Welcome to

Machine Learning for

Discrete Optimization!

About me

Ellen Vitercik
Assistant Professor at Stanford
Management Science & Engineering
Computer Science

Research revolves around
- Machine learning for discrete optimization
- Interface between economics and computation

About me

Grew up in Lincoln, Vermont

BA: Columbia
Math

PhD: Carnegie Mellon
Computer Science

Postdoc: UC Berkeley

Plan for today

1. Introduction
2. Course logistics
3. Overview of course topics

How to integrate **machine learning** into **discrete optimization**?

- **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 **discrete optimization**?

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 **discrete optimization**?

Algorithm configuration

How to tune an algorithm's parameters?

Algorithm selection

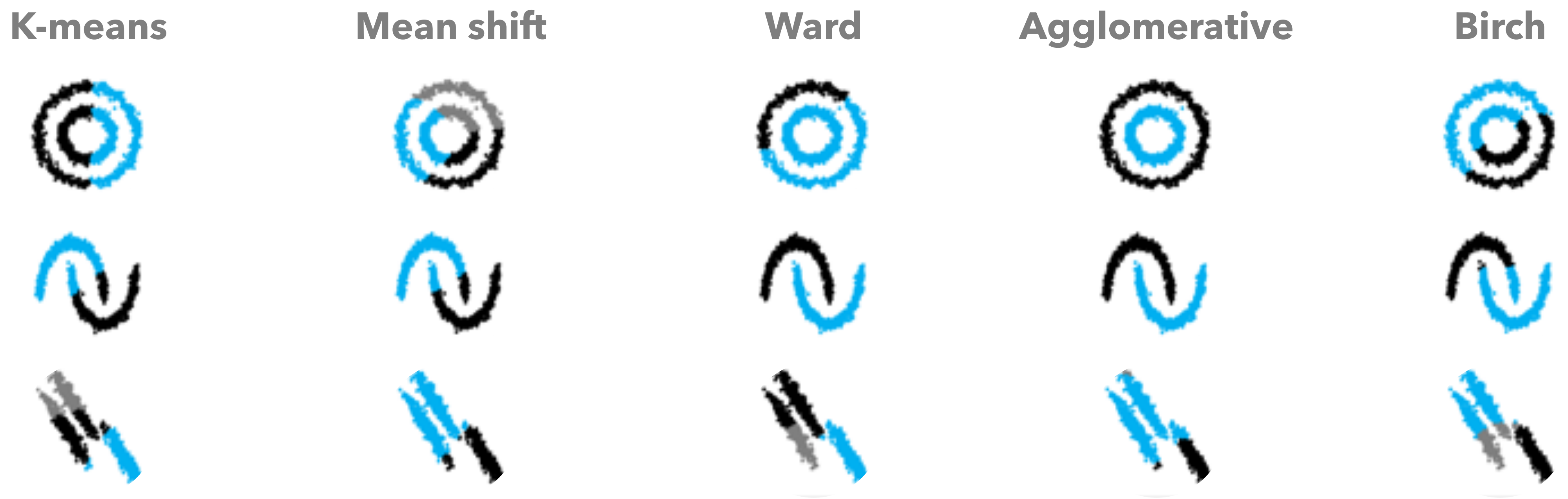
Given a variety of algorithms, which to use?

Algorithm design

Can machine learning guide algorithm discovery?

Example: Clustering

Many different algorithms



How to **select** the best algorithm for the application at hand?

Algorithm selection in theory

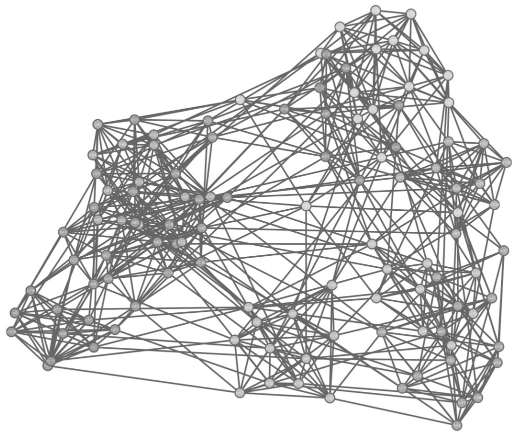
Worst-case analysis has been the main framework for decades

Has led to beautiful, practical algorithms

Worst-case analysis's approach to **algorithm selection**:

Select the algorithm that's best in worst-case scenarios

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



How to integrate **machine learning** into **discrete optimization**?

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 **discrete optimization**?

My objective:

Future engineers will have a nuanced understanding of ML's
power and **limitations**
when used to solve discrete optimization problems

How to integrate **machine learning** into **discrete optimization**?

My long-term goal:

Researchers will be empowered with **data-driven tools** to

- Conceive
- Prototype
- Validate

algorithmic ideas…

and provide theoretical guarantees for their discoveries

How to integrate **machine learning** into **discrete optimization**?

Area is built on a key observation:

In practice, we have data about the application domain

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

Scheduling problems an airline solves

In practice, we have data about the application domain

How can we use this data to guide:

- **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?

ML + discrete opt: Potential impact

Example: integer programming

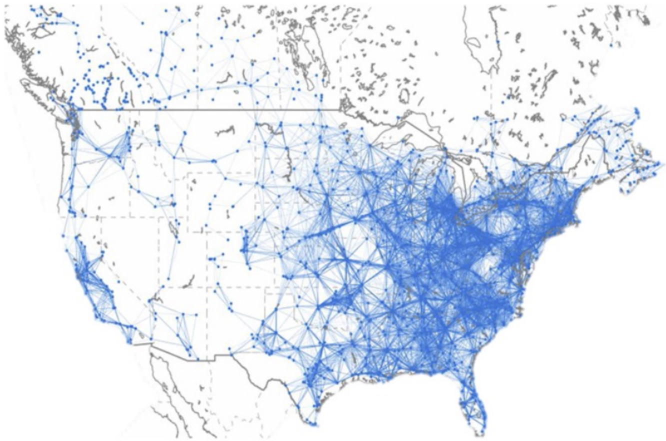
- Used heavily throughout industry and science
- **Many** different ways to incorporate **learning** into solving
- Solving is very difficult, so ML can make a huge difference

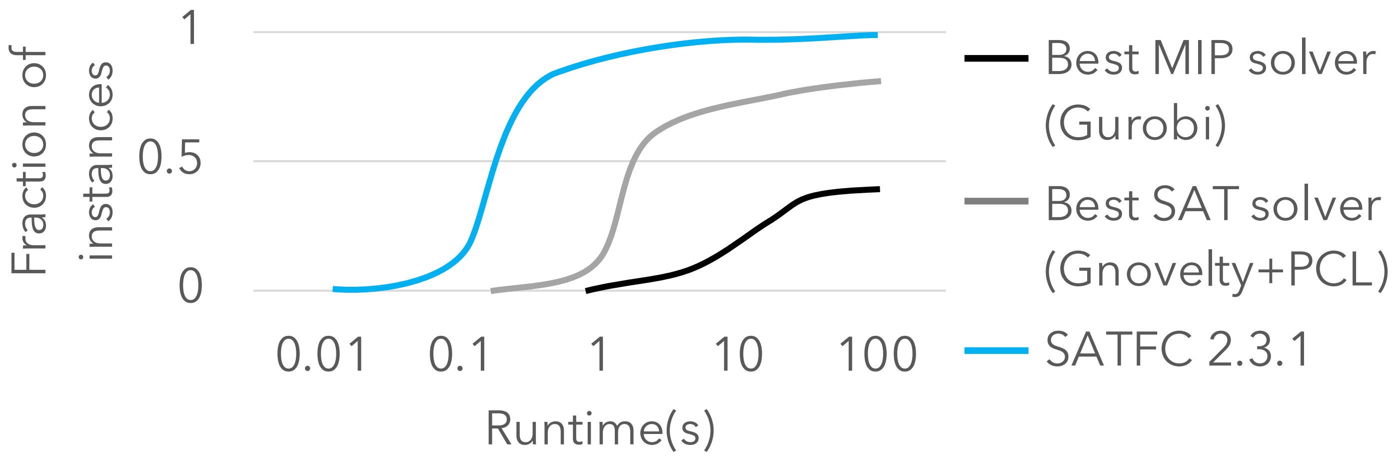




Example: Spectrum auctions

- 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

A bit of history

Important research direction in artificial intelligence for decades

Has led to **breakthroughs** in

- Combinatorial auction winner determination
- SAT
- Constraint satisfaction
- Integer programming
- Many other areas

A bit of history

Algorithm selection
[Rice '76]

RL for discrete optimization
[e.g., Zhang, Dietterich, '95]

Data-driven approaches to algorithm selection
[e.g., Lobjois, Lemaître, '98; Gomes, Selman, '01]

Runtime prediction
[e.g., Horvitz et al., '01]

Machine learning for algorithm selection
[e.g., Kadioglu et al., 2010, Leyton-Brown et al., 2009, Sandholm, 2013, Xu et al., 2008, 2010, 2011]

Machine learning for algorithm configuration
[e.g., Hutter et al. '09, '10, '11, Ansótegui et al. '09, Sandholm, 2013]

A bit of history

Course topics

Range of techniques for integrating ML into algorithm design

1. **Applied topics**
    1. Sequence-to-sequence models
    2. Graph neural networks
    3. Transformers and LLMs

2. **Theoretical topics**
    1. Statistical guarantees and online algorithm configuration
    2. Algorithms with predictions

Outline

1. Introduction
2. **Course logistics**
3. Applied topics
4. Theoretical topics

Course overview

Website: vitercik.github.io/ml4do

On the website, you can find syllabus information like:

- Office hours
- Project policy
- Homework late policy
- Schedule of topics with supplementary readings

Prerequisites

Introductory course in **algorithms/optimization**

- E.g., CS 161 or MS&E 111/211

Introductory course in **machine learning**

- E.g., CS 229
- You should be familiar with basic feed-forward neural networks

Class breakdown

10% Participation

45% Homework assignments (3 total)

45% Project

Policies

10% Participation

- In-class participation recorded using in-class polls (starting next class)
- Can’t come class?
  - Watch lecture online (posted after class on Canvas)
  - Send 100-word summary to instructors [details will be announced]
    - Must be set before the start of the next class
- 2 absent passes, no summary necessary, no questions asked

Policies

45% Weekly assignments (3 total)

- Total of 4 late days for assignments, e.g.:
  - No penalty if you submit 1 assignment 4 days late
  - Or 2 assignments 2 days late, …
- Beyond that, grade goes down by 7 points for every 12 hours it's late
  - E.g., 90% to 83%
  - Lasts until week after deadline, at which point assignment will receive grade 0%
- **Ask questions on Ed Discussion** (linked to on Canvas)
  - Fastest way to reach course staff

Policies

Policies intended to cover all

- Sicknesses
- Family events
- Sports events
- …

Use your late days carefully!

Please *come talk to me if you're struggling!*

Policies

45% Project

- Write a “mini-paper” as a final project
- Can take one of two forms:
  - Research
  - Survey

Option 1: Research project

Present progress your group made on a relevant problem

Report should adopt the structure of a research paper

(Not required to reach the standard for academic publishing)

Option 2: Survey project

Choose **2-4 papers** discussed in class. For each paper:

1. Summarize a paper that **the paper covered in class cites**
   How does the paper covered in class build on the older paper?
2. Summarize a paper that **cites the paper covered in class**
   How does the more recent paper build on the paper covered in class?
3. Imagine you're a **new researcher** working in this area
   - Propose an imaginary follow-up project
   - Not just based on the paper covered in class…
     but **only possible** due to the existence and success of that paper

Working in groups

- Welcome to work in groups on the final project
- Groups should include:
  - At most three students if it's a **research** project
  - At most two students if it's a **survey** project
- Group of two must put twice as much work into project
  - Similarly for groups of three
- The **paper length** for final write-up is:
  - 3 if solo-authored,
  - 5 if there are two authors, and
  - 7 if there are three authors

Milestones

May 1: Submit a short progress report of 1-2 pages

Describe your project and partial progress

June 5: Students will present their final project during class

June 12: Each group will submit their final report

Class format

Whiteboard!

- Studies show that students learn better from whiteboard vs. slides
- Writing down notes helps you learn
  - As opposed to just following along in slides
- I automatically go slower

Please ask questions in class!

2-minute anonymous surveys

- Watch out for an email about a 2-min anonymous survey
- Random set of students asked each week
  - You'll be asked 2-3 times during the quarter to fill it out
- It's so useful for us!

Please use it to tell us:

- What's going well 😀
- What you're confused about 🤔
- How we can best help you learn!

OAE

Let me know if you have an OAE letter as soon as possible

Thanks!

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    a. **Pointer networks for the traveling salesman problem (TSP)**
    b. Graph neural networks
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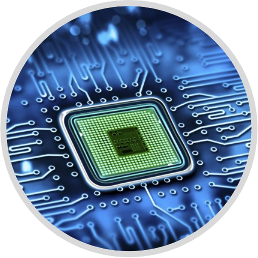
Traveling salesman problem

- One of the most famous *NP-hard* problems
- **Input:** network with n nodes, representing a map with n cities
- **Goal:** compute the shortest-distance tour

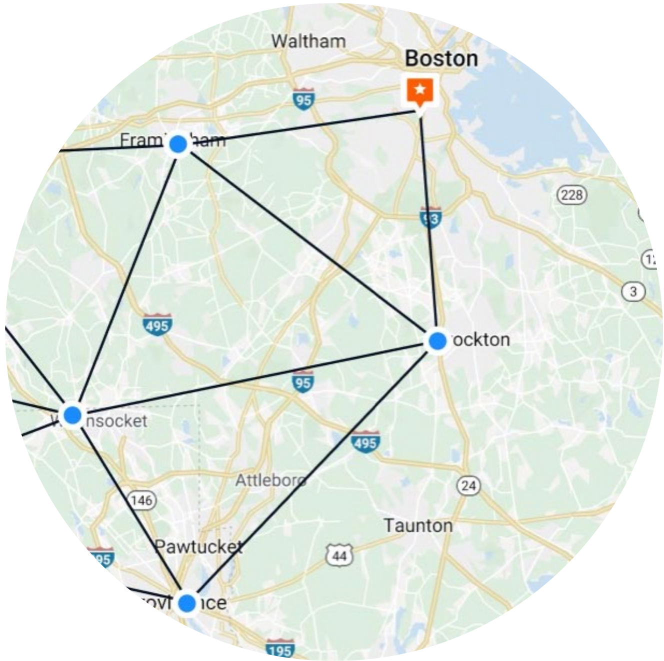
  Should pass through each city exactly once

Routing



Manufacturing

Planning

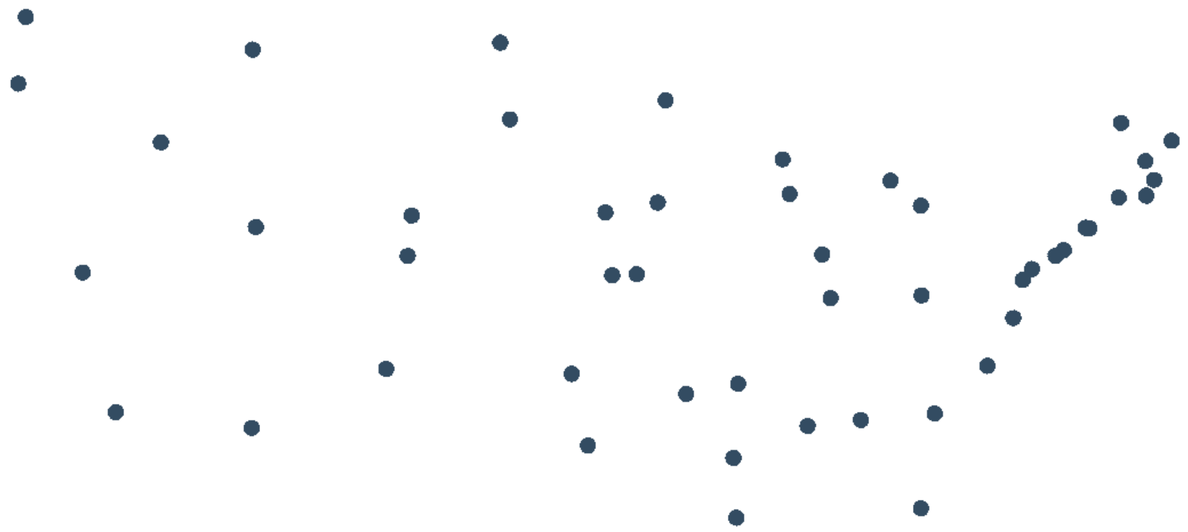


Farthest-first heuristic

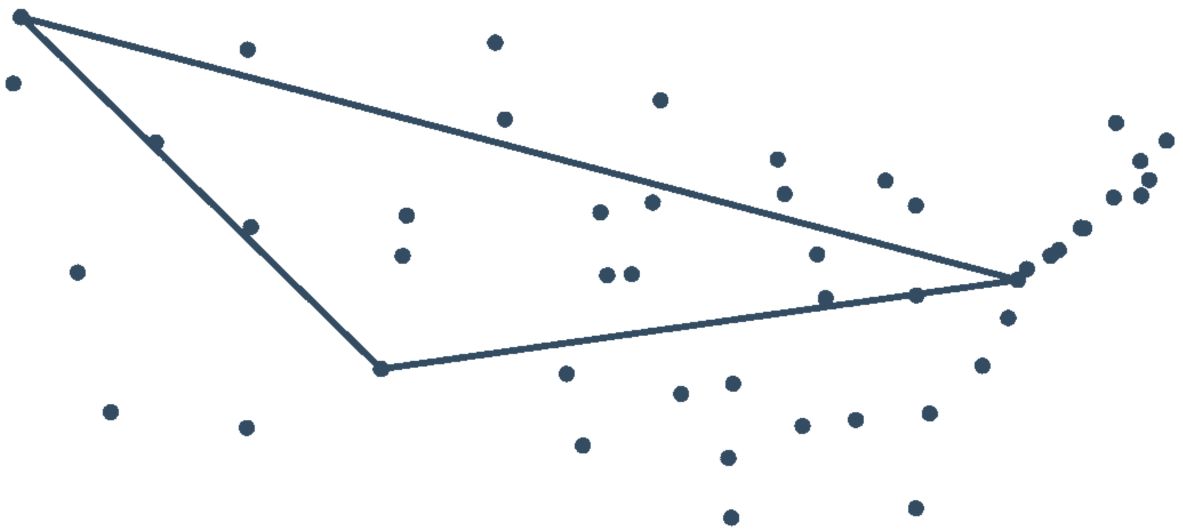
Many **heuristics** for TSP

1. Start with subtour $\{1\}$
2. Among all cities not in the subtour:
   Choose the one that's *farthest* from any city in the subtour
3. Insert it into the subtour
   Position: where it causes the smallest tour length increase

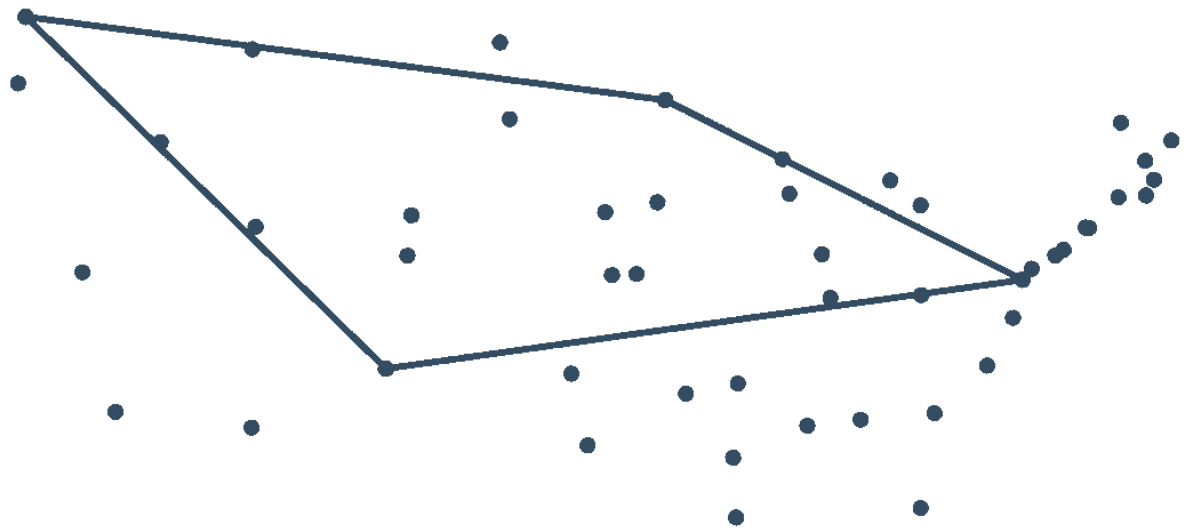
Farthest-first heuristic



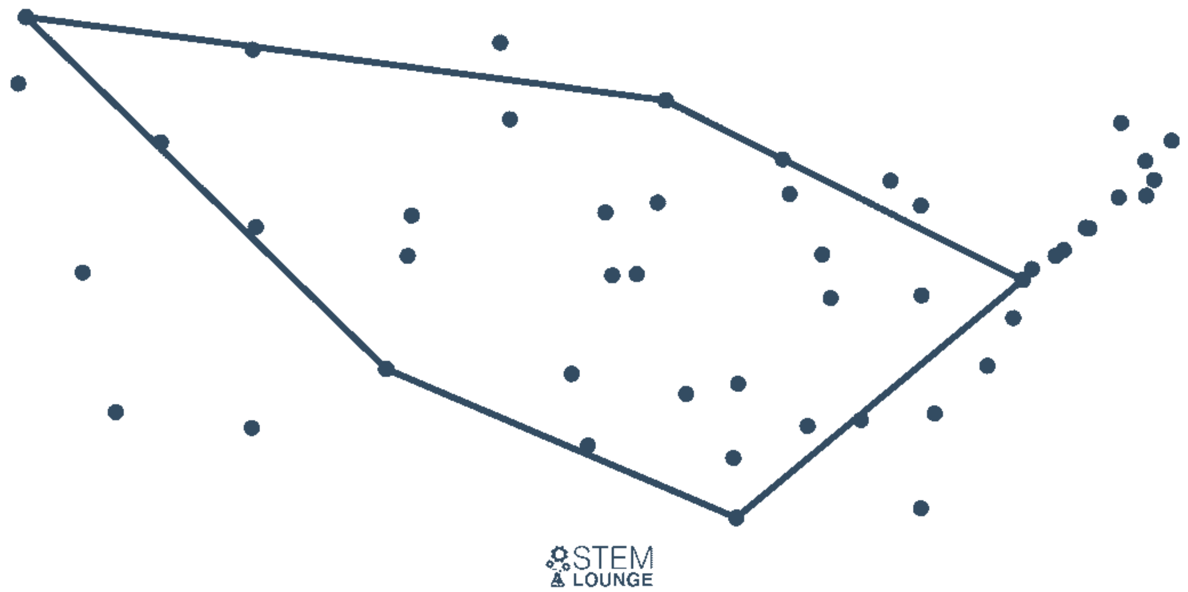
Farthest-first heuristic



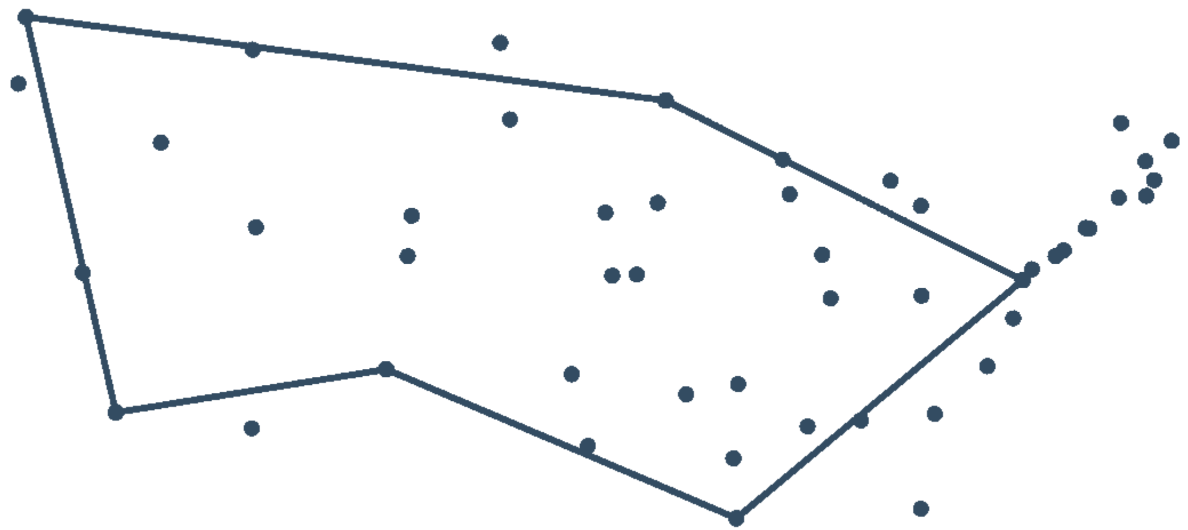
Farthest-first heuristic



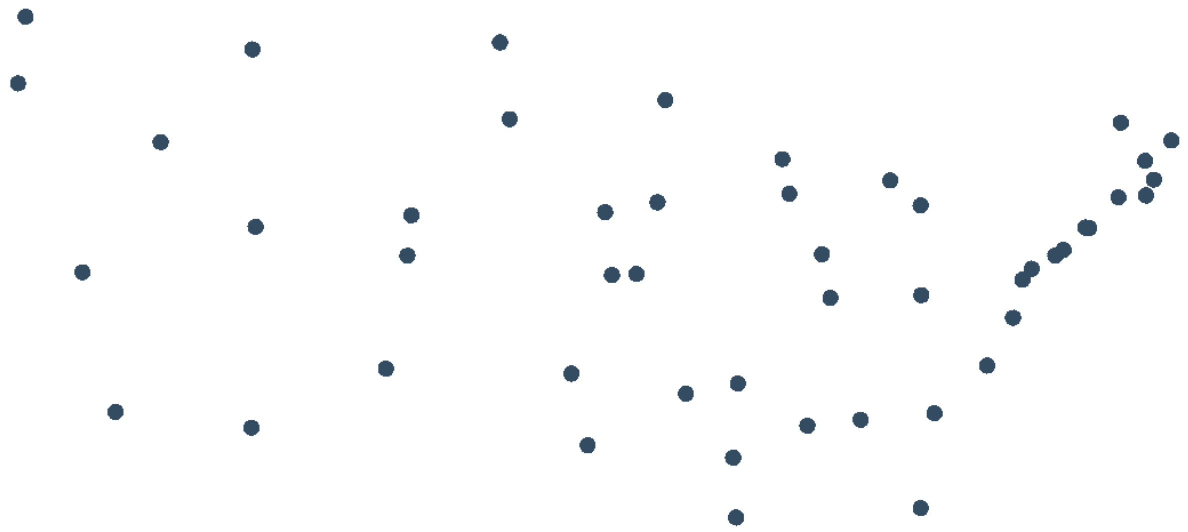
Farthest-first heuristic



Farthest-first heuristic



Farthest-first heuristic



Heuristics for TSP

Many **heuristics** for TSP

- Nearest neighbor
- Nearest insertion
- Cheapest insertion
- Random insertion
- Christofides algorithm
- …

Goal: use ML to uncover a better heuristic

Topics

This module: early approaches to DL for discrete optimization

circa '15-'17

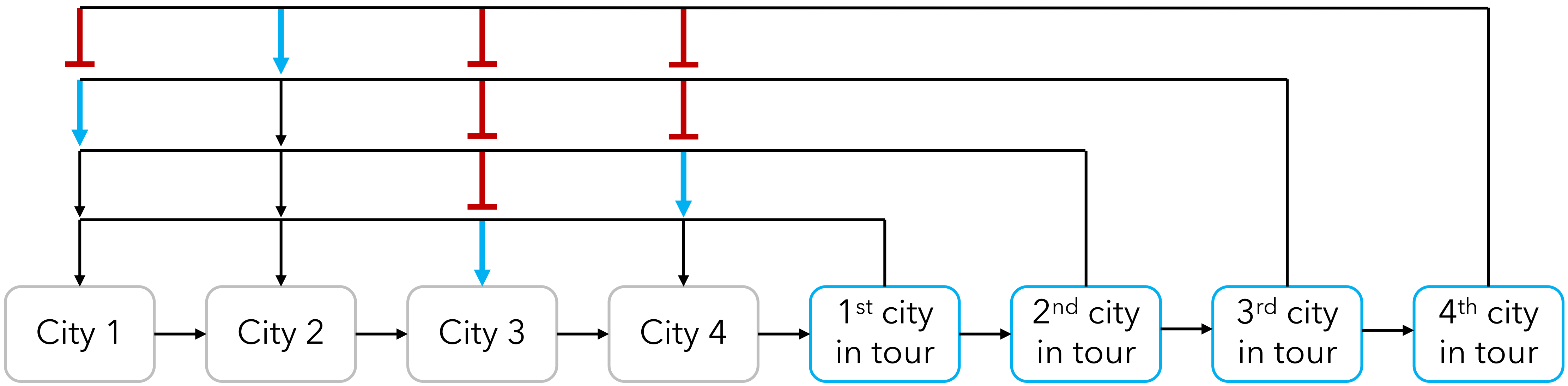
We'll cover:

- **Recurrent neural networks**

  Long-short term memories (LSTMs)
- **Pointer networks**: use LSTMs to output a permutation
- **Training** pointer networks for TSP (*policy gradient)*

Vinyals, Fortunato, Jaitly, NeurIPS'15; Bello, Pham, Le, Norouzi, Bengio, ICLR'17

Pointer networks



Shows promise that ML can be useful for discrete optimization

But treats cities as a sequence, losing the network structure 🤔

Vinyals, Fortunato, Jaitly, NeurIPS'15; Bello, Pham, Le, Norouzi, Bengio, ICLR'17

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   b. **Graph neural networks**
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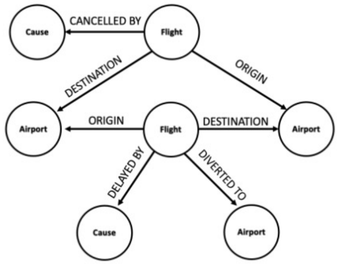
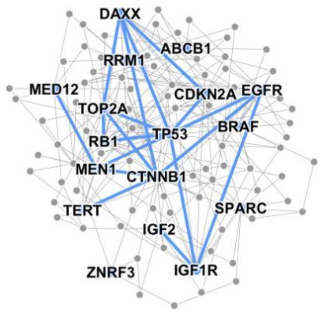
Many types of data are graphs



Event Graphs

Image credit: SalientNetworks

Computer Networks



Disease Pathways

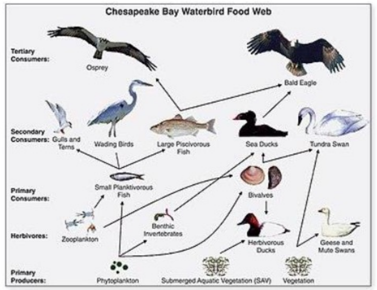


Image credit: Wikipedia

Food Webs

Image credit: Pinterest

Particle Networks

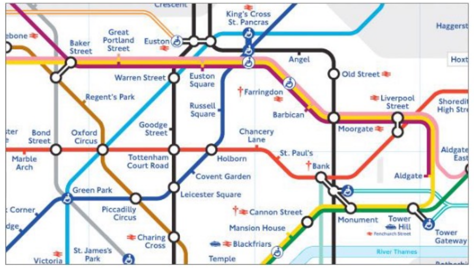
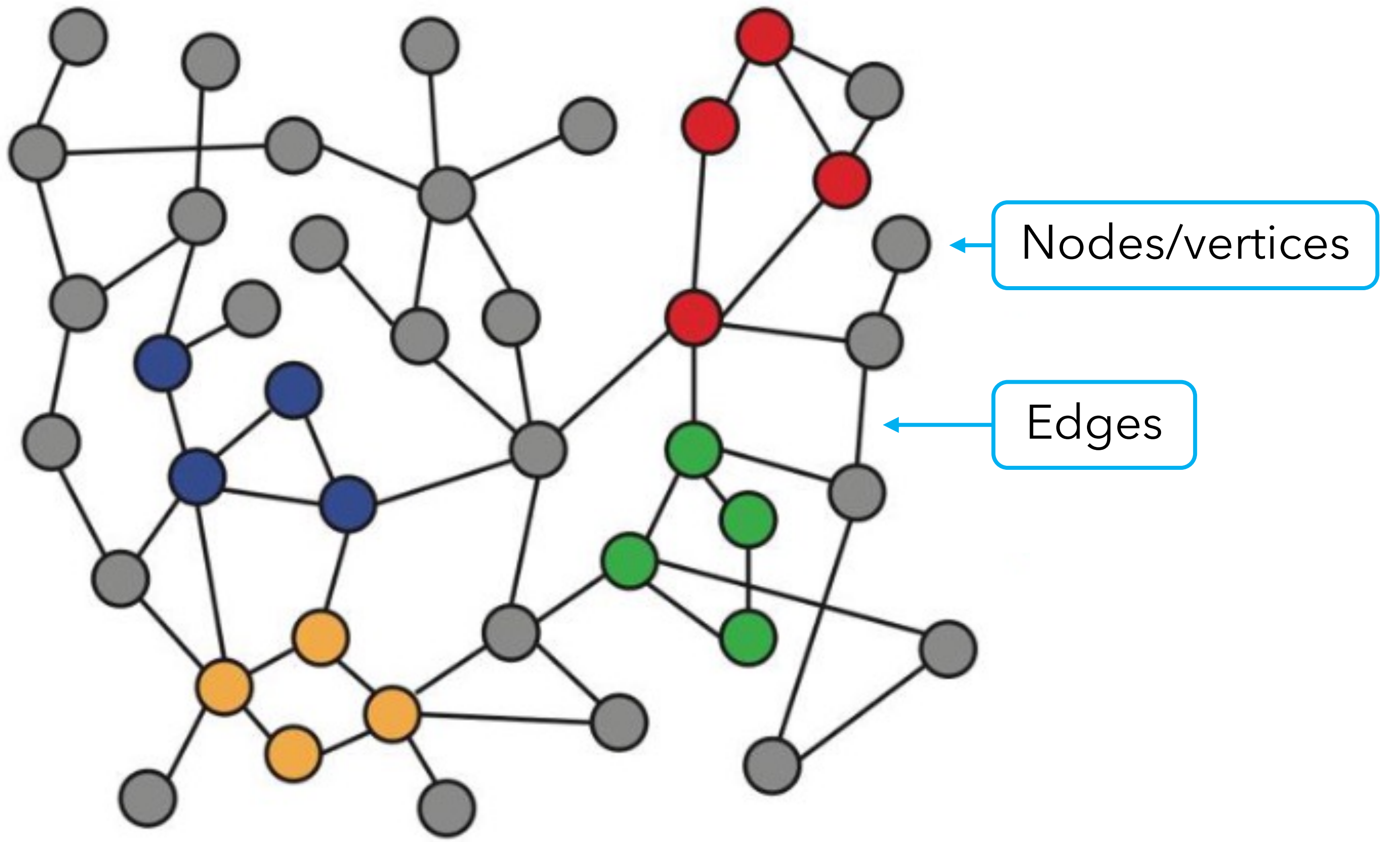


Image credit: visitlondon.com

Underground Networks

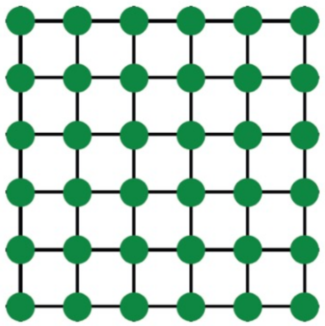
Slide by Leskovec

Graph terminology

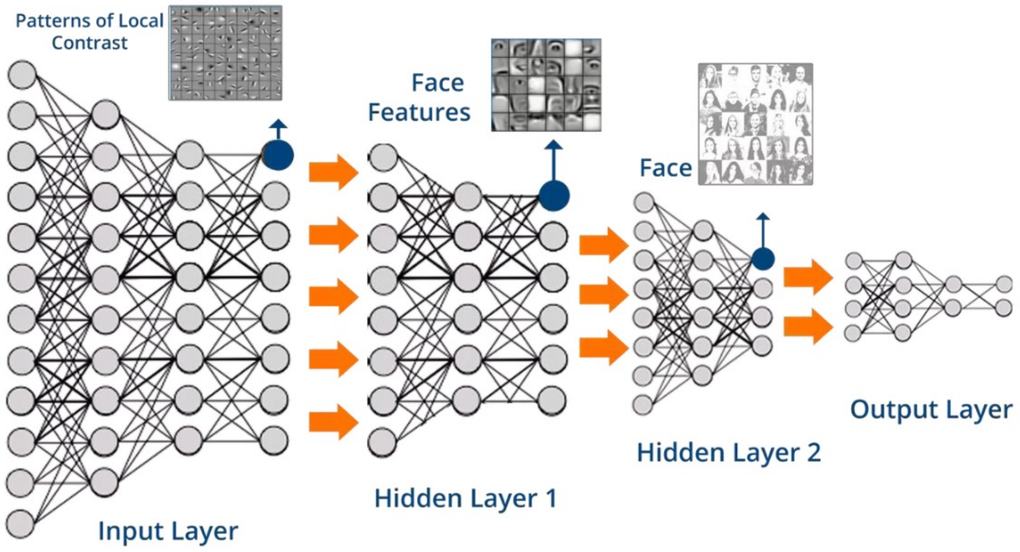


Today: Modern ML toolbox

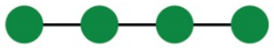
Modern DL toolbox is designed for simple sequences & grids

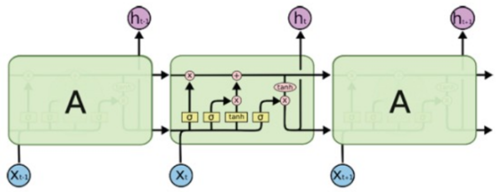


Images



Text/Speech



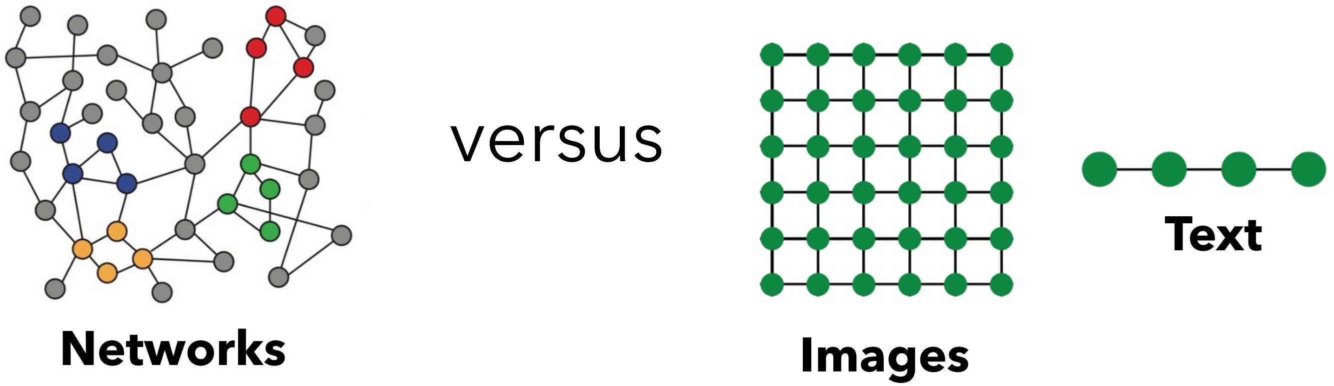


Slide by Leskovec

Why is graph deep learning hard?

Networks are complex

- Arbitrary size and complex topological structure



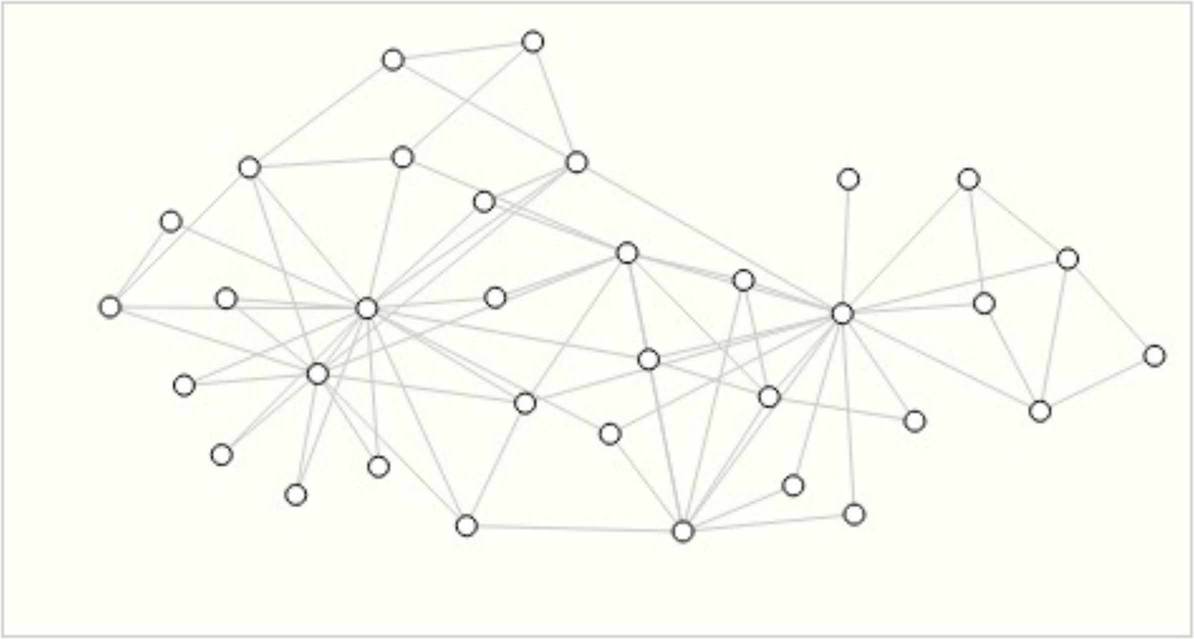
- No fixed node ordering or reference point
- Often dynamic and have multimodal features

Figure by Leskovec

GNN motivation

Special type of NN architecture for tasks involving graphs

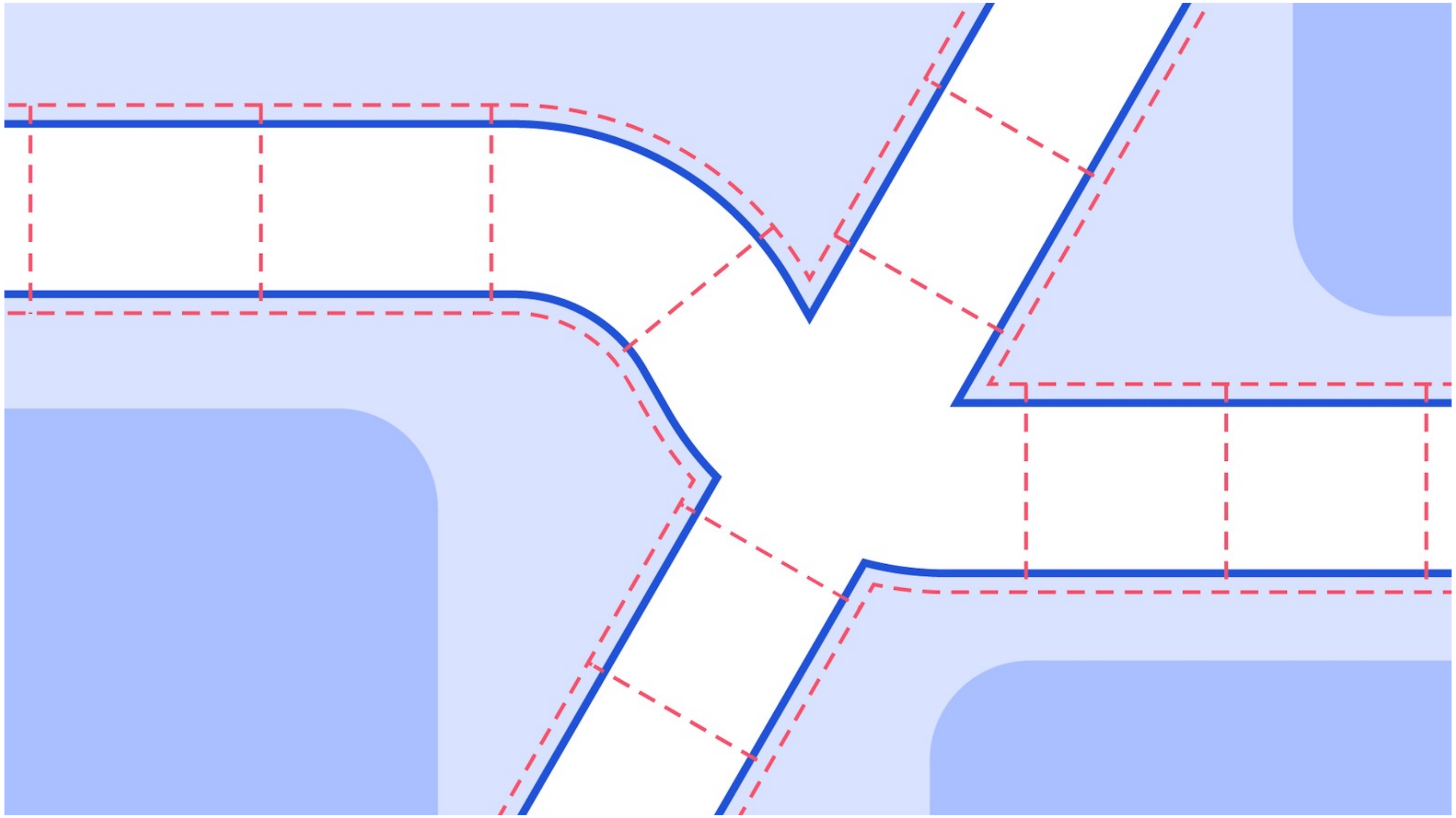
How to utilize relational structure for better prediction?



GNN overview

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

GNN overview



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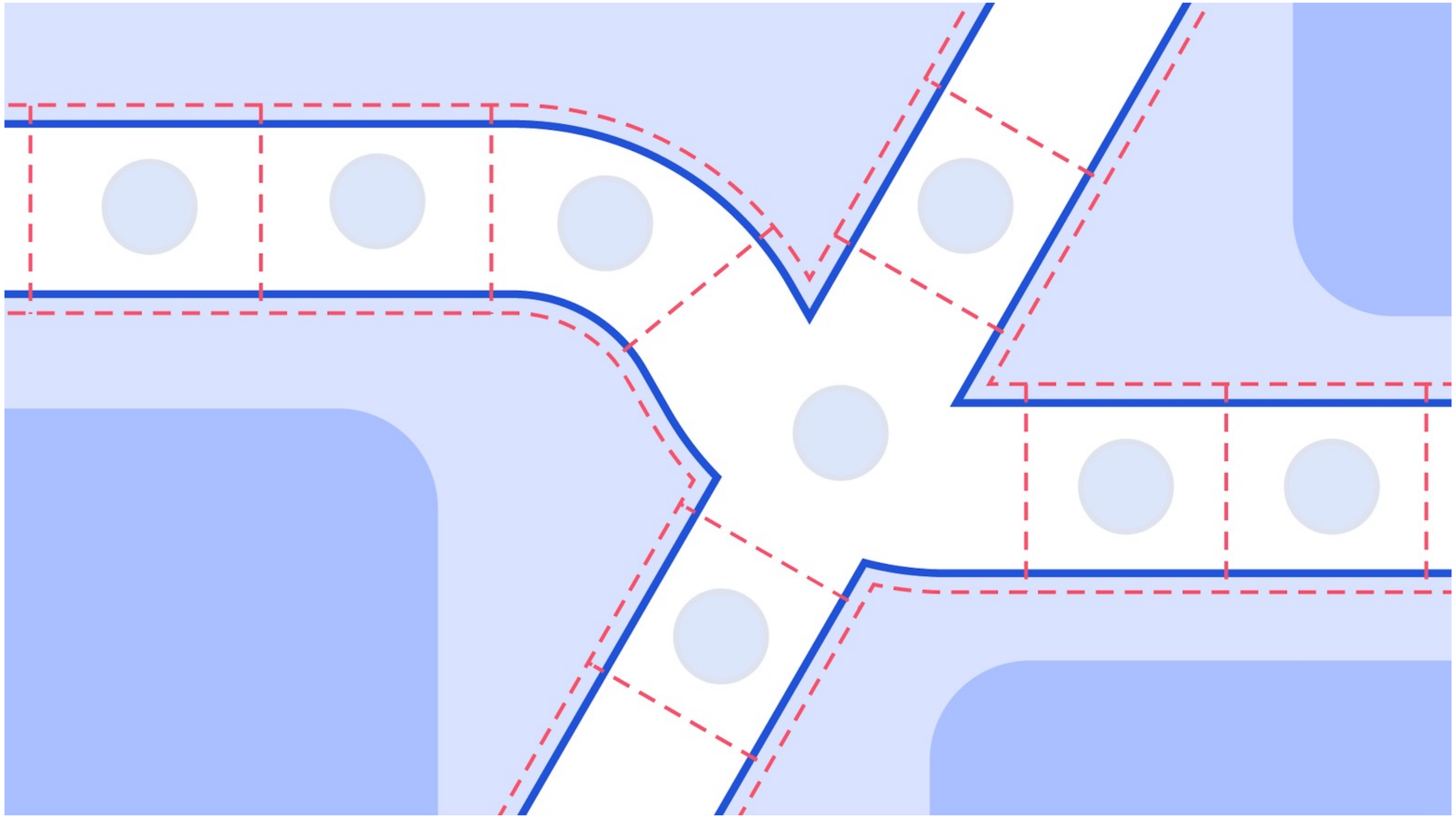

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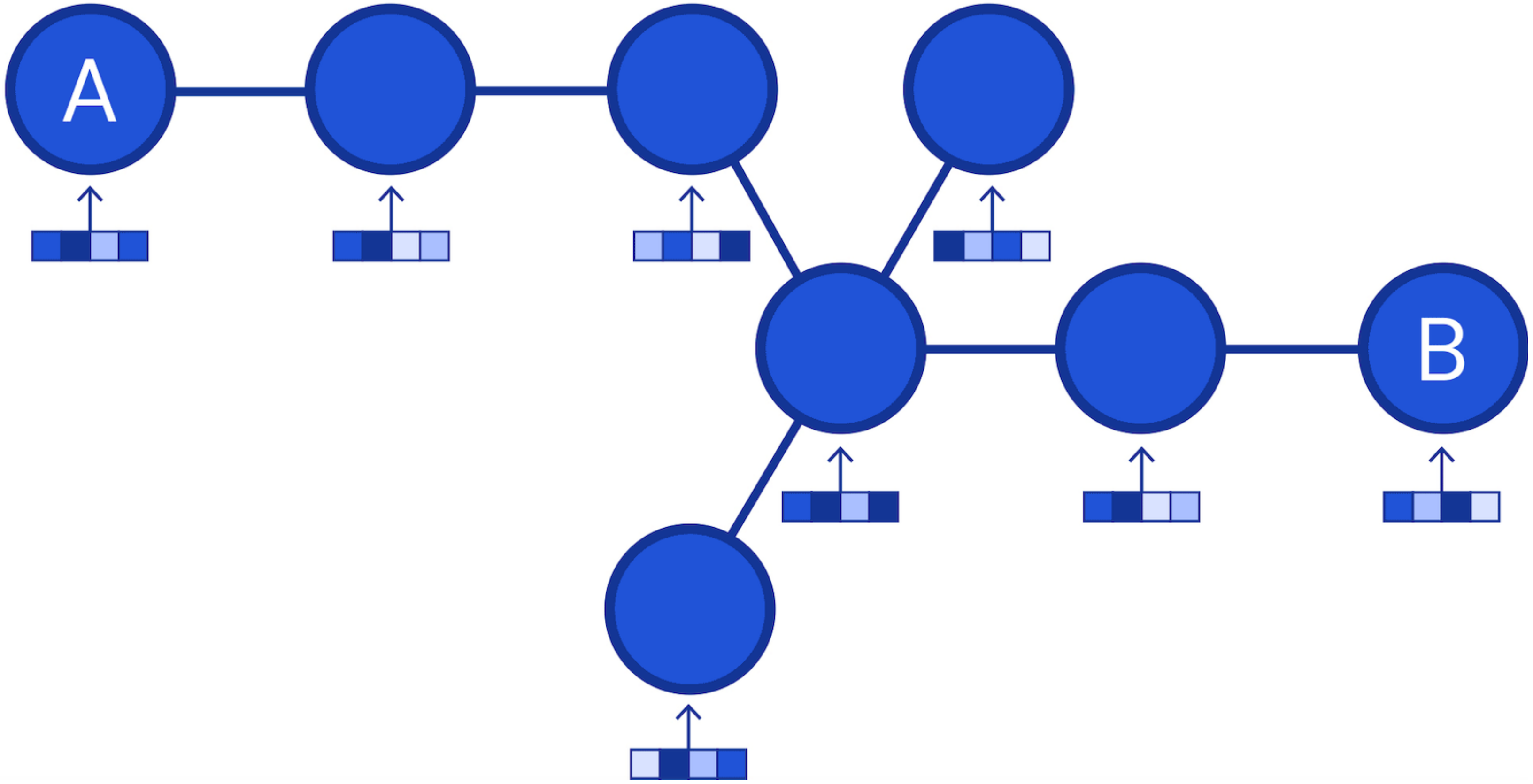

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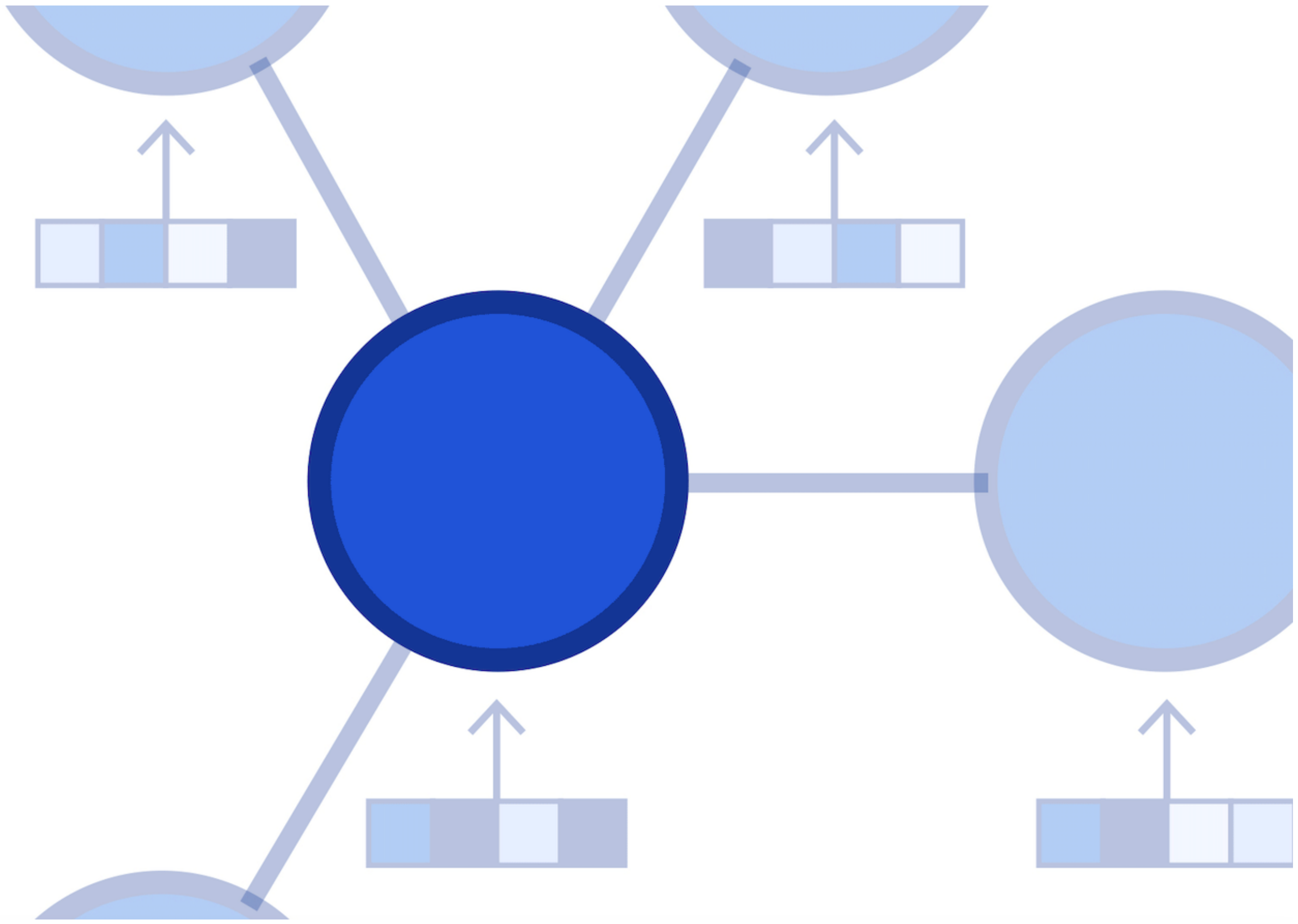

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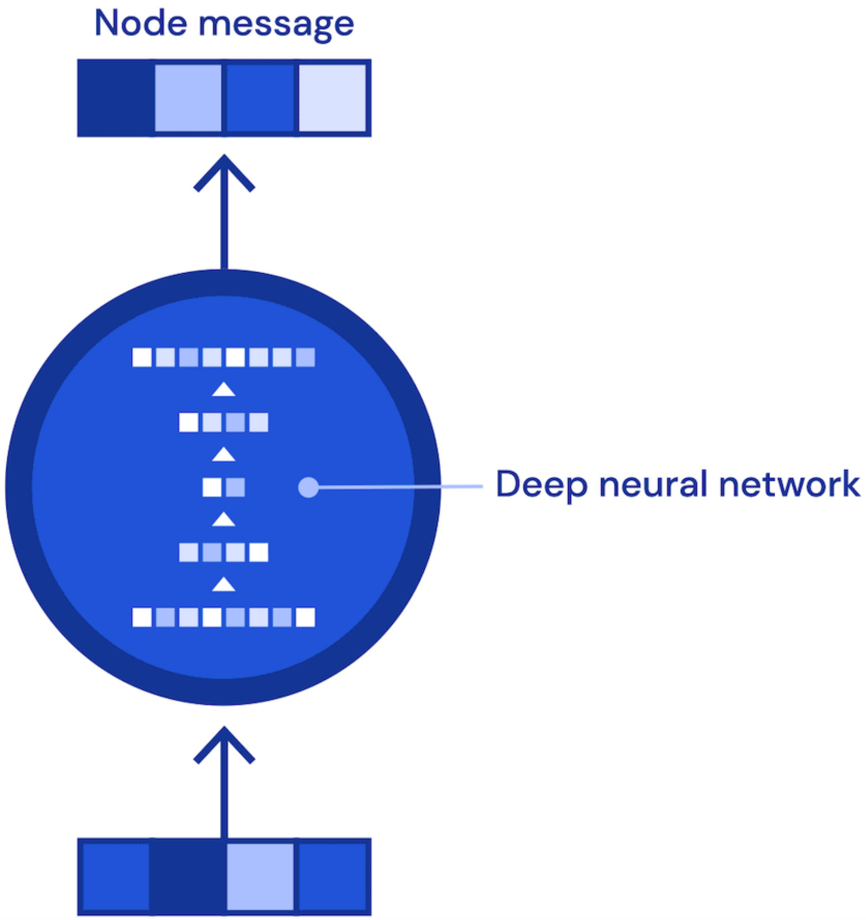

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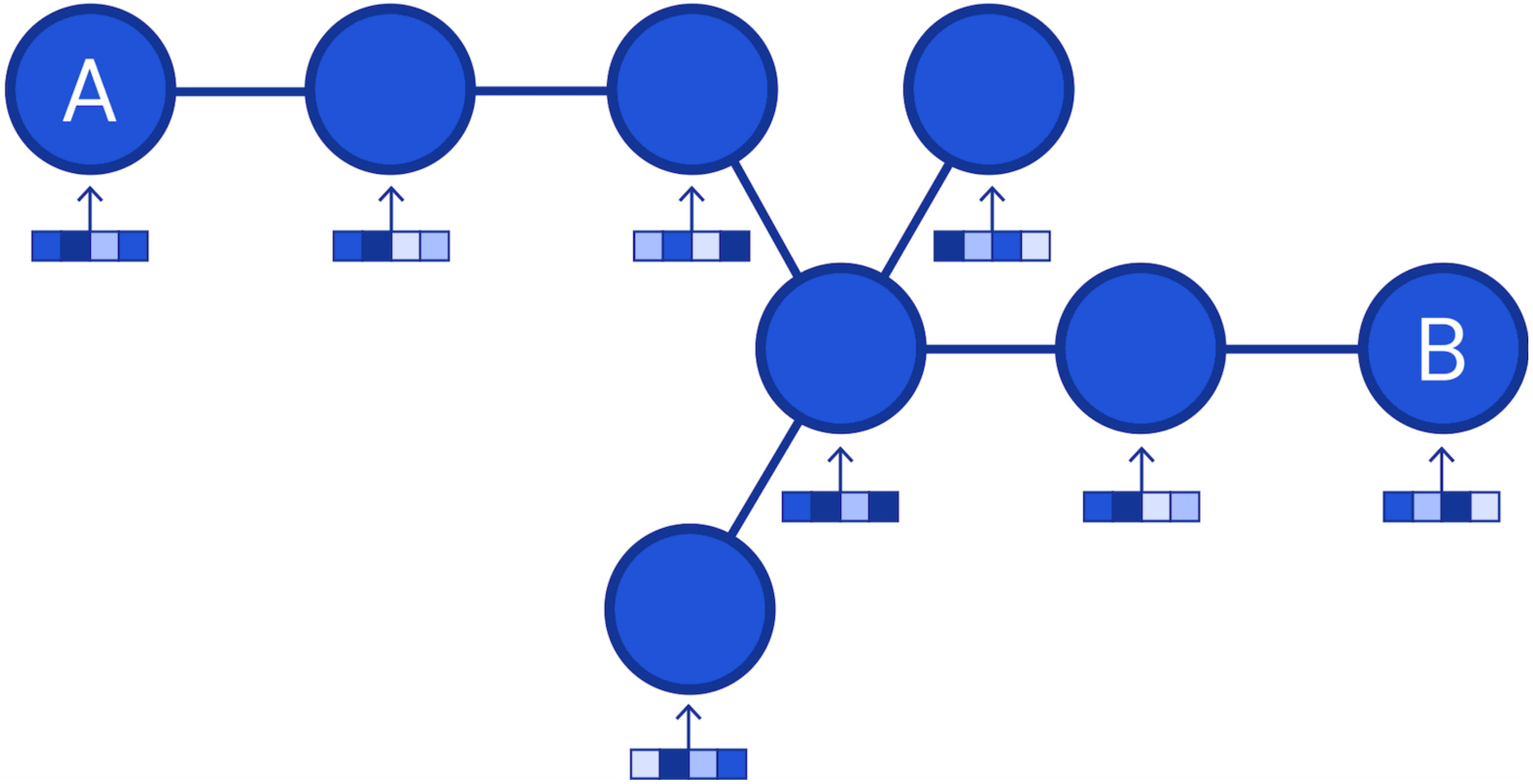

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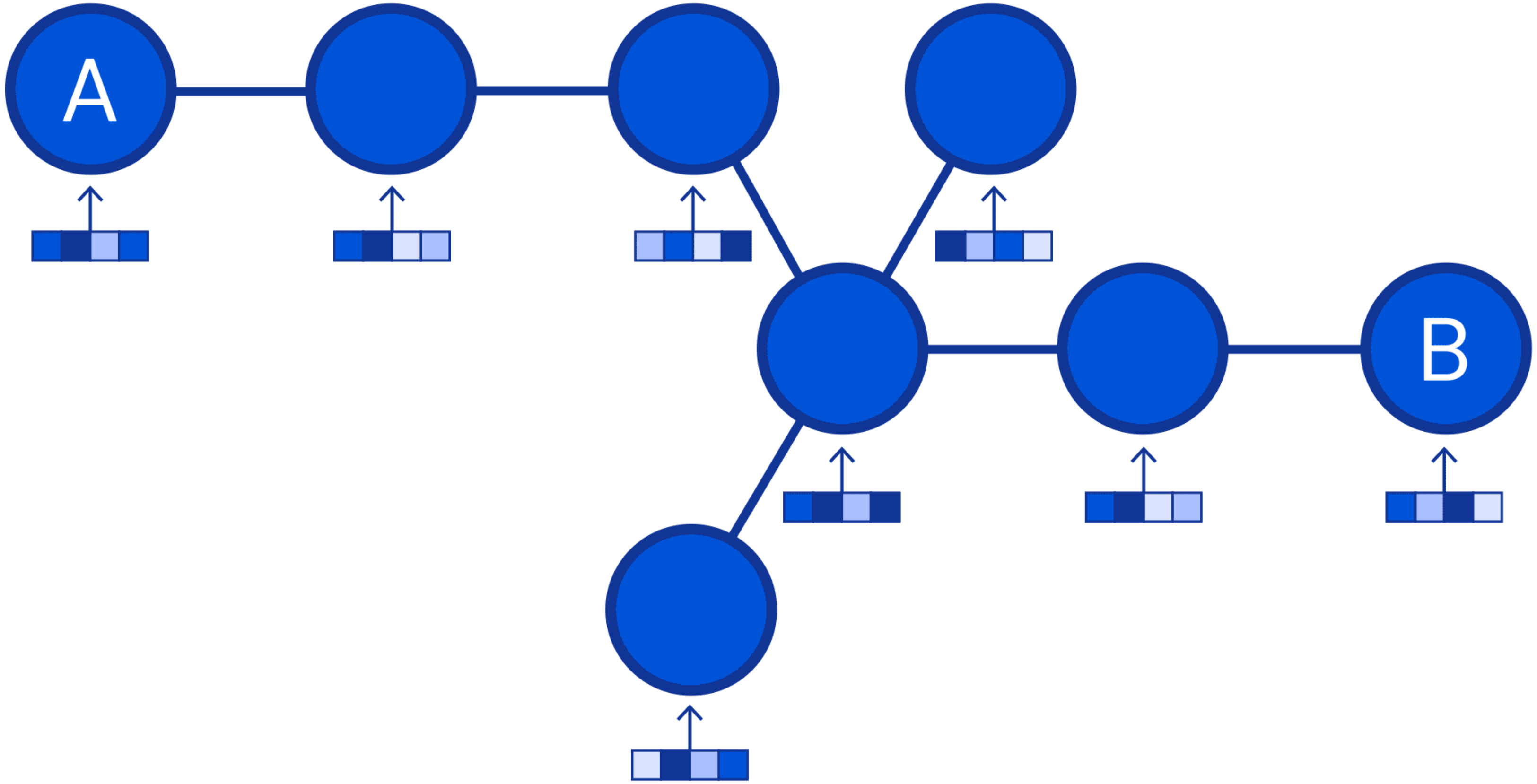

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      i. **Greedy algorithms**
      ii. Integer programming and SAT
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Greedy algorithms

Many graph problems are **NP-hard**

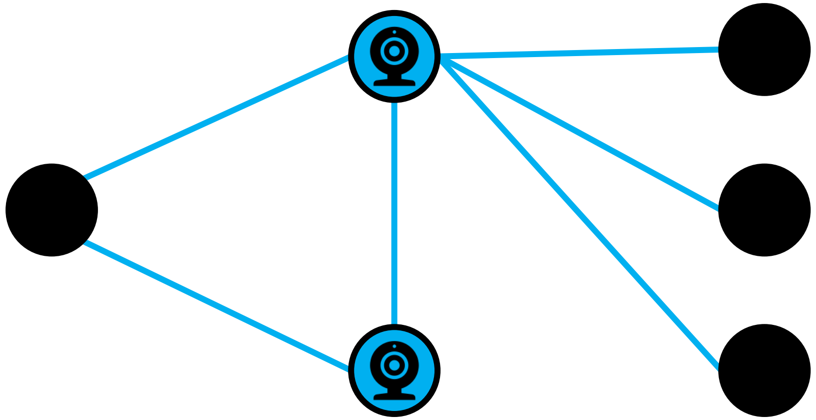
Greedy algorithms: a common type of fast heuristic algorithm

Example: minimum vertex cover

Find smallest vertex subset such that each edge is covered

Example application:

Installing cameras in corners covering all hallways on a floor



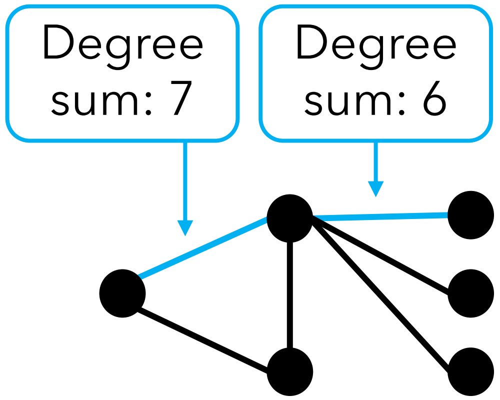
Example: minimum vertex cover

Find smallest vertex subset such that each edge is covered

Classic greedy algorithm:

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

Degree: # of edges adjacent to a vertex



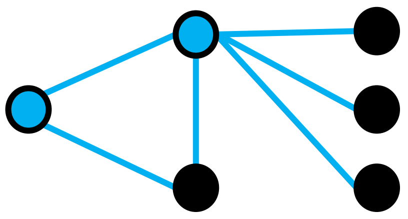
Example: minimum vertex cover

Find smallest vertex subset such that each edge is covered

Classic greedy algorithm:

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

Scoring function that guides greedy algorithm



Example: TSP

1. Among all cities not in the subtour:
   Choose the one that's *farthest* from any city in the subtour
2. Insert it into the subtour

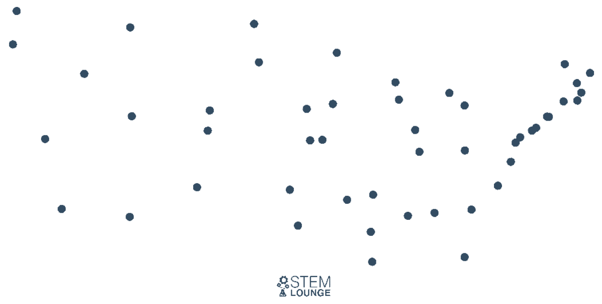
Scoring function that guides greedy algorithm

RL for combinatorial optimization

Goal: **learn** a scoring function to guide greedy algorithm

Represented by a GNN

We'll see how to use *Q-learning* to train GNN



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

ML as a toolkit for theory?

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."

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Integer programming

Integer program (IP)

$$\begin{aligned} \max \quad & \boldsymbol{c} \cdot \boldsymbol{z} \\ \text{s.t.} \quad & A\boldsymbol{z} \leq \boldsymbol{b} \\ & \boldsymbol{z} \in \mathbb{Z}^n \end{aligned}$$

Tons of applications:

Routing

Manufacturing

Scheduling

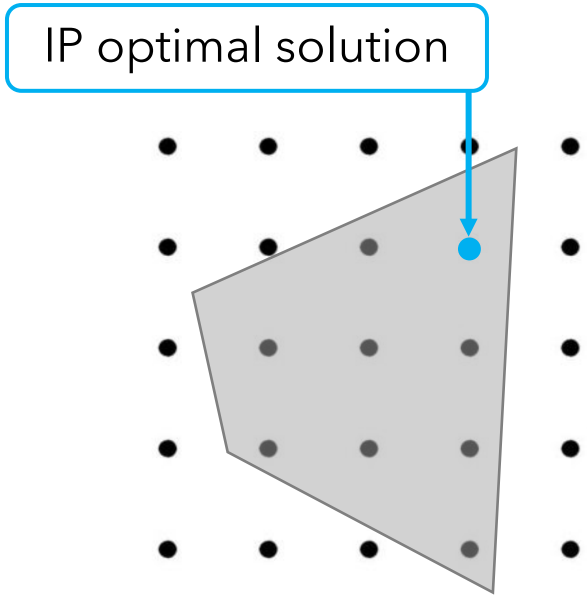
Planning

Finance

Integer programming

Integer program (IP)

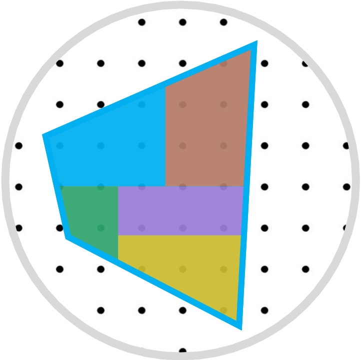
$$\begin{aligned} \max \quad & \boldsymbol{c} \cdot \boldsymbol{z} \\ \text{s.t.} \quad & A\boldsymbol{z} \leq \boldsymbol{b} \\ & \boldsymbol{z} \in \mathbb{Z}^n \end{aligned}$$



Integer programming

Recursively partitions feasible region

Partition organized with a **tree data structure**



Partitioning policy has a big impact on runtime

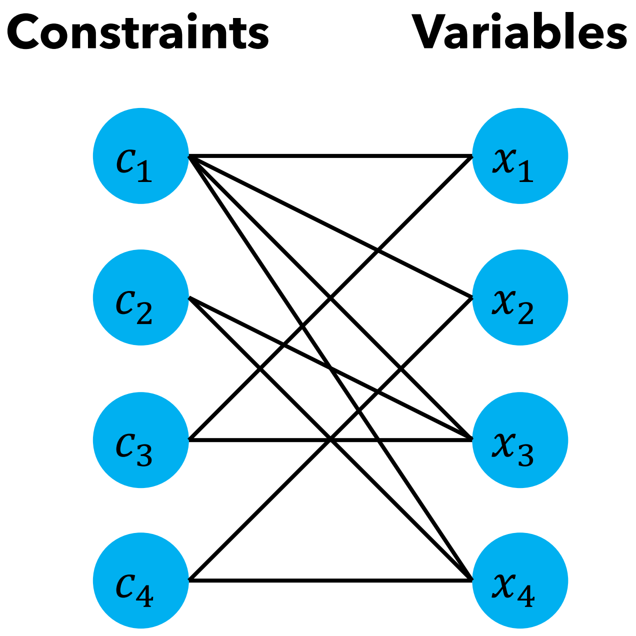
Goal: Use a GNN to guide tree search

Large improvements over leading open-source solver

GNNs for integer programming

Key insight: IP can be encoded as a **graph**

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



Goal: Use a GNN to guide tree search

Large improvements over leading open-source solver

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

SAT

$$
\begin{aligned}
& (x_1 \vee x_4) \\
\wedge\ & (x_1 \vee \bar{x}_3 \vee \bar{x}_8) \\
\wedge\ & (x_1 \vee x_8 \vee x_{12}) \\
\wedge\ & (x_2 \vee x_{11}) \\
\wedge\ & (\bar{x}_7 \vee \bar{x}_3 \vee x_9) \\
\wedge\ & (\bar{x}_7 \vee x_8 \vee \bar{x}_9) \\
\wedge\ & (x_7 \vee x_8 \vee \bar{x}_{10}) \\
\wedge\ & (x_7 \vee x_{10} \vee \bar{x}_{12})
\end{aligned}
$$

SAT: Is there an assignment of $x_1, \ldots, x_{12} \in \{0,1\}$ such that this formula evaluates to **True**?

Published as a conference paper at ICLR 2019

LEARNING A SAT SOLVER FROM SINGLE-BIT SUPERVISION

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Topics

- Graph fundamentals and famous graph algorithms
- GNNs
- Reinforcement learning (Q-learning)
- Integer programming and SAT solving

Outline

1. Introduction
2. Course logistics
3. Applied topics
   a. Pointer networks for the traveling salesman problem (TSP)
   b. Graph neural networks
   c. Integer programming
   d. **Transformers and LLMs**
4. Theoretical topics

Integer programming

$$
\begin{array}{ll}
\max & \boldsymbol{c} \cdot \boldsymbol{z} \\
\text{s.t.} & A\boldsymbol{z} \leq \boldsymbol{b} \\
 & \boldsymbol{z} \in \mathbb{Z}^n
\end{array}
$$

- Formulating a problem as an IP can be hard
- Requires a lot of domain expertise

Tons of applications:


Routing


Manufacturing


Scheduling


Planning


Finance

LLMs for discrete modeling

$$\begin{aligned} \text{max} \quad & \boldsymbol{c} \cdot \boldsymbol{z} \\ \text{s.t.} \quad & A\boldsymbol{z} \leq \boldsymbol{b} \\ & \boldsymbol{z} \in \mathbb{Z}^n \end{aligned}$$

- Formulating a problem as an IP can be hard
- Requires a lot of domain expertise
- How to use LLMs to for discrete modeling

Guest lecture by
Madeleine Udell

Topics

- Transformers
- Transformers as algorithms
  E.g., can you teach a transformer to add?
- LLMs for discrete modeling

Outline

1. Introduction
2. Course logistics
3. Applied topics
4. **Theoretical topics**
   i. **Statistical guarantees and online algorithm configuration**
   ii. Algorithms with predictions
5. Plan for the next 2 weeks

Algorithm configuration

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

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

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

Modeling the application domain

Problem instances drawn from application-specific dist. $\mathcal{D}$

E.g., **distribution over routing problems**

Widely assumed in applied research, e.g.:

Horvitz, Ruan, Gomez, Kautz, Selman, Chickering	UAI'01
Xu, Hutter, Hoos, Leyton-Brown	JAIR'08
He, Daumé, Eisner	NeurIPS'14

And theoretical research on algorithm configuration, e.g.:

Gupta, Roughgarden	ITCS'16
Balcan	Book Chapter'20

Automated configuration procedure

1. Fix parameterized algorithm
2. Receive set of "typical" inputs sampled from unknown $\mathcal{D}$

Problem instance 1

Problem instance 2

• • •

3. Return parameter setting $\hat{\boldsymbol{\rho}}$ with good avg performance

Runtime, solution quality, etc.

Automated configuration procedure

Statistical question: Will $\hat{\rho}$ have good **future** performance?

More formally: Is the expected performance of $\hat{\rho}$ also good?

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

Automated configuration procedure

1. Fix parameterized algorithm
2. Receive set of "typical" inputs sampled from unknown $\mathcal{D}$

Problem instance 1

Problem instance 2

• • •

3. Return parameter setting $\hat{\rho}$ with good avg performance

Runtime, solution quality, etc.

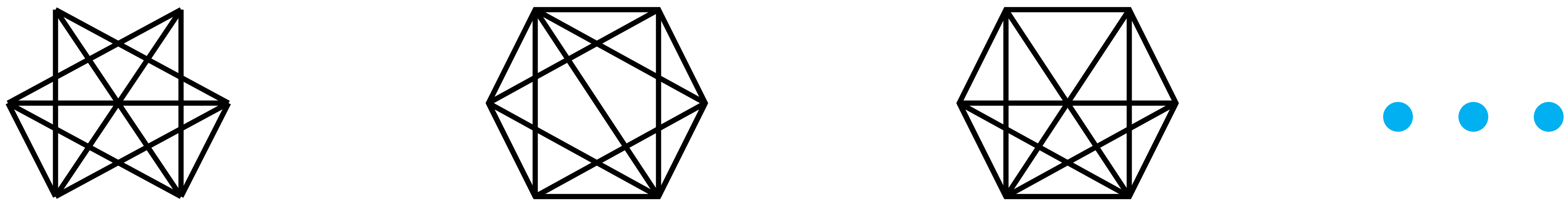
Model is known as the "**batch-learning** setting"

Optimize over a ***batch*** *of input problem instances*

Online algorithm configuration

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

Day 1: $\boldsymbol{\rho}_1$ Day 2: $\boldsymbol{\rho}_2$ Day 3: $\boldsymbol{\rho}_3$



Goal: Compete with best parameter setting in hindsight

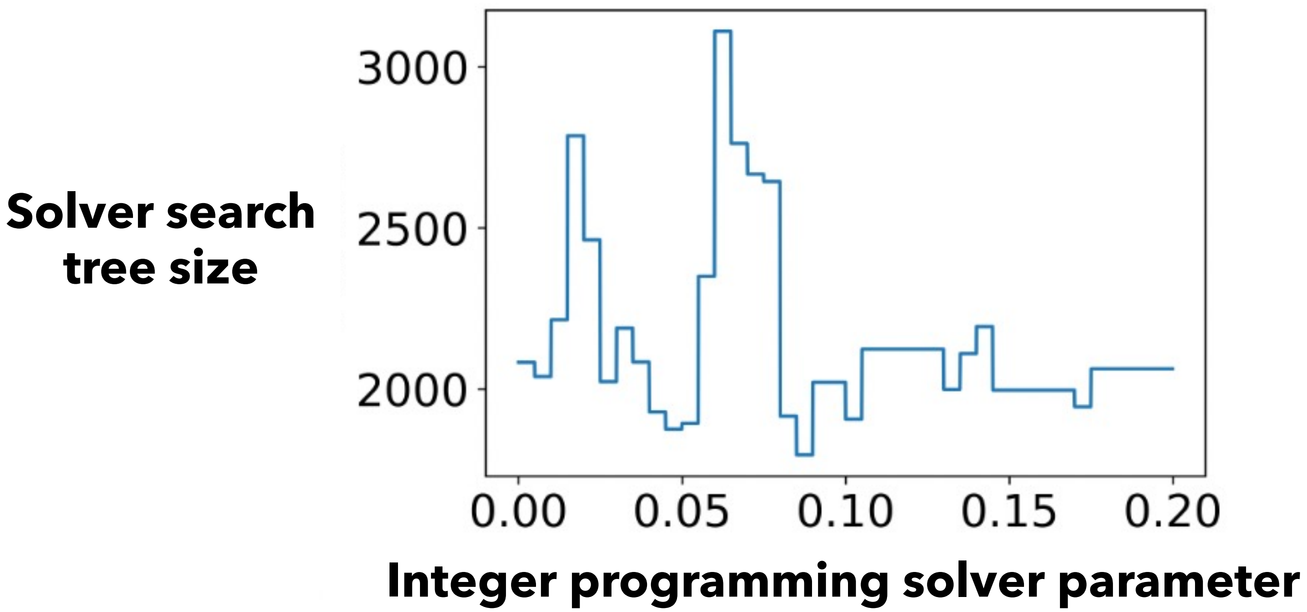
- Impossible in the worst case
- Under what conditions is online configuration possible?

Gupta and Roughgarden, ITCS'16; Cohen-Addad, Kanade AISTATS'17; Balcan, Dick, Vitercik, FOCS'18; …

Primary challenge

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

Complex connection between parameters and performance



Balcan, Prasad, Sandholm, Vitercik, NeurIPS'21

Topics

- Statistical learning theory
- Online learning

Outline

1. Introduction
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Algorithms with predictions

Assume you have some **predictions** about your problem, e.g.:

Probability any given element is in a huge database

Kraska et al., SIGMOD'18; Mitzenmacher, NeurIPS'18

In caching, the next time you'll see an element

Lykouris, Vassilvitskii, ICML'18

Main question:

How to use predictions to improve algorithmic performance?

Example: Ski rental problem

- **Problem:** Skier will ski for unknown number of days
  - Can either **rent each day** for \$1/day or **buy** for $\$b$
  - E.g., if ski for 5 days and then buy, total price is $5 + b$
- If ski x days, **opt clairvoyant** strategy pays $\mathrm{OPT} = \min\{x, b\}$
- **Breakeven strategy:** Rent for $b - 1$ days, then buy

$$\text{CR} = \frac{\mathrm{ALG}}{\mathrm{OPT}}$$

Competitive ratio

Example: Ski rental problem

Prediction y of number of skiing days, error $\eta = |x - y|$

Algorithm (with parameter $\lambda \in (0,1)$):

If $y \geq b$, buy on start of day $\lceil \lambda b \rceil$; else buy on start of day $\left\lceil \frac{b}{\lambda} \right\rceil$

Don't jump the gun… *…but don't wait too long*

Theorem: Algorithm has CR $\leq \min\left\{\frac{1+\lambda}{\lambda}, 1 + \lambda + \frac{\eta}{(1-\lambda)\mathrm{OPT}}\right\}$

- If predictor is perfect ($\eta = 0$), **CR is small** ($\leq 1 + \lambda$)
- No matter how big η is, setting $\lambda = 1$ **recovers baseline** CR $= 2$

Purohit, Svitkina, Kumar, NeurIPS'18

Design principals

Consistency:

Predictions are perfect ⇒ recover offline optimal

Robustness:

Predictions are terrible ⇒ no worse than worst-case

Lykouris, Vassilvitskii, ICML'18

Many different applications

Online advertising
Mahdian, Nazerzadeh, Saberi, EC'07; Devanur, Hayes, EC'09; Medina, Vassilvitskii, NeurIPS'17; …

Caching
Lykouris, Vassilvitskii, ICML'18; Rohatgi, SODA'19; Wei, APPROX-RANDOM'20; …

Frequency estimation
Hsu, Indyk, Katabi, Vakilian, ICLR'19; …

Learning low-rank approximations
Indyk, Vakilian, Yuan, NeurIPS'19; …

Scheduling
Mitzenmacher, ITCS'20; Moseley, Vassilvitskii, Lattanzi, Lavastida, SODA'20; …

Matching
Antoniadis, Gouleakis, Kleer, Kolev, NeurIPS'20; …

Queuing
Mitzenmacher, ACDA'21; …

Covering problems
Bamas, Maggiori, Svensson, NeurIPS'20; …

algorithms-with-predictions.github.io

Outline

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Looking forward to getting to know you this quarter!