Welcome to

Machine Learning for

Algorithm Design!

About me

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

Research revolves around
- Machine learning for algorithm design
- 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 **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

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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**

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Algorithm configuration

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

- CPLEX has **170-page** manual describing **172** parameters
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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

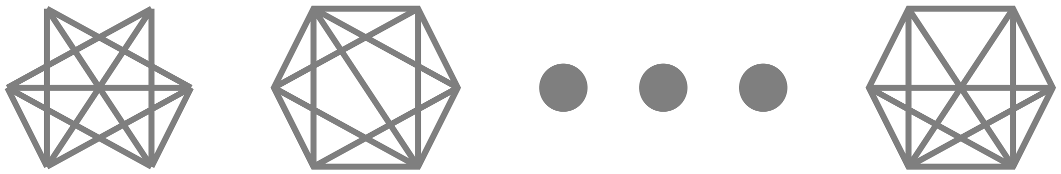
Worst-case analysis has been the main framework for decades

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

Scheduling problems an airline solves

Course topics

Range of techniques for integrating ML into algorithm design

1. **Applied topics**
   i. Graph neural networks
   ii. Integer programming and SAT
   iii. Reinforcement learning
   iv. Data structures

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

Outline

1. Introduction
2. **Course logistics**
3. Applied topics
4. Theoretical topics
5. Plan for the next 2 weeks

Course logistics

Website: vitercik.github.io/ml4algs

Office hours:

- Tuesday 11am-12pm in Huang 250
- Or by appointment, please feel free to reach out!

Course setup

1. **Lectures given by the instructor**
    - Key techniques for integrating ML into algorithm design
    - *E.g., graph neural networks, reinforcement learning, theoretical ML*

2. **Paper discussions**
    - Covering influential papers in the field

Paper discussions

- 10 paper discussion classes
- Each student will take on a **presenter role** for 5 discussions
  - Archaeologist
  - Researcher
  - Industry R&D expert
  - Private investigator
  - NeurIPS reviewer
  - (Based on a course design by Alec Jacobson and Colin Raffel)
- (Students may need to pair up depending on class size)

Paper discussions

- Presentations will be approximately 7 minutes + 5 min Q&A
- I'll distribute a Google spreadsheet next week to select roles

Presenter role: Archaeologist

- Determine where the paper sits in the context of previous and subsequent work
- Find and report on:
  1. One older paper cited by the current paper, and
  2. One newer paper citing this current paper

Presenter role: Researcher

- Propose a follow-up project on the current paper
  - Should only be possible due to the paper's existence and success

Presenter role: Industry R&D expert

- Convince your industry bosses that it's worth your time and money to implement this paper into the company's pipeline
- Choose an appropriate company and product or application

Presenter role: Private investigator

- Find out background information on one of the paper authors
  - Where have they worked?
  - What did they study?
  - What previous projects might have led to working on this one?

Presenter role: NeurIPS reviewer

Answer the questions on the NeurIPS review form

Originality, quality, clarity, significance, etc.

Non-presenter assignment

By 1pm on the day of class, post to Ed discussion:

at least one question about the paper. E.g.

- Something you're confused about
- Something you'd like to hear discussed more

Course project

- All students will write a "mini-paper" as a final project
- Can be empirical, theoretical, or both

Project policies

- Encouraged to work in groups!
  - Up to 3 people (except with special permission)
- Groups of 2 should put twice as much work into the final project than for a sole-author project
  - Similarly for groups of 3
- Paper length for a final project write-up is 3 + n where n is the number of people in the group that worked on the project
  - Not including references or the contributions paragraph
- Required to include a “contributions” paragraph in final paper that concretely lists each author's contributions

Milestones

April 17-21: All groups meet with me to discuss project ideas

- Please come prepared with ideas/interests!
- Look out for an email about scheduling this meeting

May 5: Submit a progress report of 1-2 pages

- Describe your project and partial progress

May 11: Short presentation about a paper related to your project

June 8: Present your final project during class

June 12: Submit your final report

Grading

Out of 100 points:

- Discussion: 60 points
  - Each **presentation** is worth 10 points
  - Each **non-presenter assignment** is worth 2 points
- Project: 40 points
  - **Progress report**: 7 points
  - **Midterm presentation**: 8 points.
  - **Novelty**: 5 points
    - Project should propose something new (new application, method, perspective)
  - **Writing**: 10 points
    - Final paper should be readable and complete and situate itself among related work
  - **Final presentation**: 10 points
    - Final presentation should be clear and provide a solid picture of what you did

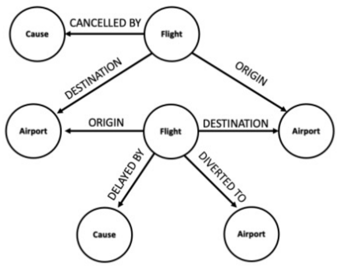
Prerequisites

- Introductory algorithms class
- Machine learning class is helpful but not required

Outline

1. Introduction
2. Course logistics
3. **Applied topics**
   1. **Graph neural networks**
   2. Integer programming and SAT
   3. Reinforcement learning
   4. Data structures
4. Theoretical topics
5. Plan for the next 2 weeks

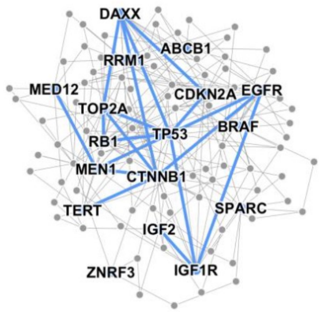
Many types of data are graphs



Event Graphs

Image credit: SalientNetworks

Computer Networks



Disease Pathways

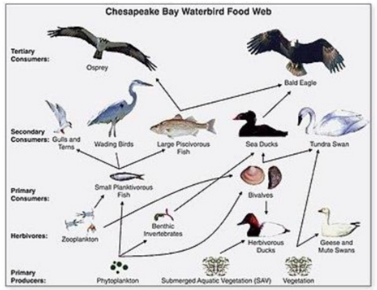


Image credit: Wikipedia

Food Webs

Image credit: Pinterest

Particle Networks

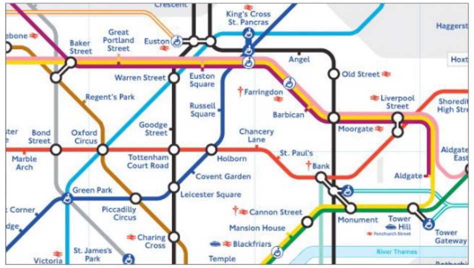


Image credit: visitlondon.com

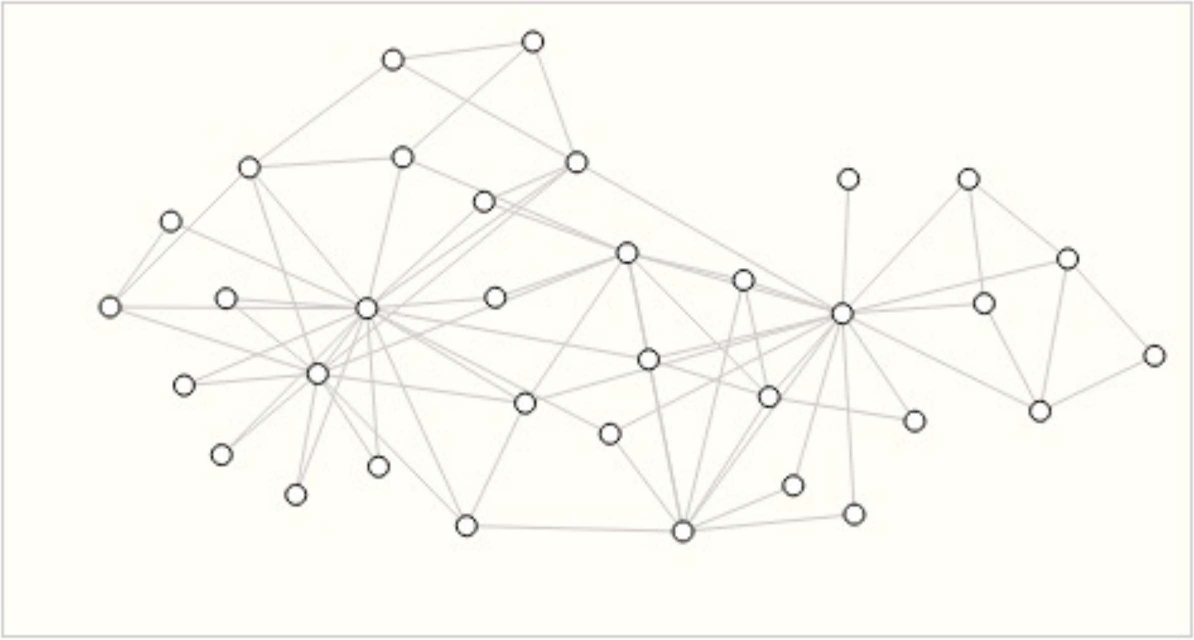
Underground Networks

Slide by Leskovec

GNN motivation

Special type of NN architecture for tasks involving graphs

How to utilize relational structure for better prediction?

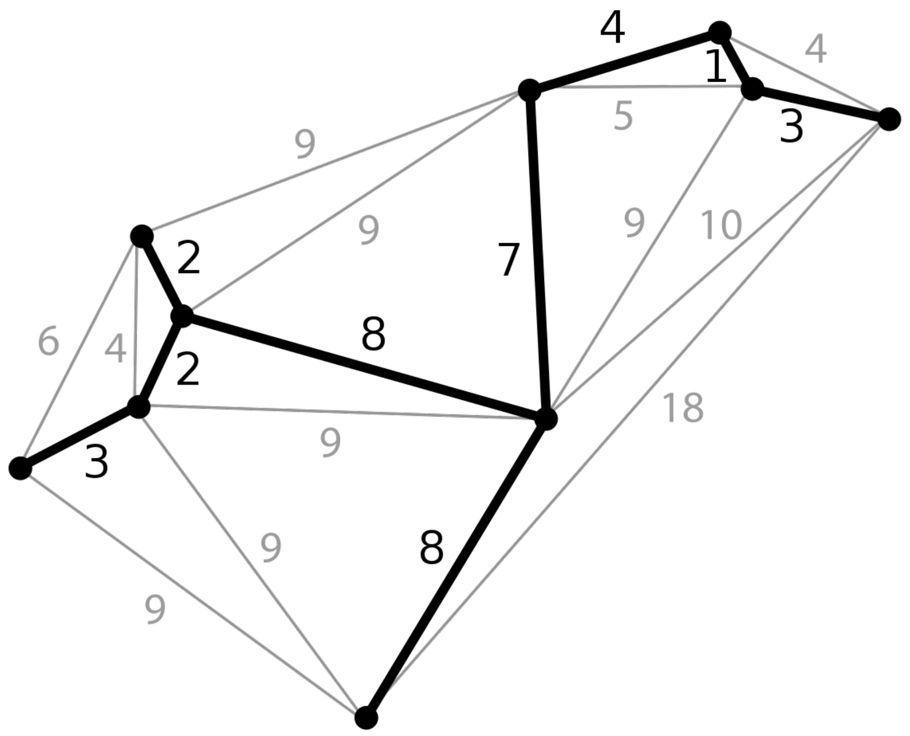


Shortest path prediction

Example: predicting the shortest path in a graph

MST prediction

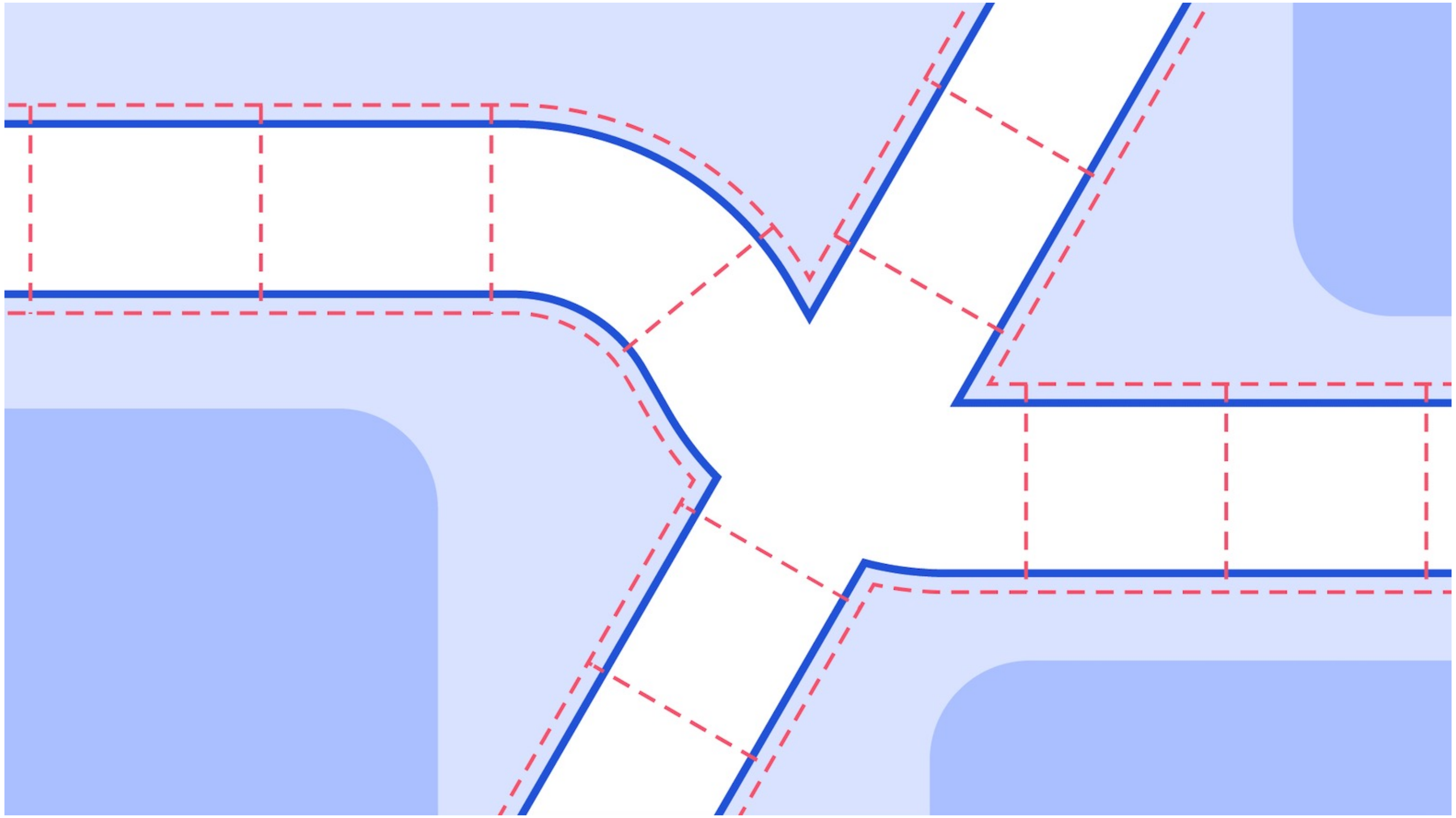
Example: predicting a minimum spanning tree



GNN: Message passing

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

GNN: Message passing



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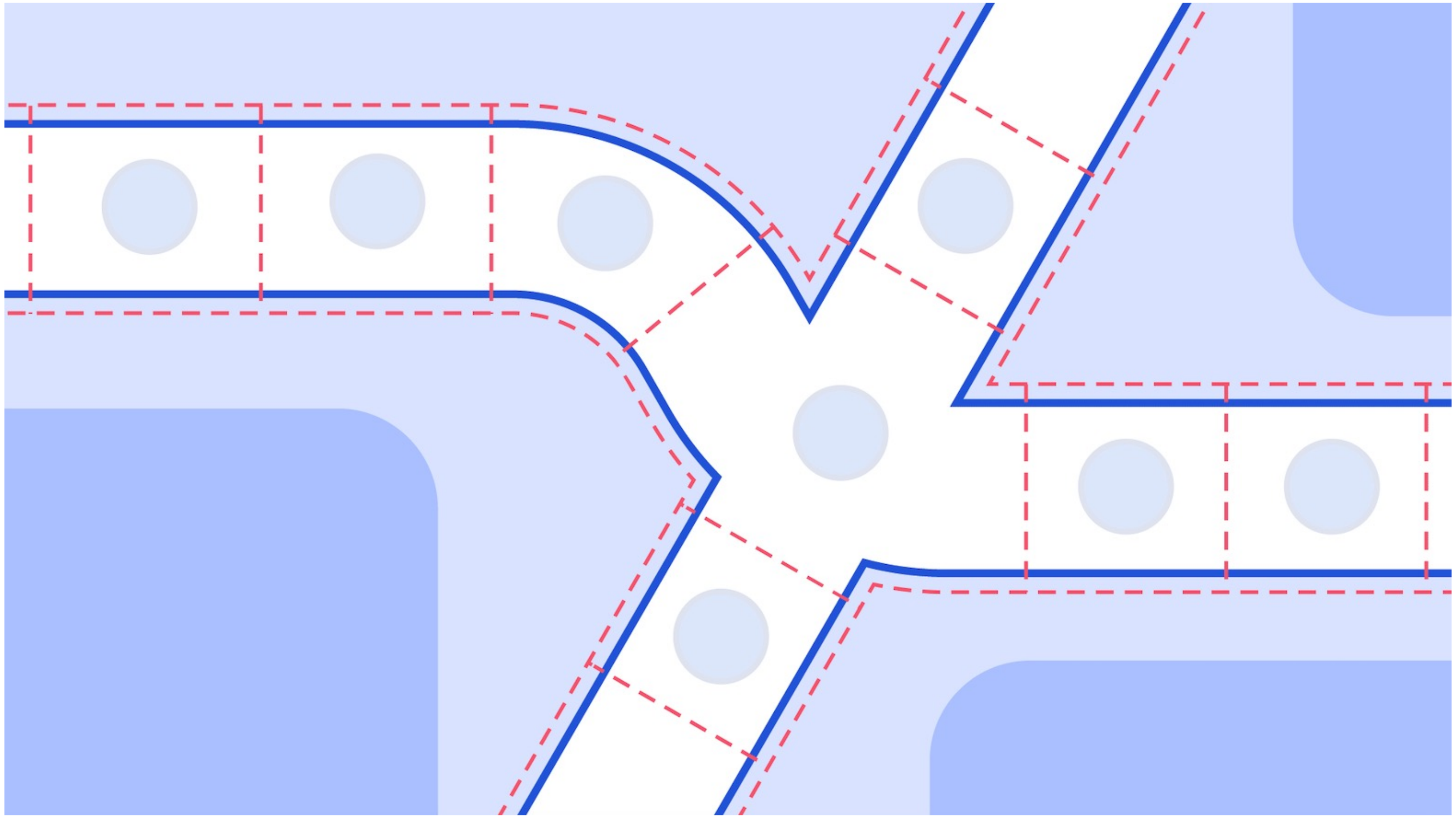
GNN: Message passing



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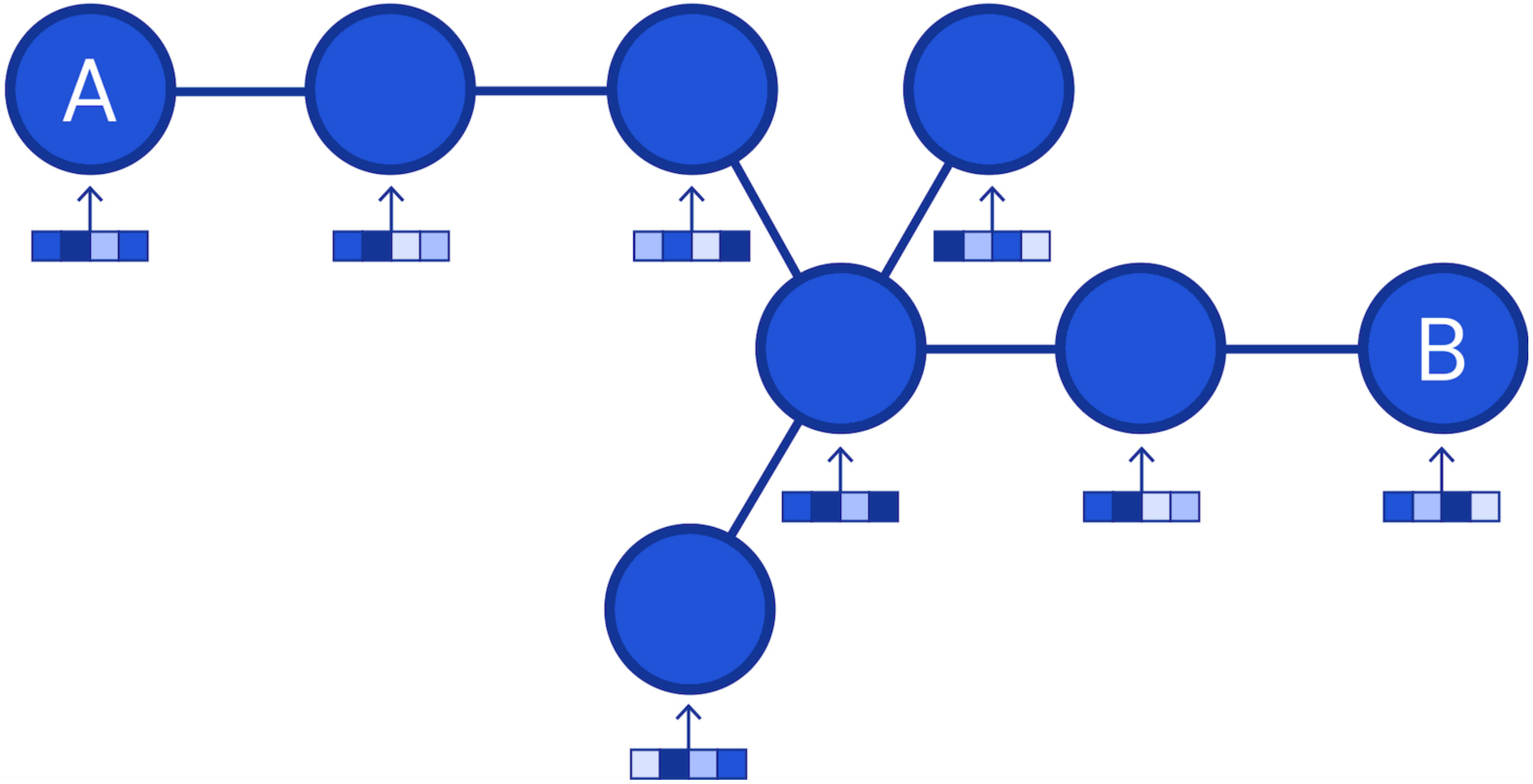

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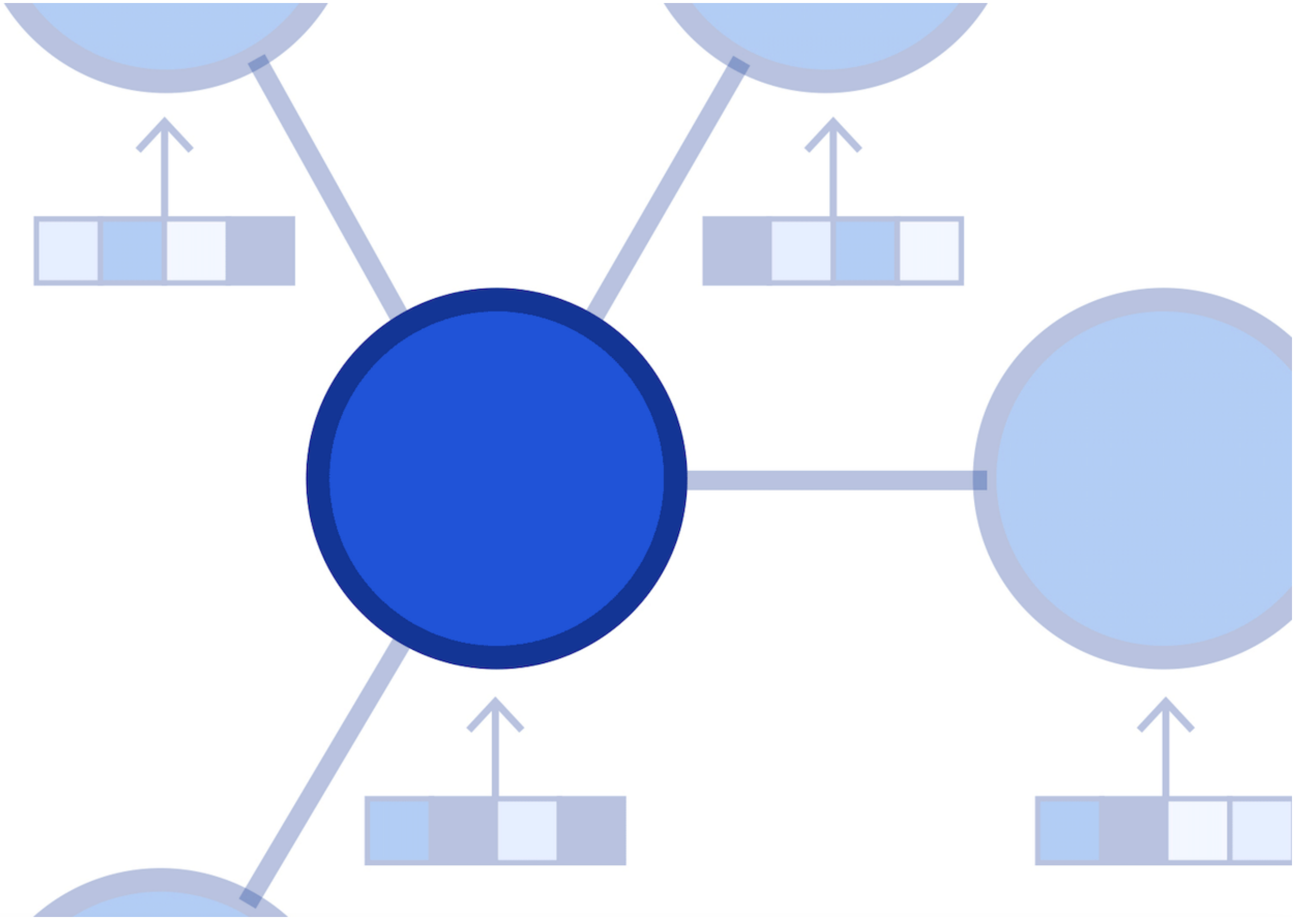

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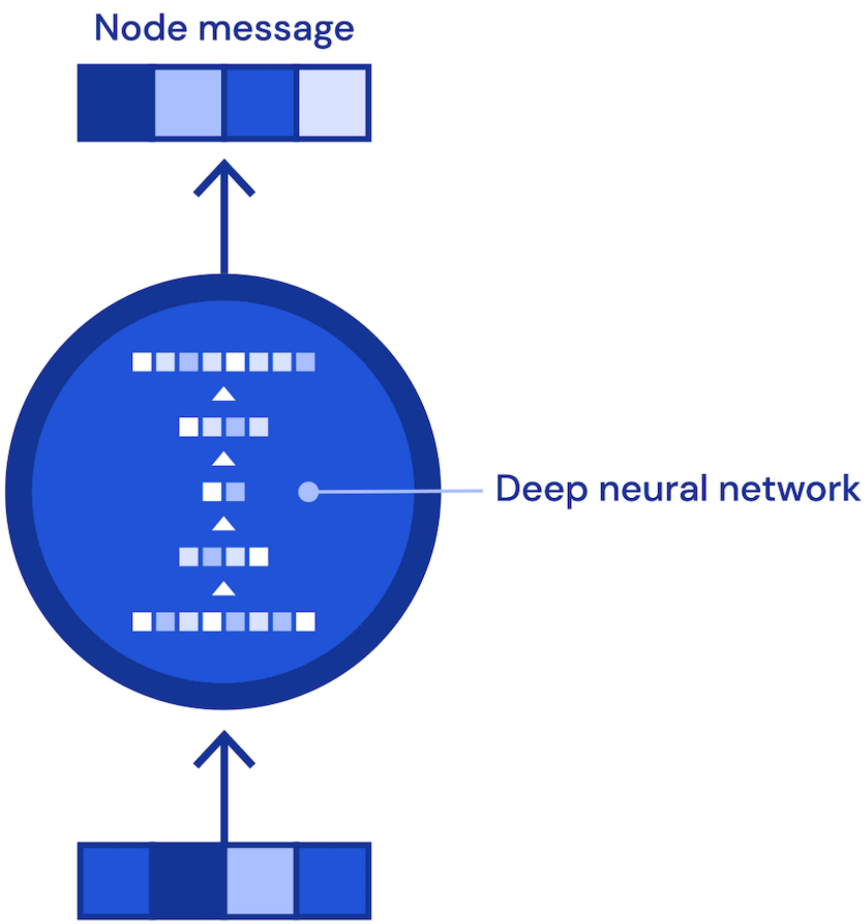

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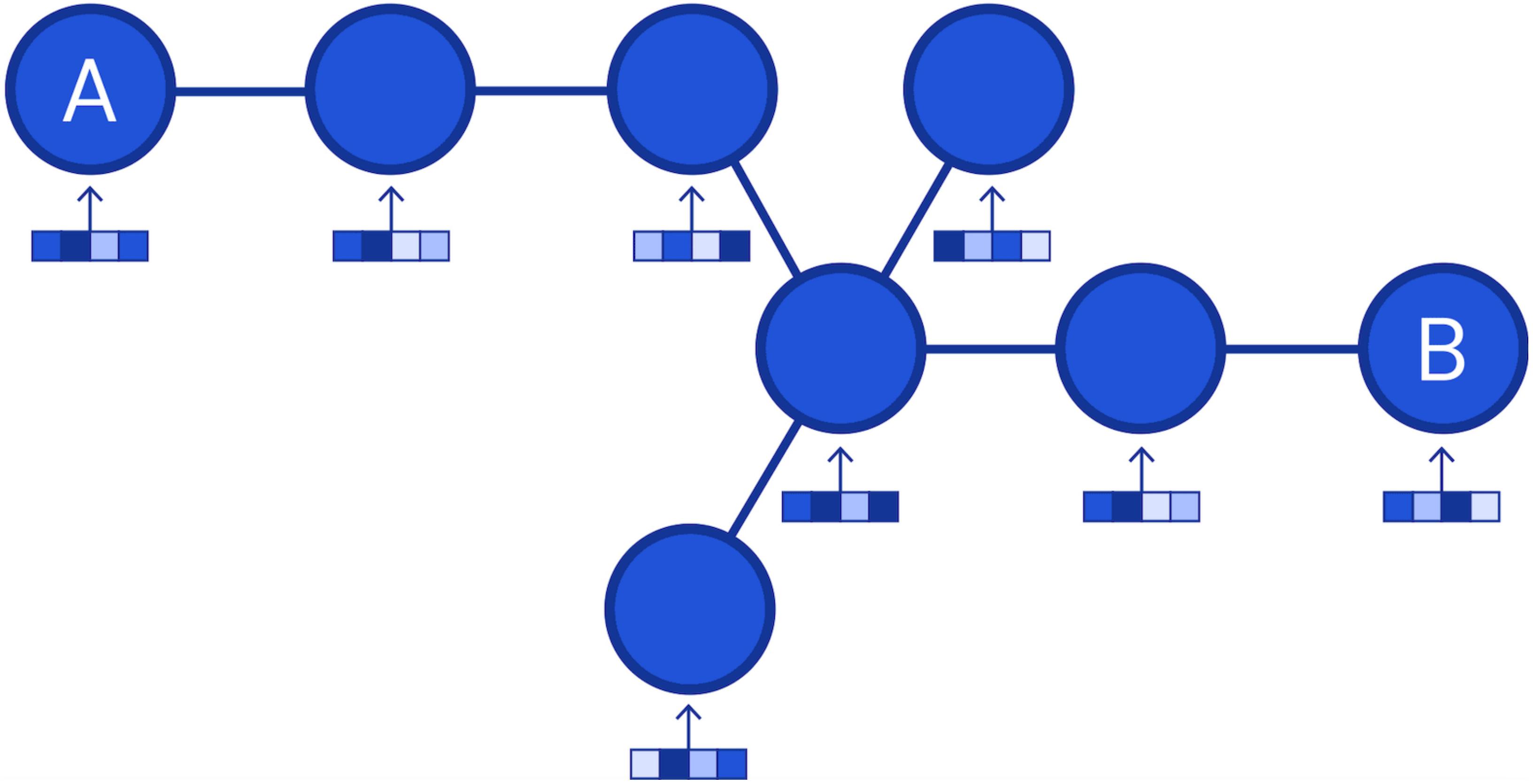
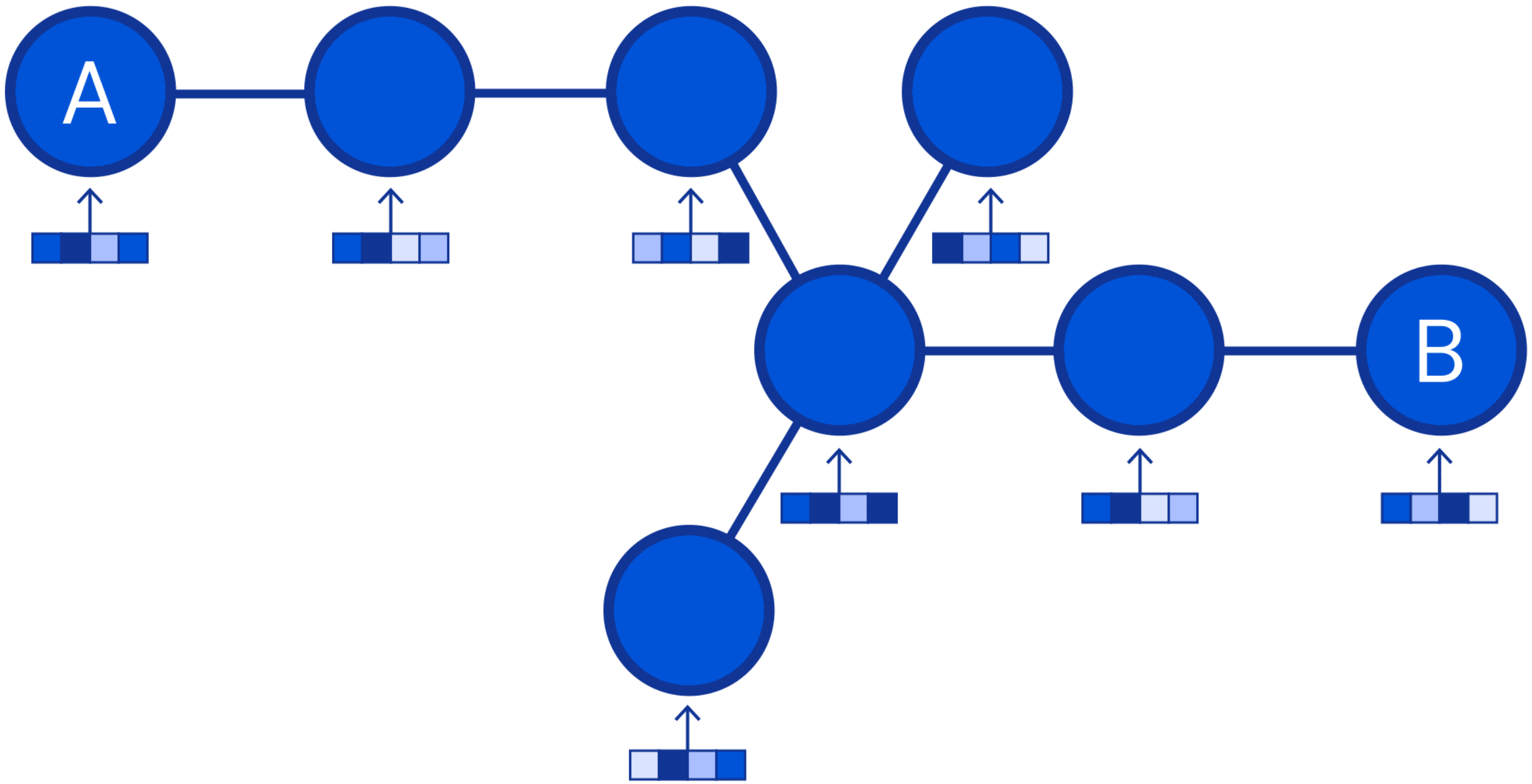
GNN: Message passing



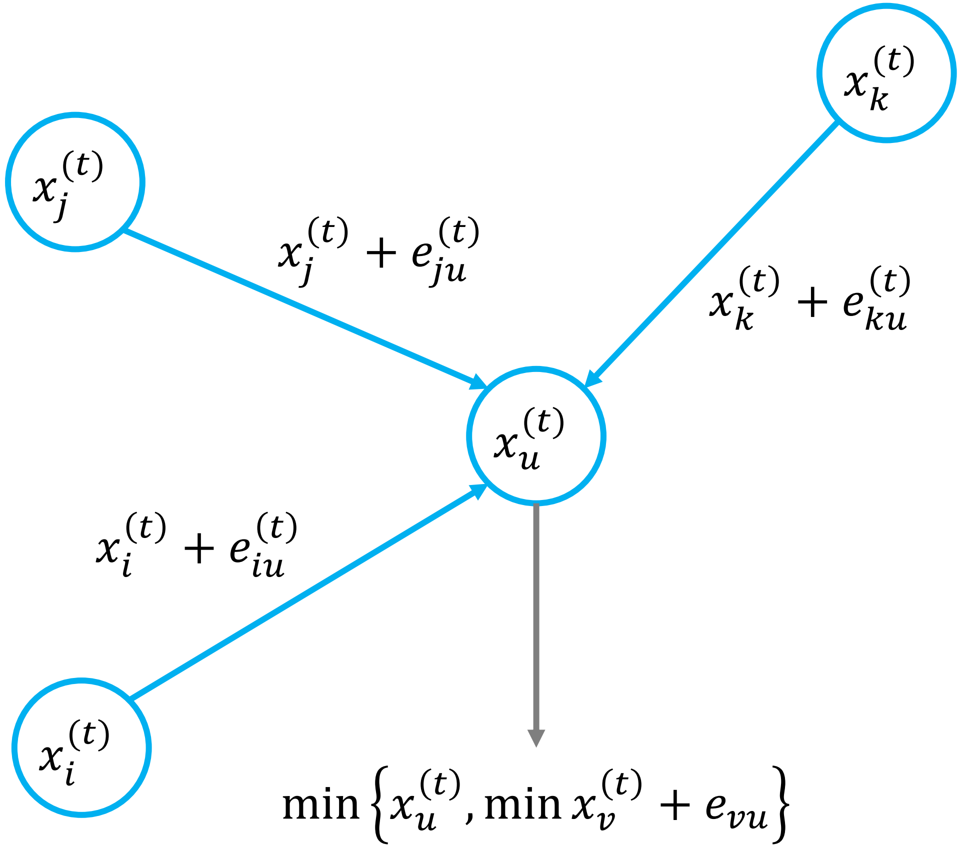
https://www.deepmind.com/blog/traffic-prediction-with-advanced-graph-neural-networks

GNN: Message passing



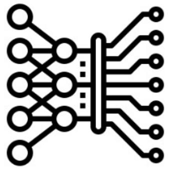
https://www.deepmind.com/blog/traffic-prediction-with-advanced-graph-neural-networks

Bellman-Ford: Message passing



Why use GNNs for algorithm design?

- Classical algorithms are designed with abstraction in mind
  - Enforce their inputs to conform to stringent preconditions
- Challenges:
  - Natural inputs may be only partially observable
  - Manually converting natural inputs into abstract inputs leads to information loss
- **Goal:** end-to-end neural pipeline which is fully differentiable

Natural inputs →  → Natural outputs

Slide inspired by Petar Veličković

Papers we'll read

Veličković, Petar, et al. "Neural execution of graph algorithms." *ICLR*. 2020.

- GNNs don't work off-the-shelf for combinatorial tasks
- How to **align** GNN architectures to these tasks

Cappart, Quentin, et al. "Combinatorial optimization and reasoning with GNNs." *arXiv*.

- **Broad overview** of the field; current & future directions

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SAT

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

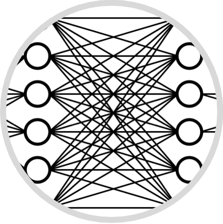
SAT: Is there an assignment of $x_1, \dots, x_{12} \in \{0,1\}$ such that this formula evaluates to **True**?

Integer program

Integer program (IP)

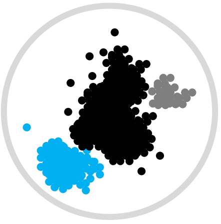
$$\begin{aligned} \text{max} \quad & \boldsymbol{c} \cdot \boldsymbol{z} \\ \text{s.t.} \quad & A\boldsymbol{z} \leq \boldsymbol{b} \\ & \boldsymbol{z} \in \mathbb{Z}^n \end{aligned}$$

Tons of applications:



Robust ML

MAP estimation



Clustering

Routing

Scheduling

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

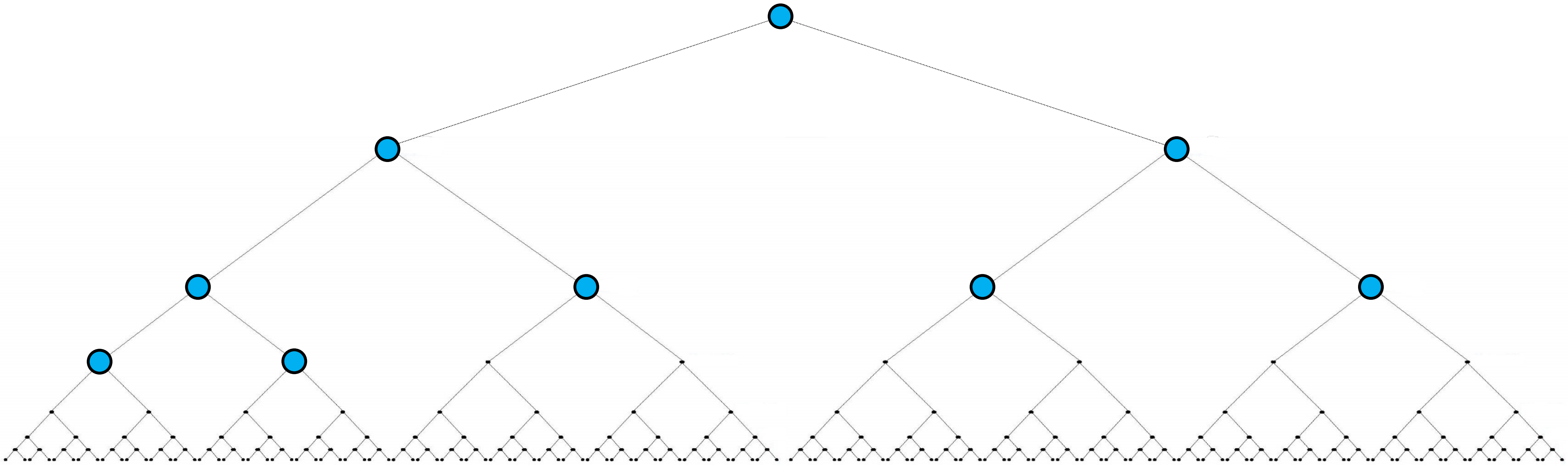
- $\boldsymbol{z} = \left(\frac{1}{2}, 1, 0, 0, 0, 0, 1\right)$ — 140
  - $z_1 = 0$: $\left(0, 1, 0, 1, 0, \frac{1}{4}, 1\right)$ — 135
    - $z_6 = 0$: $\left(0, 1, \frac{1}{3}, 1, 0, 0, 1\right)$ — 133.3
      - $z_3 = 0$: $\boxed{(0, 1, 0, 1, 1, 0, 1)}$ — $\boxed{133}$
      - $z_3 = 1$: $\left(0, \frac{4}{5}, 1, 0, 0, 0, 1\right)$ — 118
    - $z_6 = 1$: $\left(0, \frac{3}{5}, 0, 0, 0, 1, 1\right)$ — 116
  - $z_1 = 1$: $\left(1, \frac{3}{5}, 0, 0, 0, 0, 1\right)$ — 136
    - $z_2 = 0$: $\left(1, 0, 0, 1, 0, \frac{1}{2}, 1\right)$ — 120
    - $z_2 = 1$: $\left(1, 1, 0, 0, 0, 0, \frac{1}{3}\right)$ — 120

Branch and bound (B&B)

Tree-building policies

Tree-building policies can have a huge effect on tree size

E.g., node selection, variable selection, ….



Example: variable selection policies

Score-based variable selection policies:

At leaf Q, branch on variable z_i maximizing $\mathbf{score}(\boldsymbol{Q}, \boldsymbol{i}) \in \mathbb{R}$

Many options! Little known about which to use when

Gauthier, Ribière, Math. Prog. '77; Beale, Annals of Discrete Math. '79; Linderoth, Savelsbergh, INFORMS JoC '99; Achterberg, Math. Prog. Computation '09; Gilpin, Sandholm, Disc. Opt. '11; …

Example: variable selection policies

Score-based variable selection policies:

At leaf Q, branch on variable z_i maximizing $\mathbf{score}(\boldsymbol{Q}, \boldsymbol{i}) \in \mathbb{R}$

Given d scoring rules $\text{score}_1, \ldots, \text{score}_\text{d}$, possible to **learn** best convex combination $\rho_1 \text{score}_1 + \cdots + \rho_d \text{score}_\text{d}$?

History: For a specific score_1 and score_2:

- $\frac{1}{2}\text{score}_1 + \frac{1}{2}\text{score}_2$ Gauthier and Ribière '79
- score_1 Bénichou et al. '71 and Beale '71
- $\frac{1}{3}\text{score}_1 + \frac{2}{3}\text{score}_2$ Linderoth and Savelsbergh '99
- $\frac{1}{6}\text{score}_1 + \frac{5}{6}\text{score}_2$ Achterberg '09

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

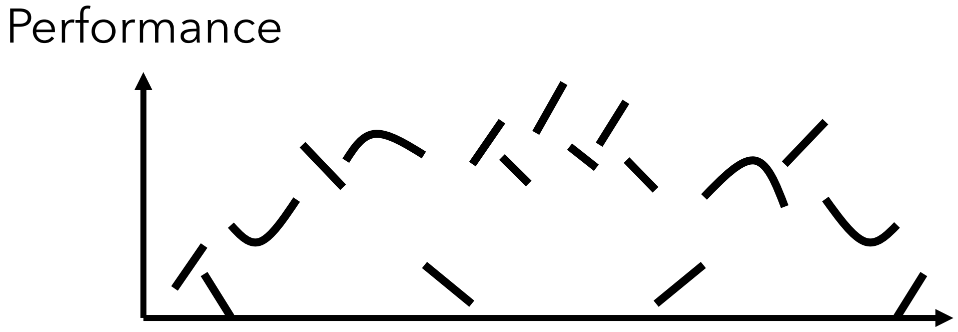




Primary challenge

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

Complex connection between parameters and performance



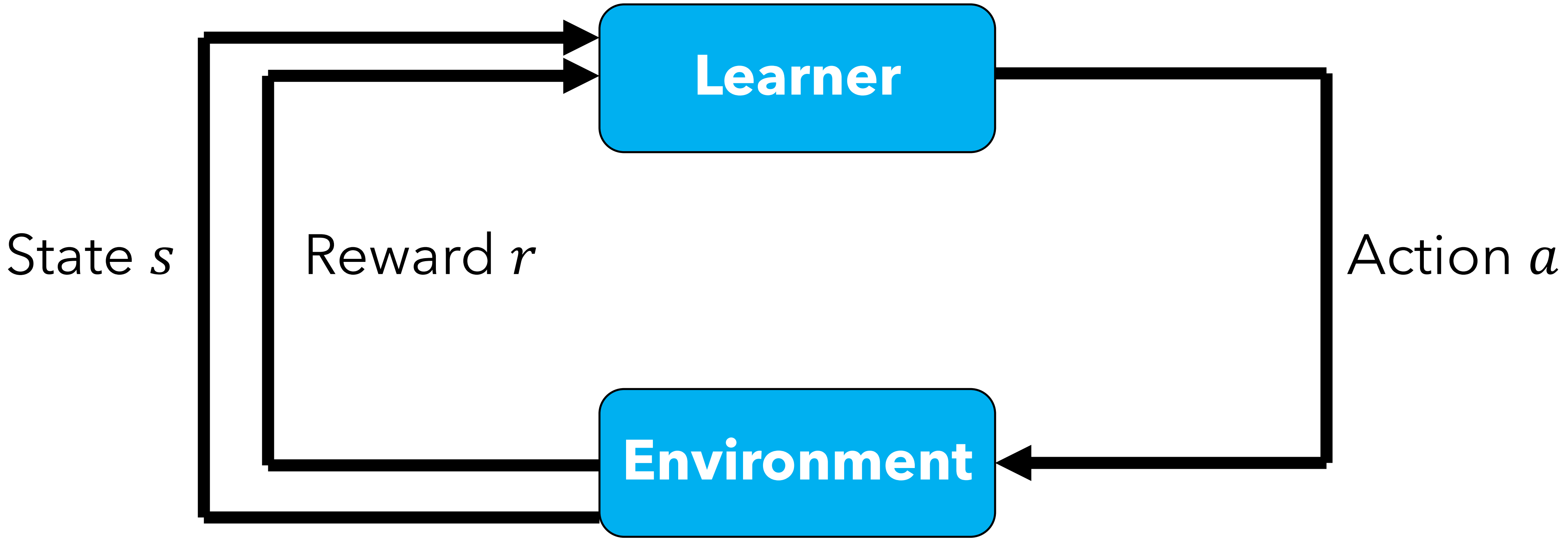
Papers we'll read

- Hutter, Frank, et al. "ParamILS: an automatic algorithm configuration framework." *JAIR* 36 (2009): 267-306.
    - Methods for **searching** through combinatorial parameter space
- Xu, Lin, et al. "SATzilla: portfolio-based algorithm selection for SAT." *JAIR* 32 (2008): 565-606.
    - How to compile a **portfolio** of algorithm configurations
    - At runtime, use **ML** to **select** a configuration from portfolio
- Gasse, Maxime, et al. "Exact combinatorial optimization with graph convolutional neural networks." *NeurIPS*. (2019).
    - Use **GNNs** to design **variable selection** policies

Outline

1. Introduction
2. Course logistics
3. Applied topics
   i. Graph neural networks
   ii. Integer programming and SAT
   iii. **Reinforcement learning**
   iv. Data structures
4. Theoretical topics
5. Plan for the next 2 weeks

Learner interaction with environment



Markov decision process

S: set of states

A: set of actions

Transition probability distribution $P(s'|s, a)$

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

RL for combinatorial optimization

[Dai et al., NeurIPS'17]

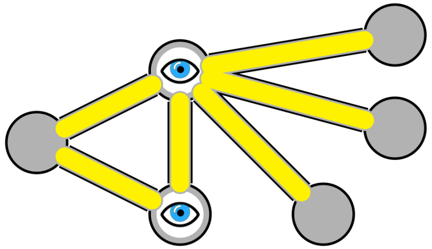
Minimum vertex cover:

Find smallest vertex subset such that each edge is covered

2-approximation:

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

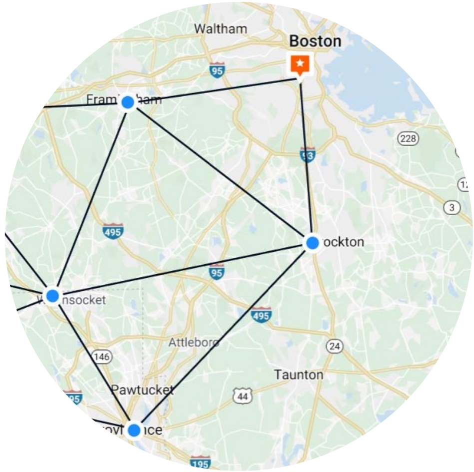
Scoring function that guides greedy algorithm



RL for combinatorial optimization

Goal: learn a scoring function to guide greedy algorithm

Problem	Greedy operation
Minimum vertex cover	Insert node into cover
Maximum cut	Insert node into subset
Traveling salesman problem	Insert node into sub-tour

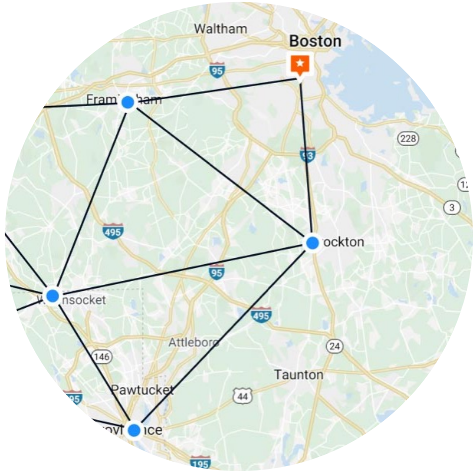


Dai et al., NeurIPS'17

RL for combinatorial optimization

Greedy algorithm	Reinforcement learning
Partial solution	State
Scoring function	Q-function
Select best node	Greedy policy

Repeat until all edges are covered:
1. Compute node scores
2. Select best node with respect to score
3. Add best node to partial solution



Dai et al., NeurIPS'17

Paper we'll read

Dai, Hanjun, Khalil, Elias, et al. "Learning combinatorial optimization algorithms over graphs." *NeurIPS'17*.

- Develop RL algorithms for a variety of combinatorial problems
- Suggest RL could be used for **algorithm discovery**

  "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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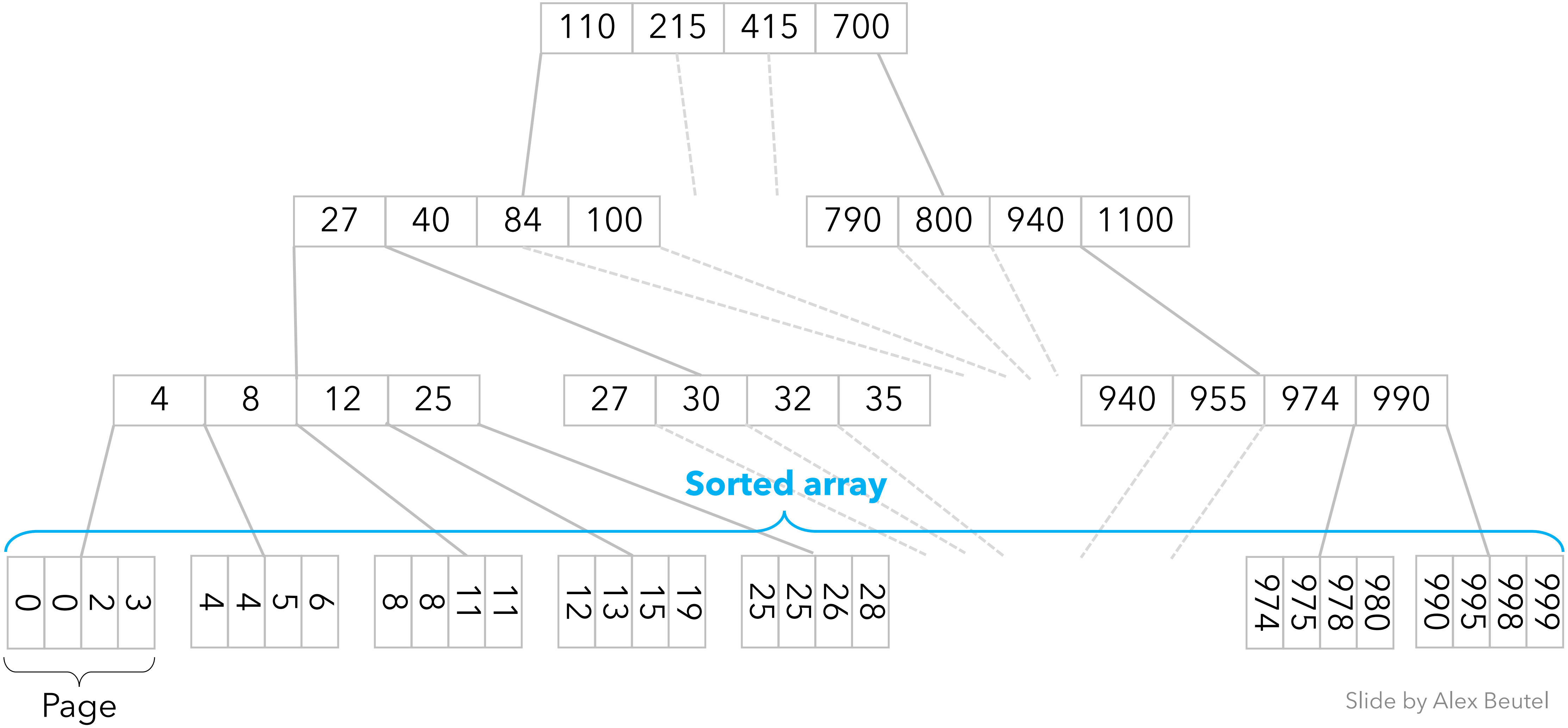
Classical databases

In classical data structures,
databases are **general purpose**. 1-size-fits all.

Example: B-trees

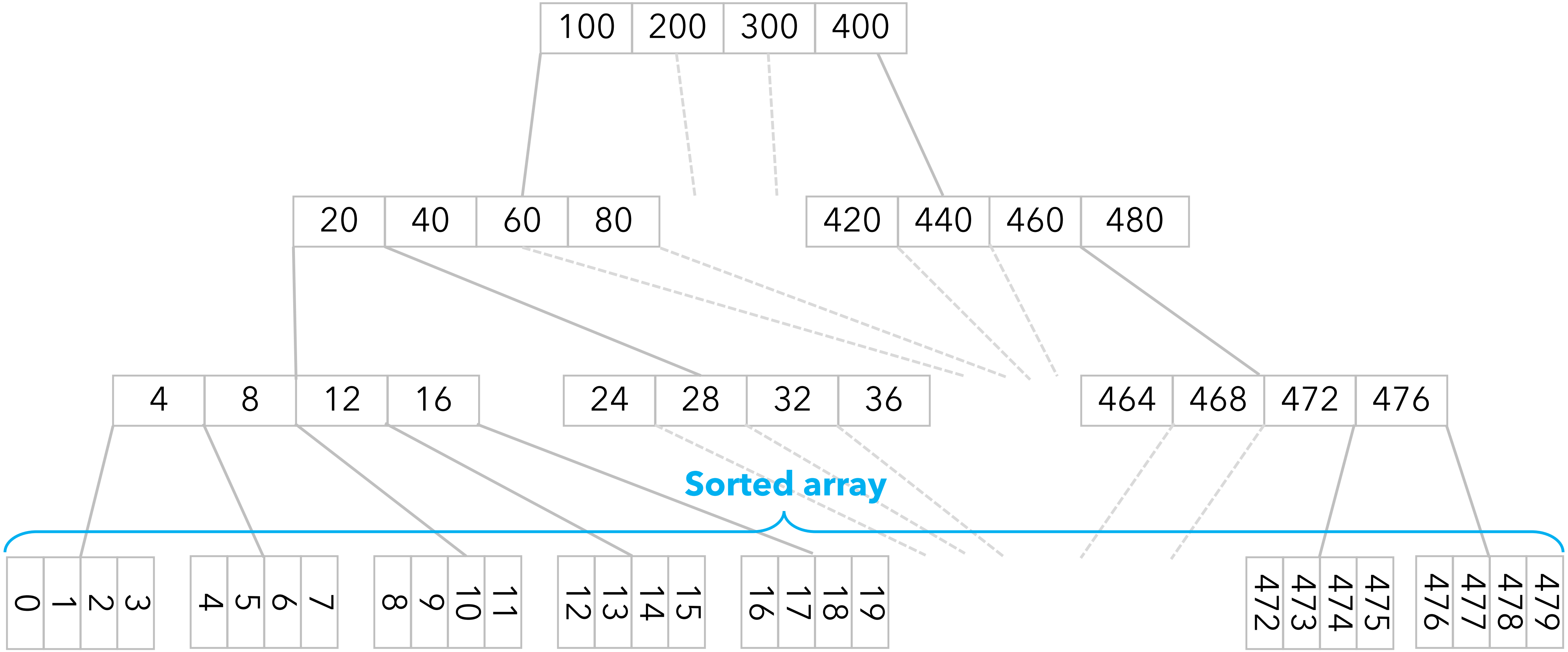
- Self-balancing **tree data structure**
- Maintains sorted data
- Searches, insertions, and deletions in **logarithmic time**

B-trees



Slide by Alex Beutel

If data is all integers from 0 to 1 million?

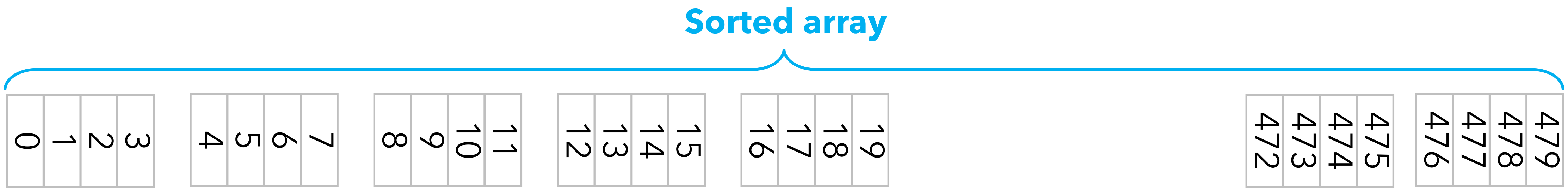


Slide by Alex Beutel

If data is all integers from 0 to 1 million?

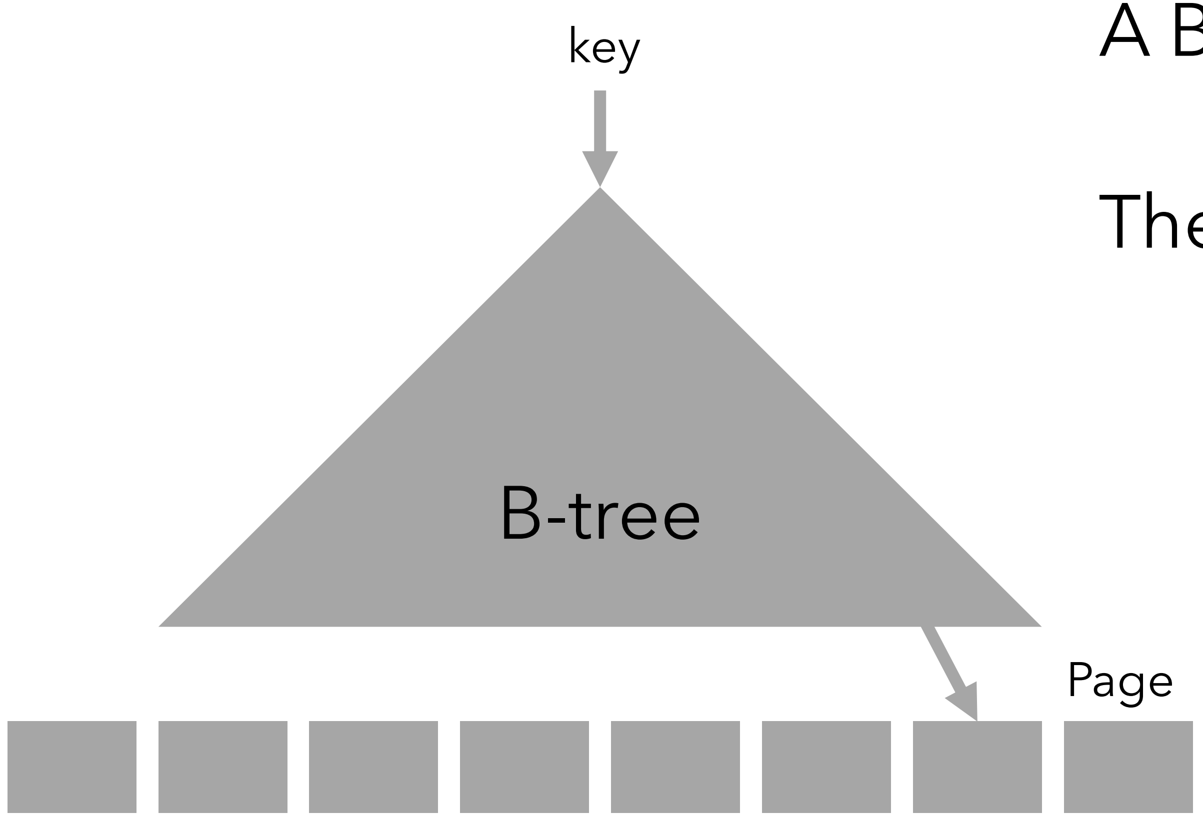
No need for B-tree

- O(1) look-up
- O(1) memory



Slide by Alex Beutel

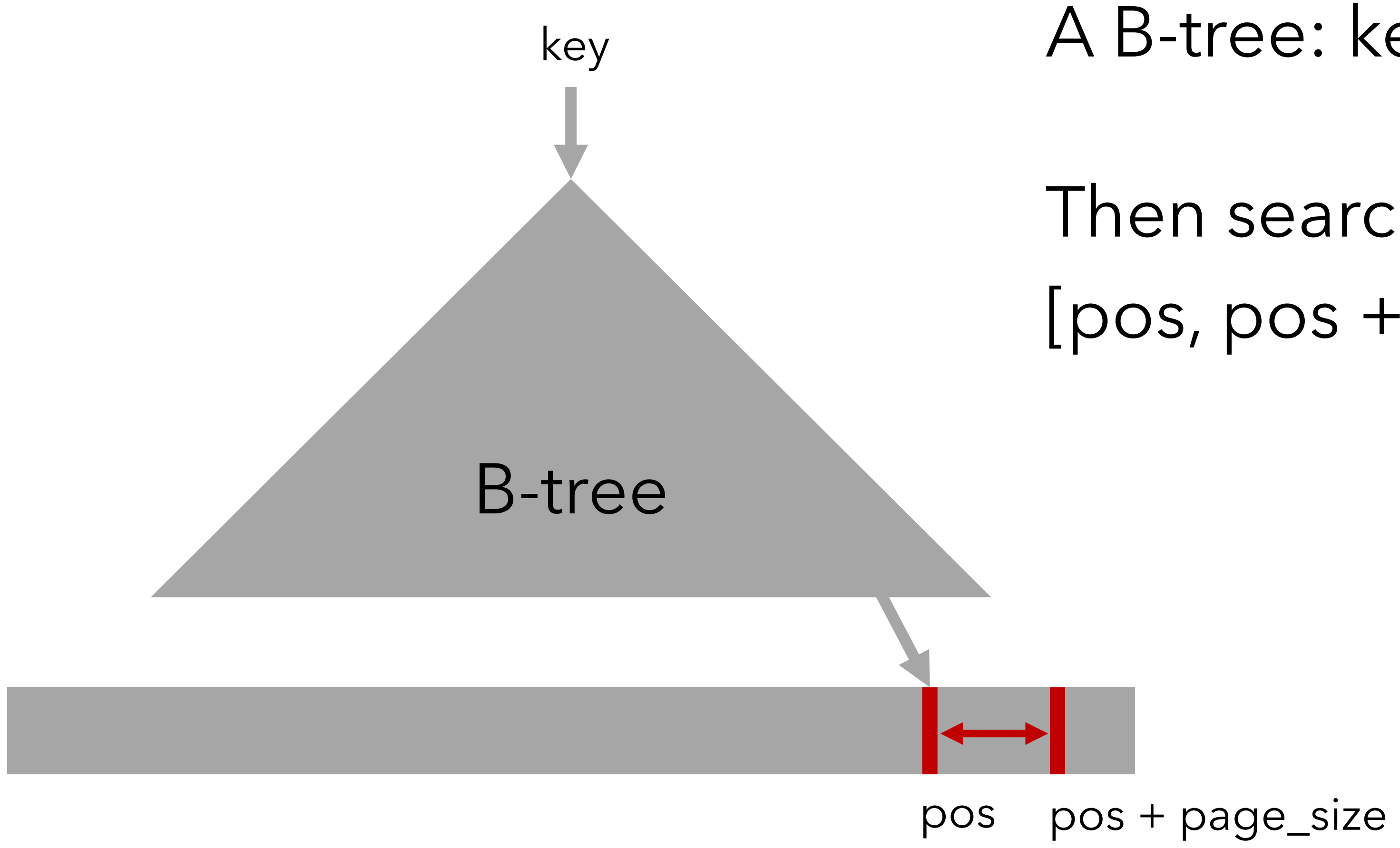
B-trees



A B-tree maps a key to a page

Then searches within the page

B-trees



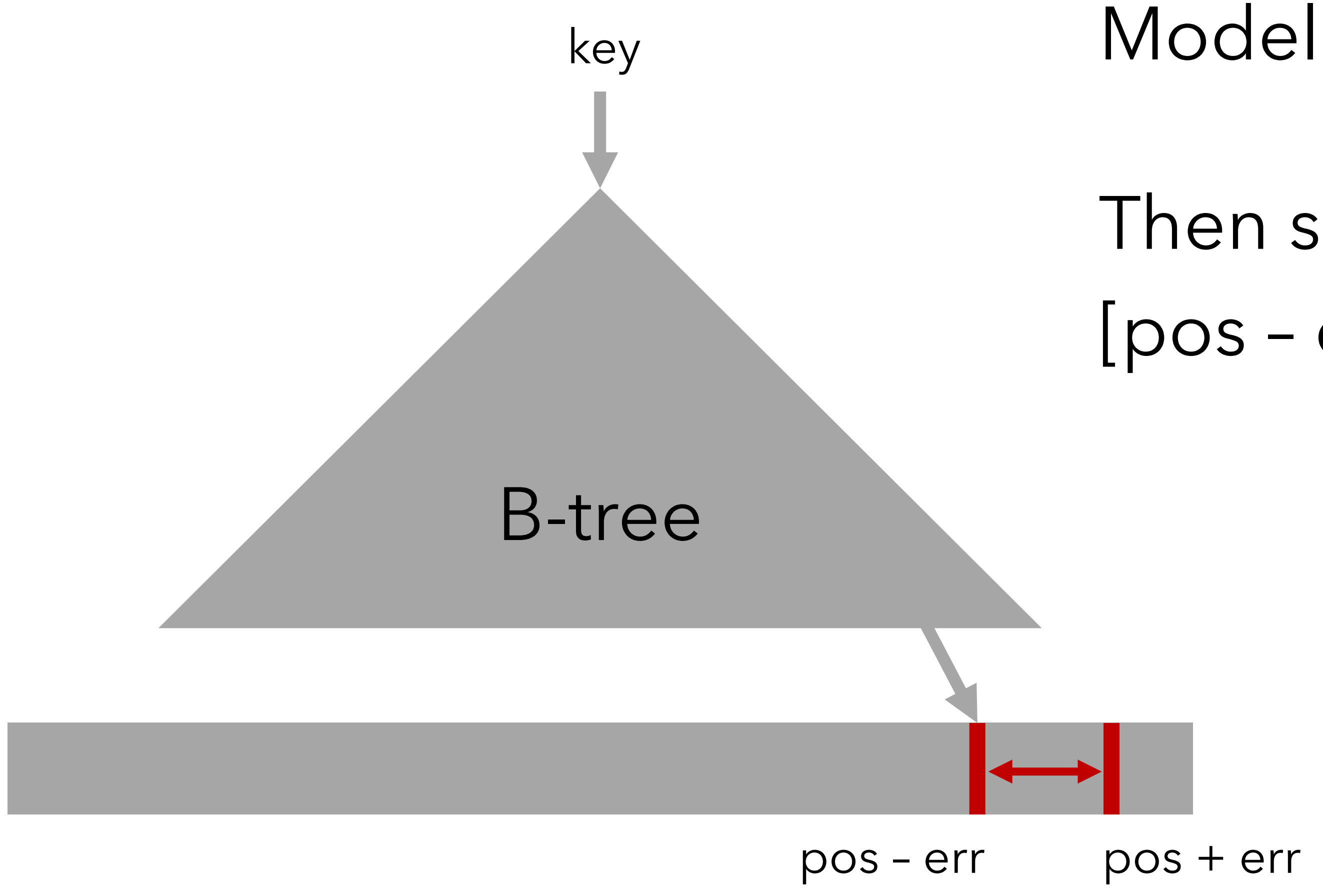
A B-tree: key → pos

Then searches from

[pos, pos + page_size]

Slide by Alex Beutel

B-trees are models



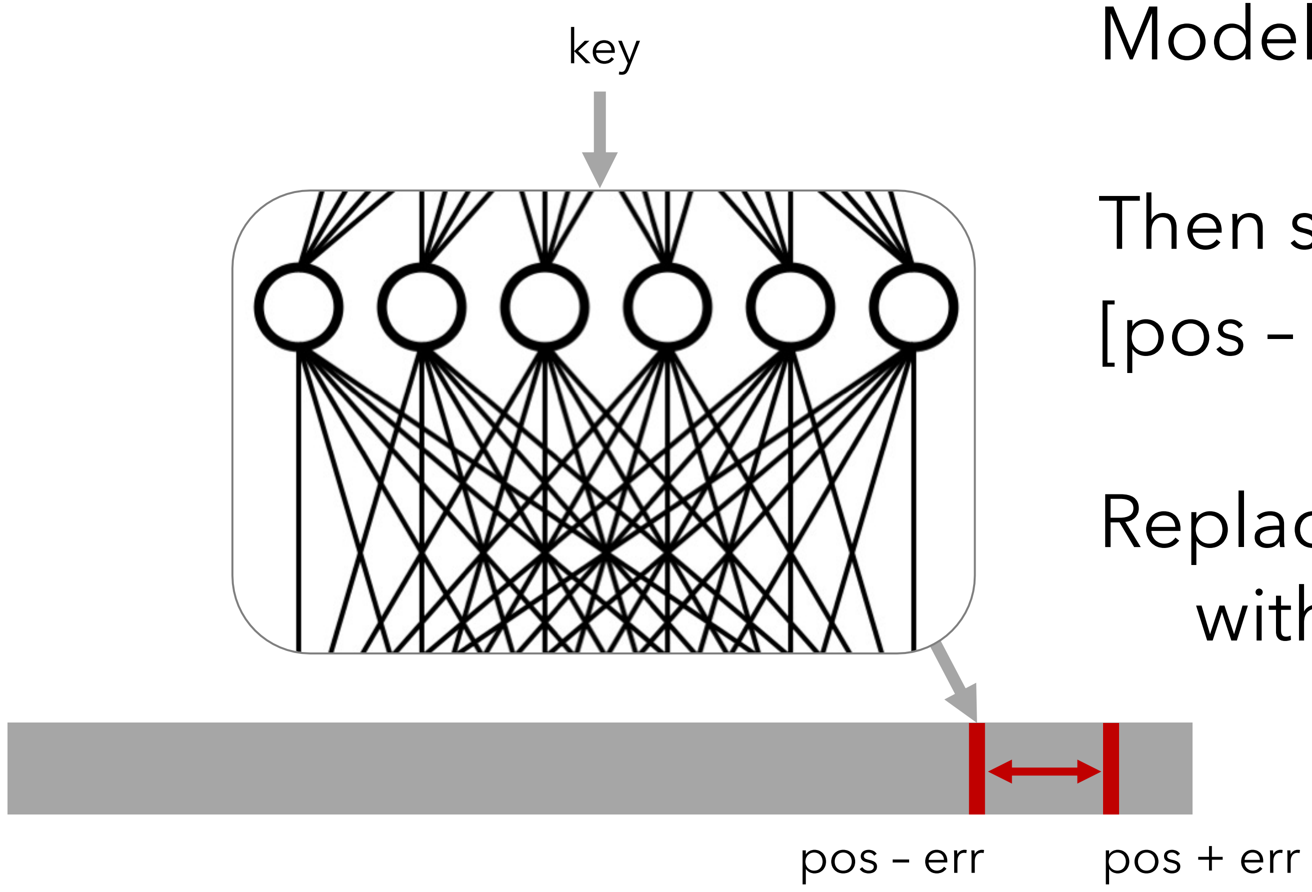
Model: f(key) → pos

Then searches from

[pos - err, pos + err]

Slide by Alex Beutel

B-trees are models



Model: f(key) → pos

Then searches from
[pos - err, pos + err]

Replace B-tree
with **neural network**?

Slide by Alex Beutel

Paper we'll read

Kraska, Tim, et al. "The case for learned index structures." *SIGMOD*. 2018.

- Naïve approach **fails**
- Investigate how to successfully **integrate** ML into databases:
    - B-trees
    - Hash maps
    - Bloom filters

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4. **Theoretical topics**
   i. **Statistical guarantees and online algorithm configuration**
   ii. Algorithms with predictions
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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?

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.

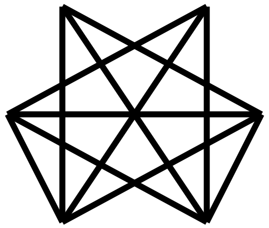
Model is known as the "**batch-learning** setting"

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

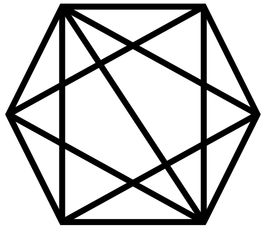
Online algorithm configuration

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

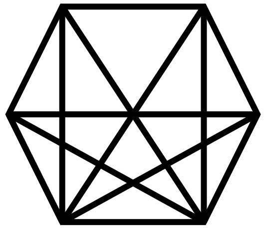
Day 1: $\boldsymbol{\rho}_1$



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?

Paper we'll read

Gupta, Rishi, and Tim Roughgarden. "A PAC approach to application-specific algorithm selection." *ITCS'16*.

Statistical guarantees for algorithm configuration

- Greedy algorithms
- Tuning the step-size of gradient decent
- Etc.

Online configuration for max-weight **independent set**

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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

$$\mathrm{CR} = \frac{\mathrm{ALG}}{\mathrm{OPT}} = \frac{x\mathbf{1}_{\{x<b\}} + (b-1+b)\mathbf{1}_{\{x\geq b\}}}{\min\{x,b\}} < 2 \text{ (best deterministic)}$$

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

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Plan for the next 2 weeks

Thursday 4/6: Machine learning crash-course

- Supervised learning model
- Regression
- Classification
- Neural networks (multi-layer perceptrons)

Plan for the next 2 weeks

Thursday 4/6: Machine learning crash-course

Tuesday 4/11: Integer programming crash-course

- Linear programming
- Integer programming solvers
- SAT solving

Plan for the next 2 weeks

Thursday 4/6: Machine learning crash-course

Tuesday 4/11: Integer programming crash-course

Thursday 4/13: GNN crash-course

Plan for the next 2 weeks

Thursday 4/6: Machine learning crash-course

Tuesday 4/11: Integer programming crash-course

Thursday 4/13: GNN crash-course

Starting Tuesday 4/18: GNN paper discussions