Machine learning for **algorithm design**

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An important property of algorithms used in practice is **broad applicability**

Example: **Integer programming solvers**

Most popular tool for solving combinatorial (& nonconvex) problems

Routing

Manufacturing

Scheduling

Planning

Finance

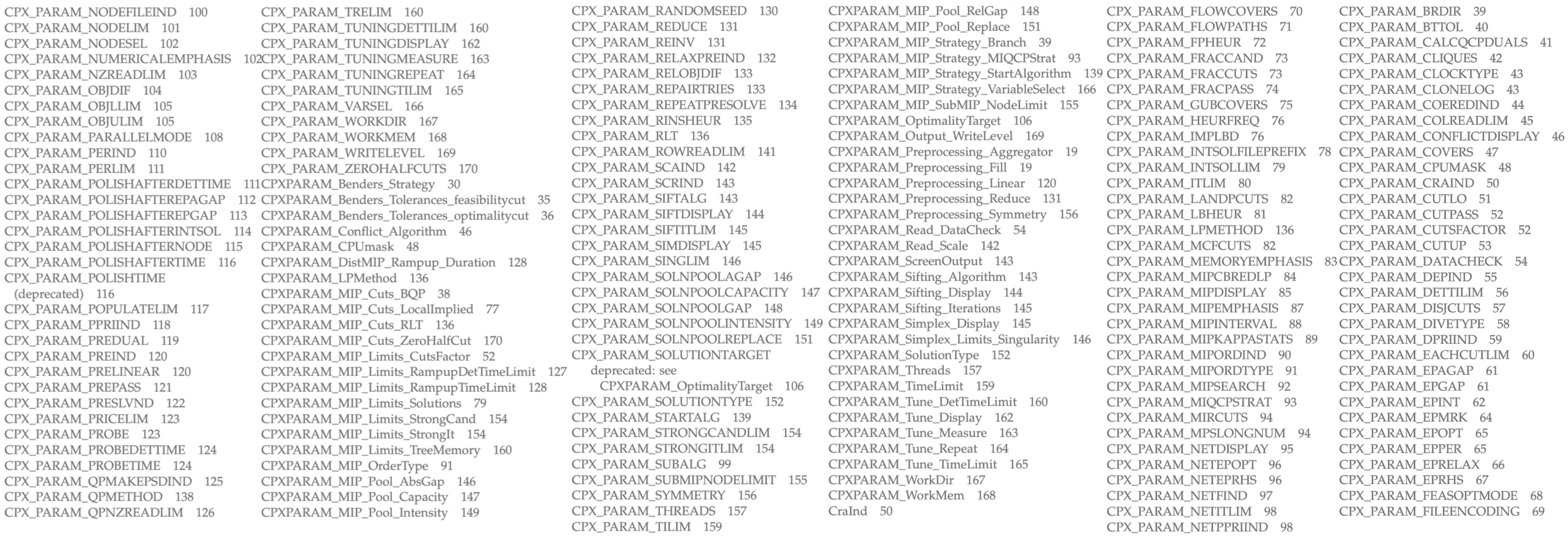
…but they can have **unsatisfactory** default performance

Slow runtime, poor solutions quality, …

Example: Integer programming (IP)

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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Example: Integer programming (IP)

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**

Example: Sequence alignment

Goal: Line up pairs of strings

Applications: Biology, natural language processing, etc.

vitterchik

Did you mean: **vitercik**

Example: Sequence alignment

Input: Two sequences S and S'

Output: Alignment of S and S'

S = A C T G

S' = G T C A

Gap

A – – C T G

– G T C A –

Insertion/deletion (*indel*)

Match

Mismatch

Example: Sequence alignment

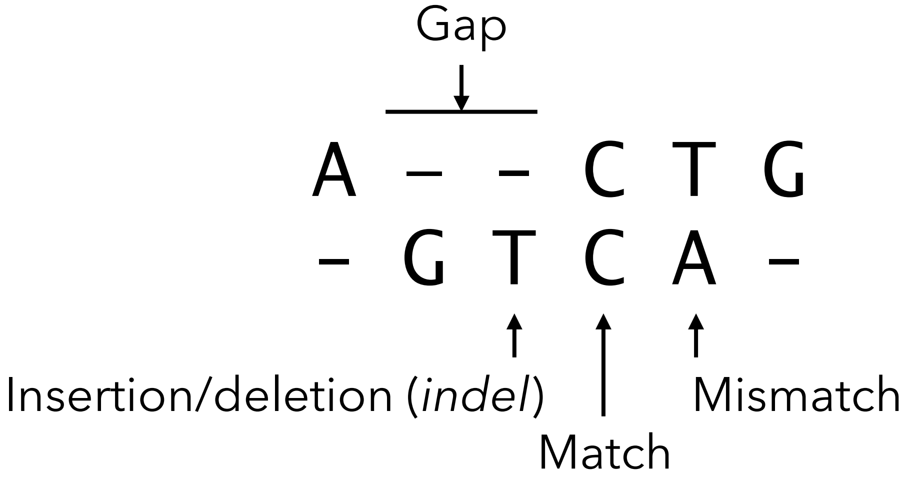
Standard algorithm with parameters $\rho_1, \rho_2, \rho_3 \geq 0$:

Return alignment maximizing:

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

$S = \mathrm{A\ C\ T\ G}$

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



Gap

A – – C T G

– G T C A –

Insertion/deletion (*indel*)

Match

Mismatch

Example: Sequence alignment

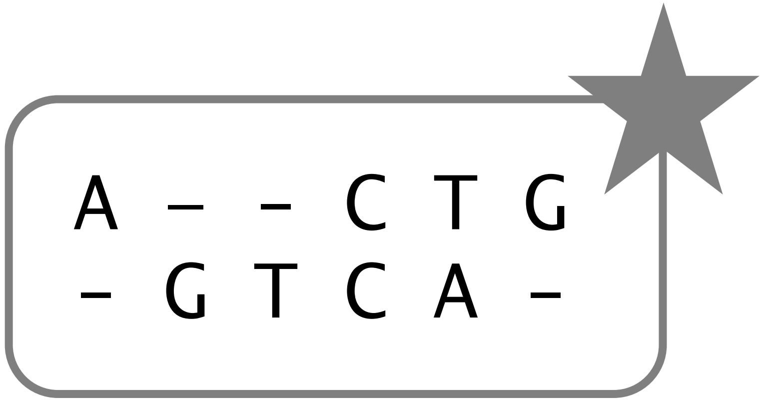
Can sometimes access **ground-truth, reference** alignment

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]



A – – C T G
– G T C A –

Example: Sequence alignment

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

Ground-truth alignment of protein sequences

Example: Sequence alignment

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-GRTCPKPDDLPFSTVVP-LKTFYEPGEEITYSCKPGYVSRGGMRKFICPLTGLWPINTLKCTP
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```

Alignment by algorithm with poorly-tuned parameters

Example: Sequence alignment

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```
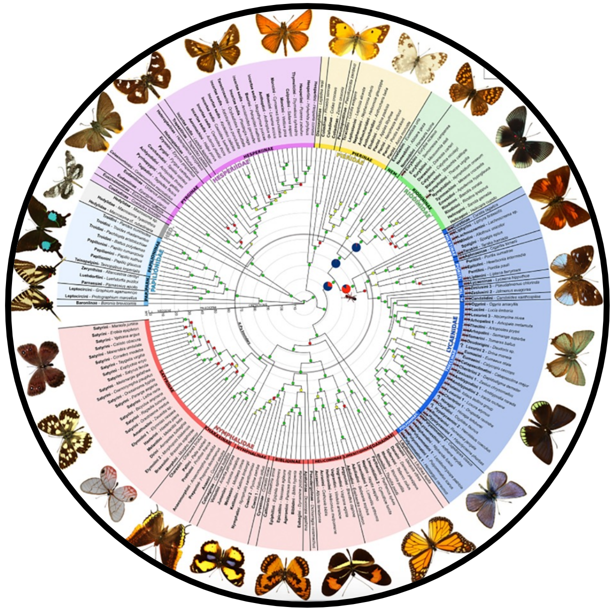
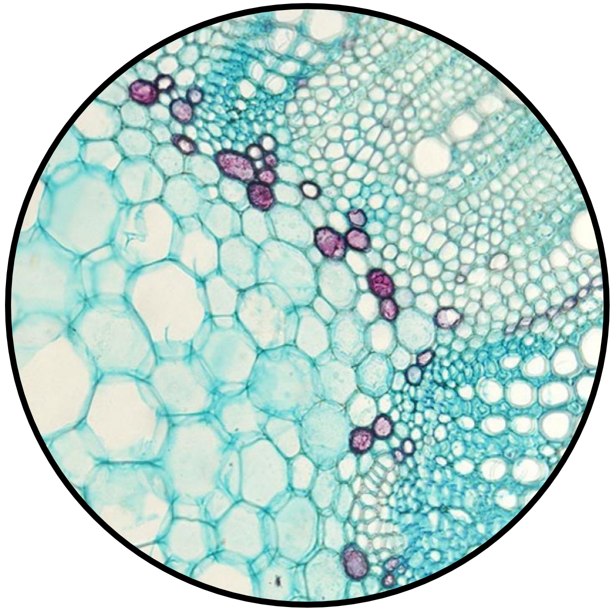

Alignment by algorithm with well-tuned parameters

Example: Clustering

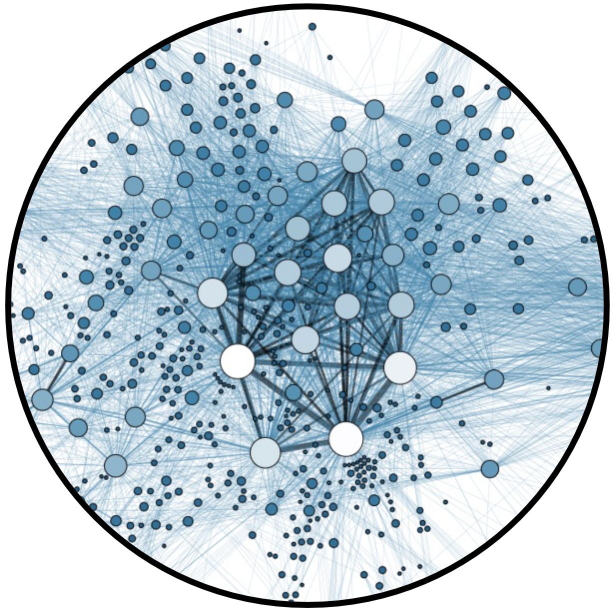
Diverse applications, including:



Ecology



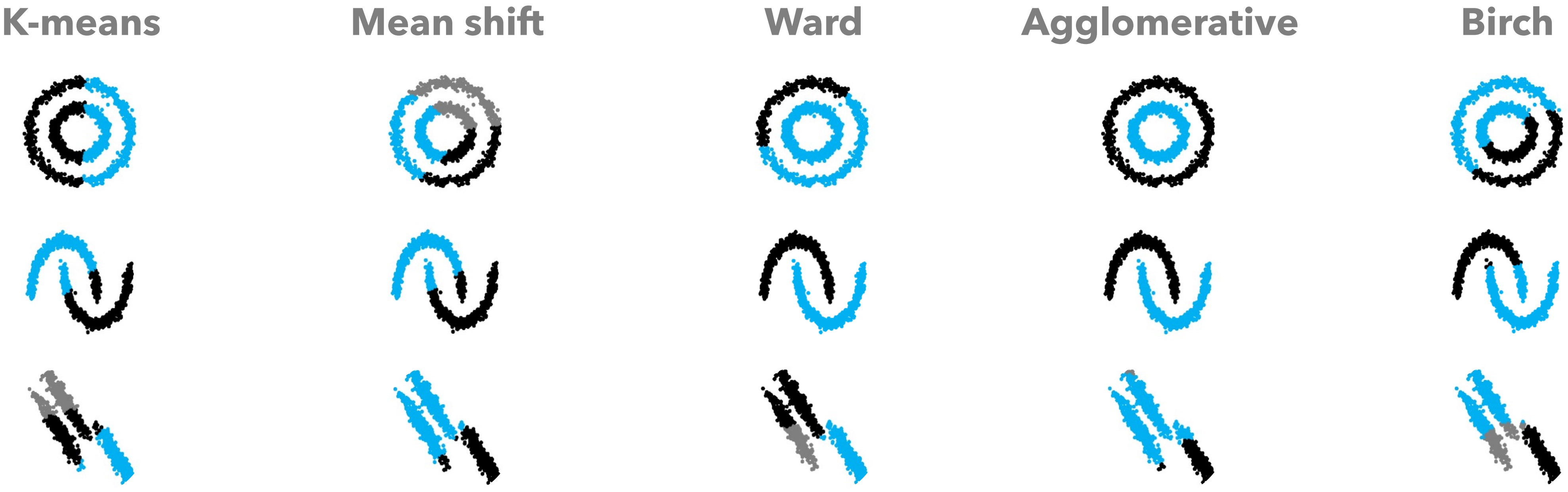
Biology



Network analysis

Example: Clustering

Many different algorithms



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

In practice, we have data about the application domain

Data we could use in the process of

- **Algorithm selection**
  - *Given a variety of algorithms, which to use?*
- **Algorithm configuration**
  - *How to tune the algorithm's parameters?*
- **Algorithm design**

In practice, we have data about the application domain

Routing problems a shipping company solves

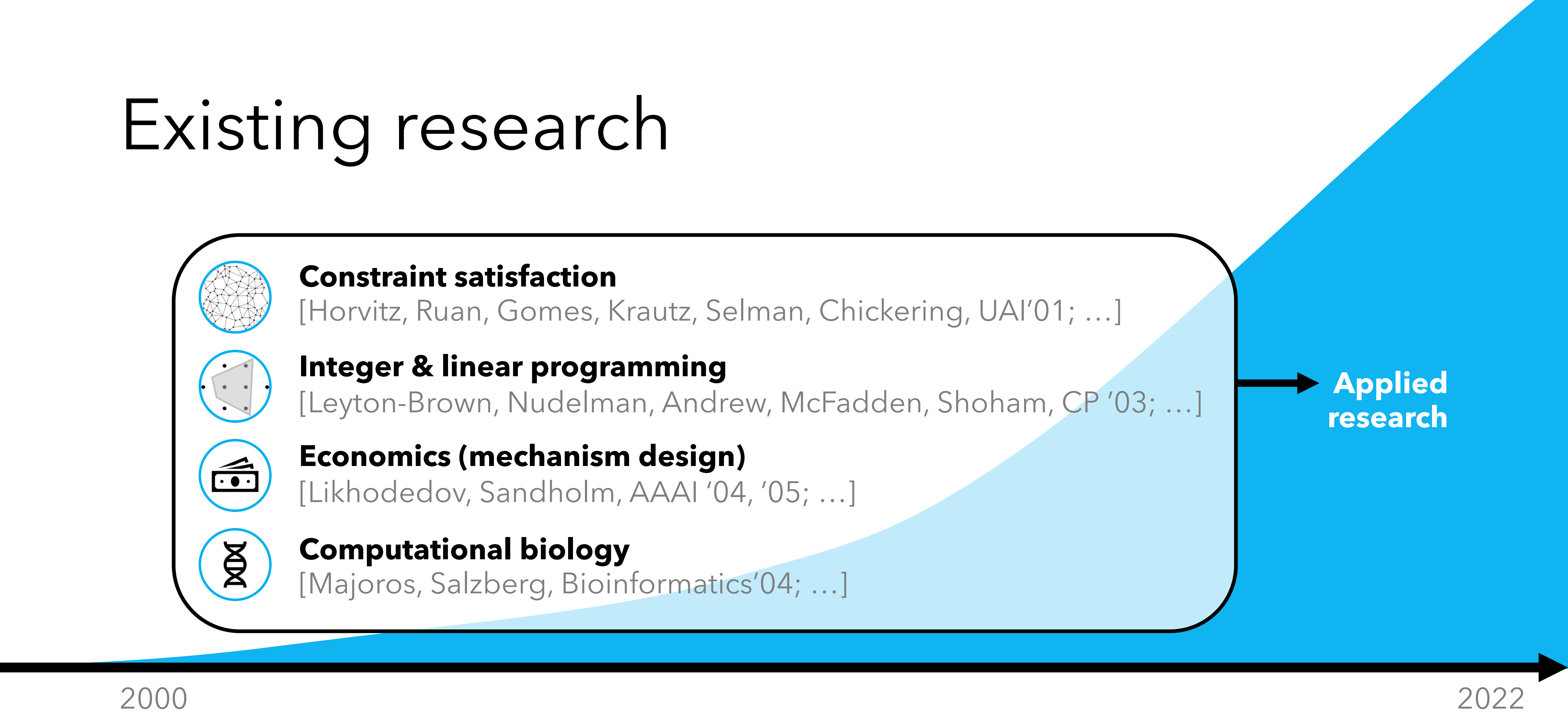
In practice, we have data about the application domain

Clustering problems a biology lab solves

In practice, we have data about the application domain

Scheduling problems an airline solves

Existing research



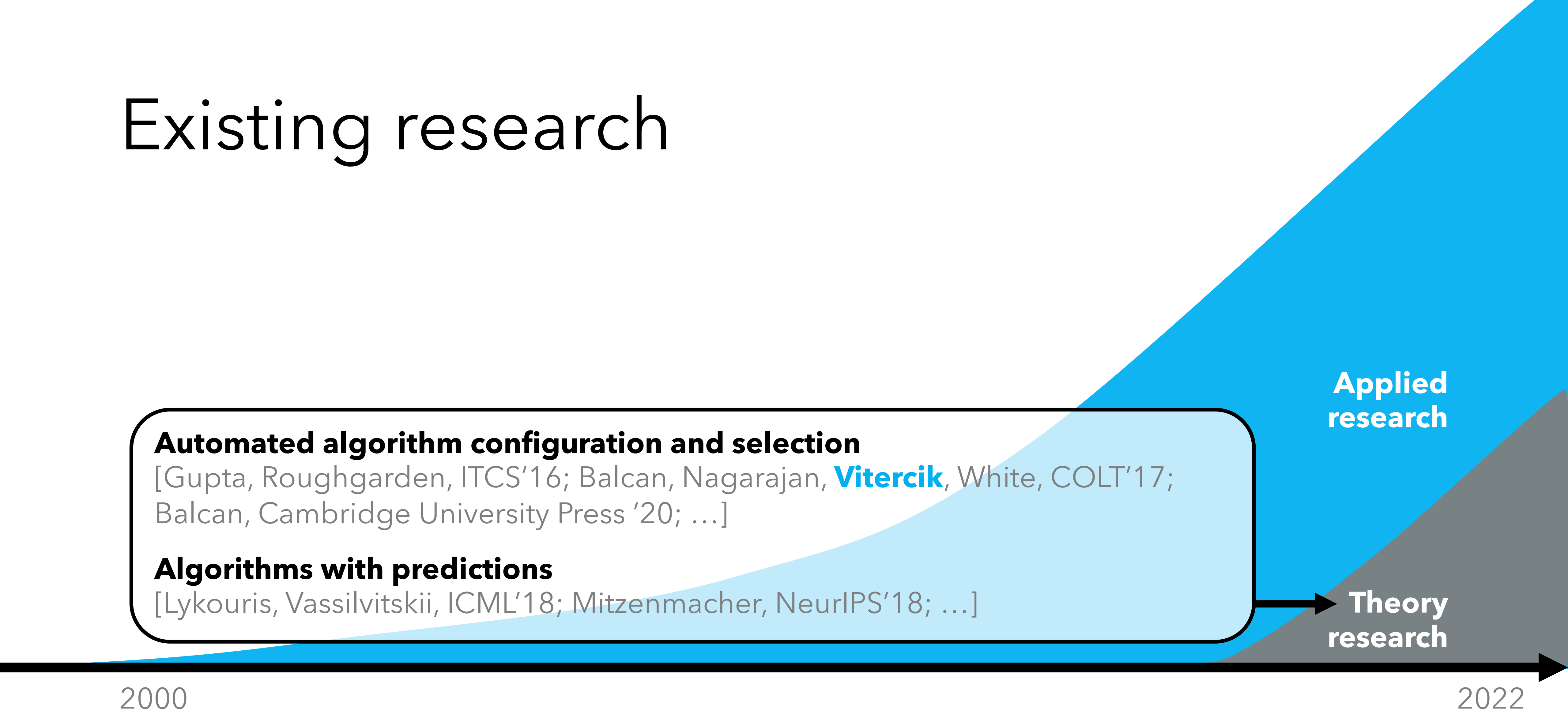
Constraint satisfaction
[Horvitz, Ruan, Gomes, Krautz, Selman, Chickering, UAI’01; …]

Integer & linear programming
[Leyton-Brown, Nudelman, Andrew, McFadden, Shoham, CP ’03; …]

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; Balcan, Cambridge University Press '20; …]

Algorithms with predictions
[Lykouris, Vassilvitskii, ICML'18; Mitzenmacher, NeurIPS'18; …]

Outline

1. Introduction
2. **Algorithm configuration**
3. Algorithms with predictions
4. Learning to prune
5. Conclusion and future directions

Gupta, Roughgarden, ITCS'16
Balcan, DeBlasio, Dick, Kingsford, Sandholm, **Vitercik**, STOC'21
Book chapter by Balcan, '20

Automated configuration procedure

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

Sequence S_1
Sequence S_1'
Reference alignment A_1

Sequence S_2
Sequence S_2'
Reference alignment A_2

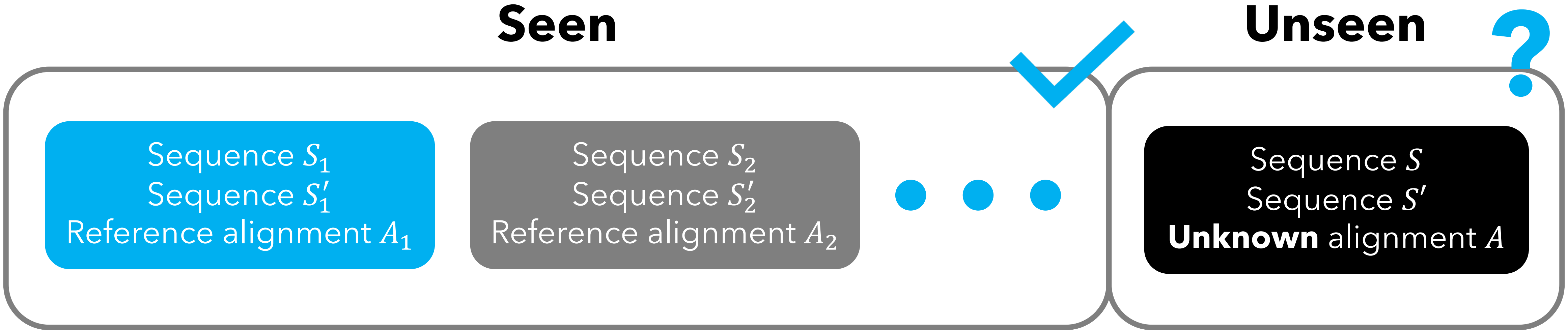
3. Return parameter setting $\hat{\boldsymbol{\rho}}$ with good avg performance

Runtime, solution quality, etc.

Key question: How to find $\hat{\boldsymbol{\rho}}$ with good avg performance?

Hutter et al. [JAIR'09, LION'11], Ansótegui et al. [CP'09], Kleinberg et al. [NeurIPS'19, IJCAI'17], Weisz et al. [ICML'19, NeurIPS'19]; Balcan, Sandholm, **V** [AAAI'20], …

Automated configuration procedure



Focus of this section: Will $\hat{\rho}$ have good **future** performance?
More formally: Is the expected performance of $\hat{\rho}$ also high?

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

Results overview

Key question **(focus of 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

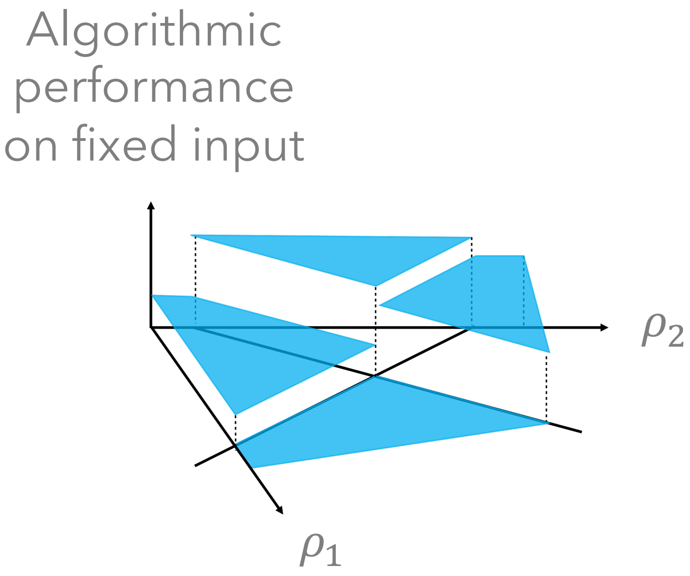
Piecewise constant, linear, quadratic, …

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

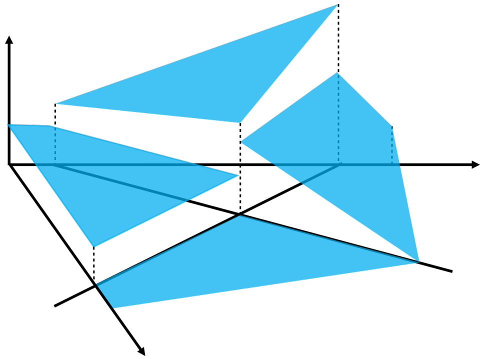
Results overview

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

Piecewise constant, linear, quadratic, …



Piecewise constant



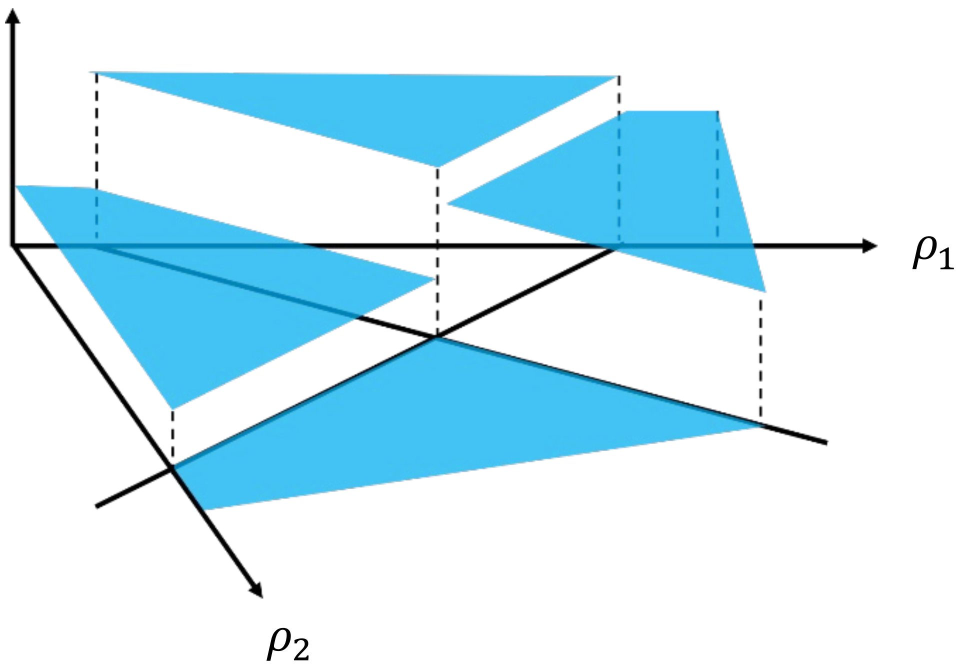
Piecewise linear

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, Nagarajan, **V**, White, COLT'17

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

Online configuration [Gupta, Roughgarden, ITCS'16, Cohen-Addad and Kanade, AISTATS'17]
Exploited piecewise-Lipschitz structure to provide regret bounds
[Balcan, Dick, **V**, FOCS'18; Balcan, Dick, Pegden, UAI'20; Balcan, Dick, Sharma, AISTATS'20]

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

Piecewise structure

Piecewise structure unifies **seemingly disparate** problems:

Integer programming
Balcan, Dick, Sandholm, **V**, ICML’18
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Computational biology
Balcan, DeBlasio, Dick, Kingsford, Sandholm, **V**, STOC’21

Greedy algorithms
Gupta, Roughgarden, ITCS’16

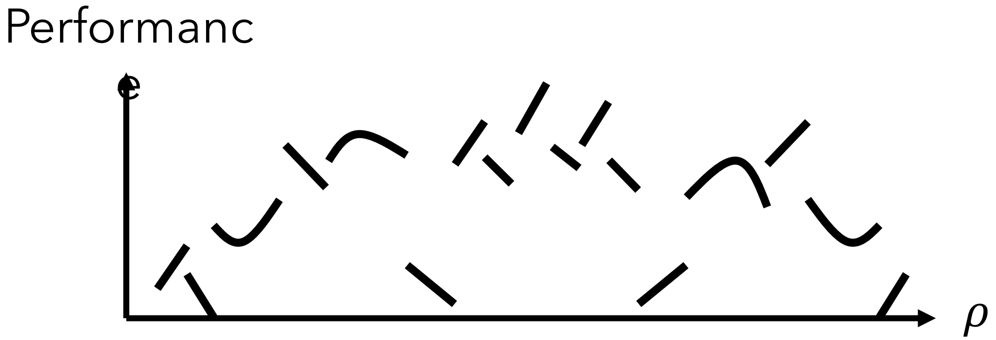
Mechanism configuration
Balcan, Sandholm, **V**, EC’18

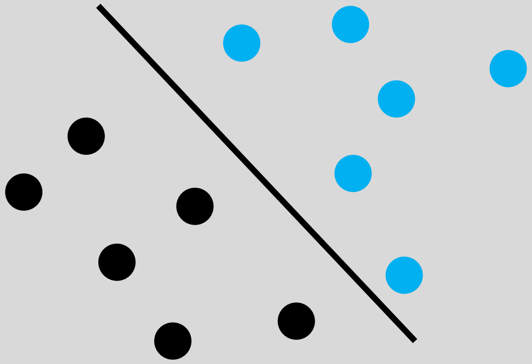
Ties to a long line of research on machine learning for **revenue maximization**
Likhodedov, Sandholm, AAAI'04, ’05; Balcan, Blum, Hartline, Mansour, FOCS’05; Elkind, SODA’07; Cole, Roughgarden, STOC’14; Mohri, Medina, ICML’14; Devanur, Huang, Psomas, STOC’16; …

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

Primary challenge:
Algorithmic performance is a **volatile** function of parameters

Complex connection between parameters and performance





For well-understood functions in machine learning theory:
Simple connection between function parameters and value

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

Outline: Algorithm configuration

1. Overview
2. **Model and problem formulation**
3. Our guarantees
   1. Example of piecewise-structured utility function
   2. Piecewise-structured functions more formally
   3. Main theorem
   4. Application: Sequence alignment
   5. 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

$$
\begin{array}{lcccc}
S = & \mathrm{A} & \mathrm{C} & \mathrm{T} & \mathrm{G} \\
S' = & \mathrm{G} & \mathrm{T} & \mathrm{C} & \mathrm{A}
\end{array}
$$

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

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

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, …

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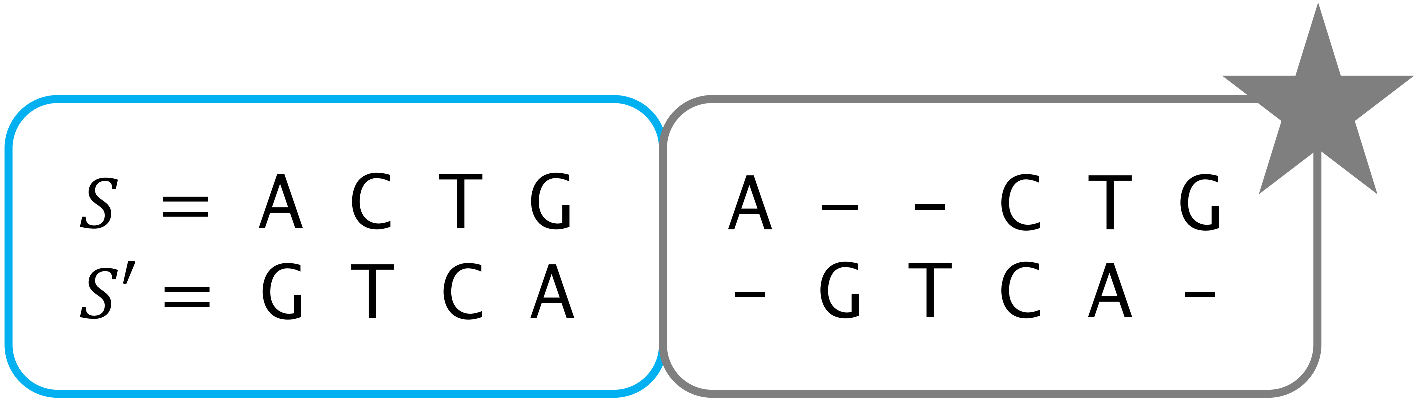
Algorithmic performance

$u_{\boldsymbol{\rho}}(x)$ = distance between algorithm’s output and ground-truth



$S = \mathrm{A\ C\ T\ G}$

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

A – – C T G

– G T C A –

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

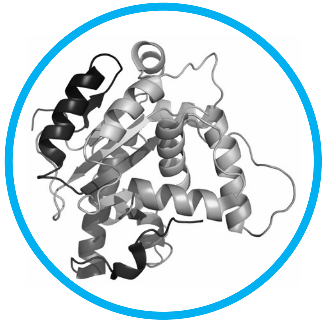
Balcan, DeBlasio, Dick, Kingsford, Sandholm, **Vitercik**, STOC’21

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

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

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 $\boldsymbol{\rho}$,

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

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

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

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

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

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

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

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

Outline: Algorithm configuration

1. Overview
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    d. Application: Sequence alignment
    e. Online algorithm configuration

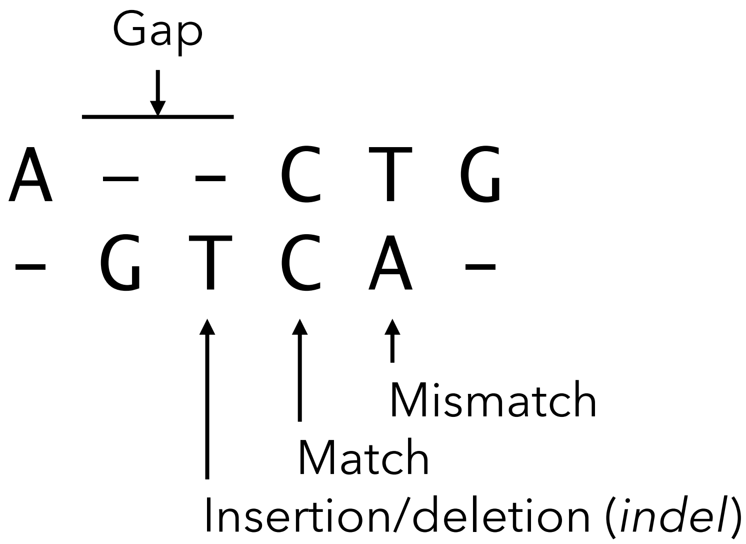
Sequence alignment algorithms

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

Return alignment maximizing:

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

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



Gap

A – – C T G

– G T C A –

Mismatch

Match

Insertion/deletion (*indel*)

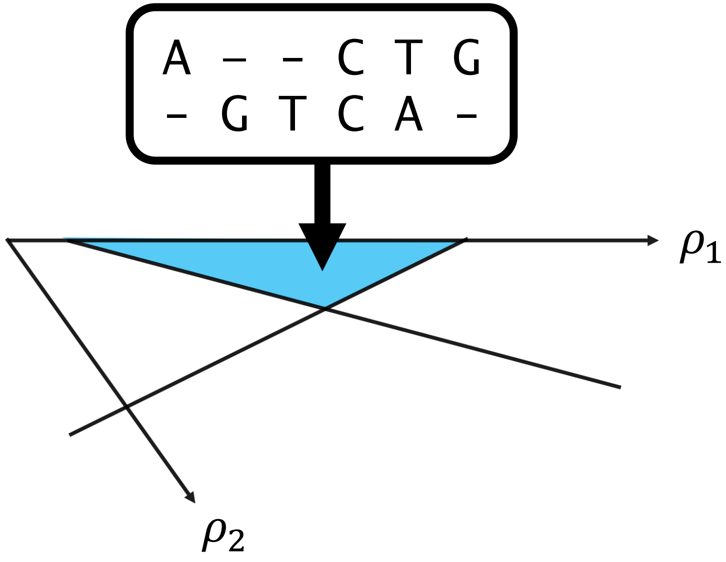
Balcan, DeBlasio, Dick, Kingsford, Sandholm, **Vitercik**, STOC’21

Sequence alignment algorithms

Lemma:

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

$S\ =$ A C T G
$S' =$ G T C A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Gusfield et al., Algorithmica '94; Fernández-Baca et al., J. of Discrete Alg. '04

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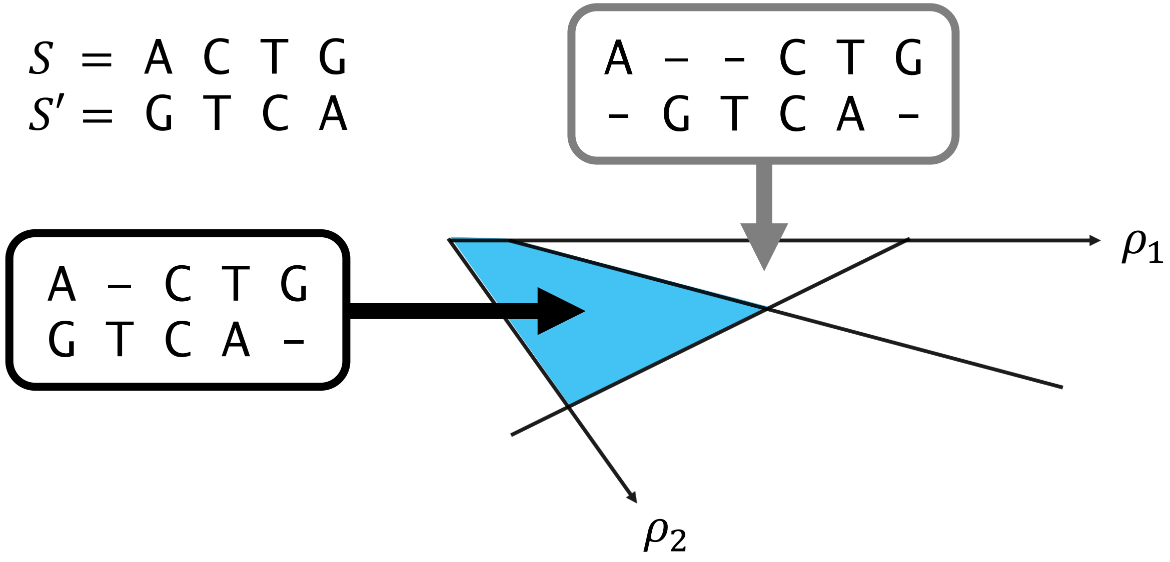


S = A C T G
S' = G T C A

A – – C T G
– G T C A –

A – C T G
G T C A –

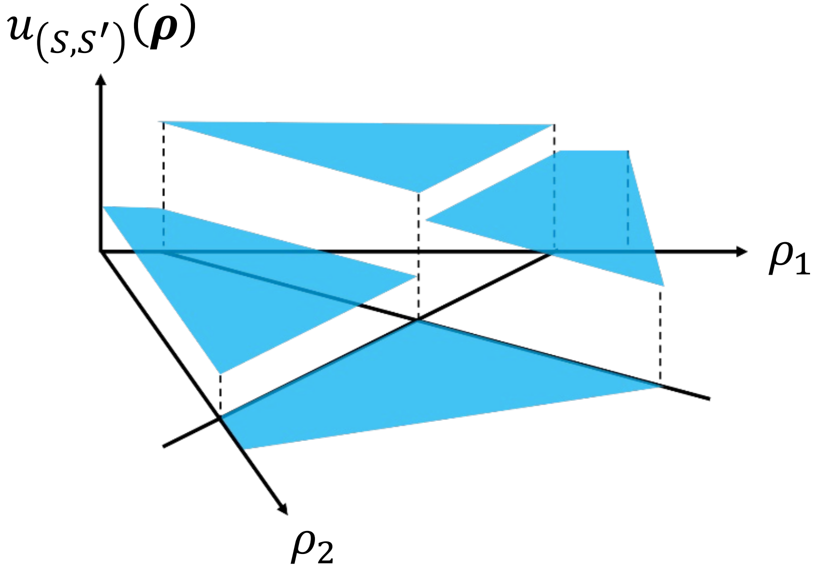
Gusfield et al., Algorithmica '94; Fernández-Baca et al., J. of Discrete Alg. '04

Piecewise-constant utility function

Corollary:

Utility is piecewise constant function of parameters

Distance between algorithm's output and ground-truth alignment



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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

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

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

VC dimension, pseudo-dimension, Rademacher complexity, …

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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

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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 $\mathcal{U}$

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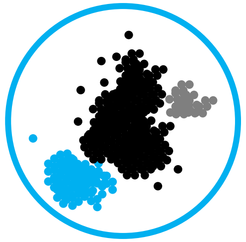
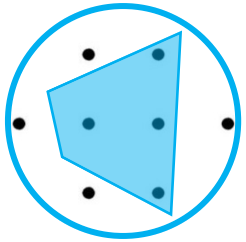
Piecewise-structured functions

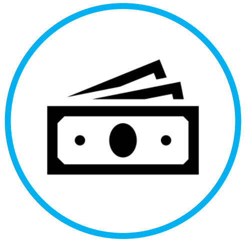
Dual functions $u_x^*: \mathbb{R}^d \rightarrow \mathbb{R}$ are piecewise-structured



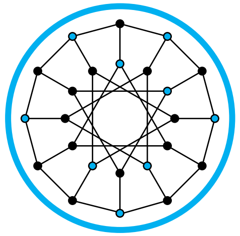
Clustering algorithm configuration



Integer programming algorithm configuration



Selling mechanism configuration



Greedy algorithm configuration

Computational biology algorithm configuration

Voting mechanism configuration

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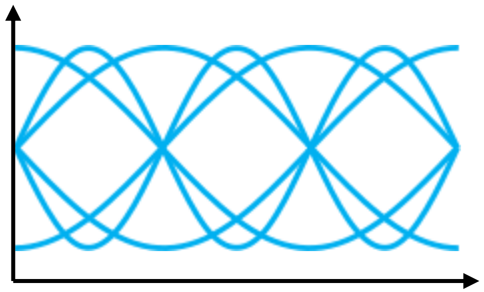
Intrinsic complexity

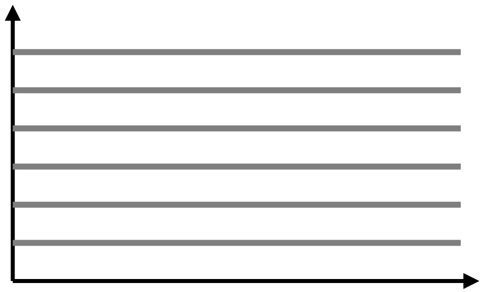
"Intrinsic complexity" of function class $\mathcal{G}$

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



More complex

Less complex



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Generalization to future inputs

With high probability, for all $\boldsymbol{\rho}$:

|**Avg** utility on training set – **expected** utility|

Intrinsic complexities of $\mathcal{F}^*$ and $\mathcal{G}^*$

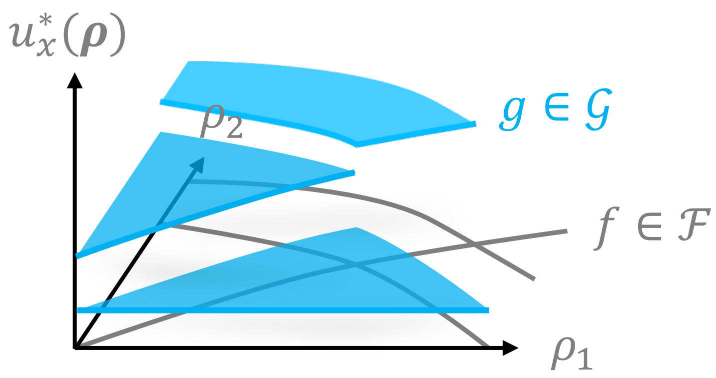
\# boundary functions

$$= \tilde{O}\left(H\sqrt{\frac{\mathrm{Pdim}(\mathcal{G}^*)+\mathrm{VC}(\mathcal{F}^*)\ln k}{N}}\right)$$

Upper bound on utility

Training set size

Revenue, runtime, solution quality, …



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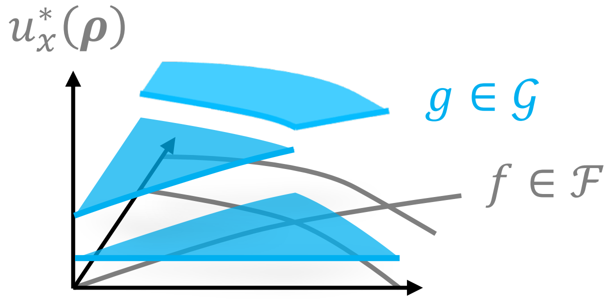
Proof sketch

Theorem: |**Avg** utility – **expected** utility| $= \tilde{O}\left(H\sqrt{\frac{\mathrm{Pdim}(\mathcal{G}^*)+\mathrm{VC}(\mathcal{F}^*)\ln k}{N}}\right)$

Proof sketch: Fix any set $S \subseteq \mathcal{X}$ of inputs

- Count regions induced by the $|S|k$ boundaries
  - Depends not on $\mathrm{VC}(\mathcal{F})$, but rather $\mathrm{VC}(\mathcal{F}^*)$
- In each region, $\{u_x^* : x \in S\}$ are simultaneously structured
  - Count # parameters in region w/ "significantly different" performance
  - Use $\mathrm{Pdim}(\mathcal{G}^*)$
- Aggregate bounds over all regions to get:

$$\mathrm{Pdim}(\mathcal{U}) = O(\mathrm{Pdim}(\mathcal{G}^*) + \mathrm{VC}(\mathcal{F}^*)\ln k)$$



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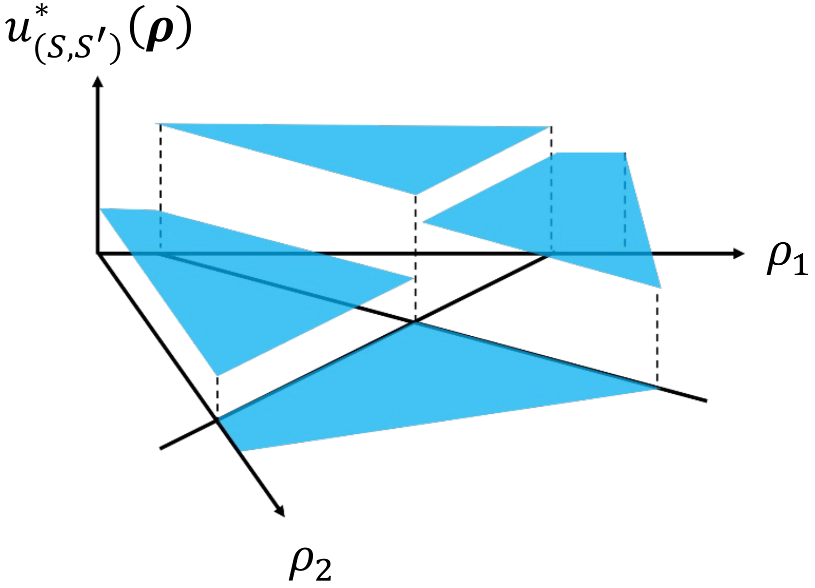
Piecewise constant dual functions

Lemma:

Utility is piecewise constant function of parameters



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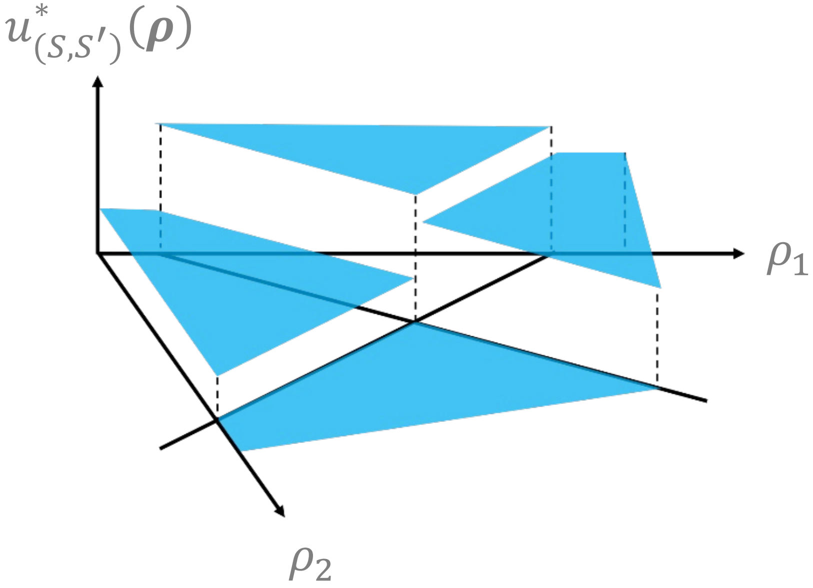
Sequence alignment guarantees

Theorem: Training set of size $\tilde{O}\left(\frac{\log(\text{seq. length})}{\epsilon^2}\right)$ implies WHP $\forall \boldsymbol{\rho}$,

|**avg** utility over training set – **exp** utility| $\leq \epsilon$



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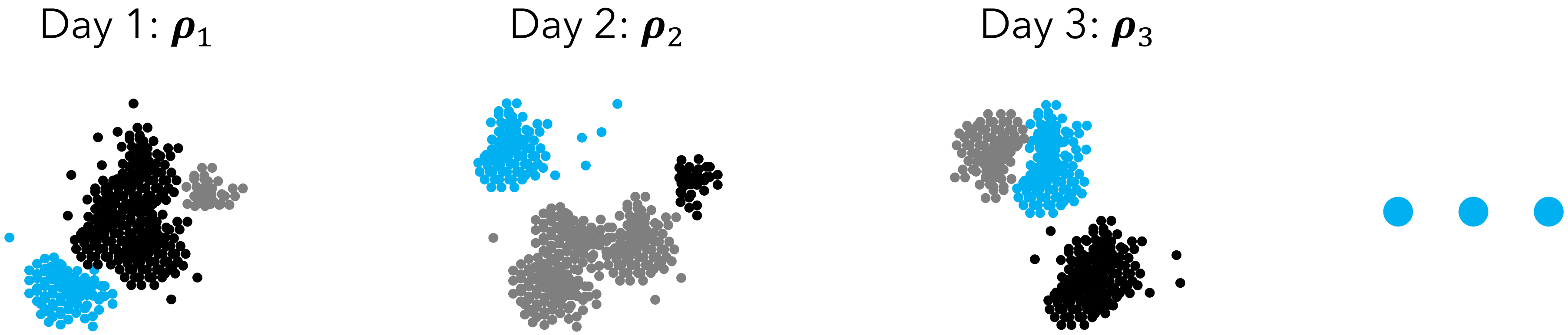
    e. **Online algorithm configuration**

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, Roughgarden, ITCS'16; Cohen-Addad, Kanade, AISTATS'17; Balcan, Dick, **Vitercik**, FOCS'18; Balcan, Dick, Pegden, UAI'20; …

Outline

1. Introduction
2. Algorithm configuration
3. **Algorithms with predictions**
4. Learning to prune
5. Conclusion and future directions

Book chapter by Mitzenmacher, Vassilvitskii, '20
Purohit, Svitkina, Kumar, NeurIPS'18

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?

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    b. Ski rental problem
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Example: Searching in a sorted array

Example:

- $q = 8$
- $h(q) = 2$

- **Goal:** Given query q & sorted array A, find q's index (if q in A)
- **Predictor:** $h(q)$ = guess of q's index
- **Algorithm:** Check $A[h(q)]$. If q is there, return $h(q)$. Else:
  - If $q > A[h(q)]$, check $A\big[h(q) + 2^i\big]$ for $i > 1$ until find something larger
    - Do binary search on interval $\big(h(q) + 2^{i-1}, h(q) + 2^i\big)$
  - If $q < A[h(q)]$, symmetric

Book chapter by Mitzenmacher, Vassilvitskii, '20

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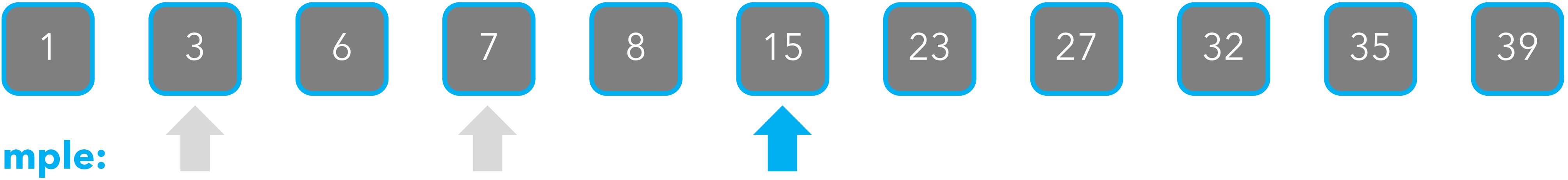

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Book chapter by Mitzenmacher, Vassilvitskii, '20

Example: Searching in a sorted array

1	3	6	7	8	15	23	27	32	35	39

Analysis:

- Let $t(q)$ be index of q in A or of smallest element larger than q
- Runtime is $O(\log\underbrace{|t(q) - h(q)|}_{\text{Prediction error}})$:
  - Finding larger/smaller element takes $O(\log|t(q) - h(q)|)$ steps
  - Binary search takes $O(\log|t(q) - h(q)|)$ steps
- Better predictions lead to **better runtime**
- Runtime **never worse than worst-case** $O(\log|A|)$

Book chapter by Mitzenmacher, Vassilvitskii, '20

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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, **optimal clairvoyant** strategy pays $\mathrm{OPT} = \min\{x, b\}$

Breakeven strategy: Rent for $b - 1$ days, then buy

- $\mathrm{CR} = \frac{\mathrm{ALG}}{\mathrm{OPT}} = \frac{x\mathbf{1}_{\{x<b\}} + (b-1+b)\mathbf{1}_{\{x\geq b\}}}{\min\{x,b\}} < 2$ (best deterministic)
- Randomized alg. $\mathrm{CR} = \frac{e}{e-1}$ [Karlin et al., Algorithmica '94]

Example: Ski rental problem

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

Baseline: Buy at beginning if $y > b$, else rent all days

Theorem: $\mathrm{ALG} \leq \mathrm{OPT} + \eta$

If y small but $x \gg b$, CR can be unbounded

Purohit, Svitkina, Kumar, NeurIPS'18

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

Example: Ski rental problem

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

Proof sketch: If $y \geq b$, buys on start of day $\lceil \lambda b \rceil$

$$\frac{\mathrm{ALG}}{\mathrm{OPT}} = \begin{cases} \dfrac{x}{x} & \text{if } x < \lceil \lambda b \rceil \\ \dfrac{\lceil \lambda b \rceil - 1 + b}{x} & \text{if } \lceil \lambda b \rceil \leq x \leq b \\ \dfrac{\lceil \lambda b \rceil - 1 + b}{b} & \text{if } x \geq b \end{cases}$$

Worst when $x = \lceil \lambda b \rceil$ and CR = $\frac{b+\lceil \lambda b \rceil - 1}{\lceil \lambda b \rceil} \leq \frac{1+\lambda}{\lambda}$; similarly for $y < b$

Purohit, Svitkina, Kumar, NeurIPS'18

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Design principals

Consistency:

- Predictions are perfect ⇒ recover offline optimal
- Algorithm is α-consistent if CR → α as error $\eta \to 0$

Robustness:

- Predictions are terrible ⇒ no worse than worst-case
- Algorithm is β-consistent if CR ≤ β for all η

E.g., ski rental: CR $\le \min\left\{\frac{1+\lambda}{\lambda}, 1+\lambda+\frac{\eta}{(1-\lambda)\mathrm{OPT}}\right\}$

$(1+\lambda)$-consistent, $\left(\frac{1+\lambda}{\lambda}\right)$-robust

Bounds are tight [Gollapudi, Panigrahi, ICML'19; Angelopoulos et al., ITCS'20]

Lykouris, Vassilvitskii, ICML'18

Design principals

E.g., ski rental: $\mathrm{CR} \leq \min\left\{\frac{1+\lambda}{\lambda}, 1+\lambda+\frac{\eta}{(1-\lambda)\mathrm{OPT}}\right\}$

$(1+\lambda)$-consistent, $\left(\frac{1+\lambda}{\lambda}\right)$-robust

Also give **randomized algorithm**:

$\left(\frac{\lambda}{1-\exp(-\lambda)}\right)$-consistent, $\left(\frac{1}{1-\exp\left(-\left(\lambda-{}^{1}/_{b}\right)\right)}\right)$-robust

Bounds are **tight** [Wei, Zhang, NeurIPS'20]

Just scratched the surface

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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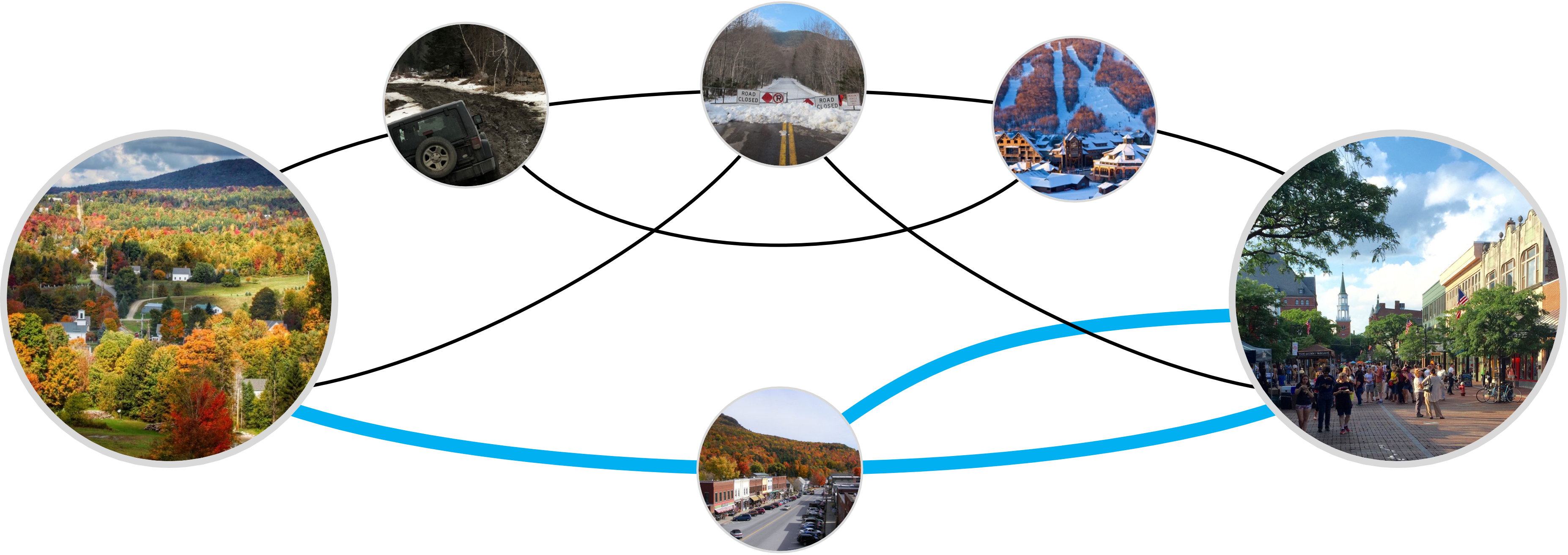
Alabi, Kalai, Ligett, Musco, Tzamos, **Vitercik**, COLT'19

Lincoln, Vermont

Burlington, Vermont

Traffic varies daily, but only a few different routes we'd take



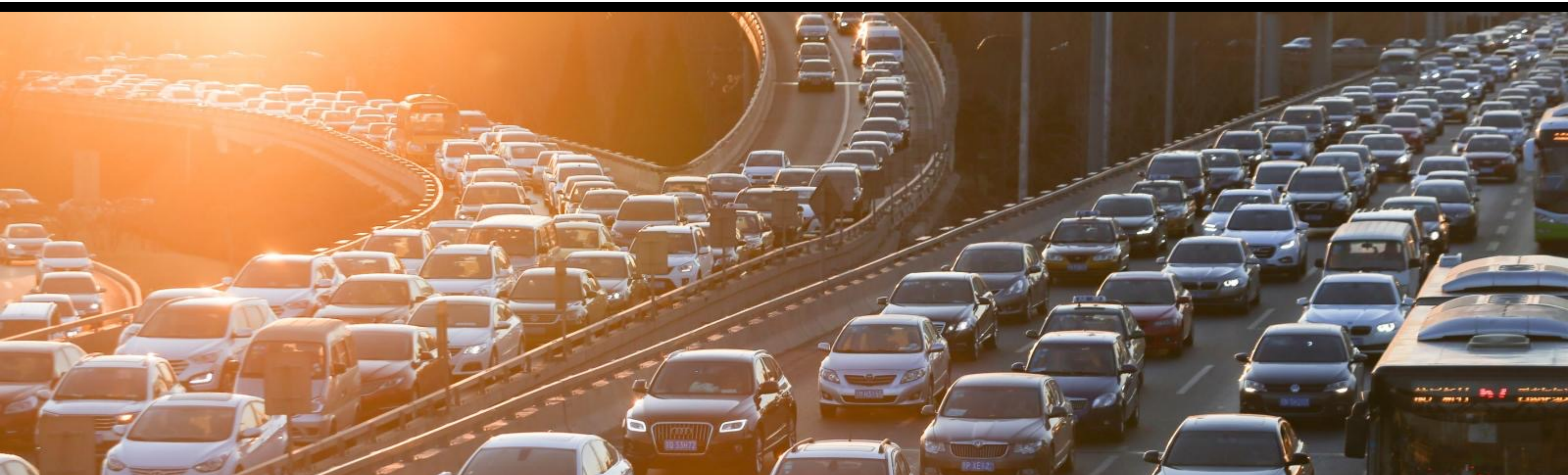
Dijkstra's algorithm wastes time searching muddy dirt roads

Alabi, Kalai, Ligett, Musco, Tzamos, **Vitercik**, COLT'19

Goal

Quickly solve sequences of similar problems

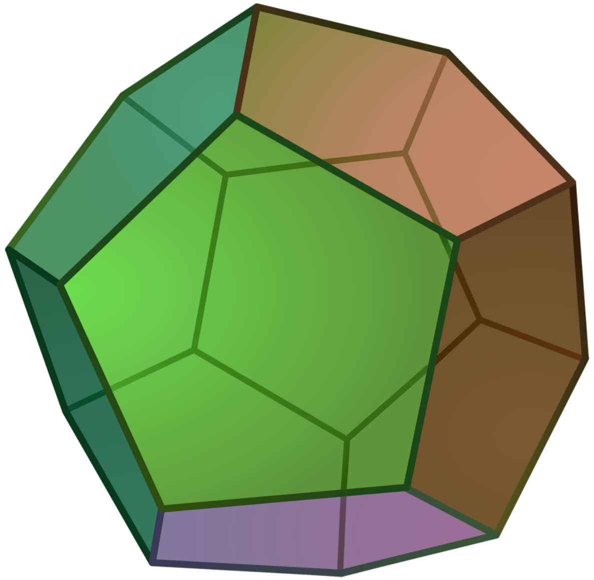
- Exploiting common structures



Speeding up repeated computations

Often, large swaths of search space **never** contain solutions…

Learn to ignore them!



Only handful of LP constraints ever bind

Large portions of DNA strings never contain patterns of interest

Alabi, Kalai, Ligett, Musco, Tzamos, **Vitercik**, COLT'19

Model

Function $f: X \to Y$ maps problem instances x to solutions y

Learning algorithm receives sequence $x_1, \ldots, x_T \in X$

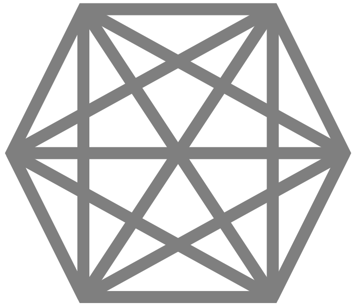
E.g., each $x_i \in \mathbb{R}^{|E|}$ equals edge weights for fixed road network

Model

Goal: Correctly compute f on *most* rounds, minimize runtime

Worst-case algorithm would compute and return $f(x_i)$ *for each* x_i

Assume access to other functions mapping $X \rightarrow Y$



- Faster to compute
- Defined by subsets (*prunings*) S of universe $\mathcal{U}$
  - Universe $\mathcal{U}$ represents entire search space
  - Denote corresponding function $f_S: X \rightarrow Y$
  - $f_{\mathcal{U}} = f$

Example:

$\mathcal{U}$ = all edges in fixed graph

S = subset of edges

Alabi, Kalai, Ligett, Musco, Tzamos, **Vitercik**, COLT'19

Model

Goal: Correctly compute f on *most* rounds, minimize runtime

Worst-case algorithm would compute and return $f(x_i)$ for each x_i

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- Defined by subsets (*prunings*) S of universe $\mathcal{U}$
  - Universe $\mathcal{U}$ represents entire search space
  - Denote corresponding function $f_S: X \to Y$
  - $f_{\mathcal{U}} = f$

Assume exists set $S^*(x) \subseteq \mathcal{U}$ where $f_S(x) = f(x)$ iff $S^*(x) \subseteq S$

- "Minimally pruned set"
- E.g., the shortest path

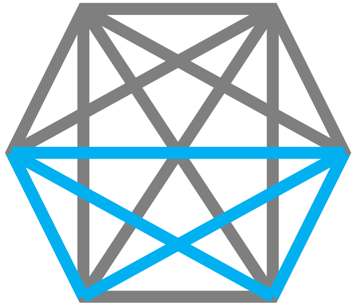
Alabi, Kalai, Ligett, Musco, Tzamos, **Vitercik**, COLT'19

Algorithm

```
1. Initialize pruned set $\bar{S}_1 \leftarrow \emptyset$
2. For each round $j \in \{1, \ldots, T\}$:
    a. Receive problem instance $x_j$
    b. With probability $1/\sqrt{j}$, explore:
        i. Output $f(x_j)$
        ii. Compute minimally pruned set $S^*(x_j)$
        iii. Update pruned set: $\bar{S}_{j+1} \leftarrow \bar{S}_j \cup S^*(x_j)$
    c. Otherwise (with probability $1 - 1/\sqrt{j}$), exploit:
        i. Output $f_{\bar{S}_j}(x_j)$
        ii. Don't update pruned set: $\bar{S}_{j+1} \leftarrow \bar{S}_j$
```

Alabi, Kalai, Ligett, Musco, Tzamos, **Vitercik**, COLT'19

Guarantees



Recap: At round j, algorithm outputs $f_{S_j}(x_j)$.

S_j depends on $x_{1:j}$.

Goal 1: Minimize $|S_j|$

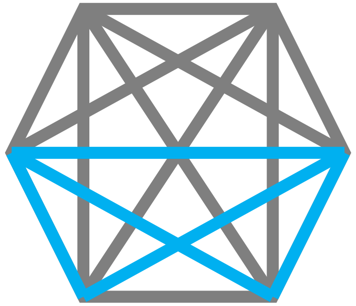
In our applications, time it takes to compute $f_{S_j}(x_j)$ grows with $|S_j|$

Theorem: Let $S^* = \bigcup_{j=1}^{T} S^*(x_j)$

Then $\mathbb{E}\left[\frac{1}{T}\sum_{j=1}^{T}|S_j|\right] \leq |S^*| + \frac{|\mathcal{U}|-|S^*|}{\sqrt{T}}$

Alabi, Kalai, Ligett, Musco, Tzamos, **Vitercik**, COLT'19

Guarantees



Recap: At round j, algorithm outputs $f_{S_j}(x_j)$.

S_j depends on $x_{1:j}$.

Goal 2: Minimize # of mistakes

Rounds where $f_{S_j}(x_j) \neq f(x_j)$

Theorem: $\mathbb{E}$[# of mistakes] $\leq \frac{|S^*|}{\sqrt{T}}$, where $S^* = \bigcup_{j=1}^{T} S^*(x_j)$

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Goal: Reach right star from left star

Grey nodes: Nodes A* explores over 30 rounds

Black nodes: Nodes in the pruned subgraph

Fraction of mistakes: 0.06 over 5000 runs of the algorithm, 30 rounds each

Alabi, Kalai, Ligett, Musco, Tzamos, **Vitercik**, COLT'19

Outline

1. Introduction
2. Algorithm configuration
3. Algorithms with predictions
4. Learning to prune
5. **Conclusion and future directions**

Conclusions

Automated configuration

Applied research dating back several decades

Horvitz et al., UAI'01; Leyton-Brown et al., CP '03; Likhodedov, Sandholm, AAAI '04, '05; …

Learning-theoretic guarantees

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

Algorithms with predictions

Lykouris, Vassilvitskii, ICML'18; Mitzenmacher, NeurIPS'18; Purohit et al., NeurIPS'18; Hsu, Indyk, Katabi, Vakilian, ICLR'19; …

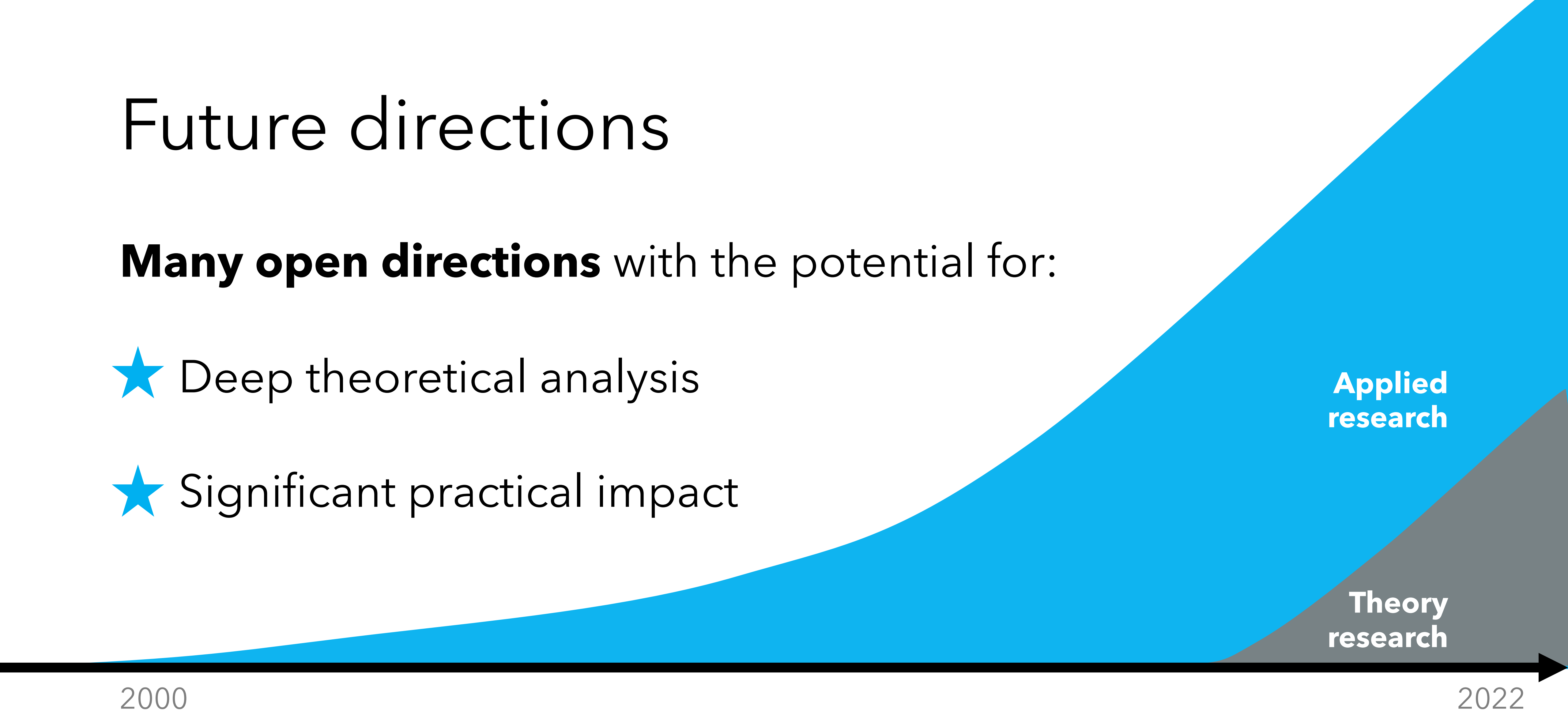
Learning to prune

Alabi, Kalai, Ligett, Musco, Tzamos, **V**, COLT'19

Future directions

Many open directions with the potential for:

- ★ Deep theoretical analysis
- ★ Significant practical impact



Future directions

What about when you don’t have enough data to learn?

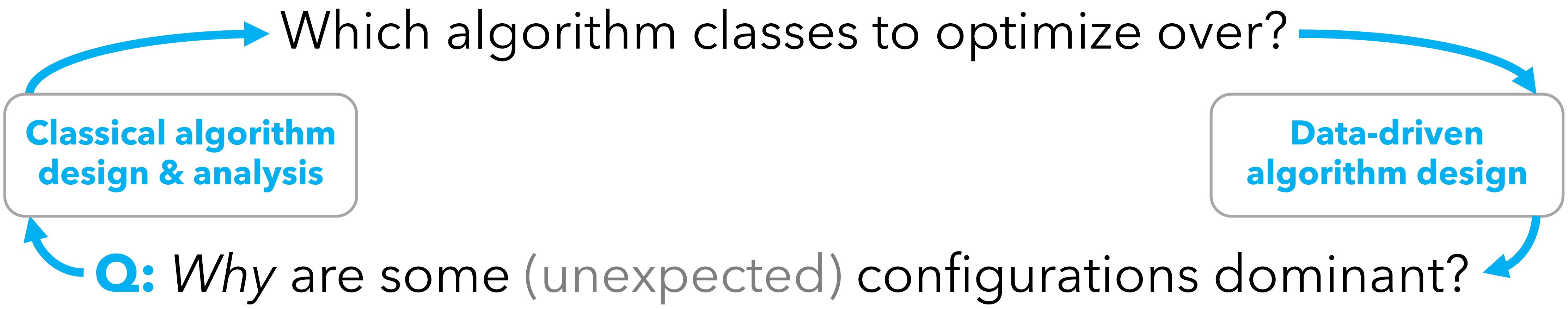
E.g., a shipping company starting out with just one routing IP

Could CPLEX still use ML to optimize performance?

Could similar problems provide guidance?

What does it mean for, say, IPs to be “similar enough”?

Future directions



Which algorithm classes to optimize over?

Classical algorithm design & analysis

Data-driven algorithm design

Q: *Why* are some (unexpected) configurations 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.”

Future directions

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.”

“extremely muscular teapot”

Similar to how DALL-E will (ideally) serve as an assistive tool for artists

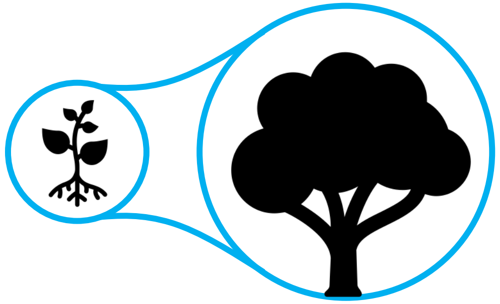
Future directions

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

Applied research: Dai et al., NeurIPS'17; Agrawal et al., ICML'20; …

Eventually, solve problems **no one's ever been able to solve**

Can theory provide guidance about how/when algs generalize?



Machine learning for **algorithm design**

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