## Theoretical foundations of machine learning for cutting plane selection

## Ellen Vitercik <br> 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


Robust ML


Routing


Manufacturing


Scheduling


Planning

## 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 $\mathbf{1 7 2}$ parameters

CPX PARAM TRELIM 160
CPX_PARAM_TUNINGDETTILIM 160
CPX_PARAM_TUNINGDISPLAY 162
CPX_PARAM_TUNINGMEASURE 163
CPX_PARAM_TUNINGREPEAT 16
CPX_PARAM_TUNINGTILIM 165
CPX_PARAM_VARSEL 166
CPX_PARAM_WORKDIR 167
CPX_PARAM_WORKMEM 168
CPX_PARAM_WRITELEVEL 169
CPX_PARAM_ZEROHALFCUTS 170
111CPXPARAM_Benders_Strategy 30
2 CPXPARAM_Benders_Tolerances_feasibilitycut 35 CPXPARAM_Benders_Tolerances_optimalitycut 3 CPXPARAM_Conflict_Algorithm 46 CPXPARAM_CPUmask 48
CPXPARAM_DistMIP_Rampup_Duration 128
CPXPARAM_LPMethod 136
CPXPARAM_MIP_Cuts_BQP 38
CPXPARAM_MIP_Cuts_LocalImplied 77
CPXPARAM_MIP_Cuts_RLT 136

CPX_PARAM_RANDOMSEED 130 CPX PARAM REDUCE 131 CPX_PARAM_REINY 131 CPX_PARAM_RELAXPREIND 132 CPX_PARAM_RELOBJDIF 133 CPX_PARAM_REPAIRTRIES 133 CPX_PARAM_REPEATPRESOLVE 134 CPX_PARAM_RINSHEUR 135 CPX_PARAM_RLT 136 CPX_PARAM_ROWREADLIM 141 CPX_PARAM_SCAIND 142 CPX_PARAM_SCRIND 143 CPX_PARAM_SIFTALG 143 CPX_PARAM_SIFTDISPLAY 144 CPX_PARAM_SIFTITLIM 14 CPX_PARAM_SIMDISPLAY 145 CPX_PARAM_SINGLIM 146 CPX_PARAM_SOLNPOOLAGAP 146 CPX_PARAM_SOLNPOOLCAPACITY CPX_PARAM_SOLNPOOLGAP 148

CPXPARAM_MIP_Pool_RelGap CPXPARAM_MIP_Pool_Replace CPXPARAM_MIP_Strategy_Branch 39 CPXPARAM_MIP_Strategy_MIQCPStrat 93 CPXPARAM_MIP_Strategy_StartAlgorithm CPXPARAM_MIP_Strategy_VariableSelect 16 CPXPARAM_MIP_SubMIP_NodeLimit CPXPARAM_OptimalityTarget 106 CPXPARAM_Output_WriteLevel 169 CPXPARAM_Preprocessing_Aggregator 19 CPXPARAM_Preprocessing_Fill 19 CPXPARAM_Preprocessing_Linear 120 CPXPARAM_Preprocessing_Reduce 131 CPXPARAM_Preprocessing_Symmetry 156 CPXPARAM_Read_DataCheck 54 CPXPARAM_Read_Scale 142 CPXPARAM_ScreenOutput 143 CPXPARAM_Sifting_Algorithm 143 CPXPARAM_Sifting_Display CPXPARAM_Sifting_Iterations 145

CPX PARAM_FLOWCOVERS 70
CPX_PARAM_FLOWPATHS
CPX_PARAM FPHEUR CPX_PARAM_PARAM_FRACCAND 73 CPX_PARAM_FRACCANTS CPX_PARAM_FRACPASS 7 CPX_PARAM_GUBCOVERS 75 CPX_PARAM_HEURFREQ 76 CPX_PARAM_IMPLBD 76 CPX_PARAM_INTSOLFILEPREFIX CPX_PARAM_INTSOLLIM 79 CPX_PARAM_ITLIM 8 CPX_PARAM_LANDPCUTS 82 CPX_PARAM_LBHEUR 81 CPX_PARAM_LPMETHOD 136 CPX_PARAM_MCFCUTS 82 CPX_PARAM_MEMORYEMPHASIS $\begin{array}{ll}\text { CPX_PARAM_MIPCBREDLP } & 84 \\ \text { CPX_PARAM MIPDISPLAY } & 85\end{array}$ CPX_PARAM_MIPDISPLAY 85
CPX_PARAM MIPEMPHASIS 87 CPX_PARAM_MIPEMPHASIS 87

CPX_PARAM_BRDIR 39 CPX_PARAM_BTTOL 40
CPX_PARAM_CALCQCPDUALS 41 CPX PARAM CLIOUES 42 CPX_PARAM_CLOCKTYPE 4 CPX_PARAM_CLONELOG 43 CPX_PARAM_COEREDIND 4
CPX_PARAM_COLREADLIM 45
CPX_PARAM_CONFLICTDISPLAY 46
CPX_PARAM_COVERS 47
CPX_PARAM_CPUMASK 4
CPX_PARAM_CRAIND 50 CPX_PARAM_CUTLO CPX_PARAM_CUTPASS 52 CPX_PARAM_CUTSFACTOR 52 CPX_PARAM_CUTUP 53

## 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 $\mathbf{1 7 2}$ parameters

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, Shoham IJCAI'03, CP'03
    Hutter,Hoos, Leyton-Brown, Stützle JAIR'09
    Sandholm
    He, Daume, Eisner
    Khalil, Le Bodic, Song, Nemhauser, Dilkina
    Song, Lanka, Yue, Dilkina
    Tang, Agrawal, Faenza
    Huang, Wang, Liu, Zhen, Zhang, Yuan, Hao, Yu, Wang
    Handbook of Market Design'13
    NeurIPS'14
    AAAI'16
    NeurIPS'20
    ICML'20
    Pattern Recognition '22
```


## This talk:

Guarantees for IP parameter optimization (cut selection)

## ML for algorithm design

## Integer \& linear programming

[Leyton-Brown, Nudelman, Andrew, McFadden, Shoham, CP '03; ...]
Constraint satisfaction
[Horvitz, Ruan, Gomes, Krautz, Selman, Chickering, UAl'01; ...]

Applied research

## Economics (mechanism design)

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


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

## ML for algorithm design

```
Automated algorithm configuration and selection
[Gupta, Roughgarden, ITCS'16; Balcan, Nagarajan, Vitercilk, White, COLT'17; ...]
Applied
Algorithms with predictions
[Lykouris, Vassilvitskii, ICML'18; Mitzenmacher, NeurIPS'18; ...]
Mechanism design via machine learning
[Elkind, SODA'07; Morgenstern, Roughgarden, NeurlPS'15, COLT'16; ...]

\section*{Outline}
1. Introduction
2. Integer programming
i. Overview
ii. Branch-and-bound
iii. Our results
3. Beyond integer programming
4. Conclusions

\section*{Integer programs}
```

maximize }\boldsymbol{c}\cdot\boldsymbol{z
subject to }A\boldsymbol{z}\leq\boldsymbol{b
z}\in\mp@subsup{\mathbb{Z}}{}{n

```
\(A \in \mathbb{Z}^{m \times n}, \boldsymbol{b} \in \mathbb{Z}^{m}\)

\section*{Modeling the application domain}

IPs drawn from unknown application-specific distribution \(\mathcal{D}\)
E.g., distribution over routing problems

Widely assumed in applied research, e.g.:

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

\section*{Automated configuration procedure}
1. Fix parameterized IP solver
2. Receive training set of "typical" IPs sampled from \(\mathcal{D}\)
\(\left\{A^{(1)}, b^{(1)}, c^{(1)}\right\}\)
\(\left\{A^{(2)}, \boldsymbol{b}^{(2)}, \boldsymbol{c}^{(2)}\right\}\)
\(\left\{A^{(3)}, \boldsymbol{b}^{(3)}, \boldsymbol{c}^{(3)}\right\}\)
\(\left\{A^{(4)}, \boldsymbol{b}^{(4)}, \boldsymbol{c}^{(4)}\right\}\)
- - -
3. Return parameter settings \(\widehat{\boldsymbol{\mu}}\) with good avg performance

Search tree size, runtime, etc.

Key question: How to find \(\widehat{\boldsymbol{\mu}}\) 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. [AAAl'16], Balcan, Sandholm, Vitercik [AAAl'20], ...

\section*{Automated configuration procedure}
1. Fix parameterized IP solver
2. Receive training set of "typical" IPs sampled from \(\mathcal{D}\)
\(\left\{A^{(1)}, b^{(1)}, c^{(1)}\right\}\)
\(\left\{A^{(2)}, \boldsymbol{b}^{(2)}, c^{(2)}\right\}\)
\(\left\{A^{(3)}, \boldsymbol{b}^{(3)}, \boldsymbol{c}^{(3)}\right\}\)
\(\left\{A^{(4)}, \boldsymbol{b}^{(4)}, \boldsymbol{c}^{(4)}\right\}\)
- - -
3. Return parameter settings \(\widehat{\boldsymbol{\mu}}\) with good avg performance

Search tree size, runtime, etc.

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

\section*{Outline}
1. Introduction
2. Integer programming
i. Overview
ii. Branch-and-bound
iii. Our results
3. Beyond integer programming
4. Conclusions


\section*{Cutting planes}

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


\section*{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

\section*{Challenges:}
- Many different types of cutting planes
- Chvátal-Gomory cuts, cover cuts, clique cuts, ...
- How to choose which cuts to apply?


\section*{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, ...

\section*{Tiny change in cut can cause major changes to tree}

-

\section*{Outline}
1. Introduction
2. Integer programming
i. Overview of results
ii. Branch-and-bound
iii. Our results
3. Beyond integer programming
4. Conclusions

\section*{Chvátal-Gomory cuts}

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

CG cut parameterized by \(\boldsymbol{\mu} \in[0,1)^{m}\) is \(\left\lfloor\boldsymbol{\mu}^{T} A\right\rfloor \mathbf{z} \leq\left\lfloor\boldsymbol{\mu}^{T} \boldsymbol{b}\right\rfloor\)

\section*{Important properties:}
- CG cuts are valid
- Can be chosen so it separates the LP opt


\section*{Key challenge: Sensitivity of B\&C}

\section*{Theorem [informal]:}

Tiny changes to \(\boldsymbol{\mu}\) can lead to exponential jumps in tree size
\[
\begin{array}{r}
\because \div \% \\
\because \because
\end{array}
\]

\section*{Key lemma}

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

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


\section*{Key lemma}

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

\section*{Proof idea:}
- CG cut parameterized by \(\boldsymbol{\mu} \in[0,1)^{m}\) is \(\left\lfloor\boldsymbol{\mu}^{T} A\right\rfloor \mathbf{z} \leq\left\lfloor\boldsymbol{\mu}^{T} \boldsymbol{b}\right\rfloor\)
- For any \(\boldsymbol{u}\) and column \(\boldsymbol{a}_{i},\left\lfloor\boldsymbol{\mu}^{T} \boldsymbol{a}_{i}\right\rfloor \in\left[-\left\|\boldsymbol{a}_{i}\right\|_{1},\left\|\boldsymbol{a}_{i}\right\|_{1}\right]\)
- For each integer \(k_{i} \in\left[-\left\|\boldsymbol{a}_{i}\right\|_{1},\left\|\boldsymbol{a}_{i}\right\|_{1}\right]\) :
\[
\left\lfloor\boldsymbol{\mu}^{T} \boldsymbol{a}_{i}\right\rfloor=k_{i} \text { iff } k_{i} \leq \boldsymbol{\mu}^{T} \boldsymbol{a}_{i}<k_{i}+1 \quad\left\{\begin{array}{c}
o\left(\|A\|_{1,1}+n\right) \\
\text { halfspaces }
\end{array}\right.
\]
- In any region defined by intersection of halfspaces:
\(\left(\left\lfloor\boldsymbol{\mu}^{T} \boldsymbol{a}_{1}\right\rfloor, \ldots,\left\lfloor\boldsymbol{\mu}^{T} \boldsymbol{a}_{m}\right\rfloor\right)\) is constant

\section*{Beyond Chvátal-Gomory cuts}

For more complex families, boundaries can be more complex


\section*{Outline}
1. Introduction
2. Integer programming
3. Beyond integer programming
4. Conclusions

\section*{Overview}

A unifying structure connects seemingly disparate problems:


Clustering algorithm configuration


Integer programming
algorithm configuration


Computational biology algorithm configuration


Mechanism configuration


Greedy algorithm configuration

Use to provide generalization bounds

\section*{General algorithm configuration model}
\(\mathbb{R}^{d}\) : Set of all algorithm parameter settings
\(x\) : Set of all algorithm inputs
E.g., integer programs

\section*{Algorithmic performance:}
\(u_{\mu}(x)=\) utility of algorithm parameterized by \(\boldsymbol{\mu}\) on input \(x\) E.g., runtime, solution quality, revenue, memory usage ...

\section*{Primal \& dual classes}
\(u_{\mu}(x)=\) utility of algorithm parameterized by \(\boldsymbol{\mu}\) on input \(x\)
\(\mathcal{U}=\left\{u_{\boldsymbol{\mu}}: \mathcal{X} \rightarrow \mathbb{R} \mid \boldsymbol{\mu} \in \mathbb{R}^{d}\right\} \quad\) "Primal" function class
Typically, prove guarantees by bounding complexity of \(\mathcal{U}\)
VC dimension, Rademacher complexity, ...

\section*{Primal \& dual classes}
\(u_{\boldsymbol{\mu}}(x)=\) utility of algorithm parameterized by \(\boldsymbol{\mu}\) on input \(x\)
\(\mathcal{U}=\left\{u_{\boldsymbol{\mu}}: \mathcal{X} \rightarrow \mathbb{R} \mid \boldsymbol{\mu} \in \mathbb{R}^{d}\right\} \quad\) "Primal" function class
Typically, prove guarantees by bounding complexity of \(\mathcal{U}\)
\(u_{x}^{*}(\boldsymbol{\mu})=\) utility as function of parameters
\(u_{x}^{*}(\boldsymbol{\mu})=u_{\mu}(x)\)
\(\mathcal{U}^{*}=\left\{u_{x}^{*}: \mathbb{R}^{d} \rightarrow \mathbb{R} \mid x \in \mathcal{X}\right\} \quad\) "Dual" function class
- Dual functions have simple, Euclidean domain
- Often have ample structure can use to bound complexity of \(\mathcal{U}\)

\section*{Piecewise-structured functions}

\section*{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

\section*{Generalization to future inputs}

\section*{Theorem:}

Pseudo-dimension \((\mathcal{U})=\tilde{O}\left(\left(\mathrm{VC}-\operatorname{dim}\left(\mathcal{F}_{\uparrow}^{*}\right)+\mathrm{P}-\operatorname{dim}\left(\mathcal{G}_{\uparrow}^{*}\right)\right) \log k\right)\)


Dual of the
piece functions

\section*{Generalization to future inputs}

With high probability, for all \(\boldsymbol{\mu}\) :
\(\mid\) Avg utility on training set - expected utility| \(=\tilde{O}\left(H \sqrt{\frac{C_{\mathcal{F}^{*}+C_{G^{*}}}^{N}}{N}}\right)\)
\(\left.\uparrow \begin{array}{c}\text { Upper bound } \\ \text { on utility }\end{array}\right] \begin{gathered}\text { Training } \\ \text { set size }\end{gathered}\)


\section*{Application to cutting planes}

\section*{Theorem:}



\section*{Outline}
1. Introduction
2. Integer programming
3. Beyond integer programming
4. Conclusions

\section*{Future directions}

Existing solvers choose cuts from finite pool using heuristics


Efficacy


Good
parallelism


Worse parallelism

Machine learning to design new cut selection policies

\section*{Future directions}

Machine-learned algorithms can scale to larger instances Applied research: Dai et al., NeurIPS'17; Agrawal et al., ICML'20; ...

\section*{Eventually, solve IPs no one's ever been able to solve}

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


\section*{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. [NeurlPS'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."

\section*{Theoretical foundations of machine learning for cutting plane selection}

\section*{Ellen Vitercik \\ Berkeley (EECS) \(\rightarrow\) Stanford (MS\&E + CS)}

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

