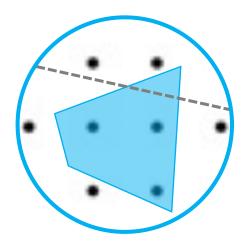
Theoretical foundations of **machine learning** for **cutting plane** selection

Ellen Vitercik

Berkeley (EECS) \rightarrow **Stanford** (MS&E + CS)

Balcan, Sandholm, Prasad, Vitercik [NeurIPS'21] Balcan, DeBlasio, Dick, Kingsford, Sandholm, Vitercik [STOC'21]



Integer programming solvers

Most popular tool for solving combinatorial problems



ML for integer programming

Used heavily throughout industry and science

Many different ways to incorporate learning into solving E.g., IP solvers (CPLEX, Gurobi) have a **ton** of parameters CPLEX has **170-page** manual describing **172** parameters

CPX_PARAM_NODEFILEIND 100 CPX PARAM TRELIM 160 CPX_PARAM_RANDOMSEED 130 CPXPARAM_MIP_Pool_RelGap 148 CPX_PARAM_REDUCE 131 CPXPARAM_MIP_Pool_Replace 151 CPX_PARAM_FLOWPATHS 71 CPX_PARAM_NODELIM 101 CPX_PARAM_TUNINGDETTILIM 160 CPX_PARAM_REINV 131 CPXPARAM_MIP_Strategy_Branch 39 CPX_PARAM_NODESEL 102 CPX_PARAM_TUNINGDISPLAY 162 CPX_PARAM_FPHEUR 72 CPX_PARAM_NUMERICALEMPHASIS 102CPX_PARAM_TUNINGMEASURE 163 CPX_PARAM_RELAXPREIND 132 CPXPARAM_MIP_Strategy_MIQCPStrat 93 CPX PARAM FRACCAND 73 CPX_PARAM_NZREADLIM 103 CPX_PARAM_TUNINGREPEAT 164 CPX PARAM RELOBIDIF 133 CPXPARAM_MIP_Strategy_StartAlgorithm 139 CPX_PARAM_FRACCUTS 73 CPX_PARAM_REPAIRTRIES 133 CPXPARAM_MIP_Strategy_VariableSelect 166 CPX_PARAM_FRACPASS 74 CPX_PARAM_OBJDIF 104 CPX_PARAM_TUNINGTILIM 165 CPX_PARAM_VARSEL 166 CPX_PARAM_REPEATPRESOLVE 134 CPXPARAM_MIP_SubMIP_NodeLimit 155 CPX_PARAM_GUBCOVERS 75 CPX_PARAM_OBJLLIM 105 CPXPARAM_OptimalityTarget 106 CPX_PARAM_RINSHEUR 135 CPX_PARAM_HEURFREQ 76 CPX_PARAM_OBJULIM 105 CPX_PARAM_WORKDIR 167 CPX_PARAM_RLT 136 CPXPARAM_Output_WriteLevel 169 CPX_PARAM_IMPLBD 76 CPX PARAM PARALLELMODE 108 CPX PARAM WORKMEM 168 CPXPARAM_Preprocessing_Aggregator 19 CPX_PARAM_ROWREADLIM 141 CPX_PARAM_PERIND 110 CPX_PARAM_WRITELEVEL 169 CPXPARAM_Preprocessing_Fill 19 CPX PARAM SCAIND 142 CPX PARAM INTSOLLIM 79 CPX_PARAM_PERLIM 111 CPX_PARAM_ZEROHALFCUTS 170 CPXPARAM_Preprocessing_Linear 120 CPX_PARAM_POLISHAFTERDETTIME 111CPXPARAM_Benders_Strategy 30 CPX_PARAM_SCRIND 143 CPX_PARAM_ITLIM 80 CPX_PARAM_SIFTALG 143 CPXPARAM_Preprocessing_Reduce 131 CPX_PARAM_LANDPCUTS 82 CPX_PARAM_POLISHAFTEREPAGAP 112 CPXPARAM_Benders_Tolerances_feasibilitycut 35 CPX_PARAM_SIFTDISPLAY 144 CPXPARAM_Preprocessing_Symmetry 156 CPX_PARAM_LBHEUR 81 CPX PARAM POLISHAFTEREPGAP CPXPARAM_Benders_Tolerances_optimalitycut 36 113 CPXPARAM_Read_DataCheck 54 CPX_PARAM_POLISHAFTERINTSOL CPXPARAM_Conflict_Algorithm 46 CPX_PARAM_SIFTITLIM 145 CPX PARAM LPMETHOD 136 114CPX_PARAM_SIMDISPLAY 145 CPXPARAM_Read_Scale 142 CPX_PARAM_MCFCUTS 82 CPX PARAM POLISHAFTERNODE 115 CPXPARAM CPUmask 48 CPX_PARAM_SINGLIM 146 CPXPARAM_ScreenOutput 143 CPX_PARAM_MEMORYEMPHASIS CPX_PARAM_POLISHAFTERTIME 116 CPXPARAM_DistMIP_Rampup_Duration 128 CPX_PARAM_SOLNPOOLAGAP 146 CPXPARAM_Sifting_Algorithm 143 CPX PARAM MIPCBREDLP 84 CPX PARAM POLISHTIME CPXPARAM_LPMethod 136 CPX_PARAM_SOLNPOOLCAPACITY 147 CPXPARAM_Sifting_Display 144 CPXPARAM_MIP_Cuts_BQP 38 CPX_PARAM_MIPDISPLAY 85 (deprecated) 116 CPX_PARAM_SOLNPOOLGAP 148 CPXPARAM_Sifting_Iterations 145 CPX_PARAM_MIPEMPHASIS 87 CPX_PARAM_POPULATELIM 117 CPXPARAM_MIP_Cuts_LocalImplied 77 149 CPXPARAM_Simplex_Display 145 CPX PARAM SOLNPOOLINTENSITY CPX_PARAM_PPRIIND 118 CPXPARAM_MIP_Cuts_RLT 136 CPX_PARAM_MIPINTERVAL 88 CPX_PARAM_PREDUAL 119 CPXPARAM_MIP_Cuts_ZeroHalfCut 170 CPX_PARAM_SOLNPOOLREPLACE 151 CPXPARAM_Simplex_Limits_Singularity 146 CPX_PARAM_MIPKAPPASTATS 89

CPX PARAM FLOWCOVERS 70 CPX PARAM BRDIR 39 CPX_PARAM_BTTOL 40 CPX_PARAM_CALCOCPDUALS 41 CPX PARAM CLIOUES 42 CPX_PARAM_CLOCKTYPE 43 CPX_PARAM_CLONELOG 43 CPX_PARAM_COEREDIND 44 CPX_PARAM_COLREADLIM 45 CPX_PARAM_CONFLICTDISPLAY 46 CPX_PARAM_INTSOLFILEPREFIX 78 CPX_PARAM_COVERS 47 CPX PARAM CPUMASK 48 CPX_PARAM_CRAIND 50 CPX_PARAM_CUTLO 51 CPX_PARAM_CUTPASS 52 CPX PARAM CUTSFACTOR 52 CPX_PARAM_CUTUP 53 83 CPX_PARAM_DATACHECK 54 CPX PARAM DEPIND 55 CPX_PARAM_DETTILIM 56 CPX PARAM DISICUTS 57 CPX_PARAM_DIVETYPE 58 CPX_PARAM_DPRIIND 59

ML for integer programming

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Solving is extremely difficult, so ML can make a huge difference

Companies often have lots of **data** about their applications E.g., all the scheduling IPs an airline solves day after day

ML for integer programming

Lots of interest from an **empirical** perspective, e.g.:

Leyton-Brown, Nudelman, Andrew, McFadden, ShohamIJCAI'03, CP'03Hutter, Hoos, Leyton-Brown, StützleJAIR'09SandholmHandbook of Market Design'13He, Daume, EisnerNeurIPS'14Khalil, Le Bodic, Song, Nemhauser, DilkinaAAAI'16Song, Lanka, Yue, DilkinaNeurIPS'20Tang, Agrawal, FaenzaICML'20Huang, Wang, Liu, Zhen, Zhang, Yuan, Hao, Yu, WangPattern Recognition '22

This talk:

Guarantees for IP parameter optimization (*cut selection*)

ML for algorithm design



[Leyton-Brown, Nudelman, Andrew, McFadden, Shoham, CP '03; ...]

Constraint satisfaction

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

Economics (mechanism design)

[Likhodedov, Sandholm, AAAI '04, '05; ...]

Computational biology

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

Applied research

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ML for algorithm design

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

Algorithms with predictions

[Lykouris, Vassilvitskii, ICML'18; Mitzenmacher, NeurIPS'18; ...]

Mechanism design via machine learning

[Elkind, SODA'07; Morgenstern, Roughgarden, NeurIPS'15, COLT'16; ...]

Applied research

→ Theory research

Outline

- 1. Introduction
- 2. Integer programming
 - i. Overview
 - ii. Branch-and-bound
 - iii. Our results
- 3. Beyond integer programming
- 4. Conclusions

Integer programs

maximize $c \cdot z$ subject to $Az \leq b$ $z \in \mathbb{Z}^n$

 $A \in \mathbb{Z}^{m imes n}$, $\boldsymbol{b} \in \mathbb{Z}^m$

Modeling the application domain

IPs drawn from unknown application-specific distribution $\ensuremath{\mathcal{D}}$



E.g., distribution over routing problems

Widely assumed in applied research, e.g.:

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

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

Gupta, Roughgarden Balcan

ITCS'16 Book Chapter'20

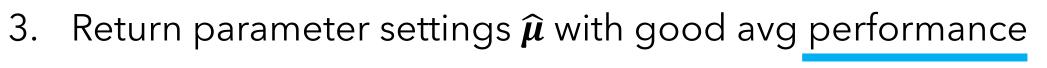
Automated configuration procedure

1. Fix parameterized IP solver

 $\{A^{(1)}, \boldsymbol{b}^{(1)}, \boldsymbol{c}^{(1)}\}$

2. Receive training set of "typical" IPs sampled from ${\cal D}$

 $\{A^{(2)}, \boldsymbol{b}^{(2)}, \boldsymbol{c}^{(2)}\}$



 $\{A^{(3)}, \boldsymbol{b}^{(3)}, \boldsymbol{c}^{(3)}\}$

Search tree size, runtime, etc.

 $\{A^{(4)}, \boldsymbol{b}^{(4)}, \boldsymbol{c}^{(4)}\}$

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

Hutter et al. [JAIR'09, LION'11], Ansótegui et al. [CP'09], Sandholm [Handbook of Market Design '13], Khalil et al. [AAAI'16], Balcan, Sandholm, **Vitercik** [AAAI'20], ...

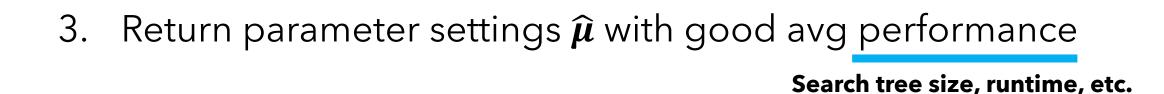
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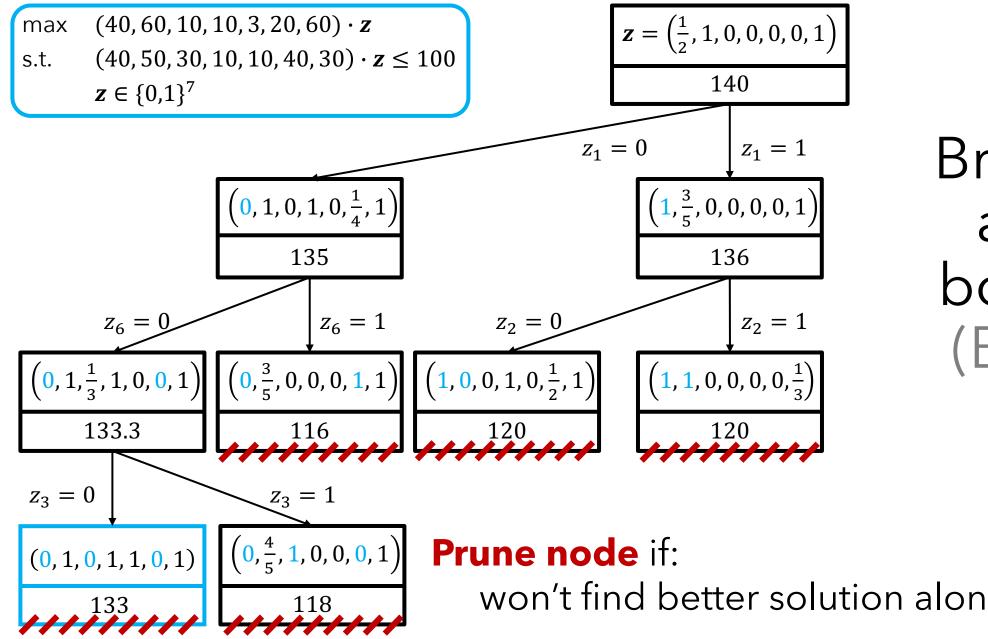
Focus of this talk: Will $\hat{\mu}$ have good future performance? More formally: Is the expected utility of $\hat{\mu}$ also high?

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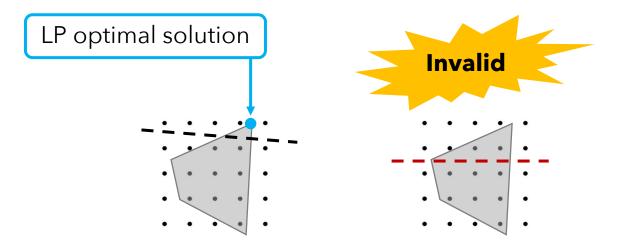
Branch and bound

won't find better solution along branch

Cutting planes

Additional constraints that:

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



Cutting planes

Modern IP solvers add cutting planes through the B&B tree *"Branch-and-cut"*

Responsible for breakthrough speedups of IP solvers Cornuéjols, Annals of OR '07

Challenges:

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



Key challenge

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

Every aspect of tree search depends on LP guidance Node selection, variable selection, pruning, ...

Tiny change in cut can cause major changes to tree



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iii. Our results

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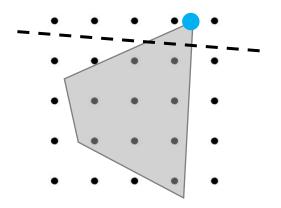
Chvátal-Gomory cuts

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

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

Important properties:

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



Key challenge: Sensitivity of B&C

Theorem [informal]:

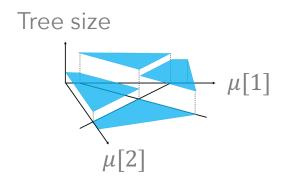
Tiny changes to μ can lead to exponential jumps in tree size





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

Tree size is a piecewise-constant function of $\mu \in [0,1)^m$



Balcan, Sandholm, Prasad, Vitercik, NeurIPS'21

Key lemma

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

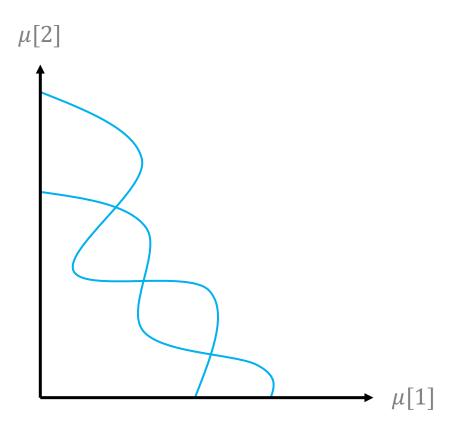
- CG cut parameterized by $\boldsymbol{\mu} \in [0,1)^m$ is $[\boldsymbol{\mu}^T A] \boldsymbol{z} \leq [\boldsymbol{\mu}^T \boldsymbol{b}]$
- For any u and column a_i , $[\mu^T a_i] \in [-\|a_i\|_1, \|a_i\|_1]$
- For each integer $k_i \in [-\|a_i\|_1, \|a_i\|_1]$:

$$[\boldsymbol{\mu}^T \boldsymbol{a}_i] = k_i \text{ iff } k_i \leq \boldsymbol{\mu}^T \boldsymbol{a}_i < k_i + 1$$

• In any region defined by intersection of halfspaces: ($[\mu^T a_1], ..., [\mu^T a_m]$) is constant $O(||A||_{1,1} + n)$ halfspaces

Beyond Chvátal-Gomory cuts

For more complex families, boundaries can be more complex

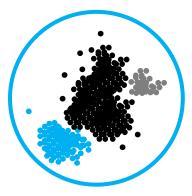


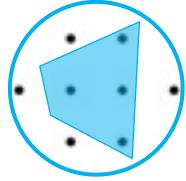
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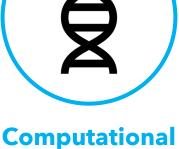
Overview

A **unifying** structure connects **seemingly disparate** problems:

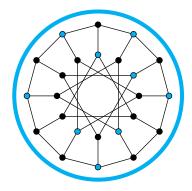




Clustering algorithm configuration Integer programming algorithm configuration



biology algorithm configuration **Mechanism** configuration



Greedy algorithm configuration

Use to provide generalization bounds

General algorithm configuration model

 \mathbb{R}^d : Set of all algorithm parameter settings

 \mathcal{X} : Set of all algorithm inputs

E.g., integer programs

Algorithmic performance:

 $u_{\mu}(x) =$ utility of algorithm parameterized by μ on input xE.g., runtime, solution quality, revenue, memory usage ...

Primal & dual classes

 $\begin{array}{l} u_{\mu}(x) = \text{utility of algorithm parameterized by } \mu \text{ on input } x \\ \mathcal{U} = \left\{ u_{\mu} \colon \mathcal{X} \to \mathbb{R} \ \middle| \ \mu \in \mathbb{R}^{d} \right\} \quad \text{"Primal" function class} \end{array}$

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

VC dimension, Rademacher complexity, ...

Primal & dual classes

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

$$u_x^*(\mu) = \text{utility as function of parameters}$$

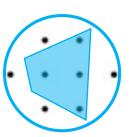
 $u_x^*(\mu) = u_\mu(x)$
 $\mathcal{U}^* = \{u_x^* : \mathbb{R}^d \to \mathbb{R} \mid x \in \mathcal{X}\}$ "Dual" function class

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

Piecewise-structured functions

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





Clustering algorithm configuration

Integer programming algorithm configuration



Selling mechanism configuration



Greedy algorithm configuration

Computational biology algorithm configuration



Voting mechanism configuration

Generalization to future inputs

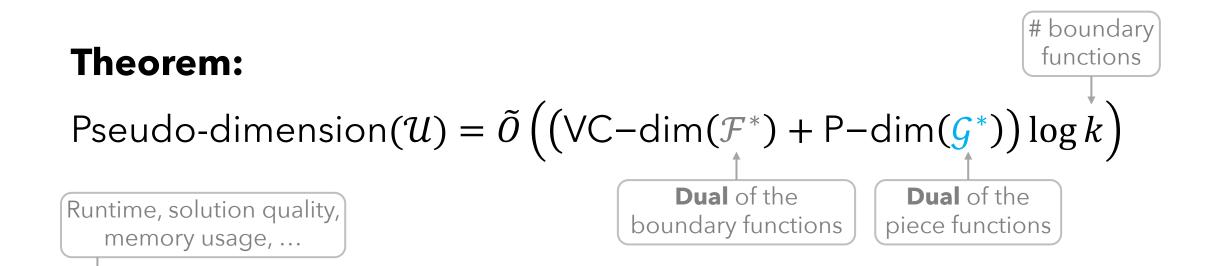
 $g \in \mathcal{G}$

 μ_1

 $\in \mathcal{F}$

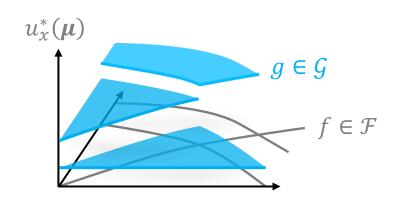
 $u_x^*(\boldsymbol{\mu})$

 μ_{2}



Generalization to future inputs

With high probability, for all μ : **Avg** utility on training set – **expected** utility = $\tilde{O}\left(H\sqrt{\frac{C_{\mathcal{F}}*+C_{\mathcal{G}}*}{N}}\right)$ Upper bound on utility Training set size

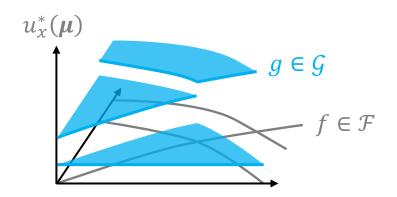


Application to cutting planes

Theorem:

$$Pseudo-dimension(\mathcal{U}) = \tilde{O}(m \log(||A||_{1,1} + ||b||_1 + n))$$

$$\ddagger constraints \qquad (Max over support) \qquad (# variables) \qquad (# variables)$$



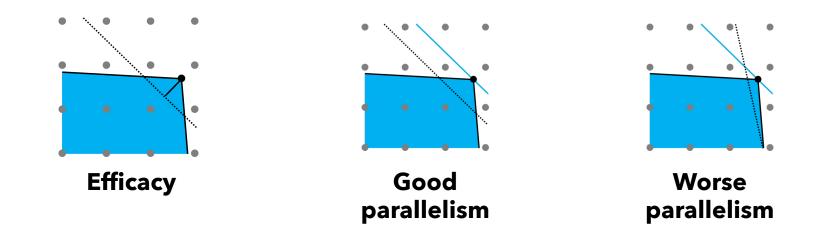
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Future directions

Existing solvers choose cuts from finite pool using heuristics



Machine learning to design new cut selection policies

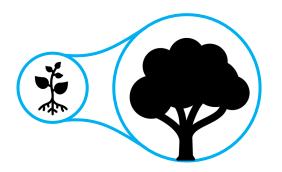
Future directions

Machine-learned algorithms can scale to larger instances

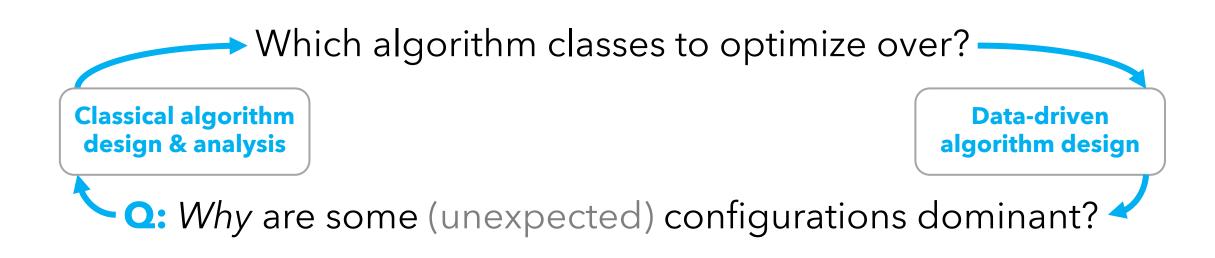
Applied research: Dai et al., NeurIPS'17; Agrawal et al., ICML'20; ...

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

More generally, given a single huge IP, how to use ML to solve?



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."

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