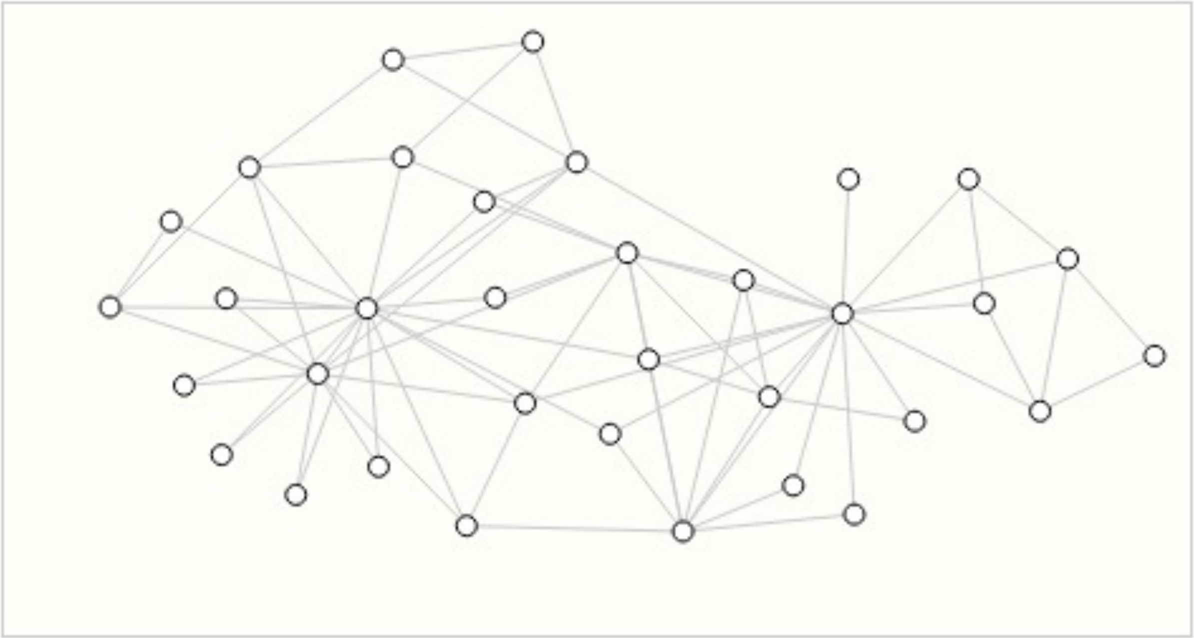
Outline (applied techniques)

1. **GNNs overview**
2. Neural algorithmic alignment
3. Reinforcement learning overview
4. Learning greedy heuristics with RL
5. Integer programming with GNNs

GNN motivation

Main question:

How to utilize relational structure for better prediction?



Graph neural networks: First step

- Design features for nodes/links/graphs
- Obtain features for all training data

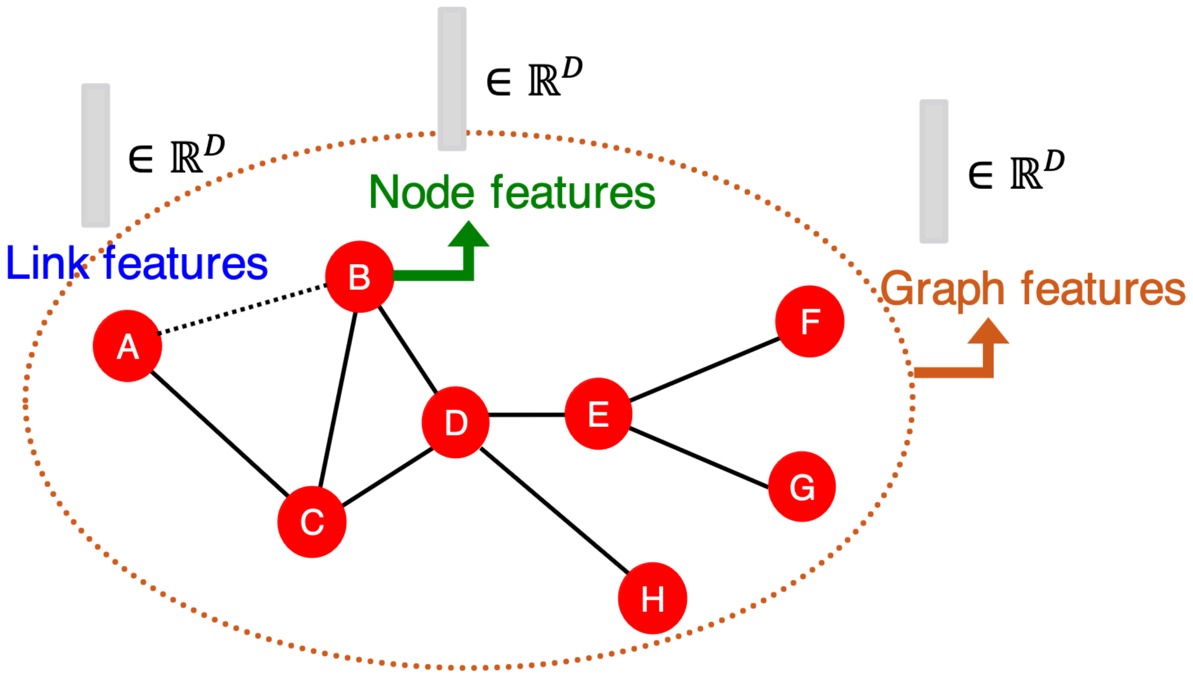


Figure by Leskovec

Graph neural networks: Objective

Idea:

1. Encode each node and its neighborhood with embedding
2. Aggregate set of node embeddings into graph embedding
3. Use embeddings to make predictions

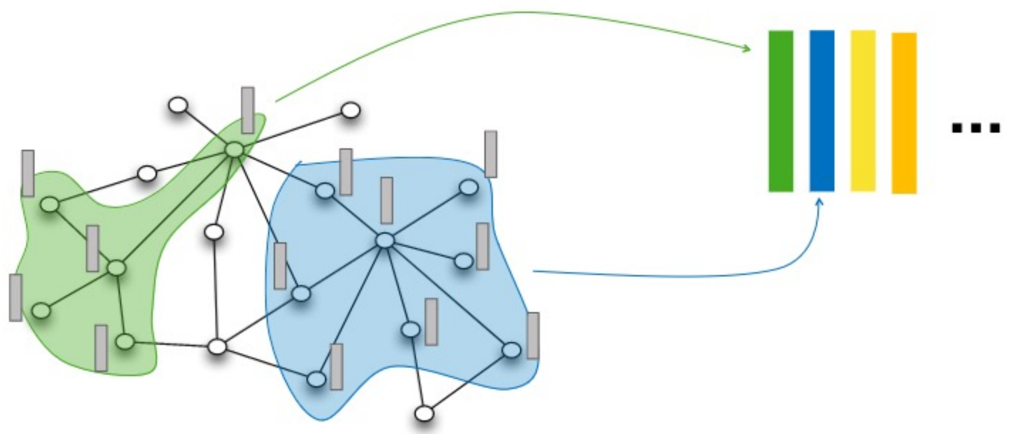
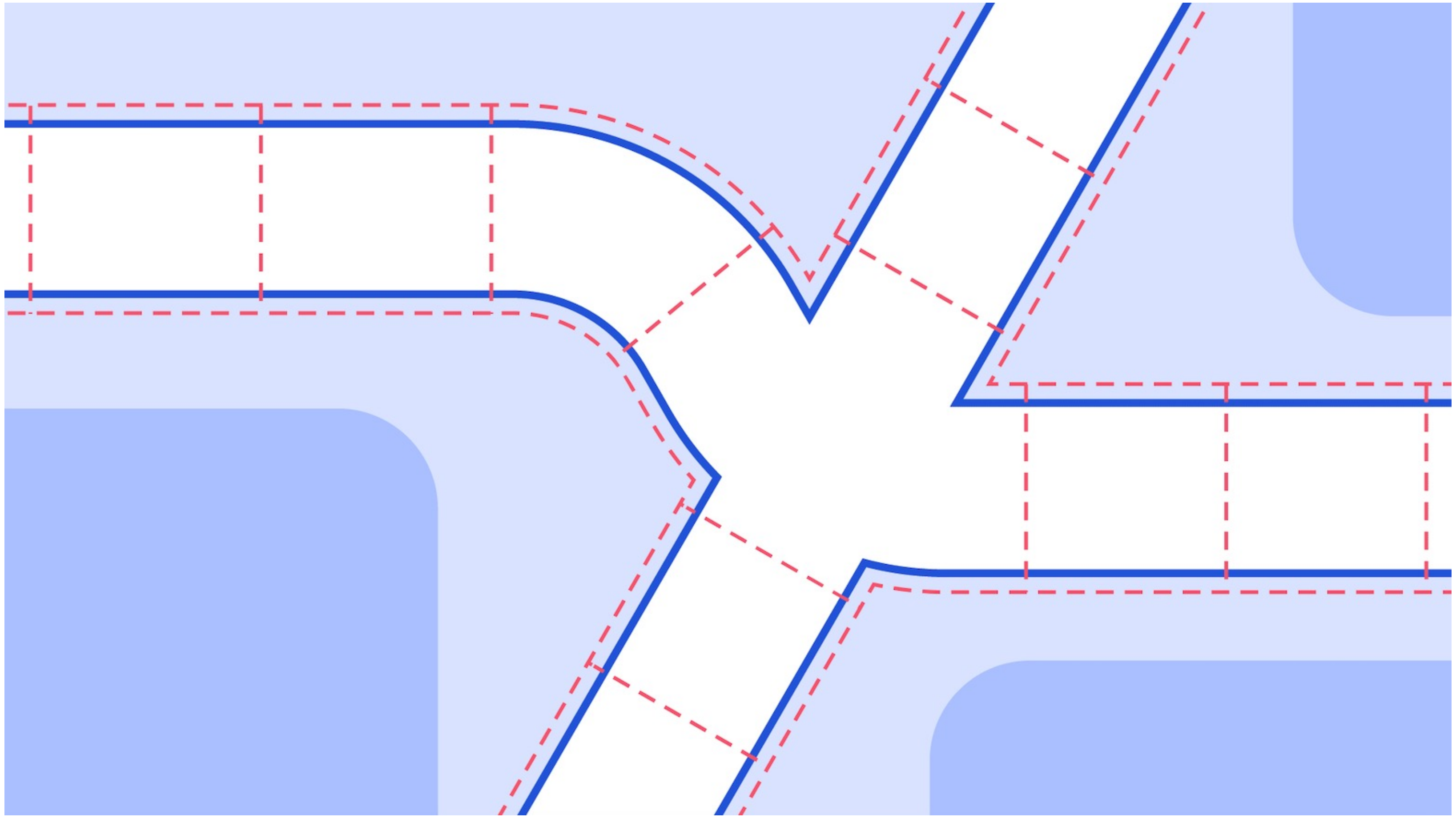


Figure by Jegelka

https://www.deepmind.com/blog/traffic-prediction-with-advanced-graph-neural-networks



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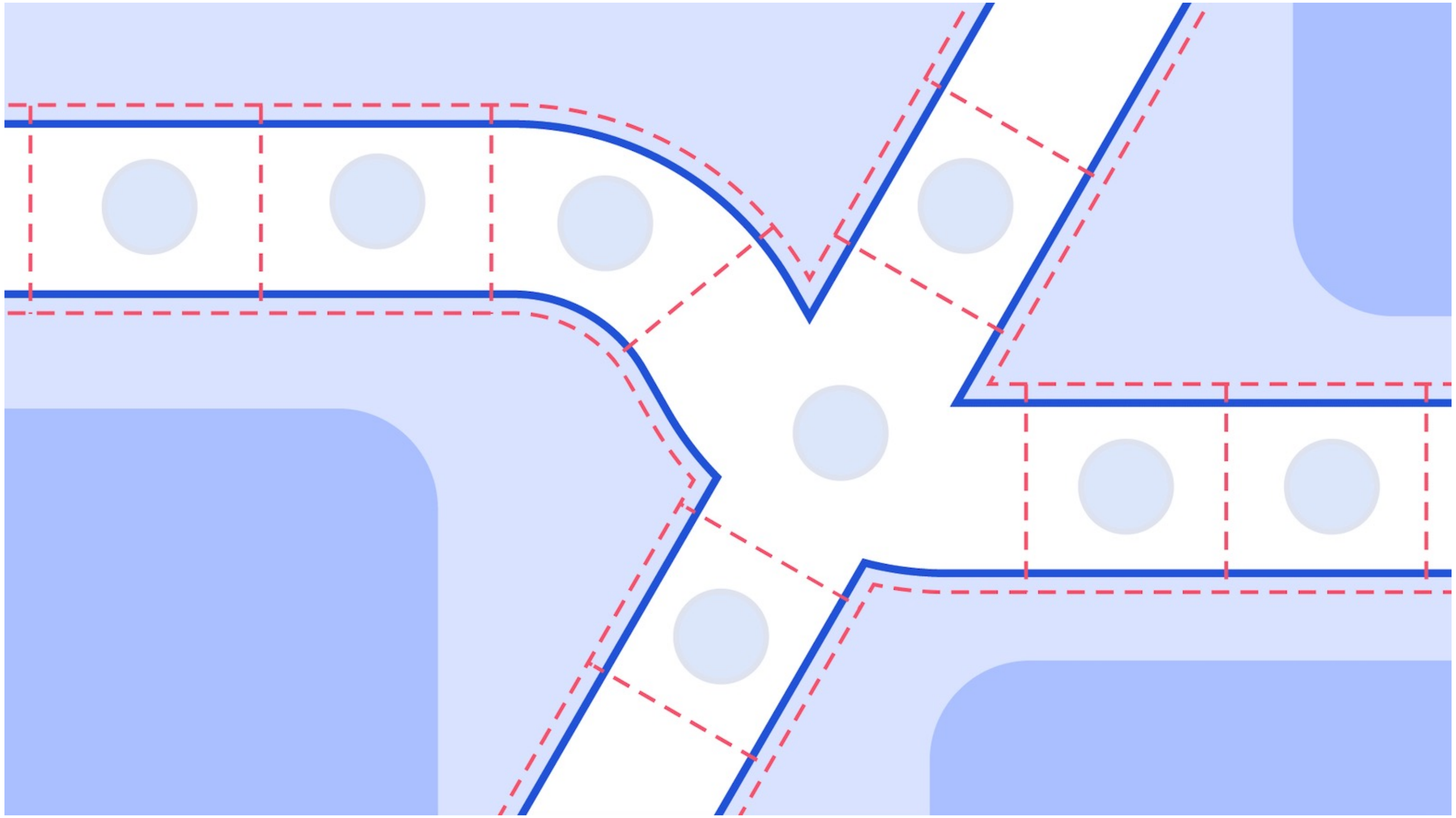

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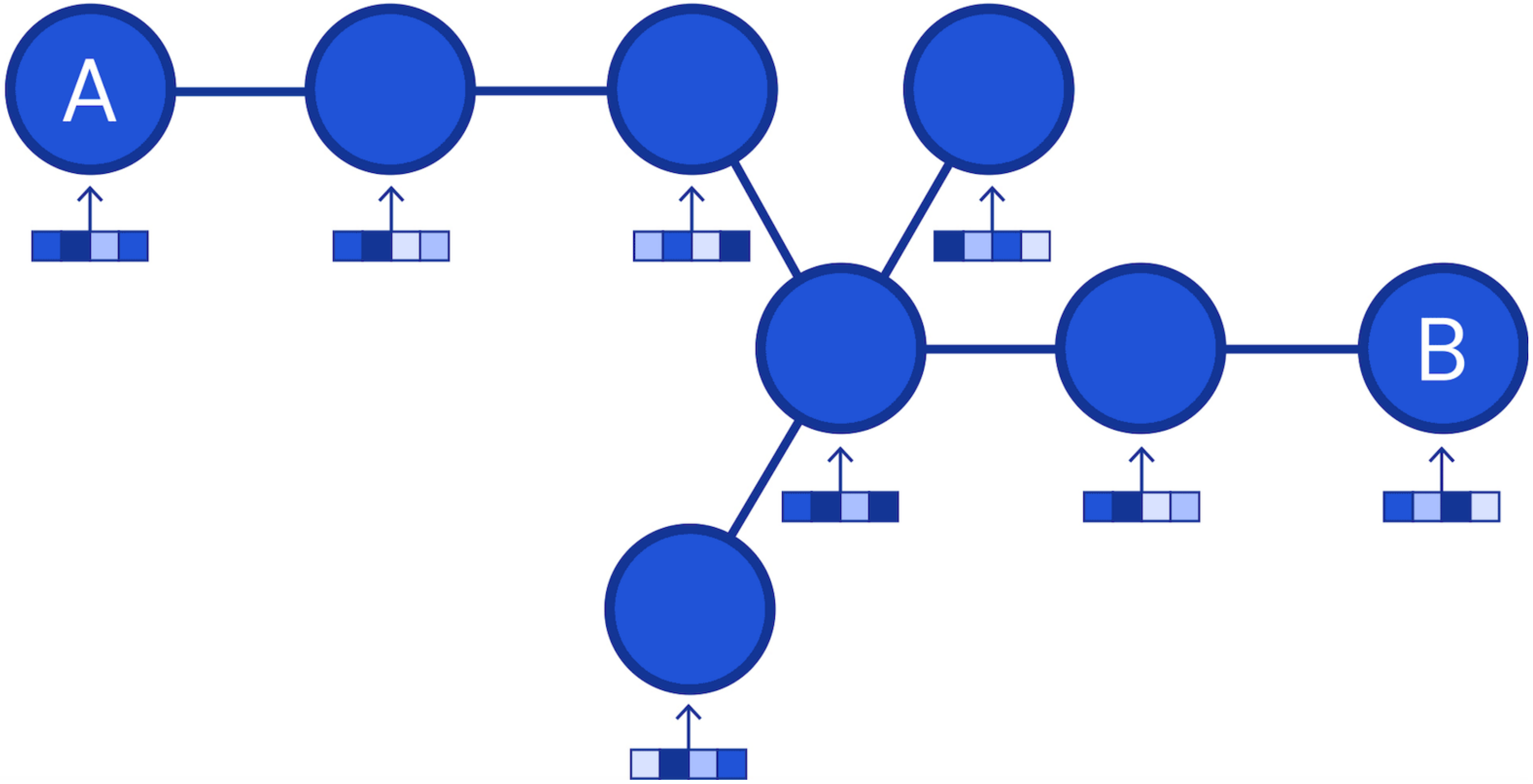

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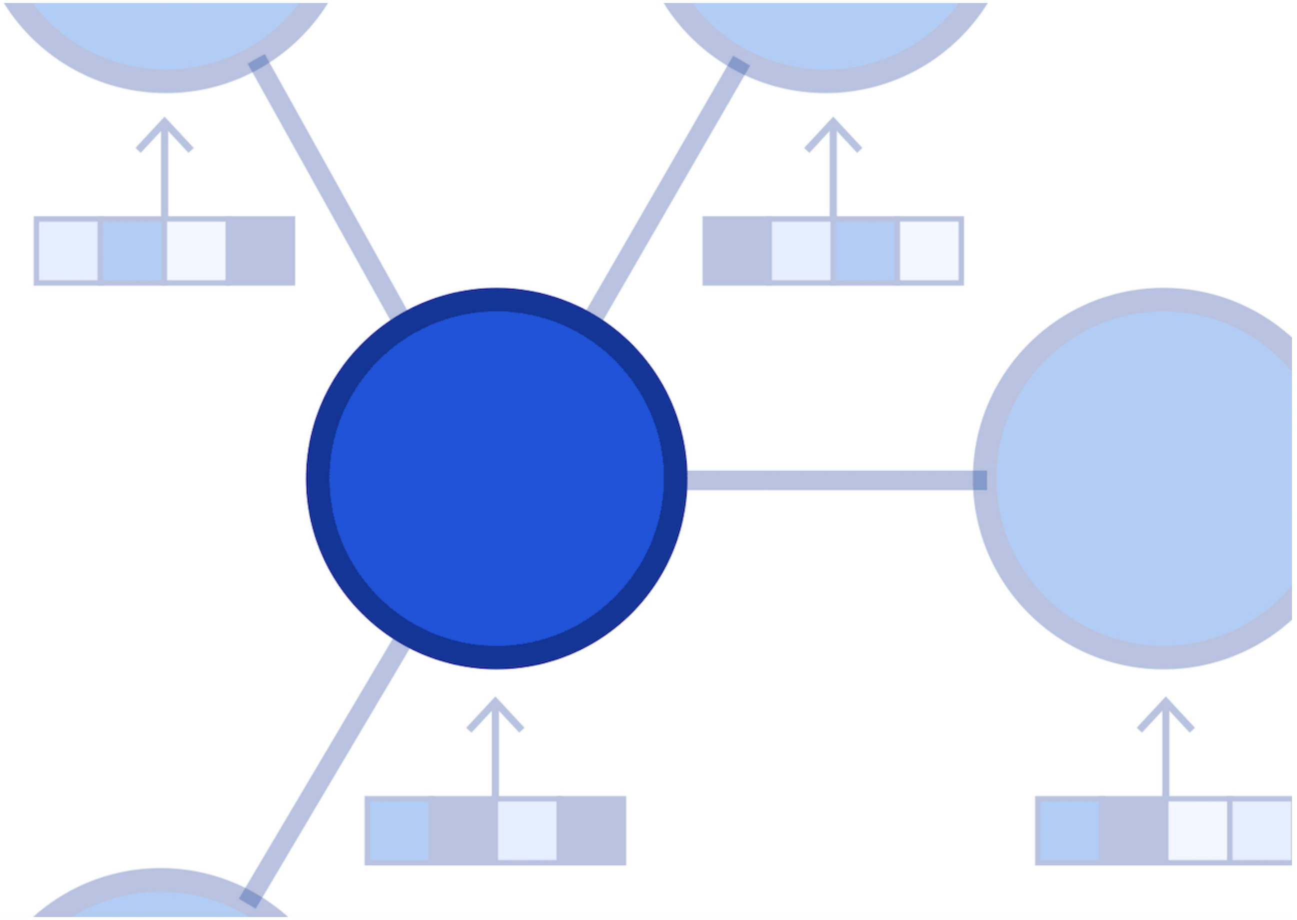

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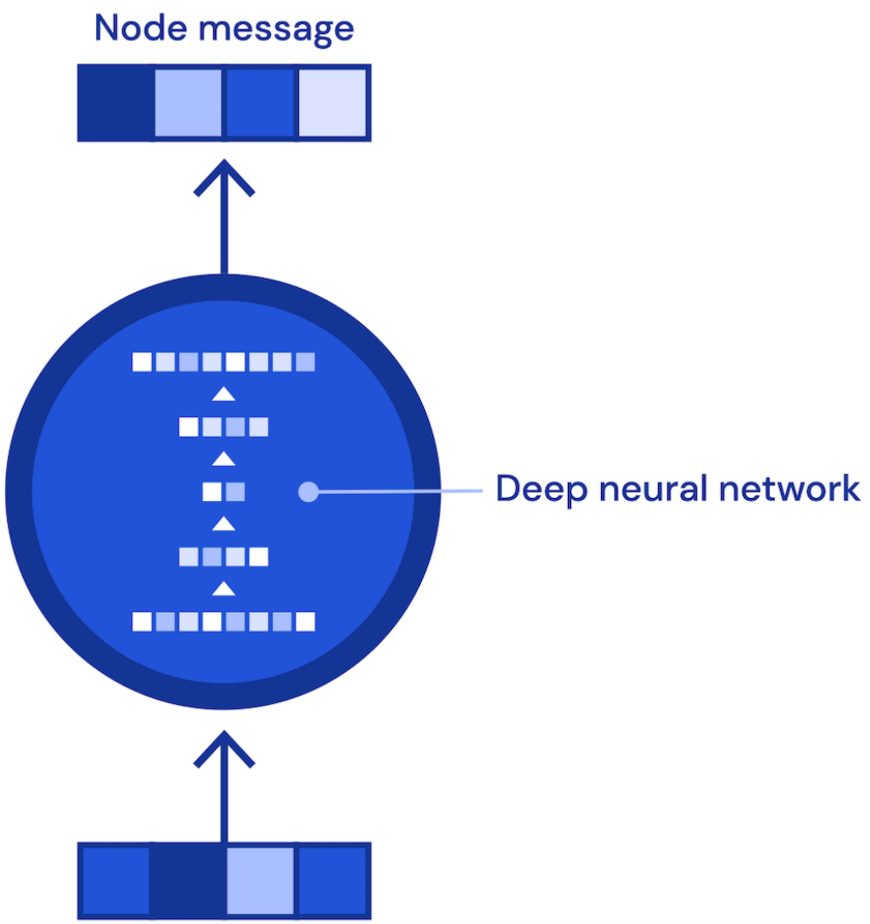

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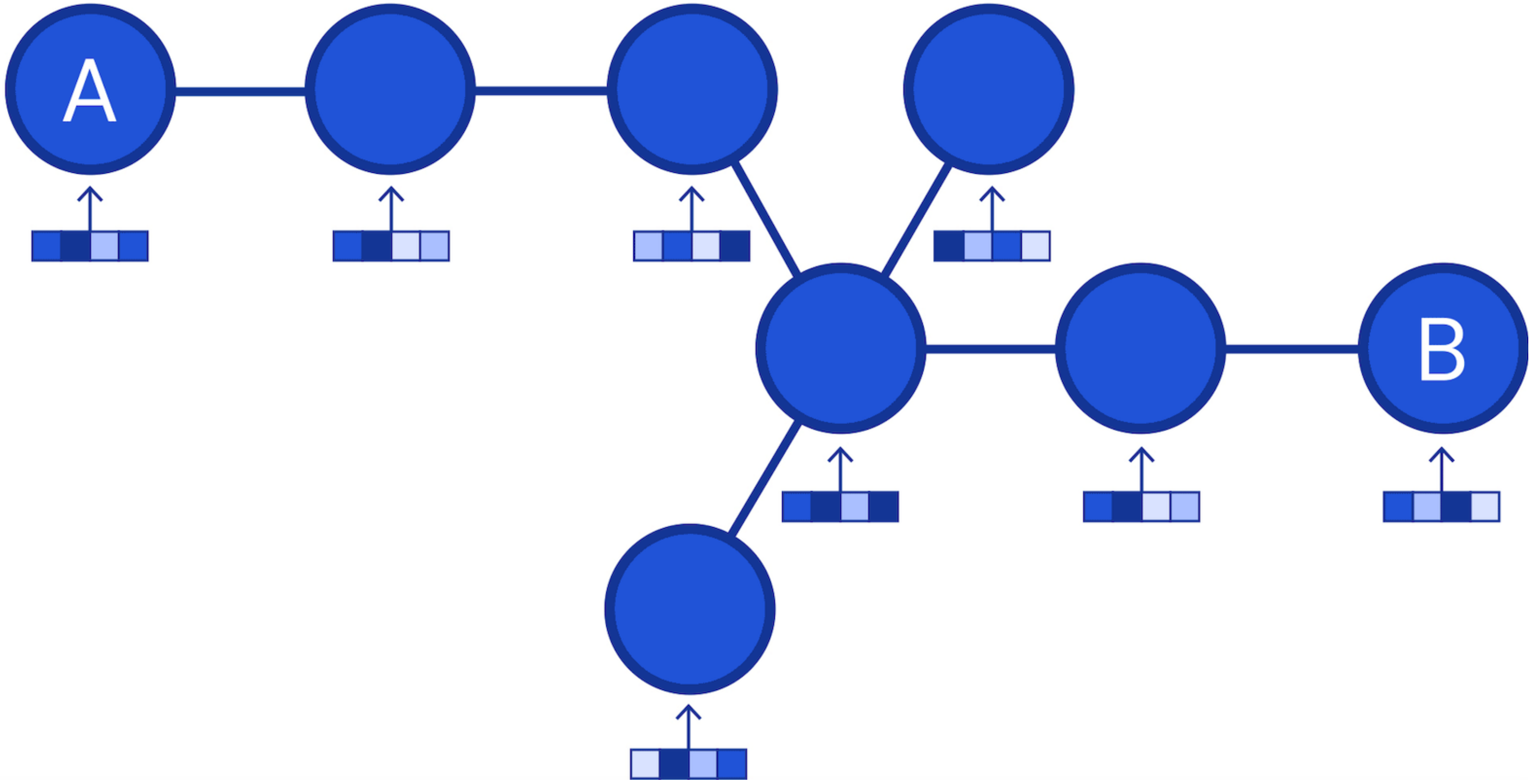

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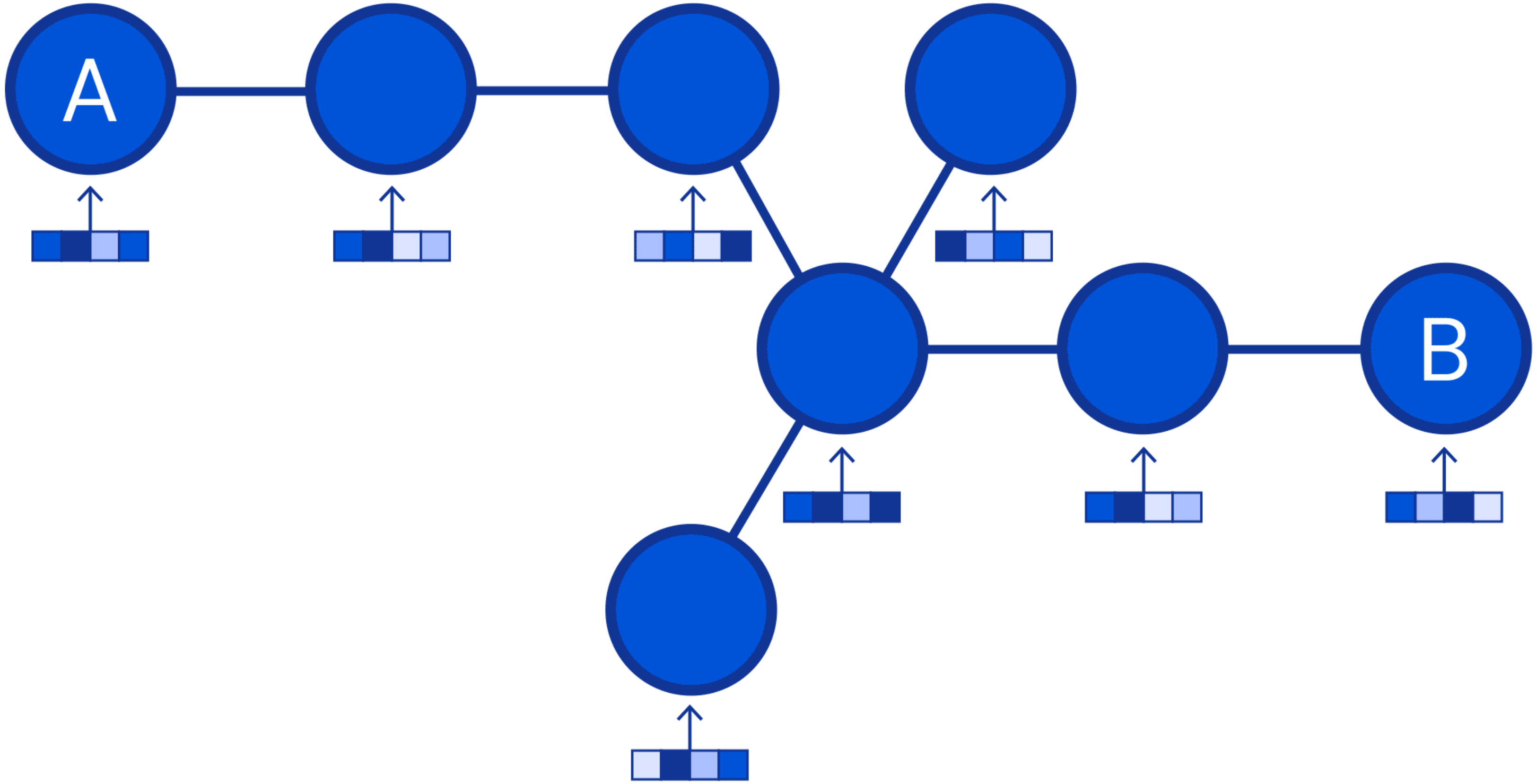

https://www.deepmind.com/blog/traffic-prediction-with-advanced-graph-neural-networks

Encoding neighborhoods: General form

$\boldsymbol{h}_u^{(0)} = \boldsymbol{x}_u$ (feature representation for node u)

In each round $k \in [K]$, for each node v:

1. **Aggregate** over neighbors

$$\boldsymbol{m}_{N(v)}^{(k)} = \text{AGGREGATE}^{(k)}\left(\left\{\boldsymbol{h}_u^{(k-1)}: u \in N(v)\right\}\right)$$

Neighborhood of v

Encoding neighborhoods: General form

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2. **Update** current node representation

$$\boldsymbol{h}_v^{(k)} = \text{COMBINE}^{(k)}\left(\boldsymbol{h}_v^{(k-1)}, \boldsymbol{m}_{N(v)}^{(k)}\right)$$

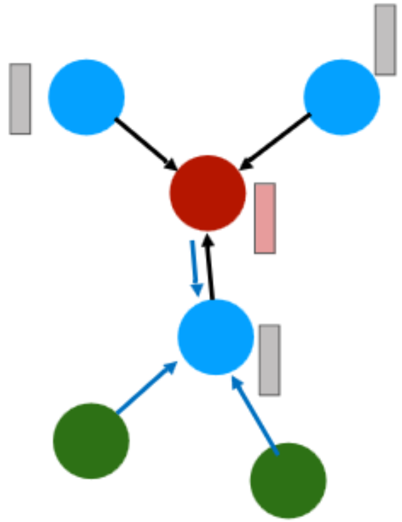
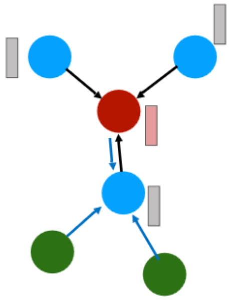


Figure by Jegelka

The basic GNN

[Merkwirth and Lengauer ‘05; Scarselli et al. ‘09]



$$\boldsymbol{m}_{N(v)} = \mathrm{AGGREGATE}(\{\boldsymbol{h}_u : u \in N(v)\}) = \sum_{u \in N(v)} \boldsymbol{h}_u$$

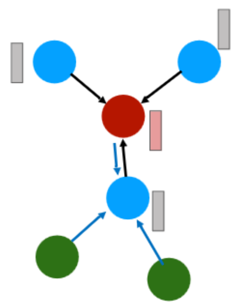
$$\mathrm{COMBINE}\left(\boldsymbol{h}_v, \boldsymbol{m}_{N(v)}\right) = \sigma\left(W_{\mathrm{self}} \boldsymbol{h}_v + W_{\mathrm{neigh}} \boldsymbol{m}_{N(v)} + \boldsymbol{b}\right)$$

Trainable parameters

Non-linearity (e.g., tanh or ReLU)

Figure by Jegelka

Aggregation functions

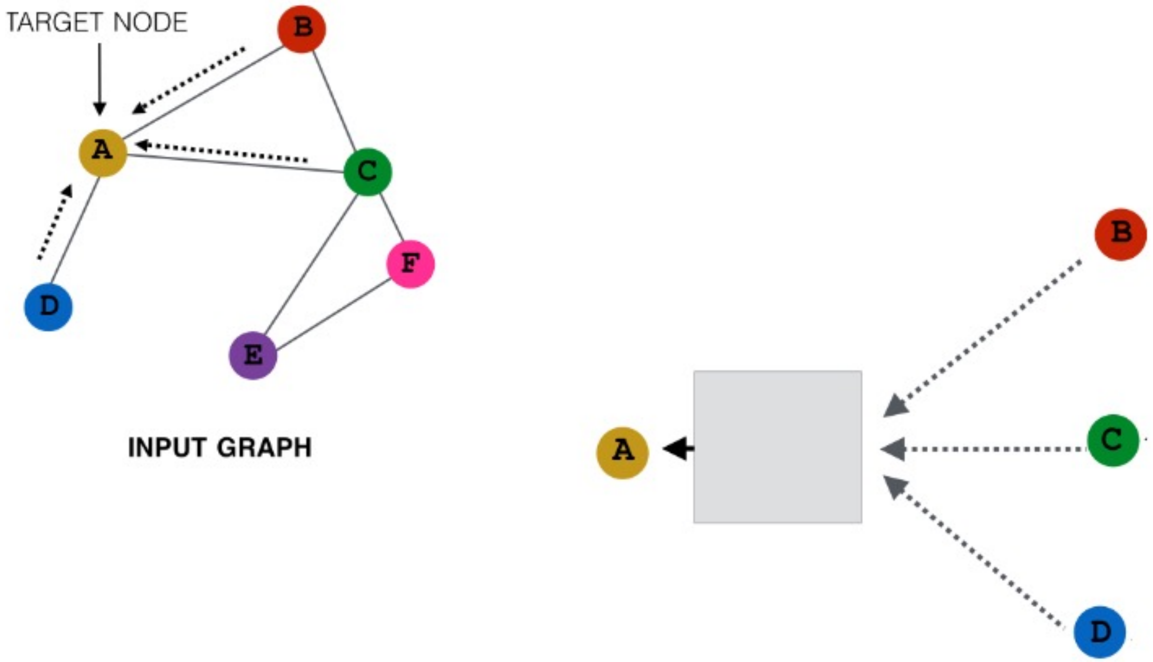


$$\boldsymbol{m}_{N(v)} = \text{AGGREGATE}(\{\boldsymbol{h}_u : u \in N(v)\}) = \bigoplus_{u \in N(v)} \boldsymbol{h}_u$$

Other element-wise aggregators, e.g.:
Maximization, averaging

Figure by Jegelka

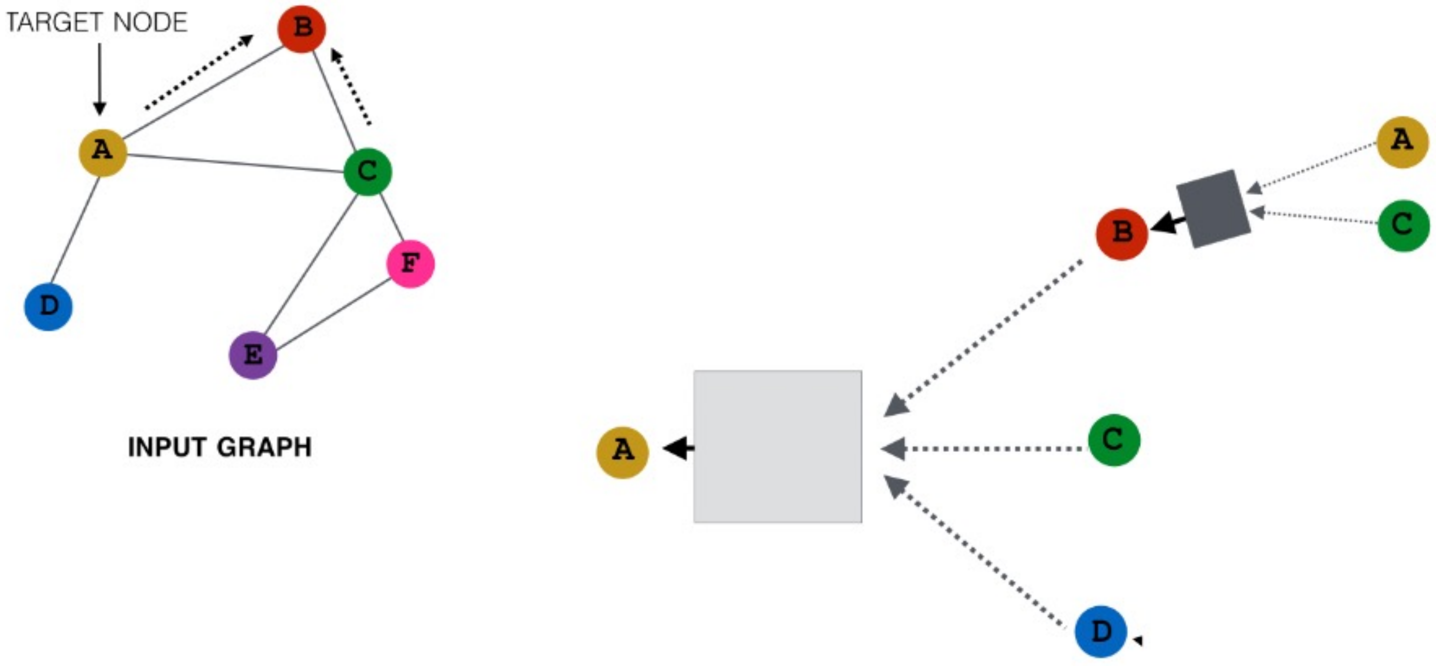
Node embeddings unrolled



Grey boxes: aggregation functions that we learn

Figures by Leskovec

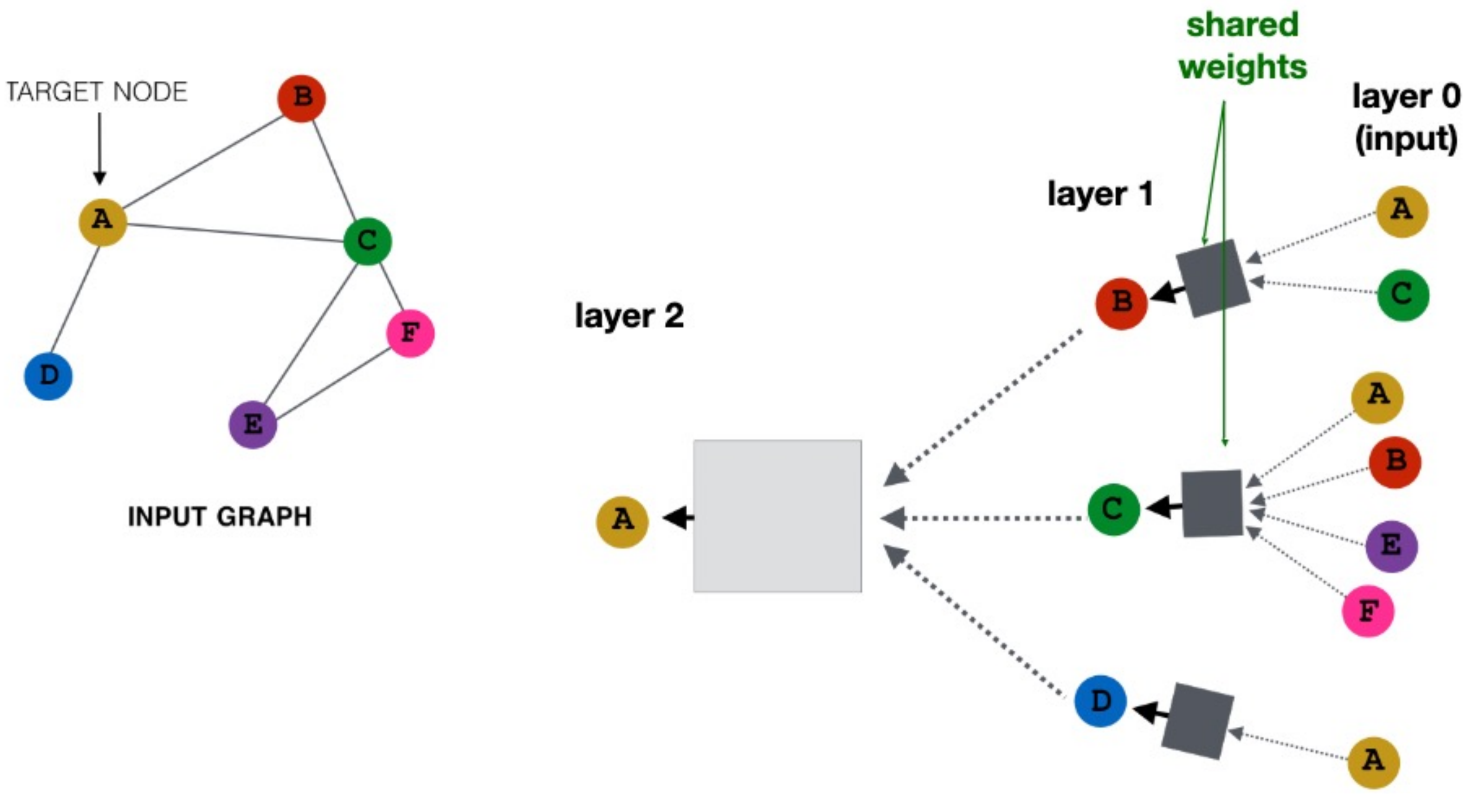
Node embeddings unrolled



Grey boxes: aggregation functions that we learn

Figures by Leskovec

Node embeddings unrolled

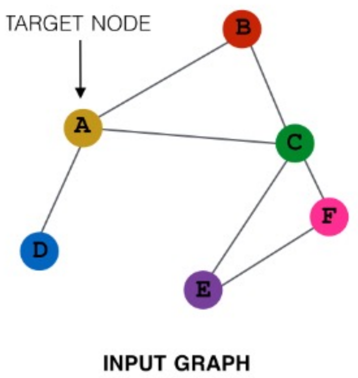


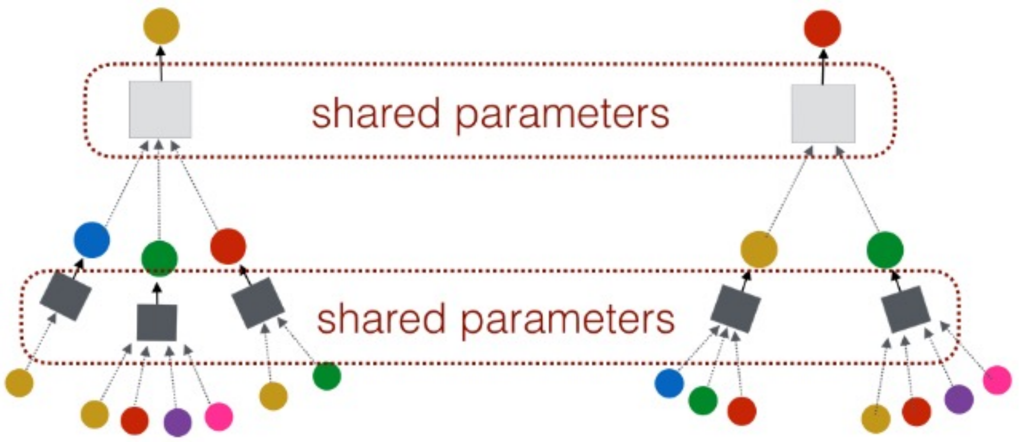
Grey boxes: aggregation functions that we learn

Figures by Leskovec

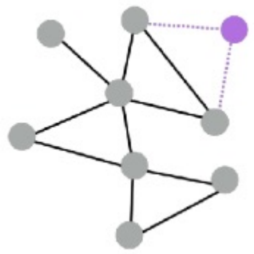
Weight sharing

Use the same aggregation functions for all nodes





Can generate encodings for previously unseen nodes & graphs!



Figures by Leskovec

Next time

1. Neural algorithmic alignment
   GNNs for discrete optimization

2. Reinforcement learning overview

3. Learning greedy heuristics with RL

4. Integer programming with GNNs

Machine learning for algorithm design:
Theoretical guarantees and applied frontiers

Part 3

Ellen Vitercik
Stanford University

Outline (applied techniques)

1. **GNNs overview (recap)**
2. Neural algorithmic alignment
3. Reinforcement learning overview
4. Learning greedy heuristics with RL
5. Integer programming with GNNs

Graph neural networks: Objective

Idea:

1. Encode each node and its neighborhood with embedding
2. Aggregate set of node embeddings into graph embedding
3. Use embeddings to make predictions

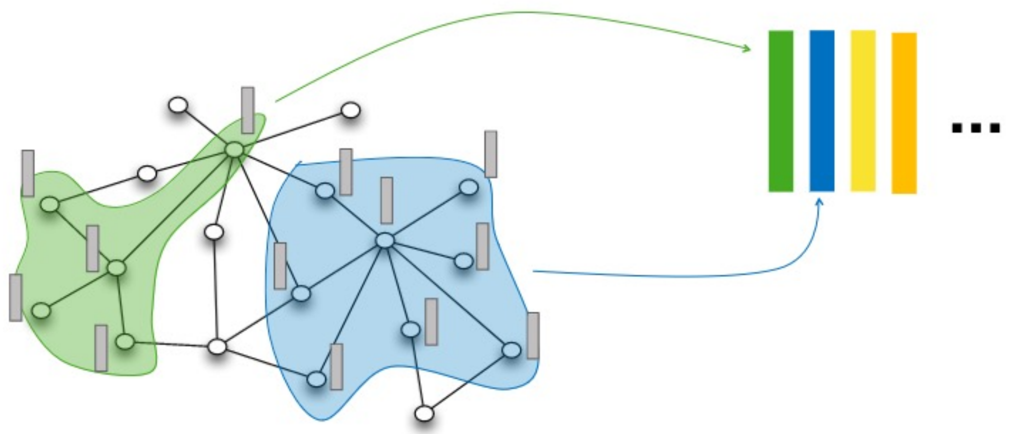


Figure by Jegelka

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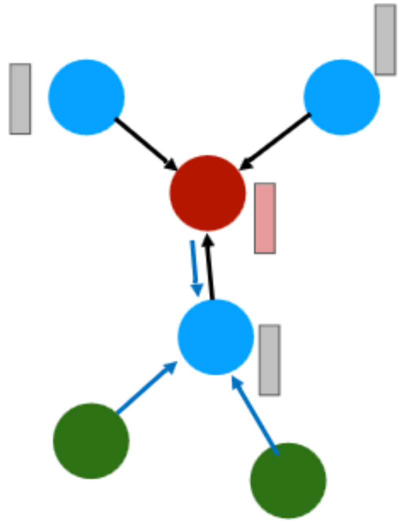


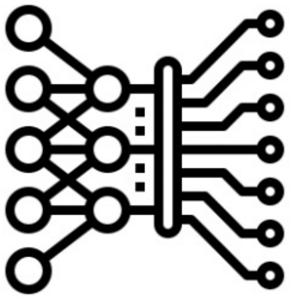
Figure by Jegelka

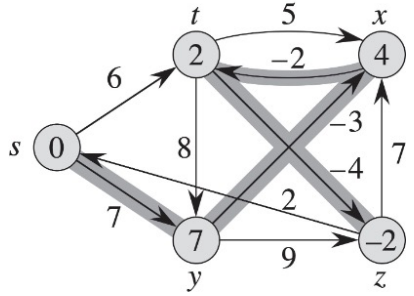
Outline (applied techniques)

1. GNNs overview
2. **Neural algorithmic alignment**
3. Reinforcement learning overview
4. Learning greedy heuristics with RL
5. Integer programming with GNNs

Veličković, Ying, Padovano, Hadsell, Blundell, ICLR'20
Cappart, Chételat, Khalil, Lodi, Morris, Veličković, arXiv'21

Problem-solving approaches





+ Operate on raw inputs
+ Generalize on noisy conditions
+ Models reusable across tasks
- Require big data
- Unreliable when extrapolating
- Lack of interpretability

+ Trivially strong generalization
+ Compositional (subroutines)
+ Guaranteed correctness
+ Interpretable operations
- Input must match spec
- Not robust to task variations

Is it possible to get the best of both worlds?

Slide by Veličković

Previous work

Previous work:

- Shortest path [Graves et al. '16; Xu et al., '19]
- Traveling salesman [Reed and De Freitas '15]
- Boolean satisfiability [Vinyals et al. '15; Bello et al., '16; …]
- Probabilistic inference [Yoon et al., '18]

Ground-truth solutions used to drive learning

Model has **complete freedom** mapping raw inputs to solutions

Neural graph algorithm execution

Key observation: Many algorithms share related **subroutines**

E.g. Bellman-Ford,BFS enumerate sets of edges adjacent to a node

Neural graph algorithm execution

- Learn several algorithms **simultaneously**
- Provide intermediate supervision signals

  Driven by how a known classical algorithm would process the input

Veličković, Ying, Padovano, Hadsell, Blundell, ICLR'20

Outline (applied techniques)

1. GNNs overview
2. Neural algorithmic alignment
    i. **Example algorithms**
    ii. Experiments
    iii. Additional motivation
    iv. Additional research
3. Reinforcement learning overview
4. Learning greedy heuristics with RL
5. Integer programming with GNNs

Breadth-first search

- Source node s
- Initial input $x_i^{(1)} = \begin{cases} 1 & \text{if } i = s \\ 0 & \text{if } i \neq s \end{cases}$
- Node is reachable from s if any of its neighbors are reachable:

$$x_i^{(t+1)} = \begin{cases} 1 & \text{if } x_i^{(t)} = 1 \\ 1 & \text{if } \exists j \text{ s.t. } (j, i) \in E \text{ and } x_j^{(t)} = 1 \\ 0 & \text{else} \end{cases}$$

- Algorithm output at round t: $y_i^{(t)} = x_i^{(t+1)}$

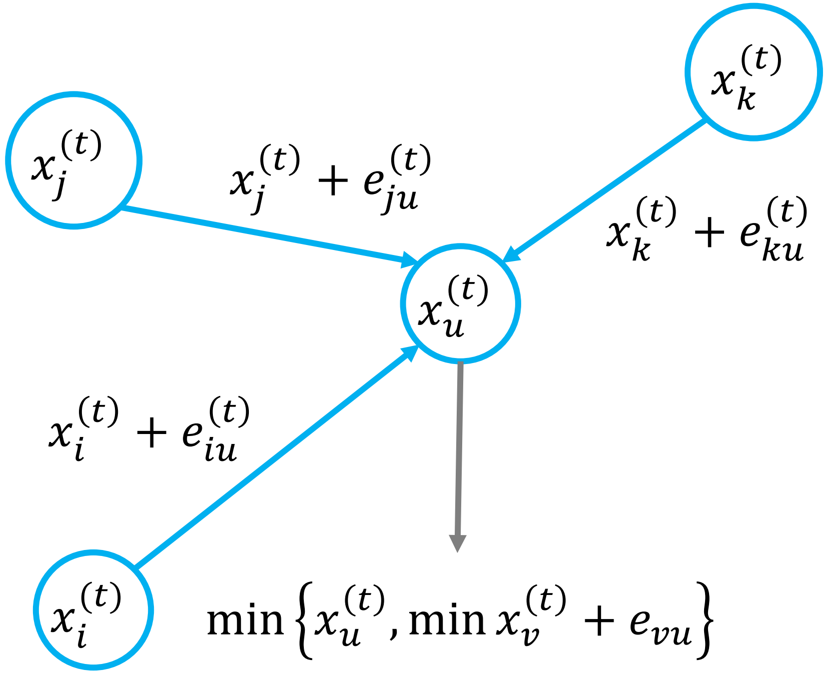
Bellman-Ford (shortest path)

- Source node s
- Initial input $x_i^{(1)} = \begin{cases} 0 & \text{if } i = s \\ \infty & \text{if } i \neq s \end{cases}$
- Node is reachable from s if any of its neighbors are reachable

  Update distance to node as minimal way to reach neighbors

$$x_i^{(t+1)} = \min\left\{x_i^{(t)}, \min_{(j,i)\in E} x_j^{(t)} + e_{ji}^{(t)}\right\}$$

Bellman-Ford: Message passing



Key idea (roughly speaking): Train GNN so that $\boldsymbol{h}_u^{(t)} \approx x_u^{(t)}, \forall t$

(Really, so that a function of $\boldsymbol{h}_u^{(t)} \approx x_u^{(t)}$)

Veličković, Ying, Padovano, Hadsell, Blundell, ICLR'20

Outline (applied techniques)

1. GNNs overview
2. Neural algorithmic alignment
   1. Example algorithms
   2. **Experiments**
   3. Additional motivation
   4. Additional research
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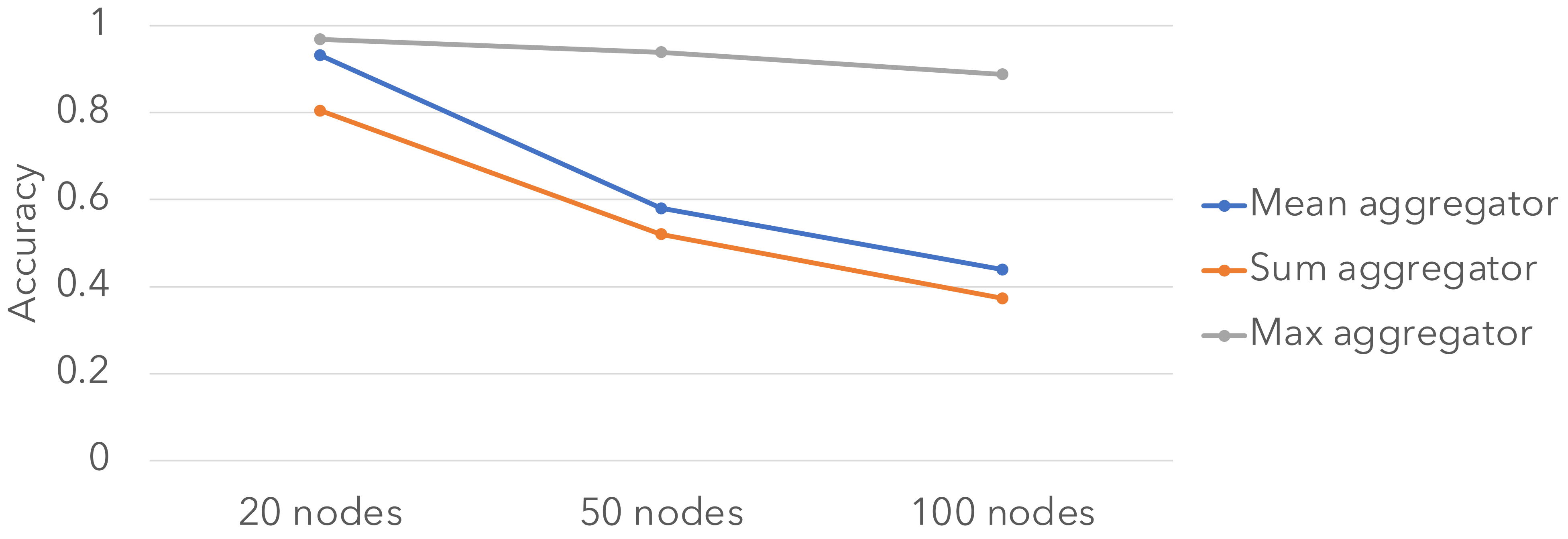
Shortest-path predecessor prediction



Improvement of max-aggregator increases with size

It **aligns** better with underlying algorithm [Xu et al., ICLR'20]

Veličković, Ying, Padovano, Hadsell, Blundell, ICLR'20

Learning multiple algorithms

Learn to execute both BFS and Bellman-Ford **simultaneously**

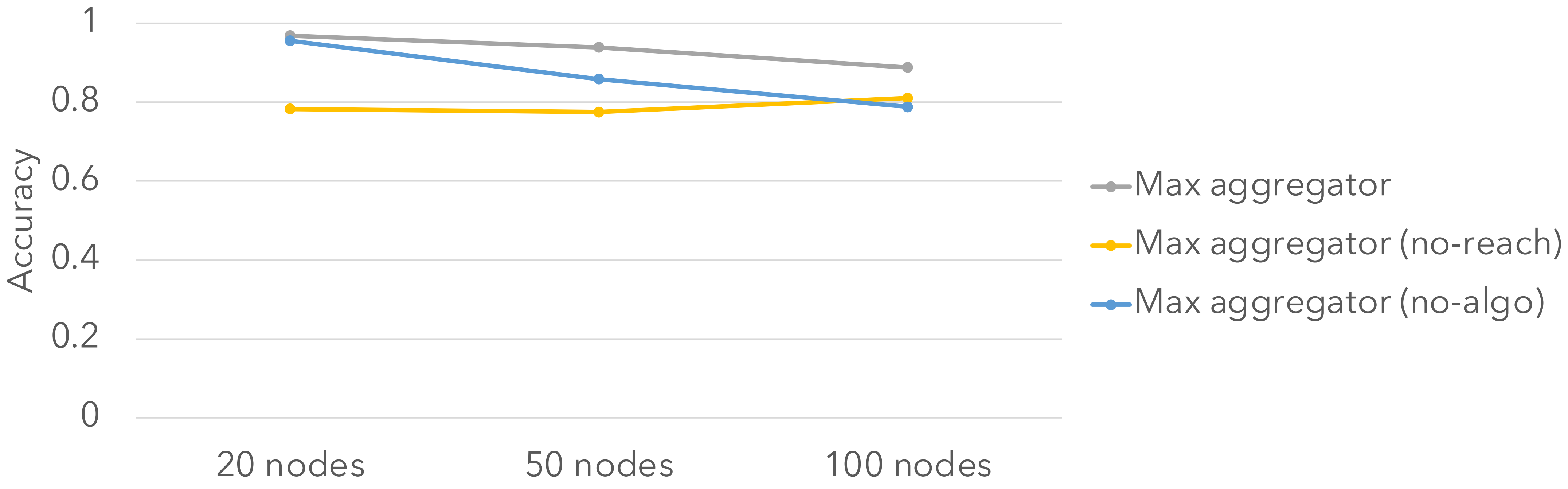
- At each step t, concatenate relevant $x_i^{(t)}$ and $\boldsymbol{y}_i^{(t)}$ values

Comparisons

- *(no-reach):* Learn Bellman-Ford alone
  - Doesn't simultaneously learn reachability
- *(no-algo):*
  - Don't supervise intermediate steps
  - Learn predecessors directly from input $x_i^{(1)}$

Veličković, Ying, Padovano, Hadsell, Blundell, ICLR'20

Shortest-path predecessor prediction



- **(no-reach) results**: positive knowledge transfer
- **(no-algo) results**: benefit of supervising intermediate steps

Veličković, Ying, Padovano, Hadsell, Blundell, ICLR'20

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Key question

Key question in neural algorithmic alignment:

If we're just teaching a NN to **imitate** a classical algorithm…

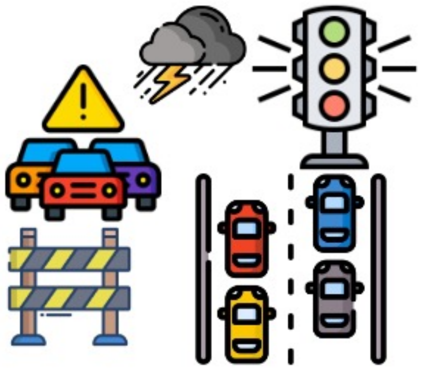
Why not just run that algorithm?

Why use GNNs for algorithm design?

Classical algorithms are designed with **abstraction** in mind

Enforce their inputs to conform to stringent preconditions

However, we design algorithms to solve **real-world** problems!

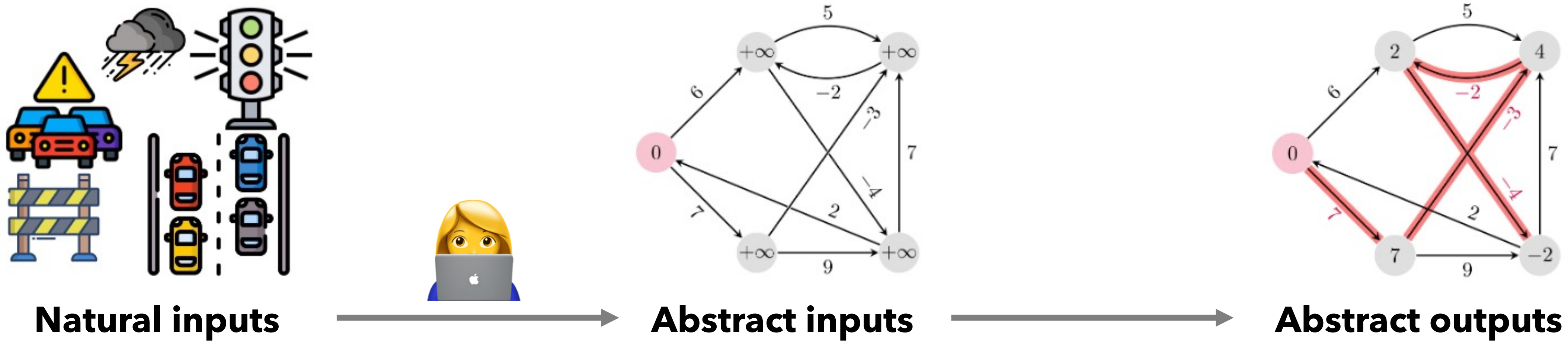


Natural inputs

Slide by Veličković

Abstractifying the core problem

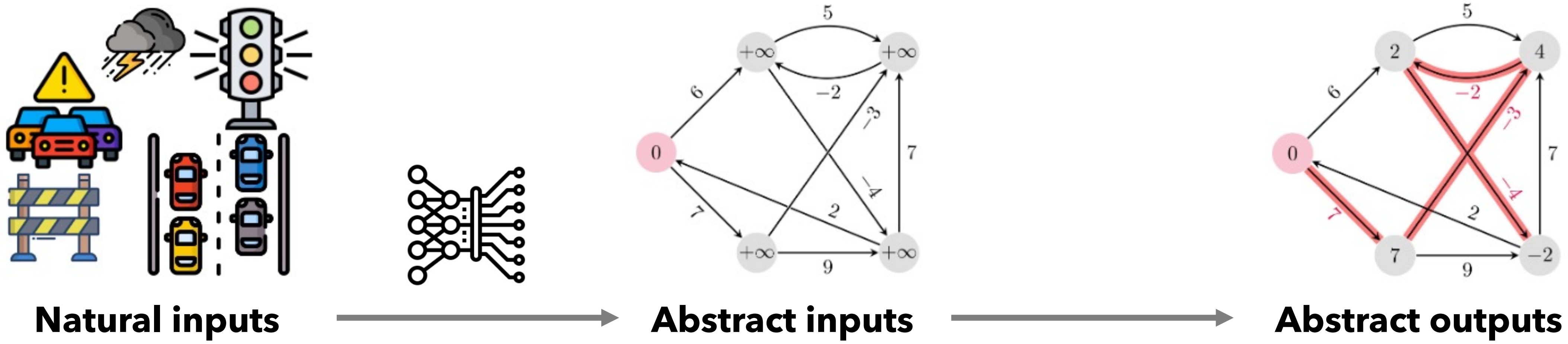
- Assume we have real-world inputs
  ...but algorithm only admits abstract inputs
- Could try **manually** converting from one input to another



Slide by Veličković

Attacking the core problem

- Alternatively, **replace** human feature extractor with NN
  - Still apply same combinatorial algorithm
- Issue: algorithms typically perform **discrete optimization**
  - Doesn't play nicely with **gradient-based** optimization of NNs



Slide by Veličković

Algorithmic bottleneck

Second (more fundamental) issue: **data efficiency**

- Real-world data is often incredibly rich
- We still have to compress it down to scalar values

The algorithmic solver commits to using this scalar

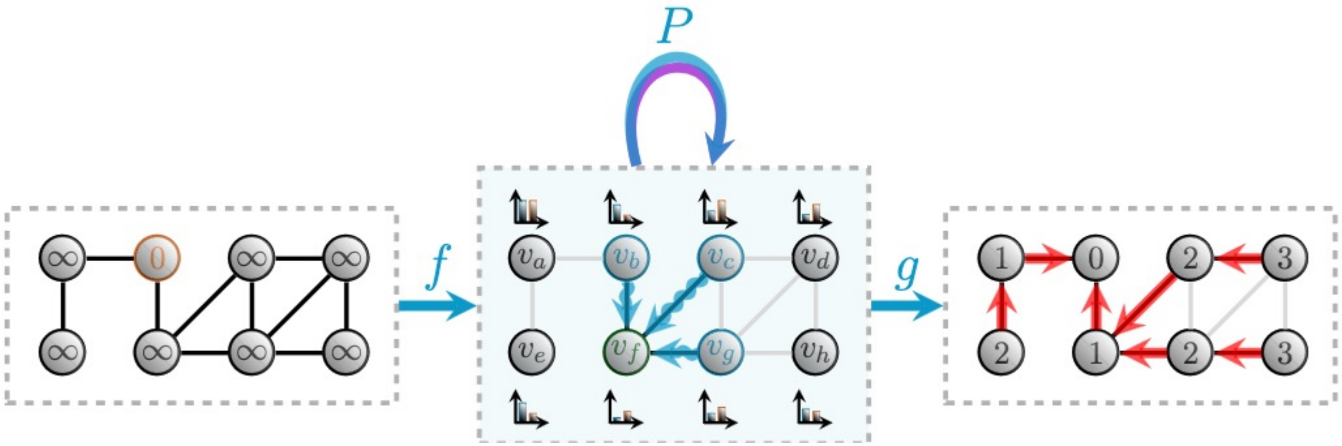
Assumes it is perfect!

If there's insufficient training data to estimate the scalars:

- Alg will give a **perfect solution**
- …but in a **suboptimal environment**

Neural algorithmic pipeline

Input $\boldsymbol{x}^{(1)}$



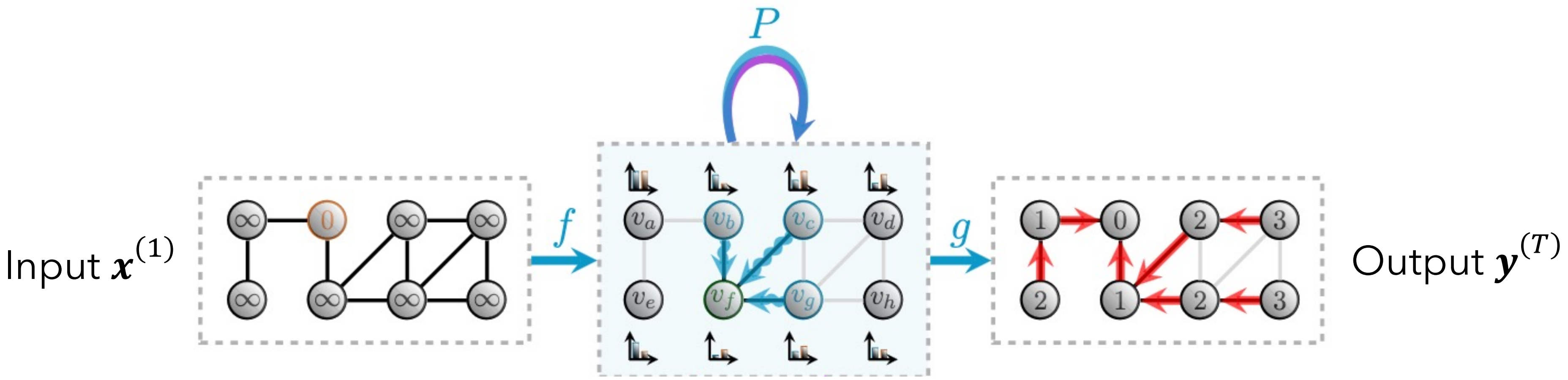
Output $\boldsymbol{y}^{(T)}$

Encoder network f

- E.g., makes sure input is in correct dimension for next step

Veličković, Ying, Padovano, Hadsell, Blundell, ICLR'20; Figure by Cappart et al.

Neural algorithmic pipeline

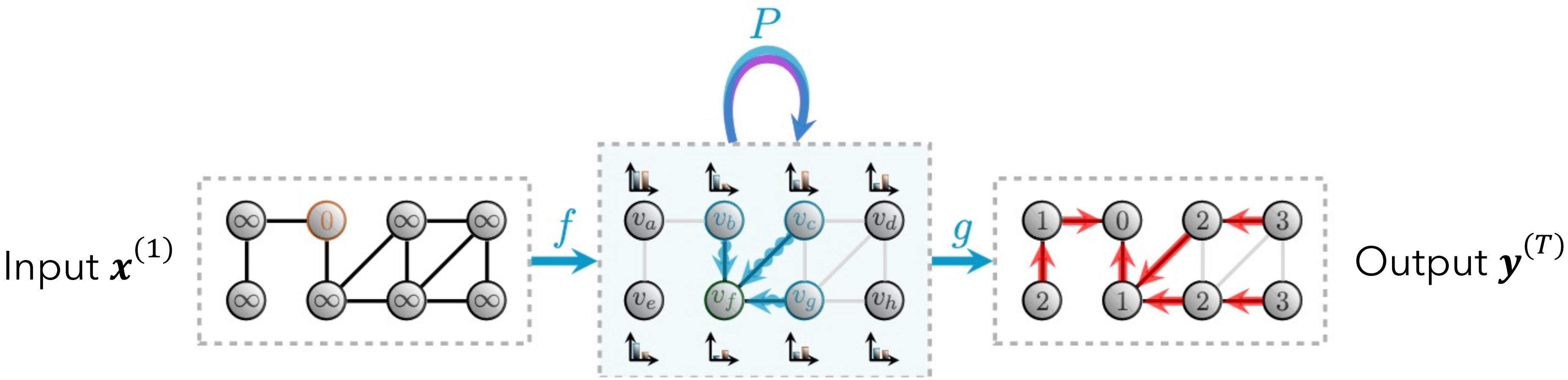


Processor network *P*

- Graph neural network
- Run multiple times (termination determined by a NN)

Veličković, Ying, Padovano, Hadsell, Blundell, ICLR'20; Figure by Cappart et al.

Neural algorithmic pipeline

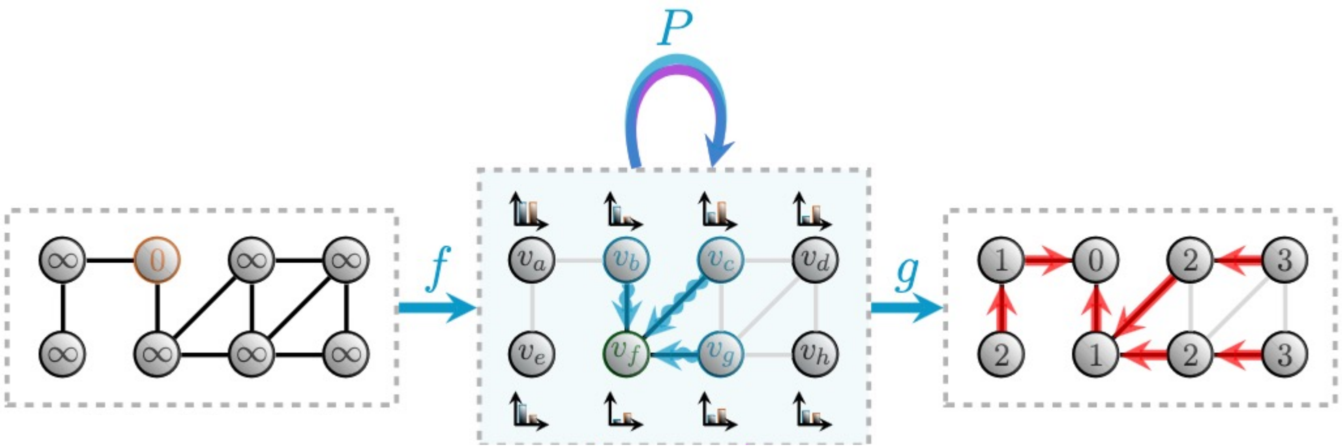


Decoder network *g*

- Transform's GNNs output into algorithmic output

Neural algorithmic pipeline

Abstract inputs $\bar{x}$



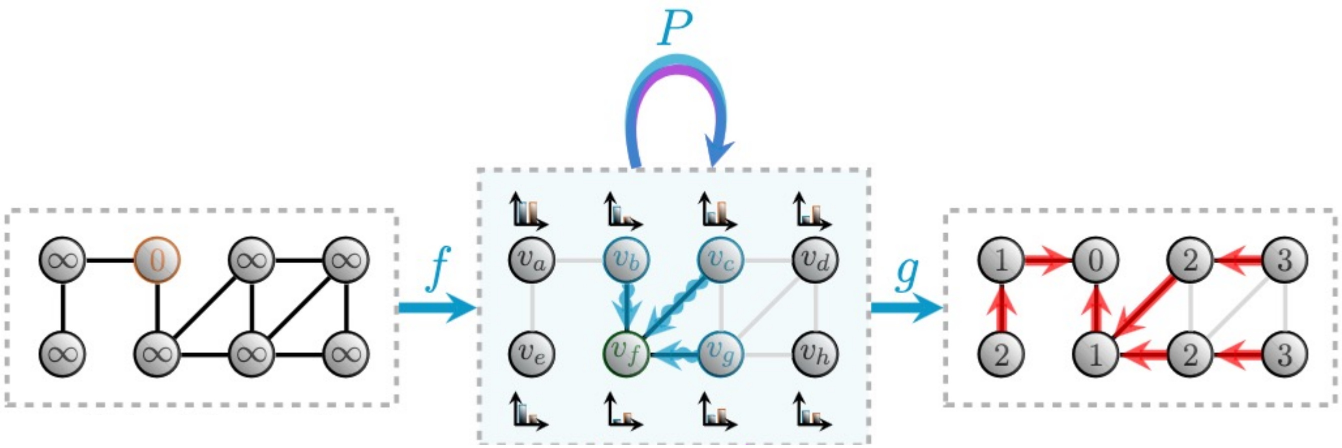
Abstract outputs
$\bar{y} \approx g\left(P\left(f(x)\right)\right)$

1. On abstract inputs, learn encode-process-decode functions

Figure by Cappart et al.

Neural algorithmic pipeline

Abstract inputs $\bar{x}$



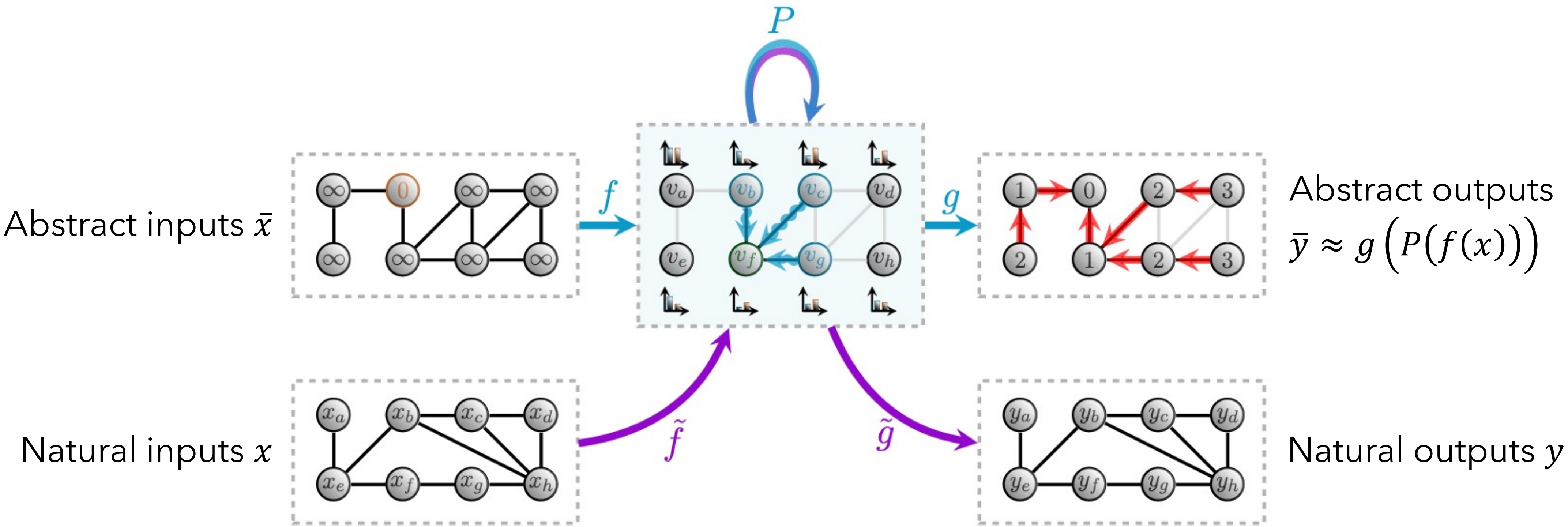
Abstract outputs
$\bar{y} \approx g\left(P\left(f(x)\right)\right)$

After training on abstract inputs, processor P:

1. Is aligned with computations of target algorithm
2. Admits useful gradients
3. Operates over high-dim latent space (better use of data)

Figure by Cappart et al.

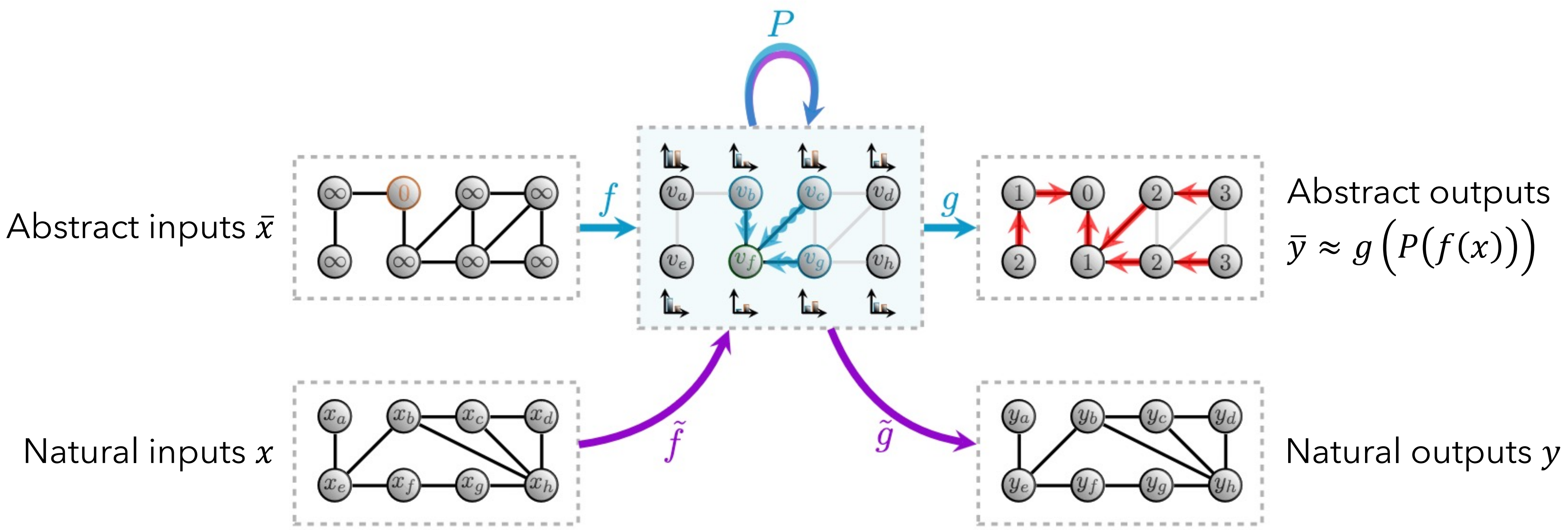
Neural algorithmic pipeline



2. Set up encode-decode functions for natural inputs/outputs

Figure by Cappart et al.

Neural algorithmic pipeline



3. Learn parameters using loss that compares $\tilde{g}\left(P\left(\tilde{f}(x)\right)\right)$ to y

Figure by Cappart et al.

Outline (applied techniques)

1. GNNs overview
2. Neural algorithmic alignment
   i. Example algorithms
   ii. Experiments
   iii. Additional motivation
   iv. Additional research
3. Reinforcement learning overview
4. Learning greedy heuristics with RL
5. Integer programming with GNNs

Additional research

Lots of research in the past few years! E.g.:

- How to achieve **algorithmic alignment** & **theory guarantees**
  - Xu et al., ICLR'20; Dudzik, Veličković, NeurIPS'22
- **CLRS** benchmark
  - Sorting, searching, dynamic programming, graph algorithms, etc.
  - Veličković et al. ICML'22; Ibarz et al. LoG'22; Bevilacqua et al. ICML'23
- **Primal-dual** algorithms
  - Numeroso et al., ICLR'23

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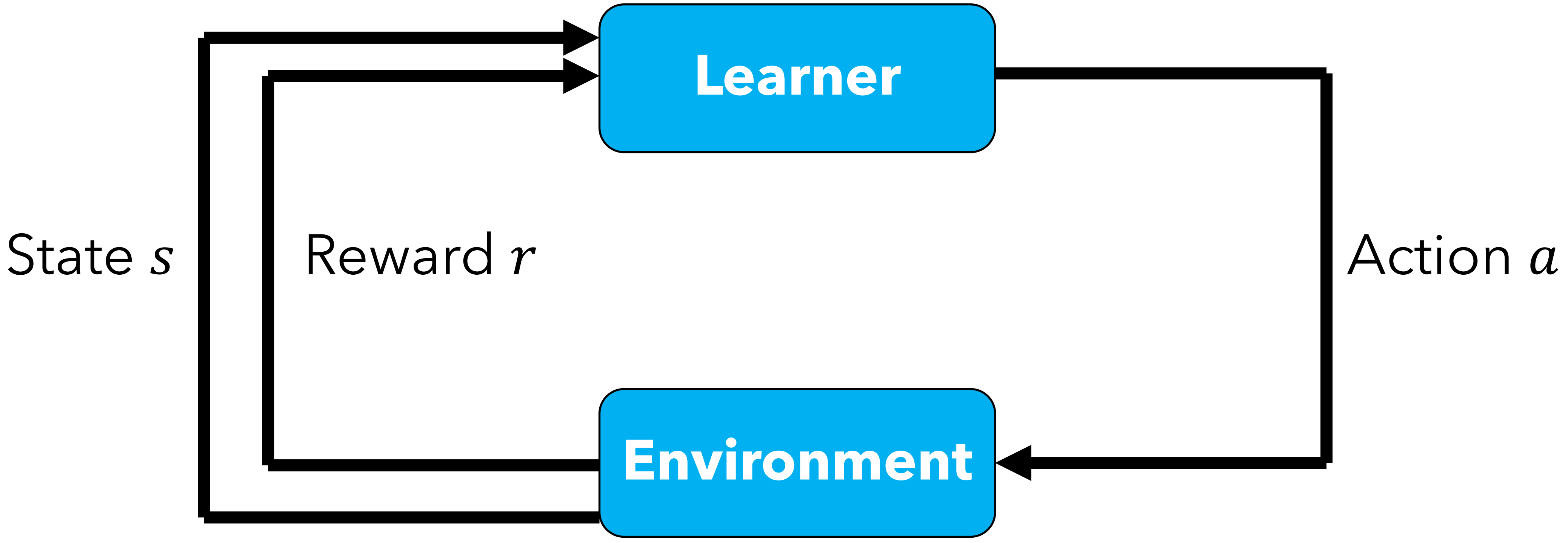
Learner interaction with environment



Slide by Kolter

Markov decision processes

S: set of states (assumed for now to be discrete)

A: set of actions

Transition probability distribution $P(s' \mid s, a)$

Probability of entering state s' from state s after taking action a

Reward function $R: S \to \mathbb{R}$

Goal: Policy $\pi: S \to A$ that maximizes total (discounted) reward

Slide by Kolter

Policies and value functions

Policy is a mapping from states to actions $\pi: S \to A$

Value function for a policy:

Expected sum of discounted rewards

$$V^\pi(s) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t R(s_t) \mid s_0 = s, a_t = \pi(s_t), s_{t+1}|s_t, a_t \sim P\right]$$

Discount factor

Slide by Kolter

Optimal policy and value function

Optimal policy $\pi^\star$ achieves the highest value for every state

$$V^{\pi^\star}(s) = \max_\pi V^\pi(s)$$

Value function is written $V^\star = V^{\pi^\star}$

Several different ways to find $\pi^\star$

- Value iteration
- Policy iteration

Slide by Kolter

Challenge of RL

MDP (S, A, P, R):

- S: set of states (assumed for now to be discrete)
- A: set of actions
- Transition probability distribution $P(s_{t+1} \mid s_t, a_t)$
- Reward function $R: S \rightarrow \mathbb{R}$

RL twist: We don't know P or R, or too big to enumerate

Q-learning

Q functions:

Like value functions but defined over state-action pairs

$$Q^{\pi}(s,a) = R(s) + \gamma \sum_{s' \in S} P(s' \mid s, a) Q^{\pi}\big(s', \pi(s')\big)$$

I.e., Q function is the value of:

1. Starting in state s
2. Taking action a
3. Then acting according to π

Slide by Kolter

Q-learning

$$Q^\star(s,a) = R(s) + \gamma \sum_{s' \in S} P(s' \mid s,a) \max_{a'} Q^\star(s',a')$$
$$= R(s) + \gamma \sum_{s' \in S} P(s' \mid s,a) V^\star(s')$$

$Q^\star$ is the value of:

1. Starting in state s
2. Taking action a
3. Then acting optimally

Slide by Kolter

Q-learning

(High-level) Q-learning algorithm

initialize $\hat{Q}(s, a) \leftarrow 0, \forall s, a$

repeat

Observe current state s and reward r

Take action $a = \operatorname{argmax} \hat{Q}(s, \cdot)$ and observe next state s'

Improve estimate $\hat{Q}$ based on s, r, a, s'

Can use *function approximation* to represent $\hat{Q}$ compactly

$$\hat{Q}(s, a) = f_\theta(s, a)$$

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Dai, Khalil, Zhang, Dilkina, Song; NeurIPS'17

RL for combinatorial optimization

Tons of research in this area

Travelling salesman

Bello et al., ICLR'17; Dai et al., NeurIPS'17; Nazari et al., NeurIPS'18; …

Bin packing

Hu et al., '17; Laterre et al., '18; Cai et al., DRL4KDD'19; Li et al., '20; …

Maximum cut

Dai et al., NeurIPS'17; Cappart et al., AAAI'19; Barrett et al., AAAI'20; …

Minimum vertex cover

Dai et al., NeurIPS'17; Song et al., UAI'19; …

This section: Example of a pioneering work in this space

Overview

Goal: use RL to learn new *greedy strategies* for graph problems

Feasible solution constructed by successively adding nodes to solution

Input: Graph $G = (V, E)$, weights $w(u, v)$ for $(u, v) \in E$

RL state representation: Graph embedding

Dai, Khalil, et al.; NeurIPS'17

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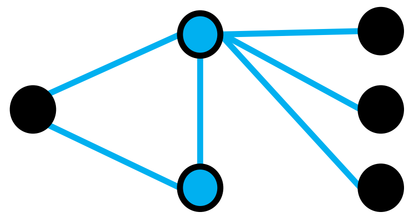
Minimum vertex cover

Find smallest vertex subset such that each edge is covered

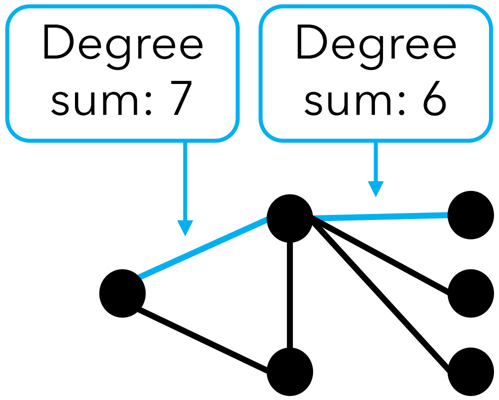


Minimum vertex cover

Find smallest vertex subset such that each edge is covered

2-approximation:

Greedily add vertices of edge with **maximum degree sum**



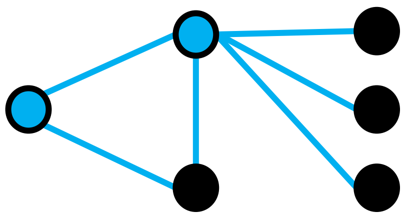
Minimum vertex cover

Find smallest vertex subset such that each edge is covered

2-approximation:

Greedily add vertices of edge with **maximum degree sum**

Scoring function that guides greedy algorithm



Maximum cut

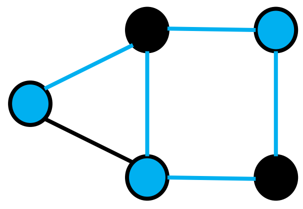
Find partition $(S, V \setminus S)$ of nodes that maximizes

$$\sum_{(u,v)\in C} w(u,v)$$

where $C = \{(u,v) \in E : u \in S, v \notin S\}$

If $w(u,v) = 1$ for all $(u,v) \in E$:

$$\sum_{(u,v)\in C} w(u,v) = 5$$



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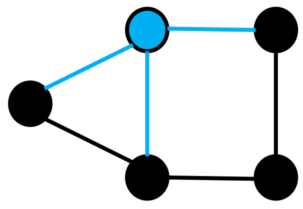
Greedy: move node from one side of cut to the other

Move node that results in the largest improvement in cut weight



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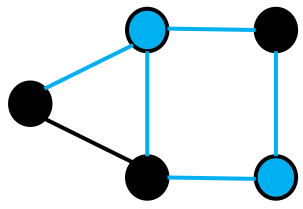

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Reinforcement learning formulation

State:

- *Goal:* encode partial solution $S = (v_1, v_2, \dots, v_{|S|}), v_i \in V$

E.g., nodes in independent set, nodes on one side of cut

Dai, Khalil, et al.; NeurIPS'17

Reinforcement learning formulation

State:

- *Goal:* encode partial solution $S = (v_1, v_2, \dots, v_{|S|}), v_i \in V$
- Use GNN to compute graph embedding $\boldsymbol{\mu}$

Initial node features $x_v = \begin{cases} 1 & \text{if } v \in S \\ 0 & \text{else} \end{cases}$

Action: Choose vertex $v \in V \setminus S$ to add to solution

Transition (deterministic): For chosen $v \in V \setminus S$, set $x_v = 1$

Dai, Khalil, et al.; NeurIPS'17

Reinforcement learning formulation

Reward: $r(S, v)$ is change in objective when transition $S \rightarrow (S, v)$

Policy (deterministic): $\pi(v|S) = \begin{cases} 1 & \text{if } v = \operatorname{argmax}_{v' \notin S} \hat{Q}(\boldsymbol{\mu}, v') \\ 0 & \text{else} \end{cases}$

Dai, Khalil, et al.; NeurIPS'17

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Min vertex cover

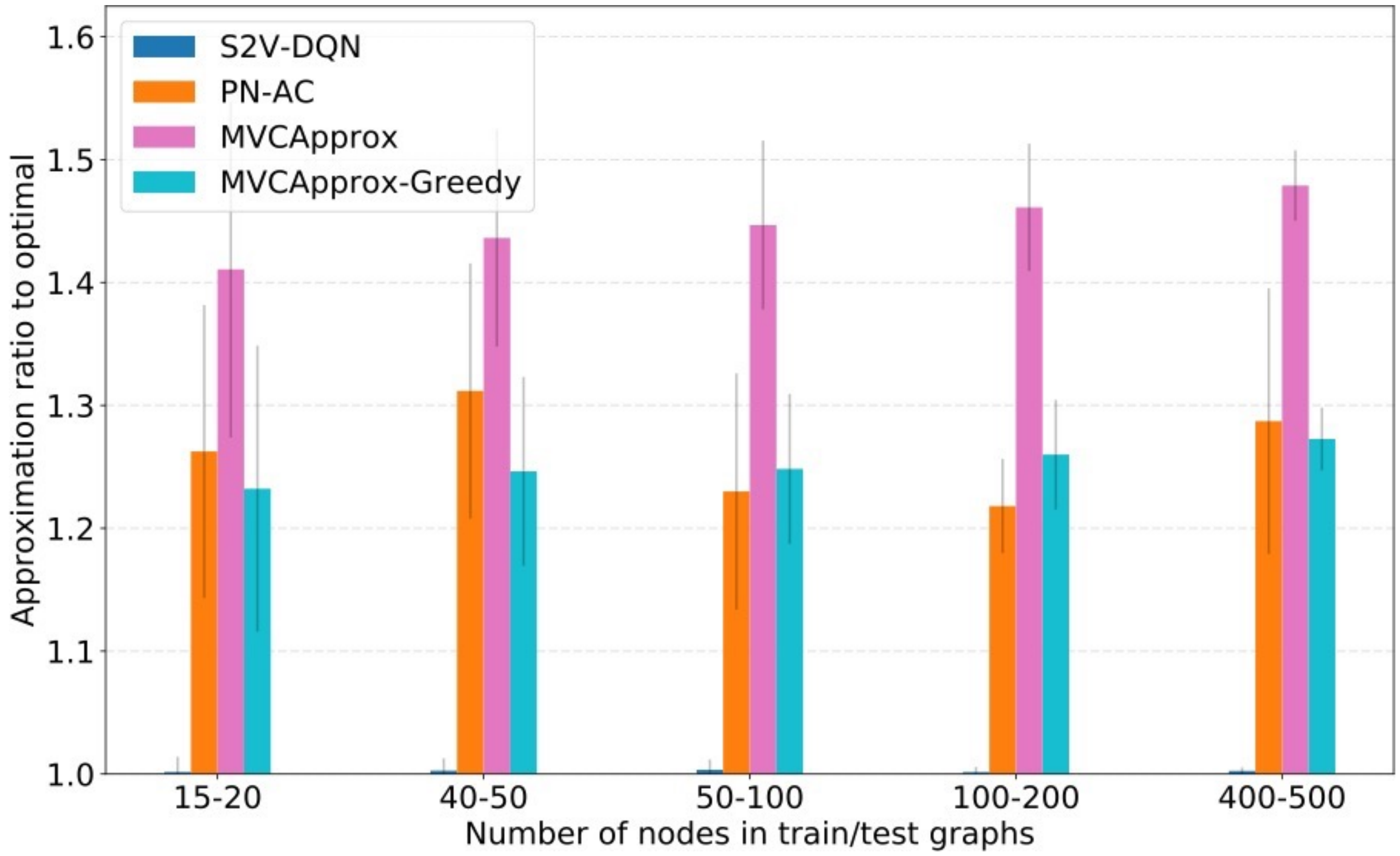
Barabasi-Albert
random graphs

Paper's approach

Another DL approach
[Bello et al., arXiv'16]

2-approximation
algorithm

Greedy algorithm
from first few slides



Dai, Khalil, et al.; NeurIPS'17

Max cut

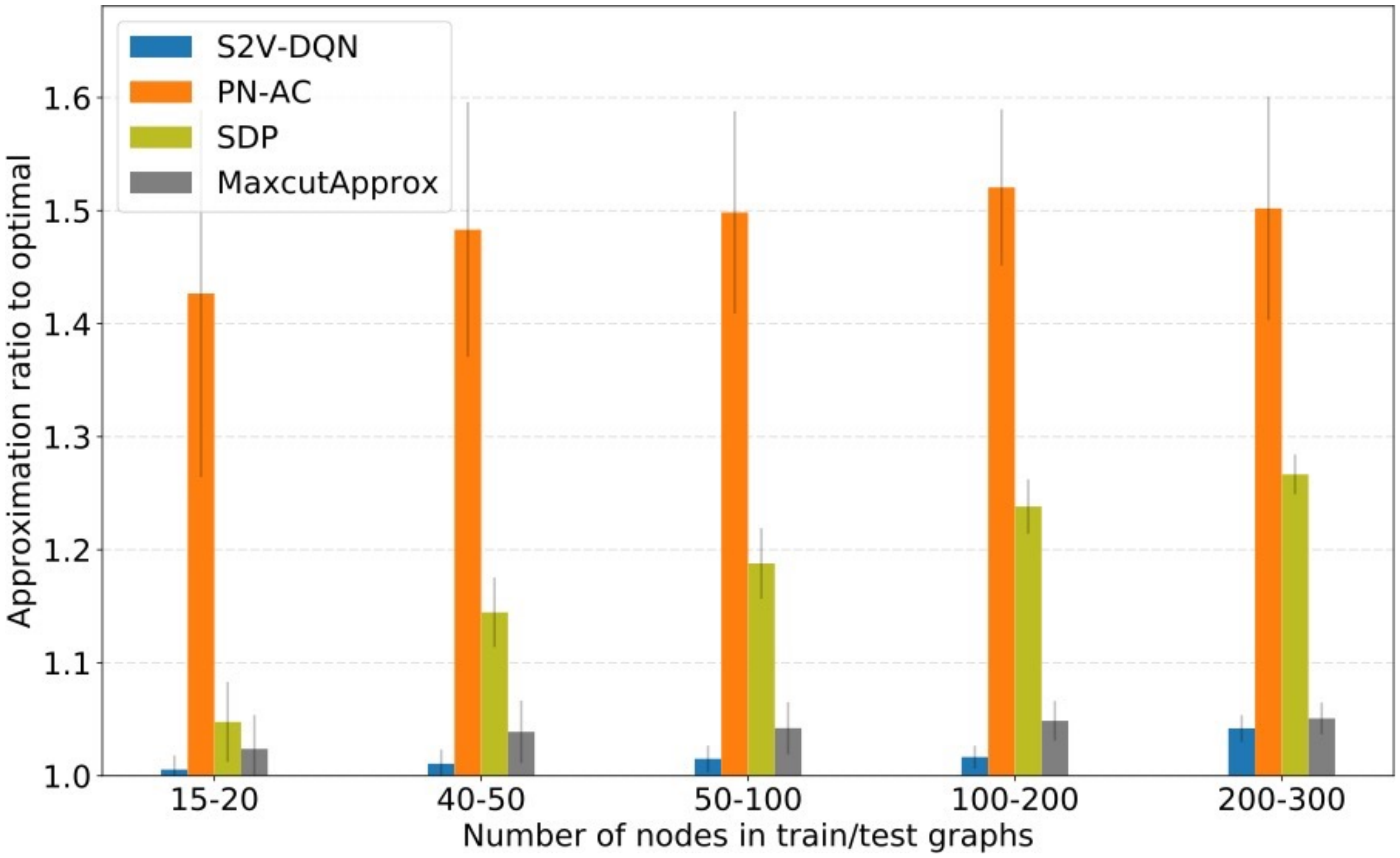
Barabasi-Albert random graphs

Paper's approach

Another DL approach [Bello et al., arXiv'16]

Goemans-Williamson algorithm

Greedy algorithm from first few slides



Dai, Khalil, et al.; NeurIPS'17

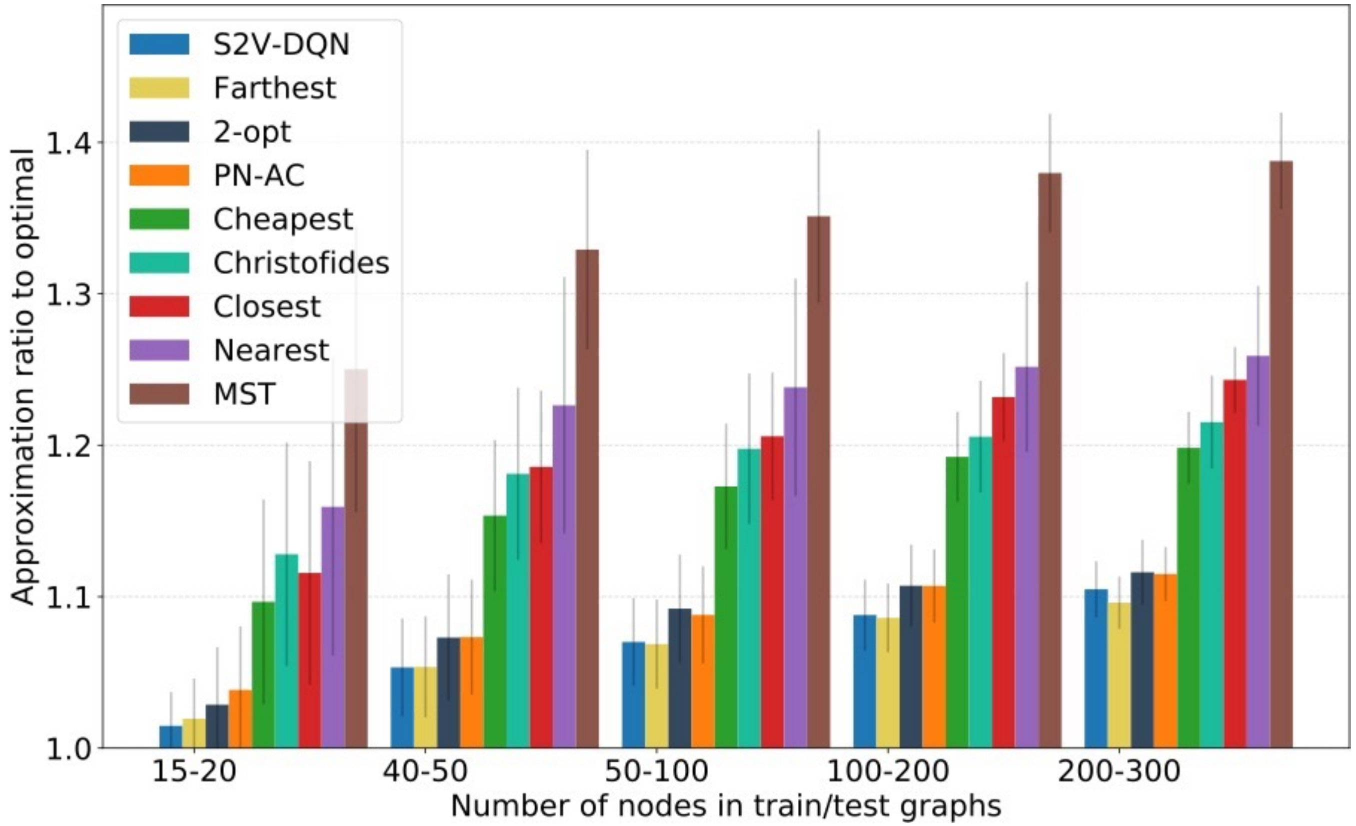
TSP

Uniform random points on 2-D grid

Paper's approach

- Initial subtour: 2 cities that are farthest apart
- Repeat the following:
  - Choose city that's *farthest* from any city in the subtour
  - Insert in position where it causes the smallest distance increase

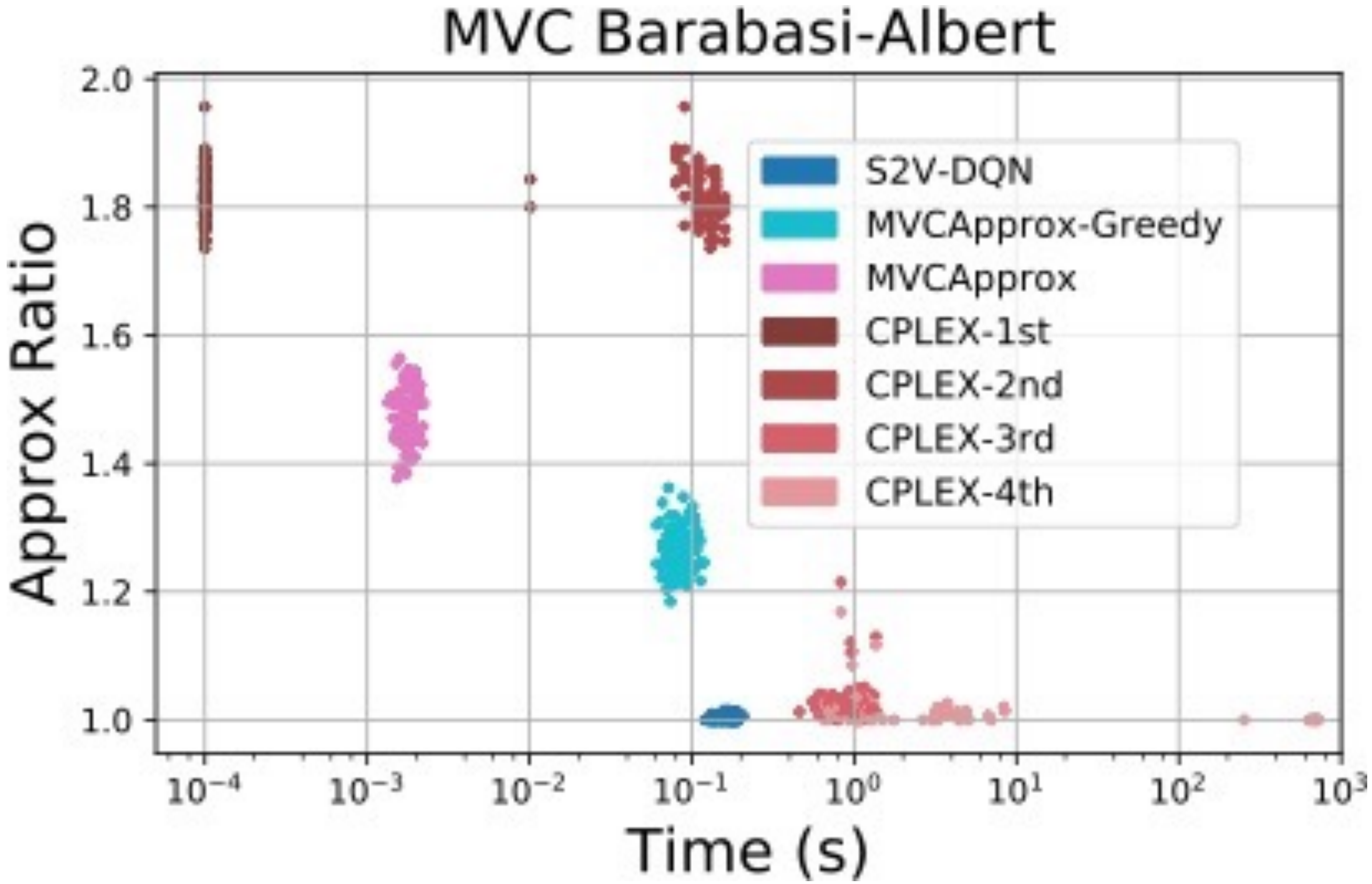
[Rosenkrantz et al., SIAM JoC'77]



Dai, Khalil, et al.; NeurIPS'17

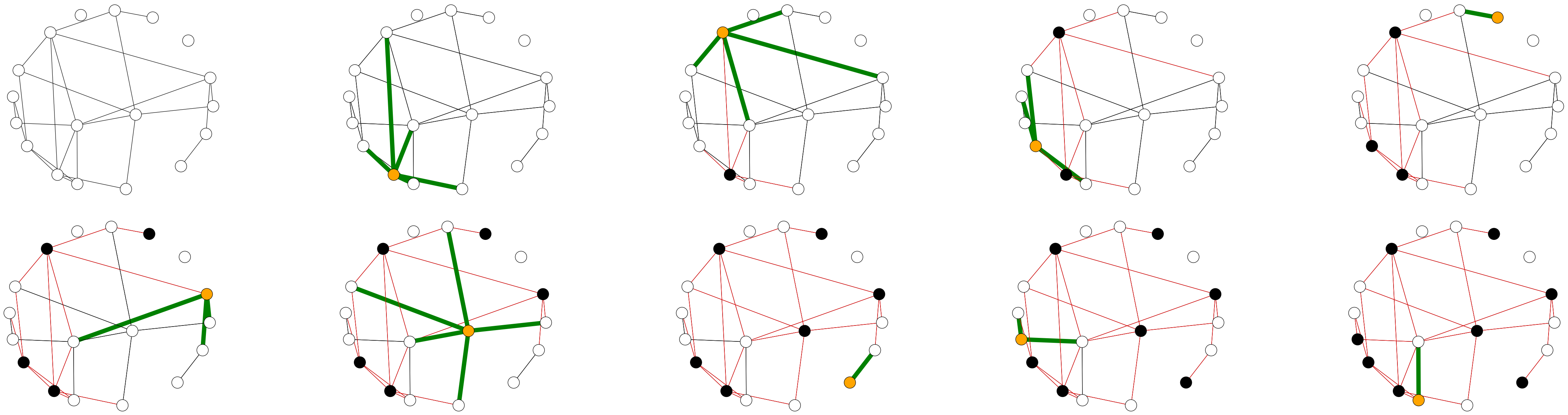
Runtime comparisons

CPLEX-1st: 1st feasible solution found by CPLEX



Dai, Khalil, et al.; NeurIPS'17

Min vertex cover visualization



Nodes seem to be selected to balance between:

- Degree
- Connectivity of the remaining graph

Dai, Khalil, et al.; NeurIPS'17

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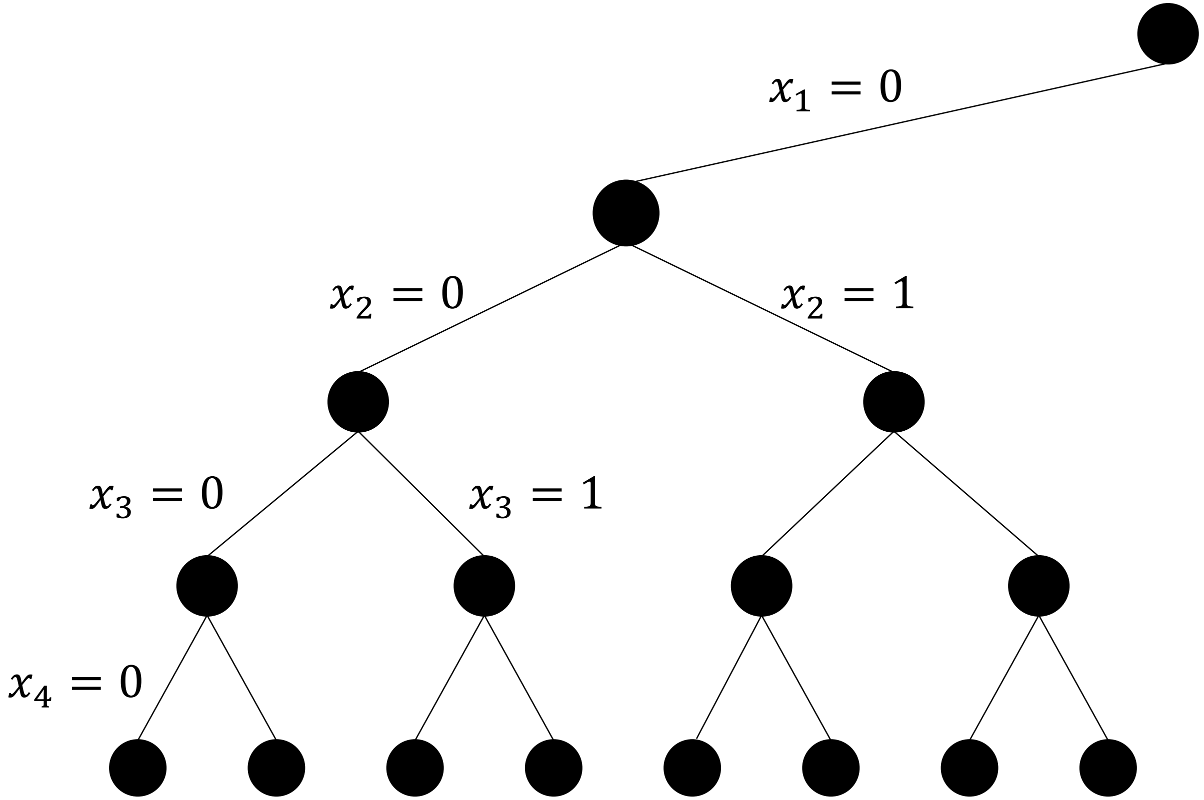
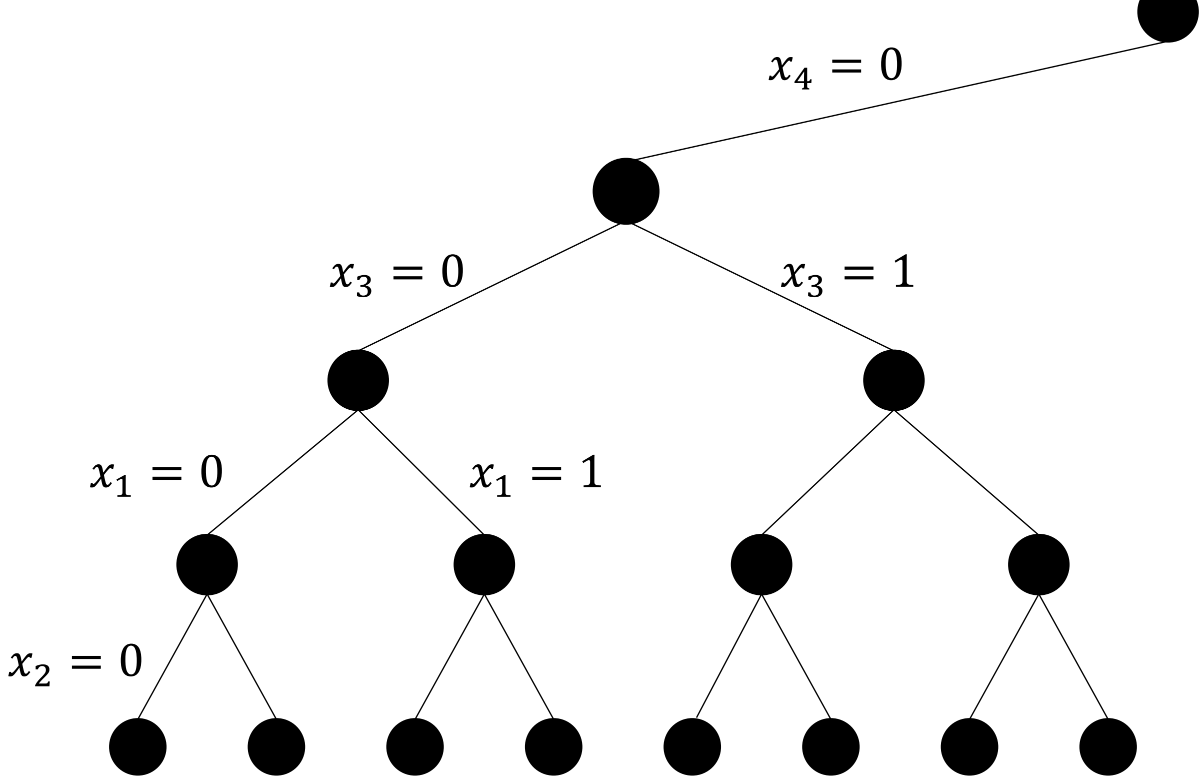
Gasse, Chételat, Ferroni, Charlin, Lodi; NeurIPS'19

Variable selection policy (VSP)



Better branching order than x_1, x_2, x_3, x_4?

Variable selection policy (VSP)

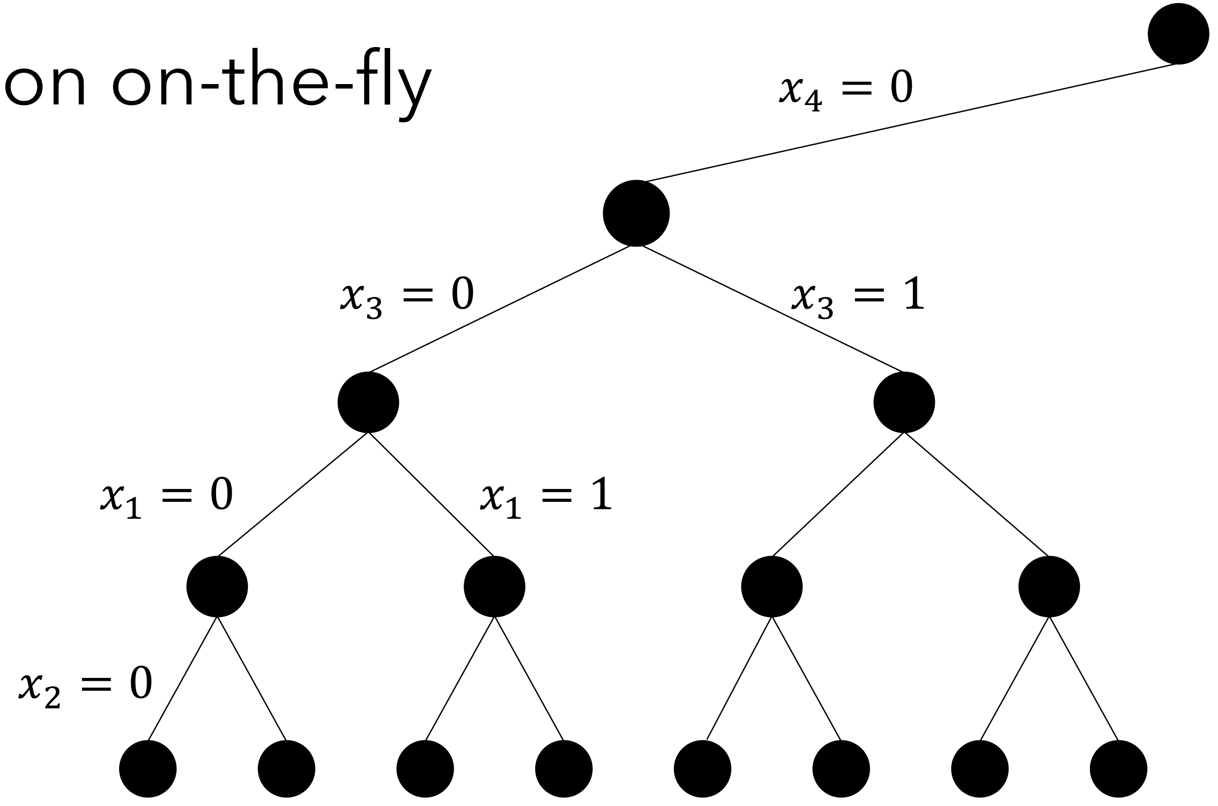


Better branching order than x_1, x_2, x_3, x_4? E.g., x_4, x_3, x_1, x_2

Variable selection policy (VSP)

Chooses variables to branch on on-the-fly

Rather than pre-defined order



Variable selection policy (VSP)

At node j with LP objective value $z(j)$:

- Let $z_i^+(j)$ be the LP objective value after setting $x_i = 1$
- Let $z_i^-(j)$ be the LP objective value after setting $x_i = 0$

VSP example:

Branch on the variable x_i that maximizes

$$\max\{z(j) - z_i^+(j), 10^{-6}\} \cdot \max\{z(j) - z_i^-(j), 10^{-6}\}$$

If score was $\left(z(j) - z_i^+(j)\right)\left(z(j) - z_i^-(j)\right)$ and $z(j) - z_i^+(j) = 0$:

would lose information stored in $z(j) - z_i^-(j)$

Strong branching

Challenge: Computing $z_i^-(j), z_i^+(j)$ requires solving a lot of LPs

- Computing all LP relaxations referred to as ***strong-branching***
- Very **time intensive**

Pro: Strong branching leads to small search trees

Idea: Train an ML model to imitate strong-branching

Khalil et al. [AAAI'16], Alvarez et al. [INFORMS JoC'17], Hansknecht et al. [arXiv'18]

This paper: using a GNN

Gasse et al.; NeurIPS'19

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Problem formulation

Goal: learn a policy $\pi(a_t \mid s_t)$

Probability of branching on variable a_t when solver is in state s_t

Approach (imitation learning)**:**

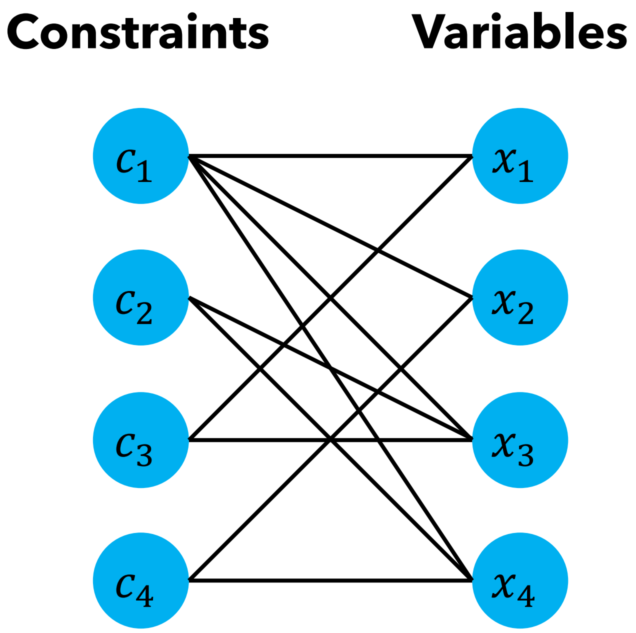
- Run strong branching on training set of instances
- Collect dataset of (state, variable) pairs $S = \{(s_i, a_i^*)\}_{i=1}^{N}$
- Learn policy $\pi_{\boldsymbol{\theta}}$ with training set S

Gasse et al.; NeurIPS'19

State encoding

State s_t of B&B encoded as a **bipartite graph** with **node** and **edge features**

$$
\begin{array}{lll}
\max & 9x_1 + 5x_2 + 6x_3 + 4x_4 & \\
\text{s.t.} & 6x_1 + 3x_2 + 5x_3 + 2x_4 \leq 10 & (c_1) \\
& x_3 + x_4 \leq 10 & (c_2) \\
& -x_1 + x_3 \leq 0 & (c_3) \\
& -x_2 + x_4 \leq 0 & (c_4) \\
& x_1, x_2, x_3, x_4 \in \{0,1\} &
\end{array}
$$

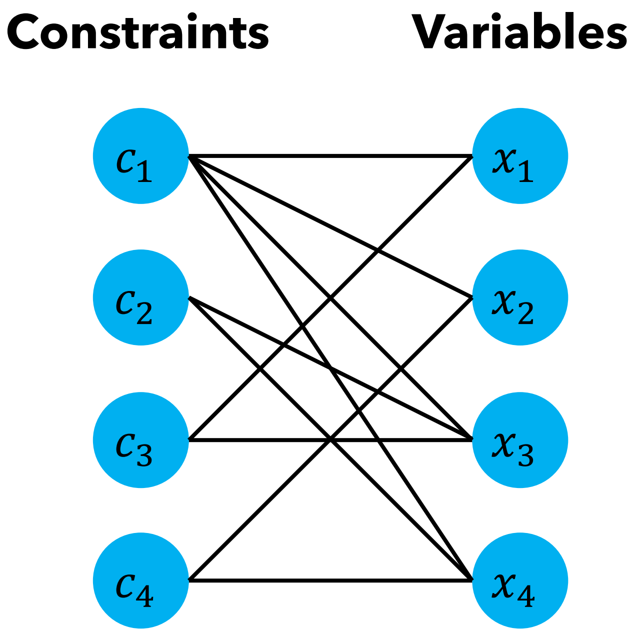


Gasse et al.; NeurIPS'19

State encoding

State s_t of B&B encoded as a **bipartite graph** with **node** and **edge features**

- **Edge feature:** constraint coefficient
- **Example node features:**
  - Constraints:
    - Cosine similarity with objective
    - Tight in LP solution?
  - Variables:
    - Objective coefficient
    - Solution value equals upper/lower bound?



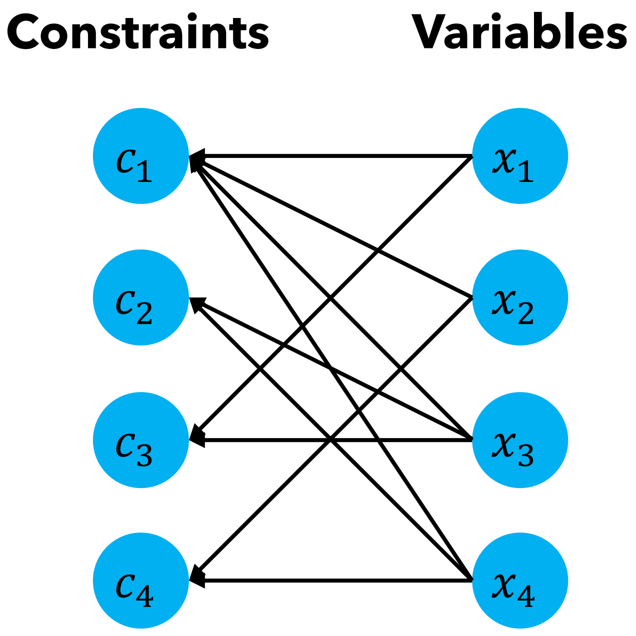
Gasse et al.; NeurIPS'19

GNN structure

1. Pass from variables → constraints

$$\boldsymbol{c}_i \leftarrow f_C\left(\boldsymbol{c}_i, \sum_{j:(i,j)\in E} g_C(\boldsymbol{c}_i, \boldsymbol{v}_j, \boldsymbol{e}_{ij})\right)$$

- $\boldsymbol{c}_i$: Constraint features
- f_C, g_C: 2-layer MLP with relu activations
- $\boldsymbol{v}_j$: Variable features
- $\boldsymbol{e}_{ij}$: Edge features



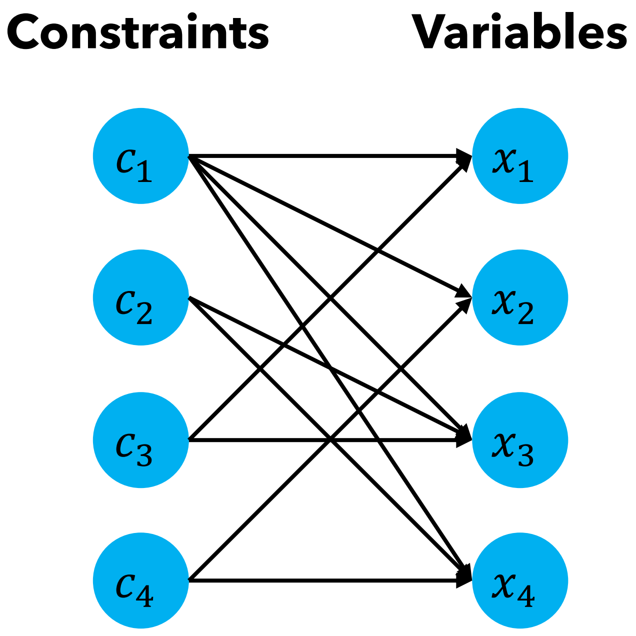
GNN structure

1. Pass from variables → constraints

$$\boldsymbol{c}_i \leftarrow f_C\left(\boldsymbol{c}_i, \sum_{j:(i,j)\in E} g_C(\boldsymbol{c}_i, \boldsymbol{v}_j, \boldsymbol{e}_{ij})\right)$$

2. Pass from constraints → variables

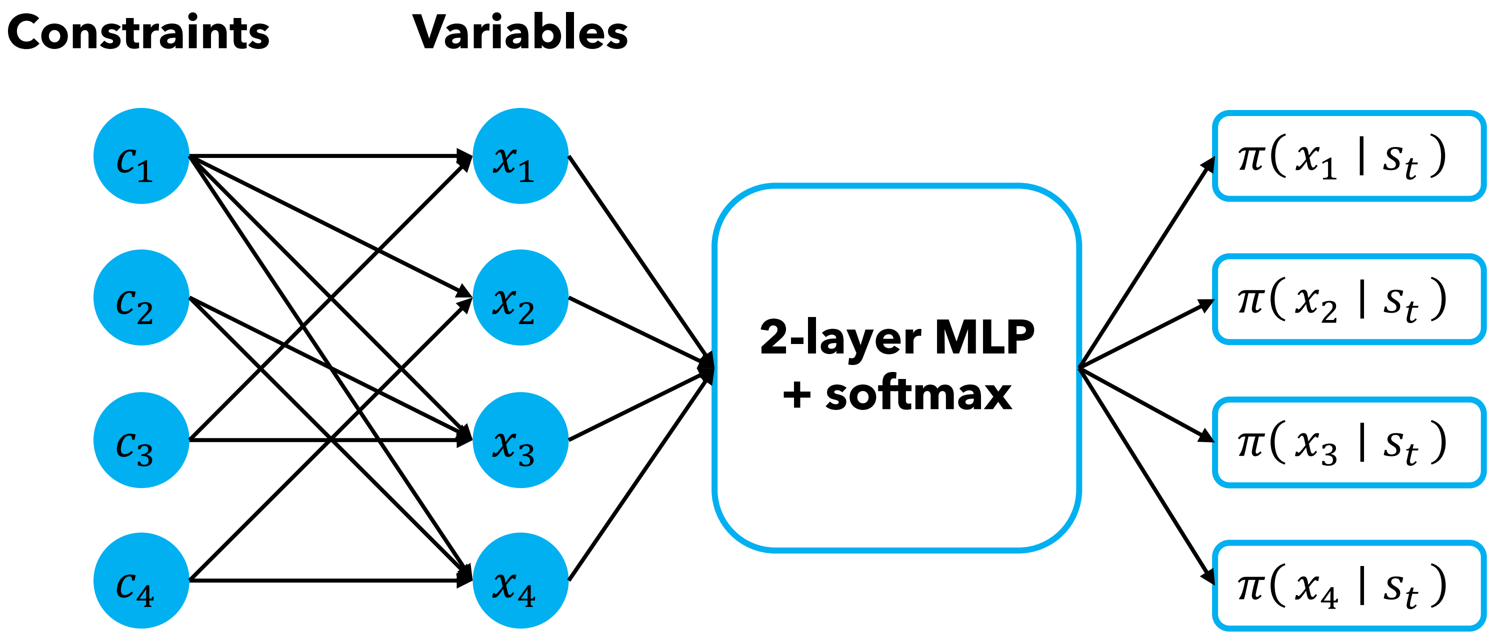
$$\boldsymbol{v}_j \leftarrow f_V\left(\boldsymbol{v}_j, \sum_{i:(i,j)\in E} g_V(\boldsymbol{c}_i, \boldsymbol{v}_j, \boldsymbol{e}_{ij})\right)$$



Gasse et al.; NeurIPS'19

GNN structure

3. Compute distribution over variables



Gasse et al.; NeurIPS'19

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Reliability pseudo-cost branching (RPB)

Rough idea:

- Goal: estimate $z(j) - z_i^+(j)$ w/o solving the LP with $x_i = 1$
- Estimate = avg change after setting $x_i = 1$ elsewhere in tree
  This is the "pseudo-cost"
- "Reliability": do strong branching if estimate is "unreliable"
  E.g., early in the tree

Default branching rule of SCIP (leading open-source solver):

$$\max\{\tilde{\Delta}_i^+(j), 10^{-6}\} \cdot \max\{\tilde{\Delta}_i^-(j), 10^{-6}\}$$

Estimate of $z(j) - z_i^+(j)$ | Estimate of $z(j) - z_i^-(j)$

Achterberg and Berthold, CPAIOR'09

Learning to rank approaches

- Predict which variable **strong branching** would rank highest
- Using a **linear model** instead of a GNN

- Khalil et al. [AAAI'16]:
  Use learning-to-rank algorithm **SVM$^{\text{rank}}$** [Joachims, KDD'06]
- Hansknecht et al. [arXiv'18]
  Use learning-to-rank alg **lambdaMART** [Burges, Learning'10]

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Set covering instances

Always train on "easy" instances

	1000 columns, 500 rows			1000 columns, 2000 rows		
		Easy			Hard	
Model	Time	Wins	Nodes	Time	Wins	Nodes
FSB	17.30 ± 6.1%	0 / 100	17 ±13.7%	3600.00 ± 0.0%	0 / 0	n/a ± n/a %
RPB	8.98 ± 4.8%	0 / 100	**54** ±20.8%	1677.02 ± 3.0%	4 / 65	47 299 ± 4.9%
TREES	9.28 ± 4.9%	0 / 100	187 ± 9.4%	2869.21 ± 3.2%	0 / 35	59 013 ± 9.3%
SVMRANK	8.10 ± 3.8%	1 / 100	165 ± 8.2%	2389.92 ± 2.3%	0 / 47	42 120 ± 5.4%
LMART	7.19 ± 4.2%	14 / 100	167 ± 9.0%	2165.96 ± 2.0%	0 / 54	45 319 ± 3.4%
GCNN	**6.59** ± 3.1%	**85** / 100	134 ± 7.6%	**1489.91** ± 3.3%	**66** / 70	**29 981** ± 4.9%

Gasse et al.; NeurIPS'19

Set covering instances

Runtime in seconds with a timeout of 1 hour

Number instances with fastest runtime / number solved

Size of B&B tree

Model	Easy Time	Easy Wins	Easy Nodes	Hard Time	Hard Wins	Hard Nodes
FSB	17.30 ± 6.1%	0 / 100	17 ±13.7%	3600.00 ± 0.0%	0 / 0	n/a ± n/a %
RPB	8.98 ± 4.8%	0 / 100	**54** ±20.8%	1677.02 ± 3.0%	4 / 65	47 299 ± 4.9%
TREES	9.28 ± 4.9%	0 / 100	187 ± 9.4%	2869.21 ± 3.2%	0 / 35	59 013 ± 9.3%
SVMRANK	8.10 ± 3.8%	1 / 100	165 ± 8.2%	2389.92 ± 2.3%	0 / 47	42 120 ± 5.4%
LMART	7.19 ± 4.2%	14 / 100	167 ± 9.0%	2165.96 ± 2.0%	0 / 54	45 319 ± 3.4%
GCNN	**6.59** ± 3.1%	**85** / 100	134 ± 7.6%	**1489.91** ± 3.3%	**66** / 70	**29 981** ± 4.9%

Gasse et al.; NeurIPS'19

Set covering instances

- GNN is **faster than SCIP** default VSP (RPB)
- Performance generalizes to **larger instances**
- Similar results for auction design & facility location problems

Model	Easy Time	Easy Wins	Easy Nodes	Hard Time	Hard Wins	Hard Nodes
FSB	17.30 ± 6.1%	0 / 100	17 ±13.7%	3600.00 ± 0.0%	0 / 0	n/a ± n/a %
RPB	8.98 ± 4.8%	0 / 100	**54** ±20.8%	1677.02 ± 3.0%	4 / 65	47 299 ± 4.9%
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Gasse et al.; NeurIPS'19

Max independent set instances

RPB is catching up to GNN on MIS instances

Model	Easy Time	Easy Wins	Easy Nodes	Hard Time	Hard Wins	Hard Nodes
FSB	23.58 ±29.9%	9 / 100	7 ±35.9%	3600.00 ± 0.0%	0 / 0	n/a ± n/a %
RPB	8.77 ±11.8%	7 / 100	**20** ±36.1%	2045.61 ±18.3%	22 / 42	**2675** ±24.0%
TREES	10.75 ±22.1%	1 / 100	76 ±44.2%	3565.12 ± 1.2%	0 / 3	38 296 ± 4.1%
SVMRANK	8.83 ±14.9%	2 / 100	46 ±32.2%	2902.94 ± 9.6%	1 / 18	6256 ±15.1%
LMART	7.31 ±12.7%	30 / 100	52 ±38.1%	3044.94 ± 7.0%	0 / 12	8893 ± 3.5%
GCNN	**6.43** ±11.6%	**51** / 100	43 ±40.2%	**2024.37** ±30.6%	**25** / 29	2997 ±26.3%

Gasse et al.; NeurIPS'19

Outline (applied techniques)

1. GNNs overview
2. Neural algorithmic alignment
3. Reinforcement learning overview
4. Learning greedy heuristics with RL
5. Integer programming with GNNs
   i. Machine learning formulation
   ii. Baselines
   iii. Experiments
   iv. **Additional research**

Additional research

CPU-friendly approaches

Gupta et al., NeurIPS'20

Bipartite representation inspired many follow-ups

Nair et al., '20; Sonnerat et al., '21; Wu et al., NeurIPS'21; Huang et al. ICML'23; …

Survey on *Combinatorial Optimization & Reasoning w/ GNNs*:

Cappart, Chételat, Khalil, Lodi, Morris, Veličković, JMLR'23

Conclusions and future directions

Overview

1 **Theoretical guarantees**

a. Statistical guarantees for algorithm configuration
   i. Broadly applicable theory for deriving generalization guarantees
   ii. Proved using connections between primal and dual classes
b. Online algorithm configuration
   a. Impossible in the worst cases
   b. Introduced *dispersion* to provide no-regret guarantees

Overview

1 Theoretical guarantees

a. Statistical guarantees for algorithm configuration
b. Online algorithm configuration

2 Applied techniques

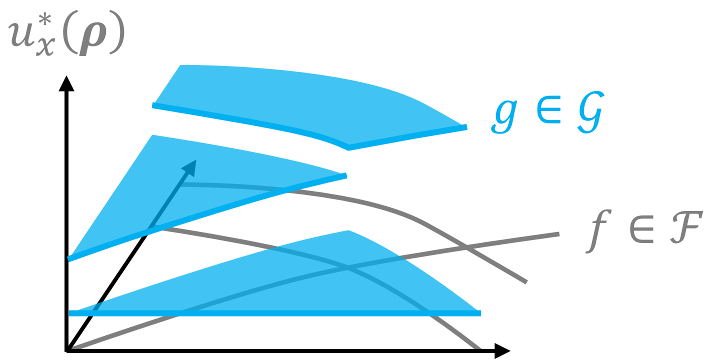
a. Graph neural networks
    i. Neural algorithmic alignment
    ii. GNNs for variable selection in branch-and-bound
b. Reinforcement learning
    i. Design new greedy heuristics for NP-hard problems

Future work: Tighter statistical bounds

WHP $\forall \boldsymbol{\rho}$, |**avg** utility over training set – **exp** utility| $\leq \epsilon$

given training set of size $\tilde{O}\left(\frac{1}{\epsilon^2}\left(\mathrm{Pdim}(\mathcal{G}^*) + \mathrm{VCdim}(\mathcal{F}^*)\log k\right)\right)$

Number of boundary functions



k is often exponential

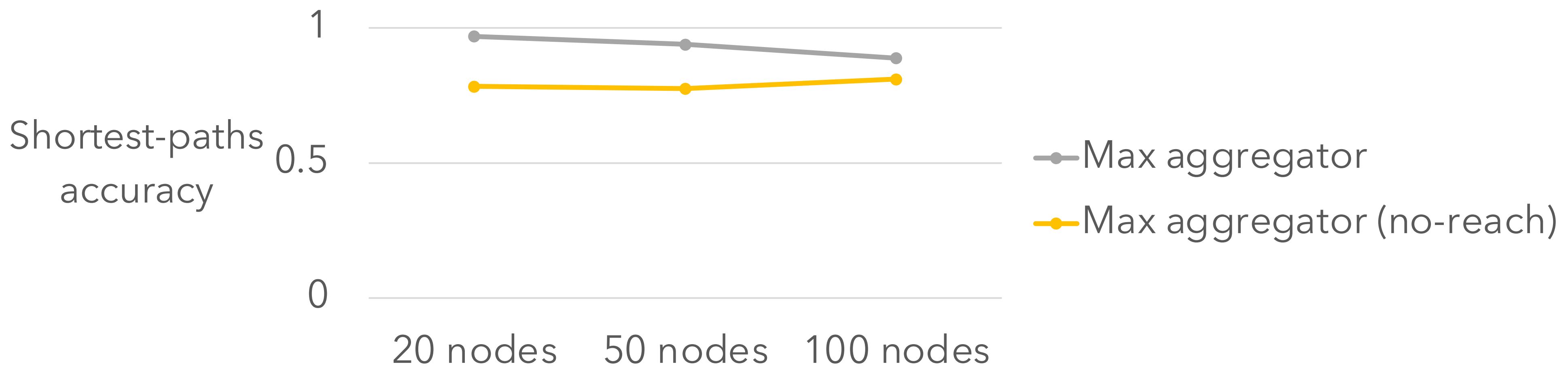
Can lead to large bounds

I expect this can sometimes be avoided!

Would require more information about duals

Future work: Knowledge transfer

- Training a GNN to solve multiple related problems…
  can sometimes lead to better **single-task** performance
- E.g., training reachability and shortest-paths (grey line)
  v.s. just training shortest-paths (yellow line)



Veličković, Ying, Padovano, Hadsell, Blundell, ICLR'20

Future work: Knowledge transfer

- Training a GNN to solve multiple related problems…
  can sometimes lead to better **single-task** performance
- Can we understand **theoretically** why this happens?
  - For which sets of algorithms can we expect **knowledge transfer**?

Future work: Size generalization

Machine-learned algorithms can **scale to larger instances**

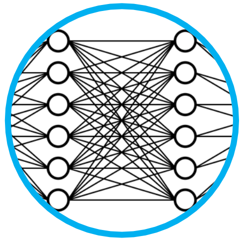
Applied research: Dai et al., NeurIPS'17; Veličković, et al., ICLR'20; …

Goal: eventually, solve problems **no one's ever been able to solve**

However, size generalization is not immediate! It depends on:

- The **machine-learned algorithm**

  Is the algorithm scale sensitive?



Example [Xu et al., ICLR'21]:

- Algorithms represents by GNNs **do generalize**
- Algs represented by MLPs **don't generalize** across size

Future work: Size generalization

Machine-learned algorithms can **scale to larger instances**

Applied research: Dai et al., NeurIPS'17; Veličković, et al., ICLR'20; …

Goal: eventually, solve problems **no one's ever been able to solve**

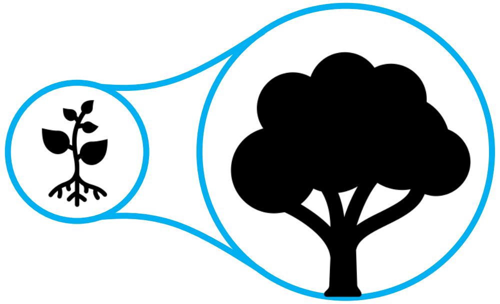
However, size generalization is not immediate! It depends on:

- The **machine-learned algorithm**

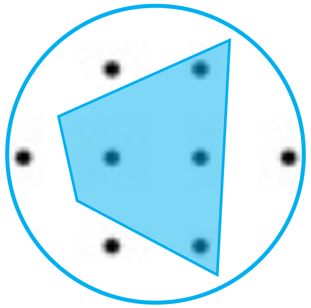
  Is the algorithm scale sensitive?

- The **problem instances**

  As size scales, what features must be preserved?



Future work: Size generalization



Can you:

1. **Shrink** a set of big integer programs
   graphs
   …
2. **Learn** a good algorithm on the **small** instances
3. **Apply** what you learned to the **big** instances?

Future work: ML as a toolkit for theory

Which algorithm classes to optimize over?

Classical algorithm design & analysis

Data-driven algorithm design

Q: *Why* are some machine-learned algs so dominant?

E.g., Dai et al. [NeurIPS'17] write that their RL alg discovered:

"New and interesting" greedy strategies for MAXCUT and MVC

"which **intuitively make sense** but have **not been analyzed** before,"

thus could be a "good **assistive tool** for discovering new algorithms."