

Machine learning in MI(NL)P solvers

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Director, Mixed-Integer Optimization @ FICO

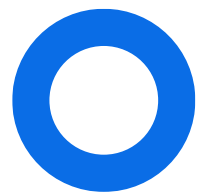
Exam

- Exam dates
 - September 11, September 25, October 5
 - 10-17, every 45min. Target length: 30min
- Contents
 - All lectures, and algorithmic/mathematical material from exercises, basic concepts
 - You will not need to do C++ coding (or discuss code)
 - Describe algorithms, intuitions behind them, the mathematical concepts, apply them to concrete examples, provide or explain visualizations
 - Ask yourself: How would you set up an exam for this course?
- Room: ZIB, 3104 (first floor Langbau)

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Agenda

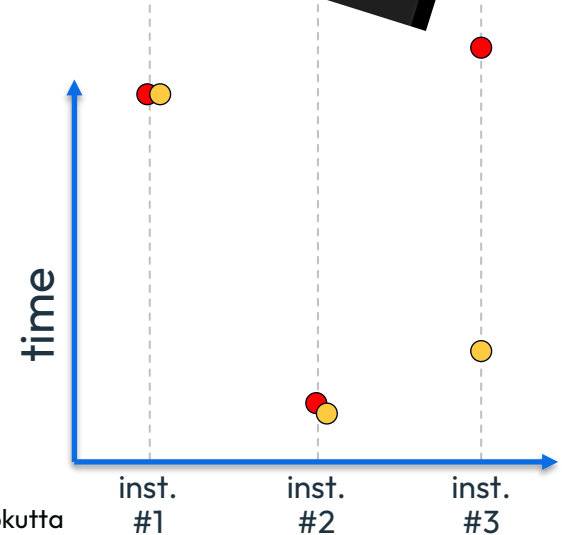
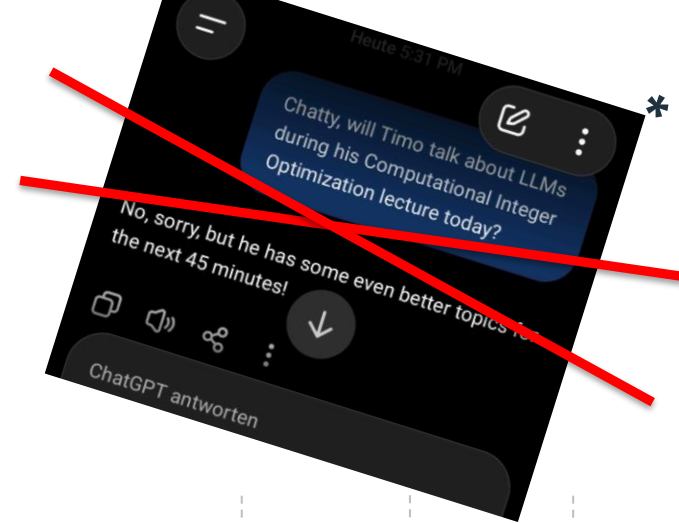
1. What do I mean by ML?
2. Learning to Scale
3. Learning to Use Local Cuts
4. Learning to Select Branching Rules



What do I mean by ML?

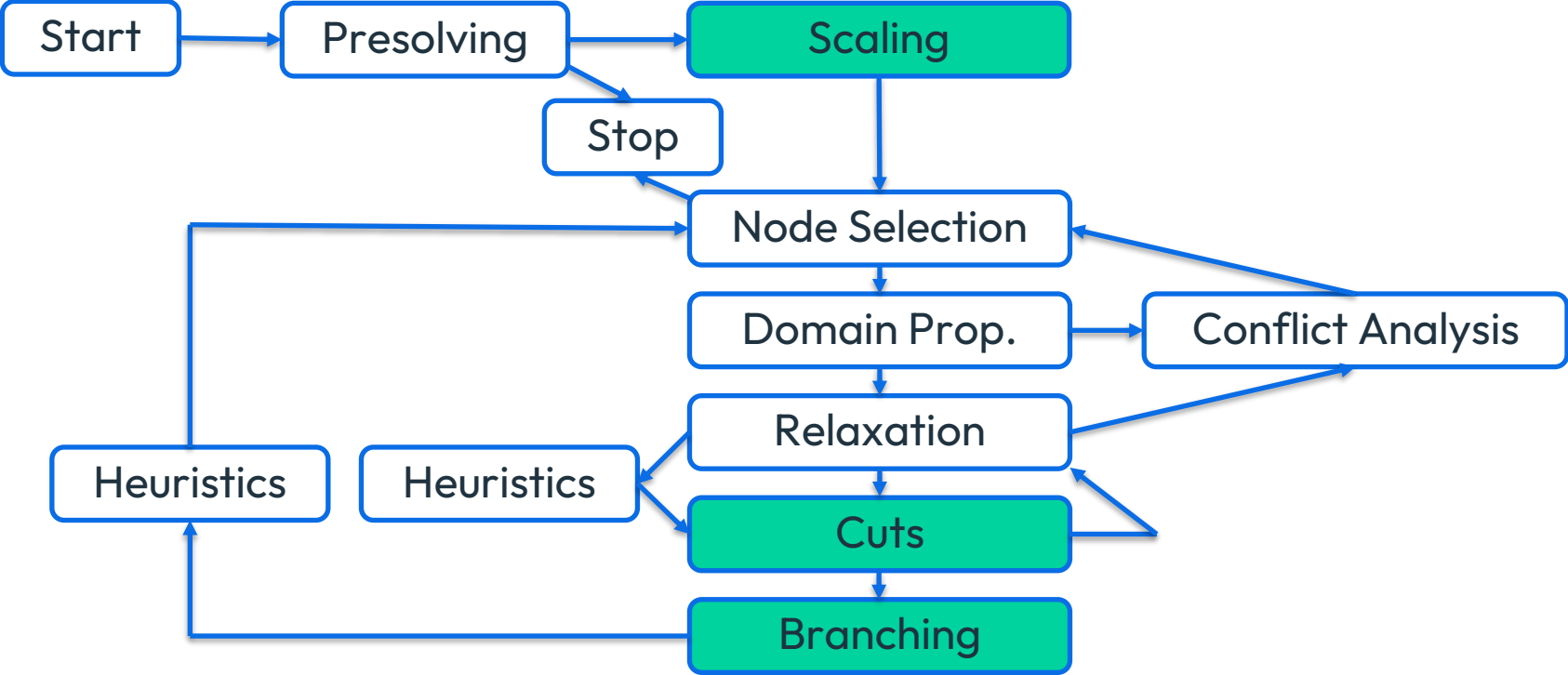
What do I mean by Machine Learning?

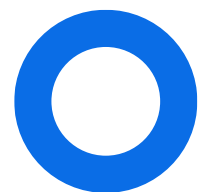
- Most of the cases: Learning a (binary) **decision** on which action to take **inside a MIP solver**
- „Classic“ offline, supervised learning
- Trained on general, heterogeneous test sets, not individually trained for application
- Easy-to-evaluate, ideally interpretable model
- **Use regression for „classification“ w.r.t. a continuous measure**
 - Labels are **improvement factors**, not „this one worked better“
 - Draws are a typical case
 - Misclassifications not too bad on instances where methods perform similar
 - But fatal when there is a huge difference



*Side-track: “Global Optimization for Combinatorial Geometry Problems Revisited in the Era of LLMs”, <https://arxiv.org/html/2601.05943v1>, joint work with Dominik Kamp, Gioni Mexi, Imre Polik & Sebastian Pokutta

MIP Solver Flowchart





Learning to Scale

Proc. of AAAI 2021, joint work with Gregor Hendel

Huge Activity in Machine Learning for Mathematical Optimization

Ding et al.	Accelerating Primal Solution Findings for Mixed Integer Programs Based on Solution Prediction	2019
Bertsimas & Stellato	Online Mixed-Integer Optimization in Milliseconds	2019
Fischetti & Fraccaro	Machine learning meets mathematical optimization to predict the optimal production of offshore wind parks	2018
Misra et al.	Learning for constrained optimization: Identifying optimal active constraint sets	2018
Bertsimas & Stellato	The Voice of Optimization	2018
Tang et al.	Reinforcement Learning for Integer Programming: Learning to Cut	2019
Baltea-Lugoian et al.	Selecting cutting planes for quadratic semidefinite outer-approximation via trained neural networks	2018
Etheve et al.	Reinforcement Learning for Variable Selection in a Branch and Bound Algorithm	2020
Zarpellon et al.	Parameterizing Branch-and-Bound Search Trees to Learn Branching Policies	2020
Yang et al.	Learning Generalized Strong Branching for Set Covering, Set Packing, and 0-1 Knapsack Problems	2020
Song et al.	Learning to Search via Retrospective Imitation	2019
Gasse et al.	Exact Combinatorial Optimization with Graph Convolutional Neural Networks	2019
Lee et al.	Learning to Branch: Accelerating Resource Allocation in Wireless Networks	2019
Hansknecht et al.	Cuts, Primal Heuristics, and Learning to Branch for the Time-Dependent Traveling Salesman Problem	2018
Balcan et al.	Learning to branch	2018
Václavík et al.	Accelerating the branch-and-price algorithm using machine learning	2018
Hottung et al.	Deep Learning Assisted Heuristic Tree Search for the Container Pre-marshalling Problem	2017
Lodi & Zarpellon	On learning and branching: a survey	2017
Alvarez et al.	A Machine Learning-Based Approximation of Strong Branching	2017
Alvarez et al.	Online Learning for Strong Branching Approximation in Branch-and-Bound	2016
Khalil et al.	Learning to branch in mixed integer programming	2016
Khalil	Machine Learning for Integer Programming	2016
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Di Liberto et al.	Dynamic Approach for Switching Heuristics	2013
Sabharwal et al.	Guiding Combinatorial Optimization with UCT	2012

Khalil et al.	Learning to Run Heuristics in Tree Search	2017
Hutter et al.	Algorithm Runtime Prediction: Methods & Evaluation	2012
Hutter et al.	Automated Configuration of Mixed Integer Programming Solvers	2010
Ferber et al.	MIpaal: Mixed Integer Program as a Layer	2019
Wilder et al.	End to end learning and optimization on graphs	2019
Wang et al.	SATNet: Bridging deep learning and logical reasoning using a differentiable satisfiability solver	2019
Wilder et al.	Melding the Data-Decisions Pipeline: Decision-Focused Learning for Combinatorial Optimization	2018
Elmachtoub & Grigas	Smart "Predict, then Optimize"	2017
Kool et al.	Attention, Learn to Solve Routing Problems!	2018
Li et al.	Combinatorial Optimization with Graph Convolutional Networks and Guided Tree Search	2018
Dai et al.	Learning Combinatorial Optimization Algorithms over Graphs	2017
Bello et al.	Neural Combinatorial Optimization with Reinforcement Learning	2016
Bowly et al.	Generation techniques for linear programming instances with controllable properties	2017
Bowly	Stress testing mixed integer programming solvers through new test instance generation methods	2019
François et al.	How to Evaluate Machine Learning Approaches for Combinatorial Optimization: Application to the Travelling Salesman Problem	2019
Fischetti et al.	Learning MILP Resolution Outcomes Before Reaching Time-Limit	2018
Kuhlmann	Learning to steer nonlinear interior-point methods	2019
Kruber et al.	Learning when to use a decomposition	2018
Bengio et al.	Machine Learning for Combinatorial Optimization: a Methodological Tour d'Horizon	2018
Hendel	Adaptive Large Neighborhood Search for Mixed Integer Programming	2018
Bonami et al.	Learning a Classification of Mixed-Integer Quadratic Programming Problems	2017
Amos & Kolter	OptNet: Differentiable Optimization as a Layer in Neural Networks	2017
Schweidtmann & Mitsos	Global Deterministic Optimization with Artificial Neural Networks Embedded	2018
Sculley	Large Scale Learning To Rank	2020
Song et al.	A General Large Neighborhood Search Framework for Solving Integer Programs	2020

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Saltean-Lugan	Machine Learning for Mixed Integer Programming	2018	Yang et al.	SATNet: Bridging deep learning and logical reasoning using a differentiable SAT solver	2019
Etcheve et al.	Machine Learning for Mixed Integer Programming	2018	Meldinger et al.	Model-Agnostic Meta-Learning for Mixed Integer Programming	2018
Zarpellon et al.	Machine Learning for Mixed Integer Programming	2018	Chetoui & Grigoriadis	Machine Learning for Mixed Integer Programming	2018
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Only few of these
implemented in general
purpose MIP solvers!
(and activated by
default)

(at the time)



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Huge variability,
no ground truth

Sophisticated rules
already in place

Heterogeneity...

We don't even
know good
features

[illegible]

Numeric Stability (Somewhat Outdated Slide)

- Numeric stability of MIP solving is a **crucial topic** in many OR applications
 - Blog series on Numerics:
 - Numerics I: Solid Like a Rock or Fragile Like a Flower?
 - Numerics II: Zoom Into the Unknown
 - Numerics III: Learning to Scale
 - Numerics IV: Learning to pay attention
 - Numerics V: Integrality – When Being Close Enough is not Always Good Enough
- Real-life applications often complex and numerically challenging to handle:
 - In the past (2019), more than **half of client problems** had some numeric issues
 - After performance, numeric failures are the **most common support request**
 - Unexpected solution status
 - Inconsistent results
 - Performance issues (e.g., simplex cycling)

This number has dropped significantly
due to the work presented here.

Recall

- Spread of nonzero matrix coefficient, rhs and objective coefficients

Coefficient range	original	solved
Coefficients	[min,max] : [9.17e-05, 4.20e+02]	/ [1.17e-02, 1.31e+01]
RHS and bounds	[min,max] : [3.00e-02, 1.00e+04]	/ [5.00e-01, 4.35e+02]
Objective	[min,max] : [1.00e+00, 7.16e+00]	/ [1.56e-02, 1.86e+02]

- Difference in the exponents (aka **orders of magnitude**) more relevant than the actual numbers
- **Attention level** gives a [0,1]-measure of the expected numerical difficulty
 - 0.0 = no major issues expected
 - The larger, the worse
 - 1.0 = Good luck...

Two scaling methods

Equilibrium scaling (Tomlin 1975):

- Divide rows by largest coefficient
- Then divide columns by largest coefficient
- Potentially iterate

Curtis-Reid (1972):

- Minimize least-squares deviation from 1:
- $\min \sum_{i=1}^m \sum_{j=1}^n (\log R_{ii} C_{jj} |A_{ij}|)^2$
- Positive semidefinite, unconstrained $\rightarrow$ conjugate gradient
- Binary logarithm, round scaling factors to powers of two

$$\begin{array}{ll} \max & (cC)^T(C^{-1}x) \\ \text{s. t.} & (RAC)(C^{-1}x) \leq Rb \end{array}$$



$$\begin{array}{l} c' = cC, A' = RAC, b' = Rb \\ x' = C^{-1}x \end{array}$$



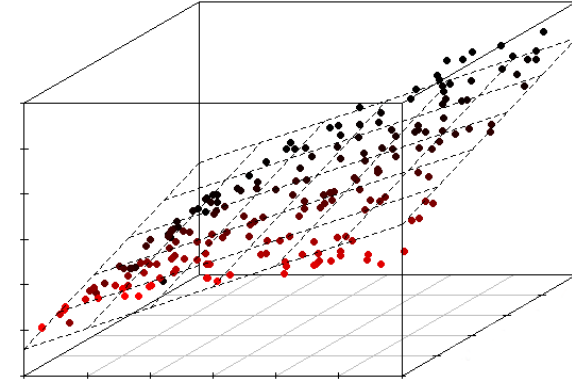
$$\begin{array}{ll} \max & c'^T x' \\ \text{s. t.} & A' x' \leq b' \end{array}$$

Learning to Scale

- One fixed method not always best
- New approach: **Learn to Scale**
 - Try each scaling method: **Equilibrium** and **Curtis-Reid**
 - Try to predict which method will result in the smaller **attention level**
 - Or rather: The **factor** by which the attention level differs (**label**)
- **Features** drawn from coefficient distributions
 - **Coefficient spread**: $\gamma := \log \frac{\max_{i,j} |A_{ij}|}{\min_{i,j} |A_{ij}|}$
 - Use $\gamma_{Equi} - \gamma_{Curtis}$ as a feature
 - Same procedure to get features for objective spread and right-hand side spread

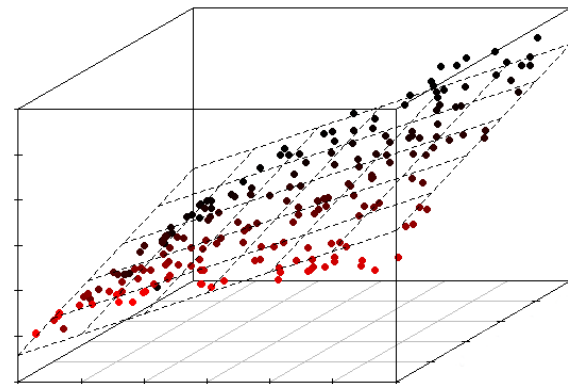
Learning to Scale

- New approach: **Learn to Scale**
 - Use **linear regression** model to predict which method will result in the smaller **attention level**
 - Tried random forests, neural nets, ...
 - Use matrix spread, objective spread, rhs spread as features
- Trained on thousands of customer MIP instances
- Validation outcome:



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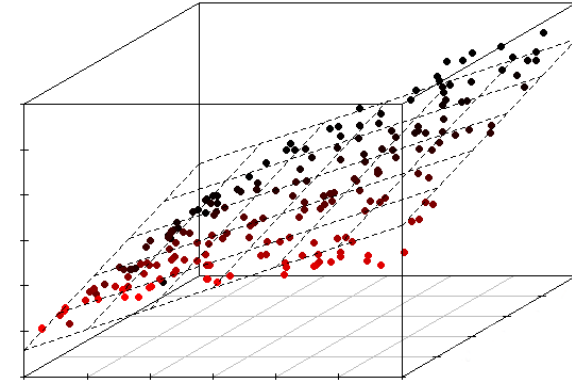


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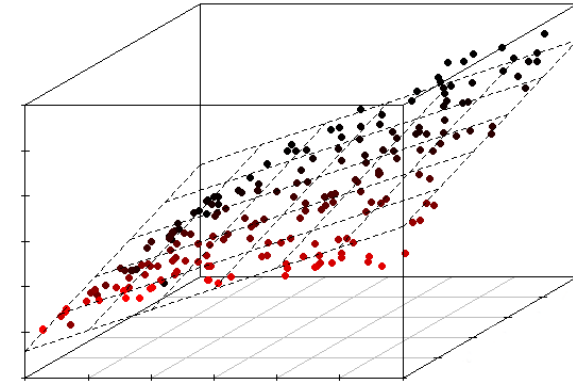
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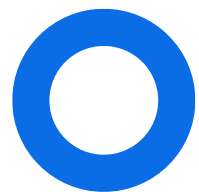


Computational Results

- On our set of numerically Challenging instances:
 - Tremendous improvements in all stability criteria

Dual Fails	-64%	Primal Fails	-67%	Singular Inverts	-48%
Infeasibilities	-26%	Inconsistencies	-35%	Violated Sols	-12%
Kappa Stable	+148%	Max. Condition	-979%	Attn. Level	-88%

- ≈10% performance improvements on Xpress simplex test sets



Learning to Use Local Cuts

Mathematical Programming Computation, 2025
joint work with Matteo Francobaldi & Gregor Hendel

Solving Integer Optimization Problems

- **Example MIP:**

$$\max x + 5y$$

$$x - 3y \leq 3.6 \quad -x - 3y \leq -7.2$$

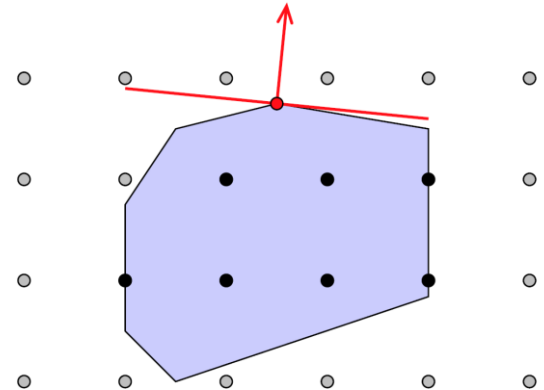
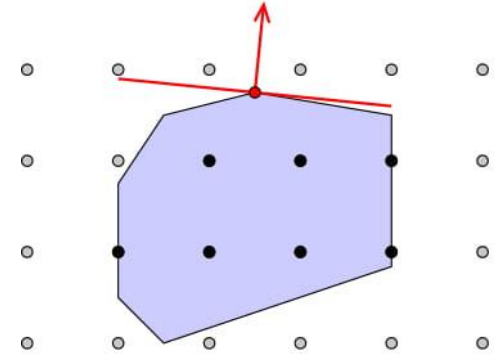
$$-x - 3y \leq 0.5 \quad 0 \leq x \leq 3$$

$$-2x + 3y \leq 0.8 \quad x, y \in \mathbb{Z}$$

$$-x + 3y \leq 4.2$$

- Two principal algorithms to solve such problems:

- **Branch-and-Bound**



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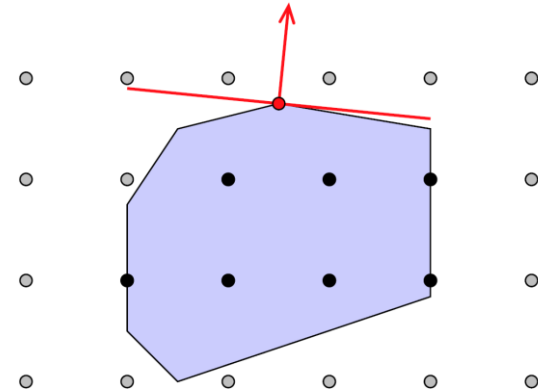
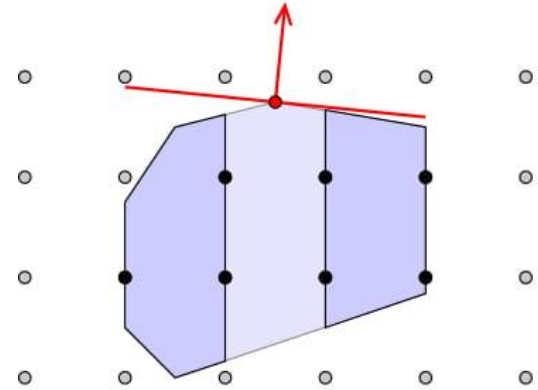
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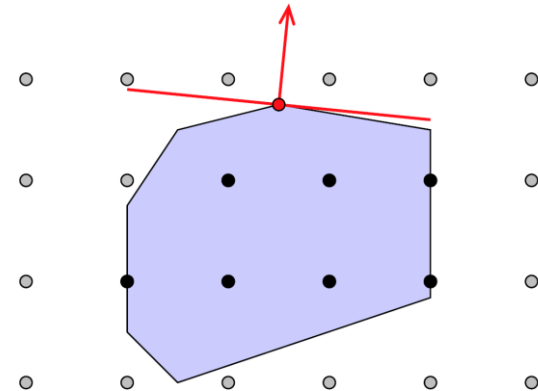
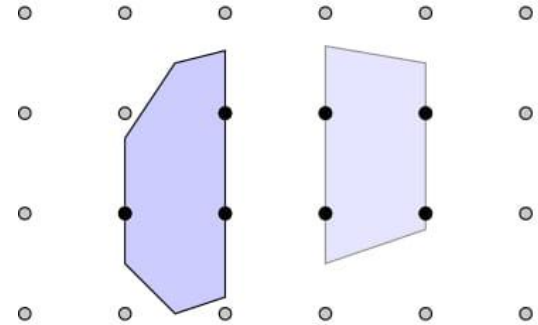
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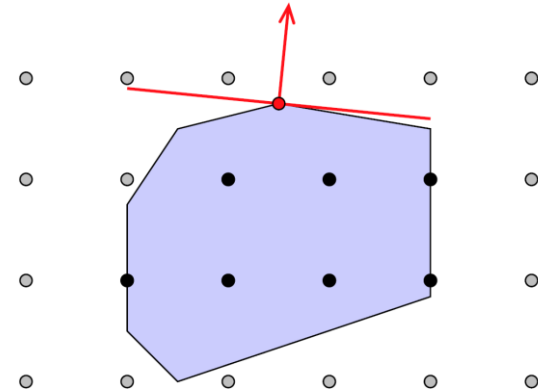
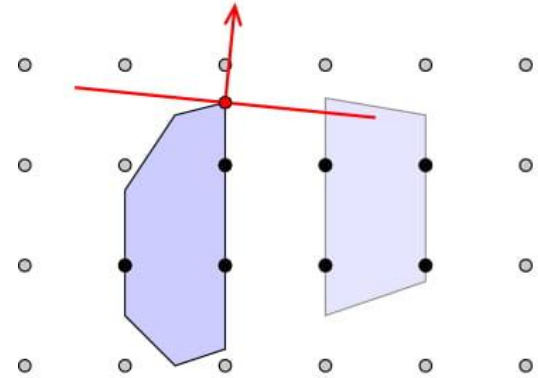
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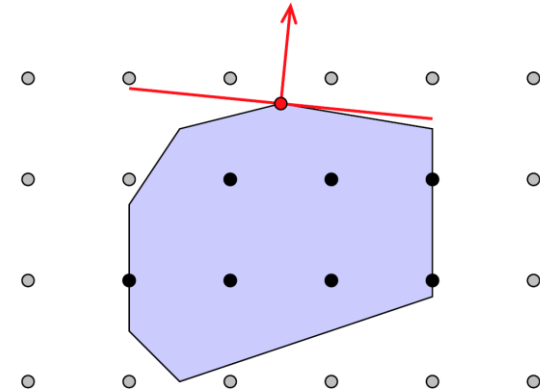
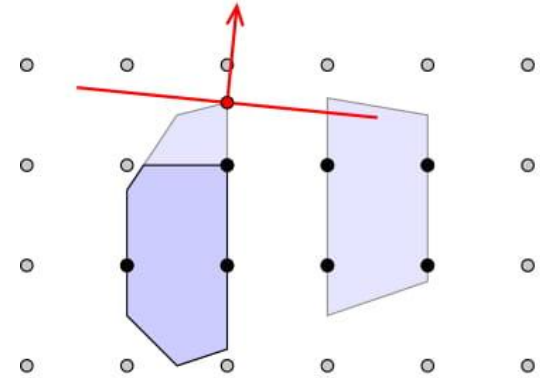
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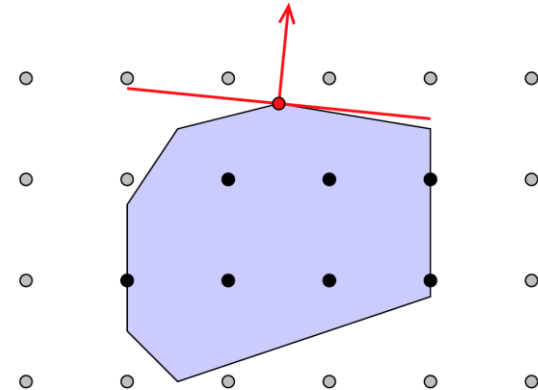
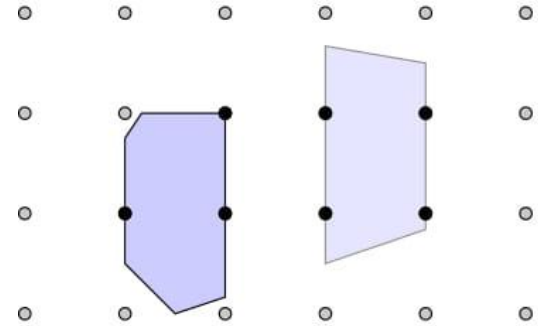
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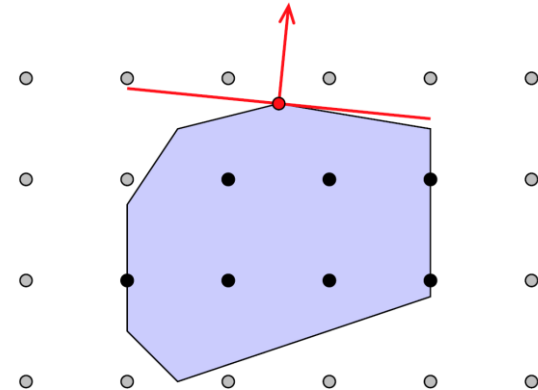
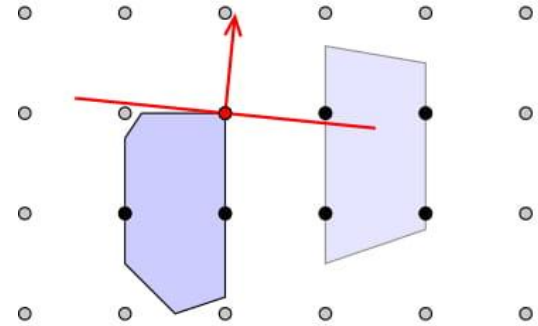
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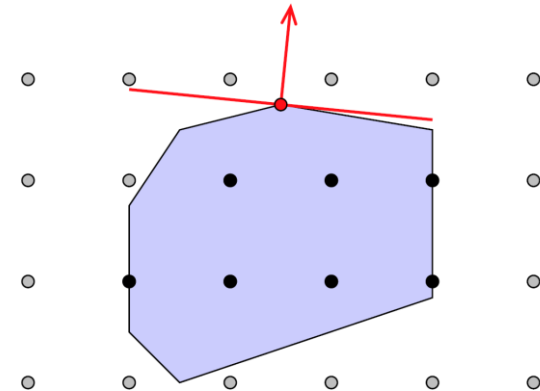
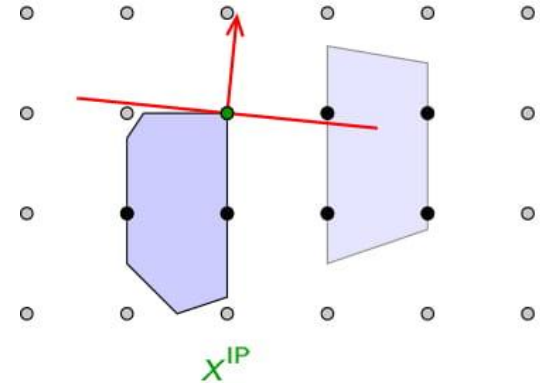
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- Two principal algorithms to solve such problems:

- **Branch-and-Bound**



Solving Integer Optimization Problems

- **Example** MIP:

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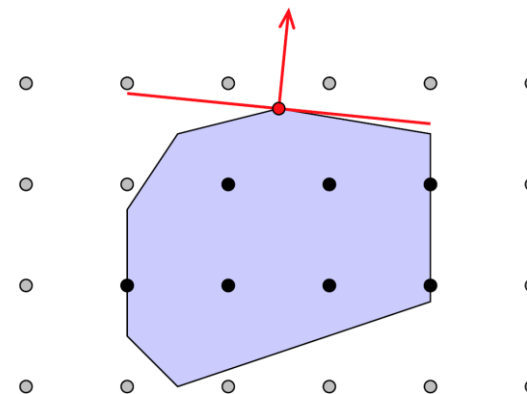
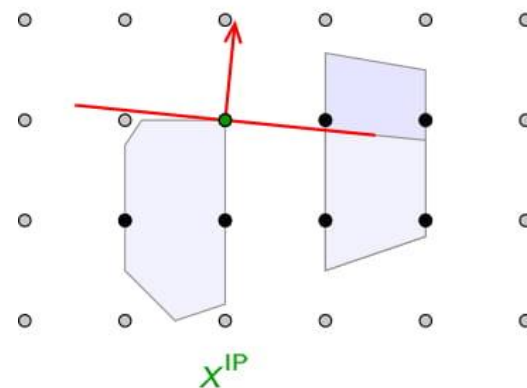
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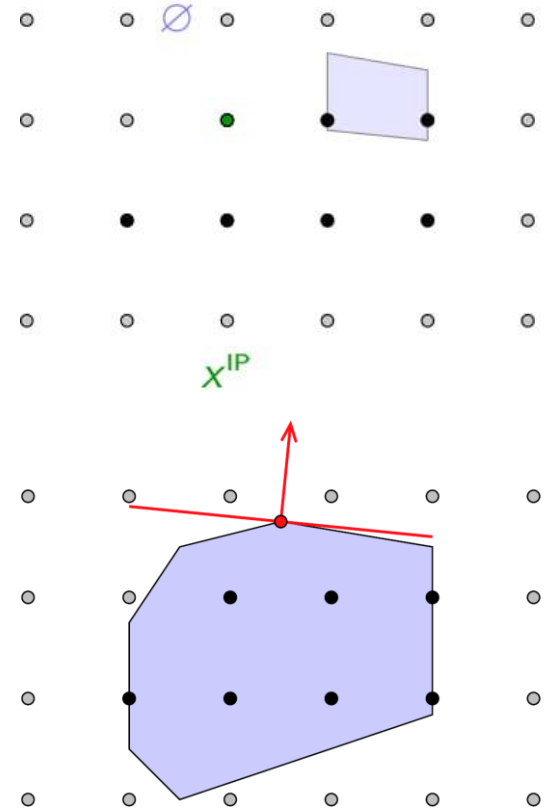
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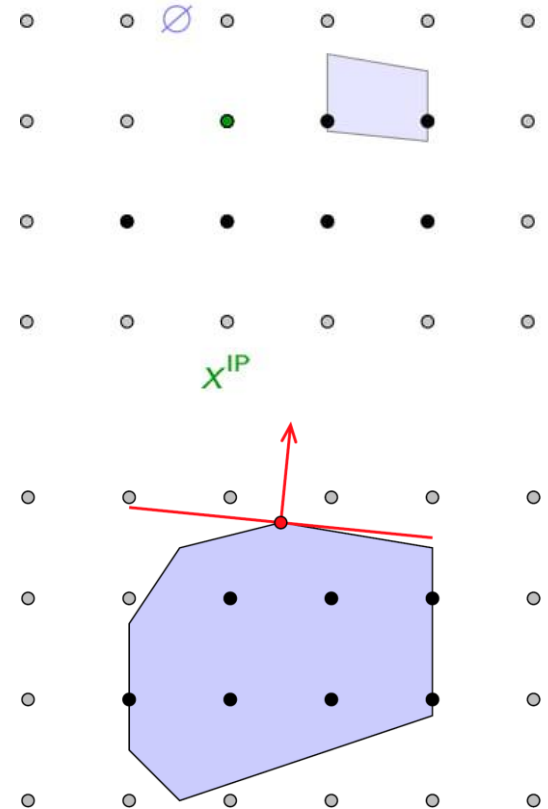
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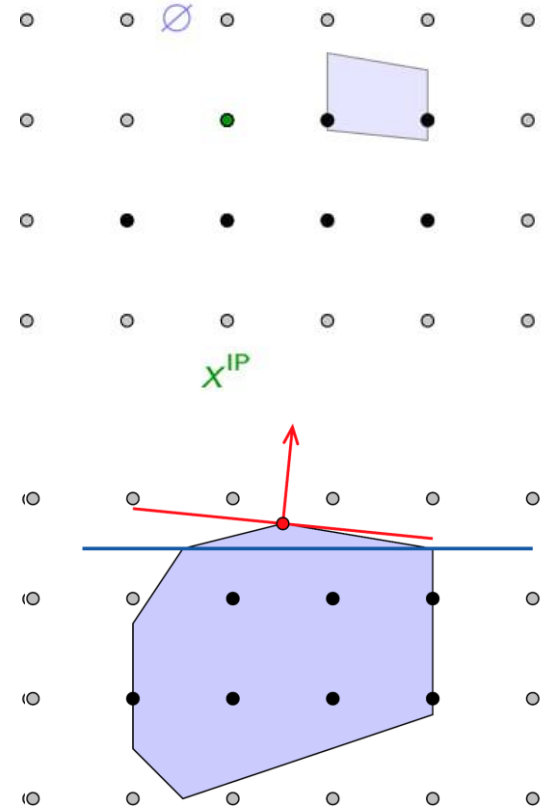
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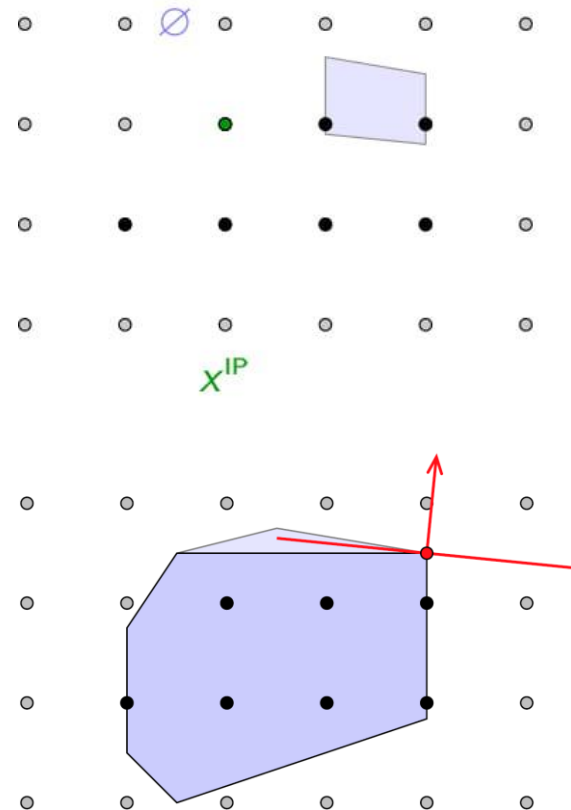
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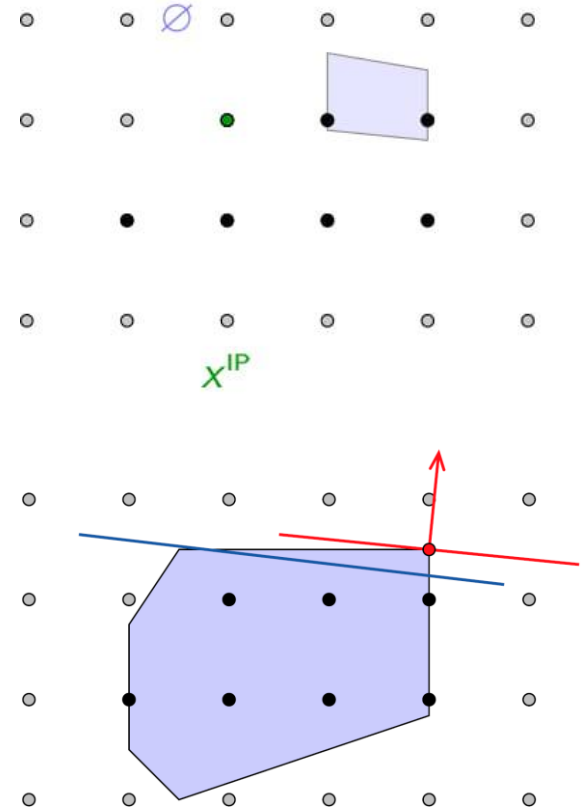
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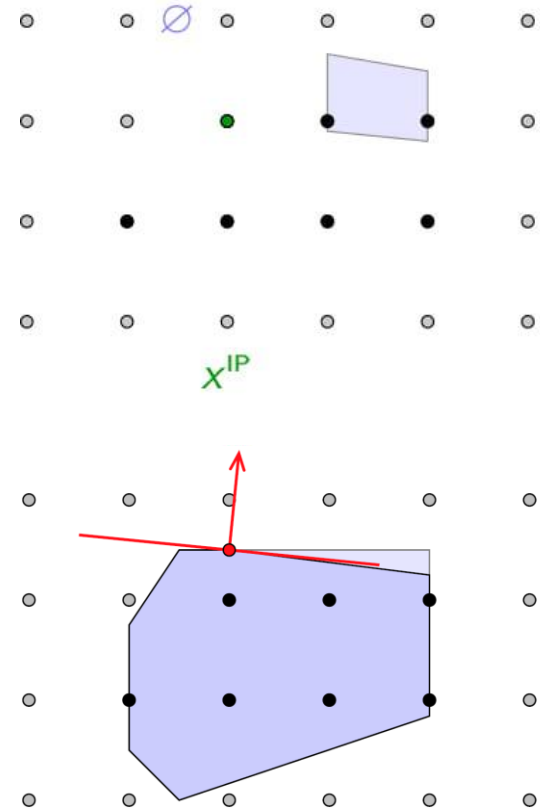
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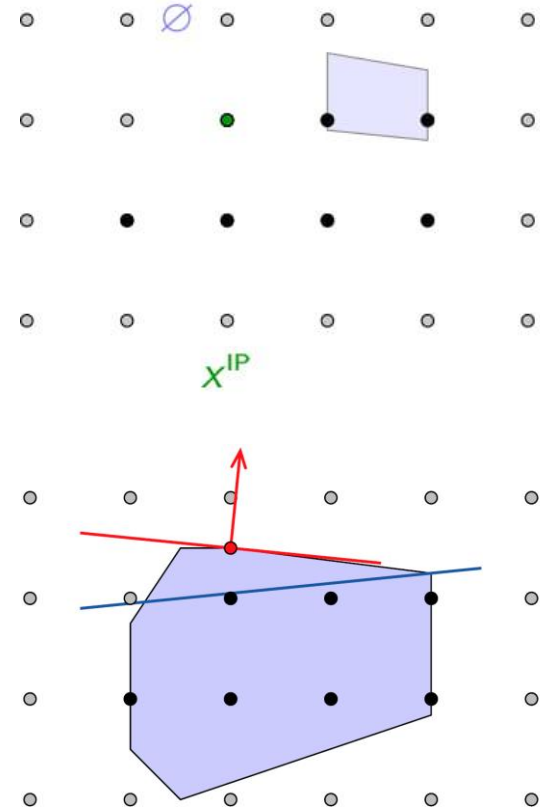
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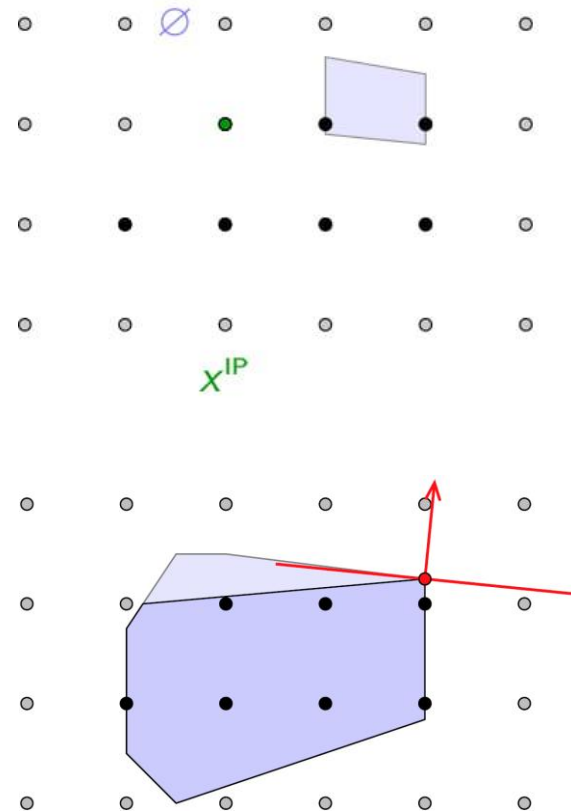
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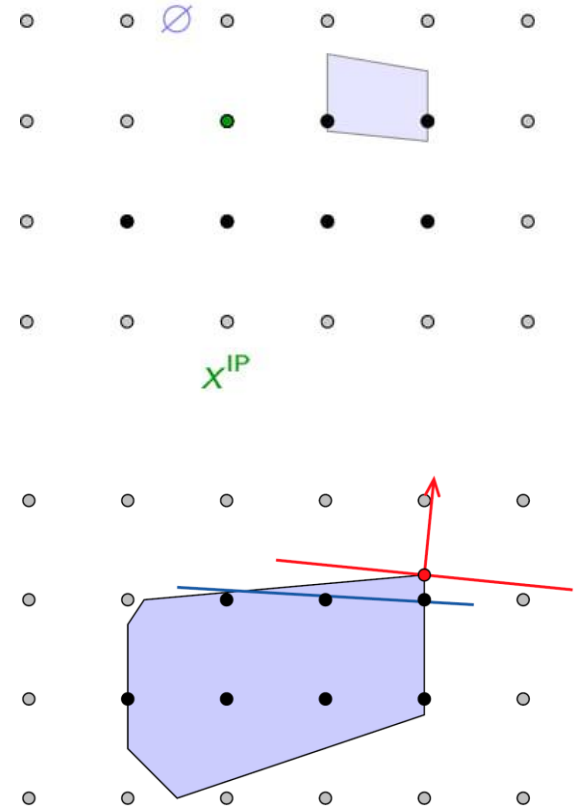
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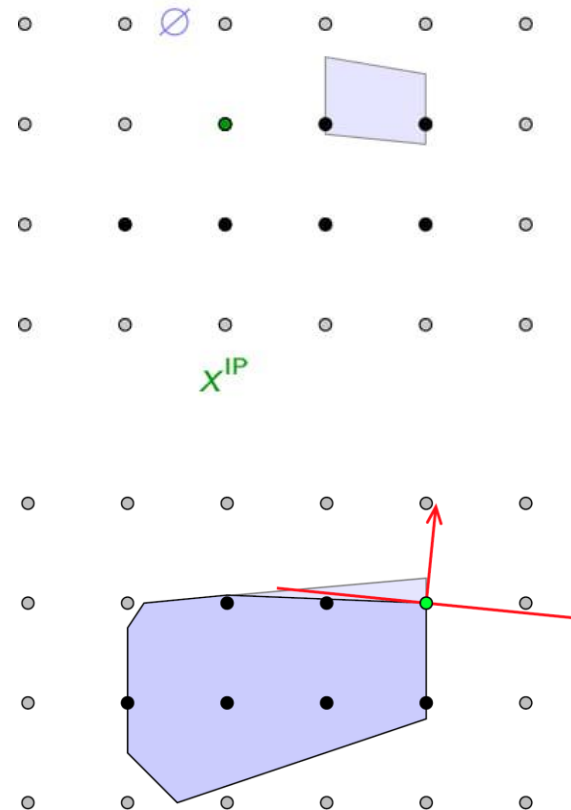
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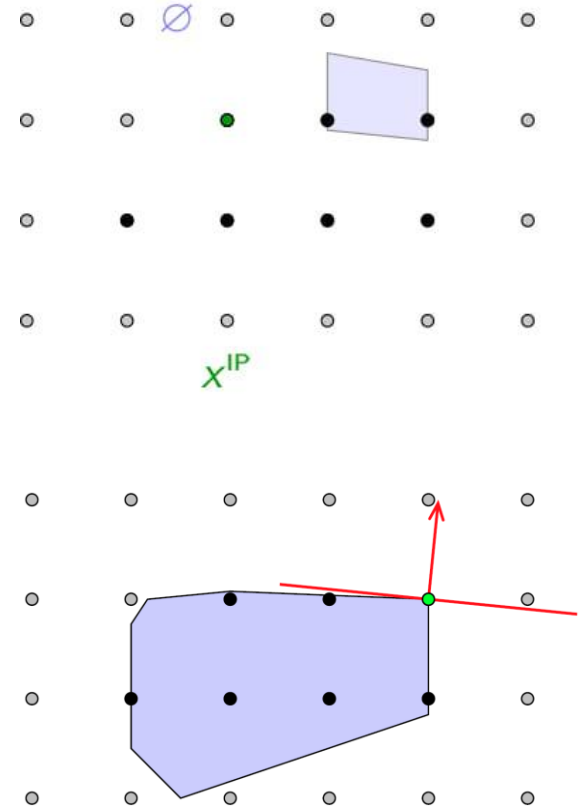
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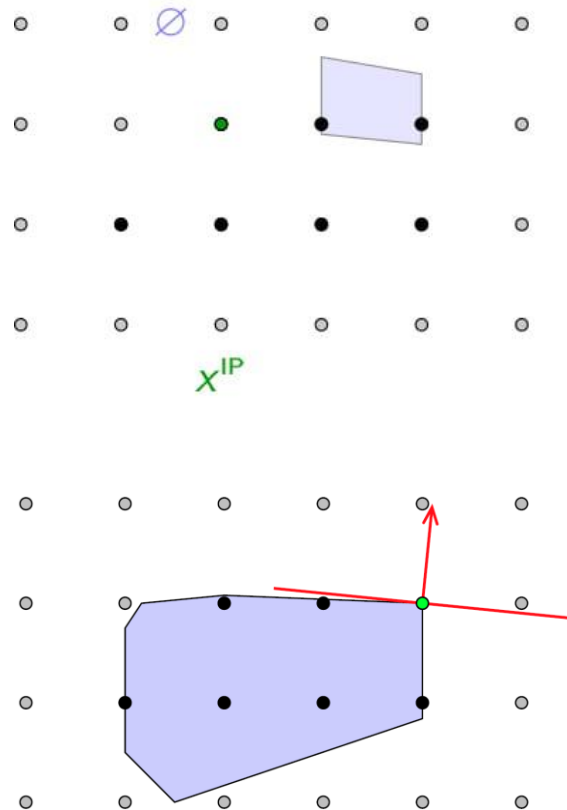
- Two principal algorithms to solve such problems:

- Branch-and-Bound
- Cutting Plane Method

- Two meaningful combinations of those algorithms:

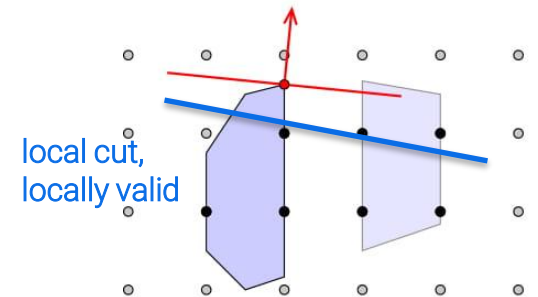
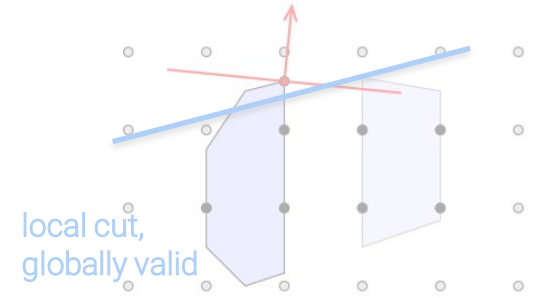
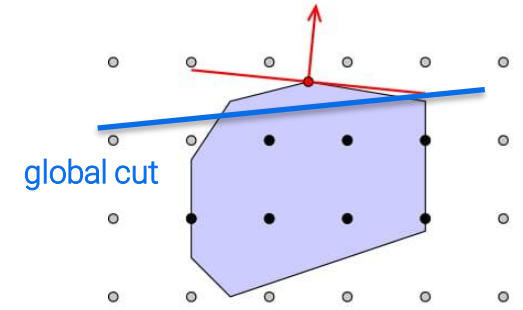
- Cut & Branch
- Branch & Cut

Which one
is better?



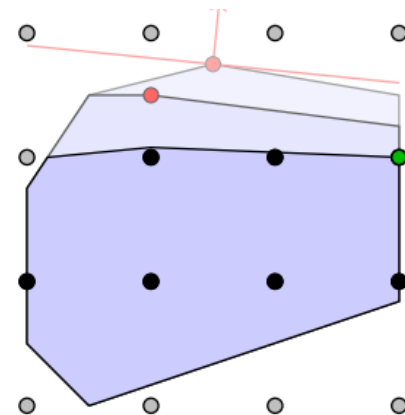
Local Cuts

- Global cuts
 - Generated at the **root node**
 - Hence globally valid by construction
- Local cuts
 - Generated at **internal nodes**
 - Either globally valid
 - When only using global information (e.g. bounds)
 - Can be re-used in other parts of the tree
 - Or **locally valid**
 - When using local bounds
 - Potentially stronger



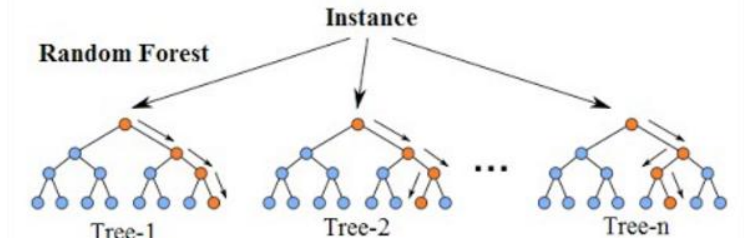
To Cut or Not to Cut?

- Crucial question: Should we generate **cutting planes at tree nodes or only at the root?**
 - Cuts are an essential part of branch-and-cut algorithms, many problems unsolvable without them
 - Local cuts complicate some other solver features (e.g., conflict analysis)
 - Cutting plane generation costs time and makes LPs slower to solve
 - When cuts do not make a difference, they slow down the solve
- How good are local cuts?
 - **45%** of instances significantly **benefit** from local cuts
 - **23%** of instances **suffer** from local cuts
- Idea: Try to **predict at the beginning of tree search** whether local cuts will work



Learning to Use Local Cuts

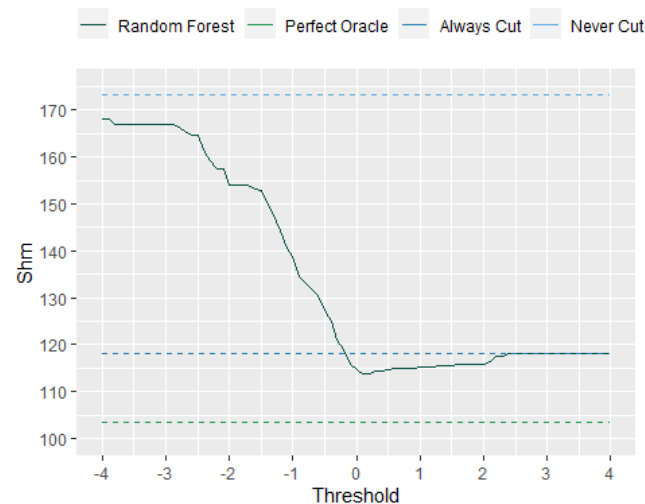
- Train a **random regression forest** to predict speed-up factor from deactivating cuts
 - On more than 3000 customer instances
 - Final decision by an average and a majority vote
- **Static Features**: Row types, percentage binaries
 - Indicate whether this is a combinatorial problem
- **Semi-static features**: Density, numeric conditioning
 - Indicate whether cuts might lead to expensive LPs
- **Dynamic feature**: Gap closed by root cuts
 - Indicates the potential of cuts to raise the best bound



Computational results

Benchmark	#Instances	Δ Solved	Time	Nodes	PDI
MIP – Benchmark	5331	+9	-2%	+2%	-1%
→ > 100 sec	2226	+9	-2%	0	-1%
→ affected	480	+9	-15%	+19%	-10%

- Opposite effect on Time and Nodes (to be expected)
- **Conservative setting**, failed predictions are rare



Learning to Select Branching Rules for MINLP

Proceedings of CPAIOR 2026,
joint work with Fritz Geis



Learning to Select Branching Rules for MINLP

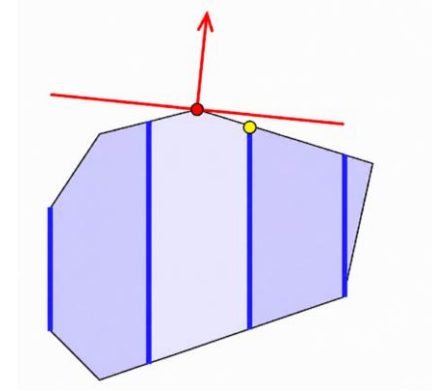
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From MIP to MINLP

- General MIP:

- maximizing a **linear objective** function over a set of **linear constraints**
- Some or all variables have to take **integral values**, some or all are bounded

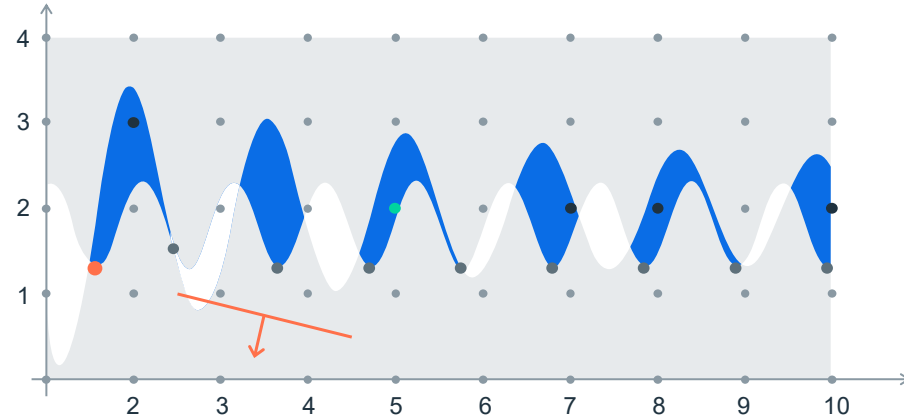
- $\max c^T x$
 $s.t. Ax \leq b$
 $x \in \mathbb{Z}^I \times \mathbb{R}^{N \setminus I}$
 $\ell \leq x \leq u$



- Solution algorithm: (supercharged) LP-based **branch-and-bound** (on integer variables)
 - Once the integer variables take integral value in the LP solution, the solution is feasible and optimal for the branching subproblem

From MIP to MINLP

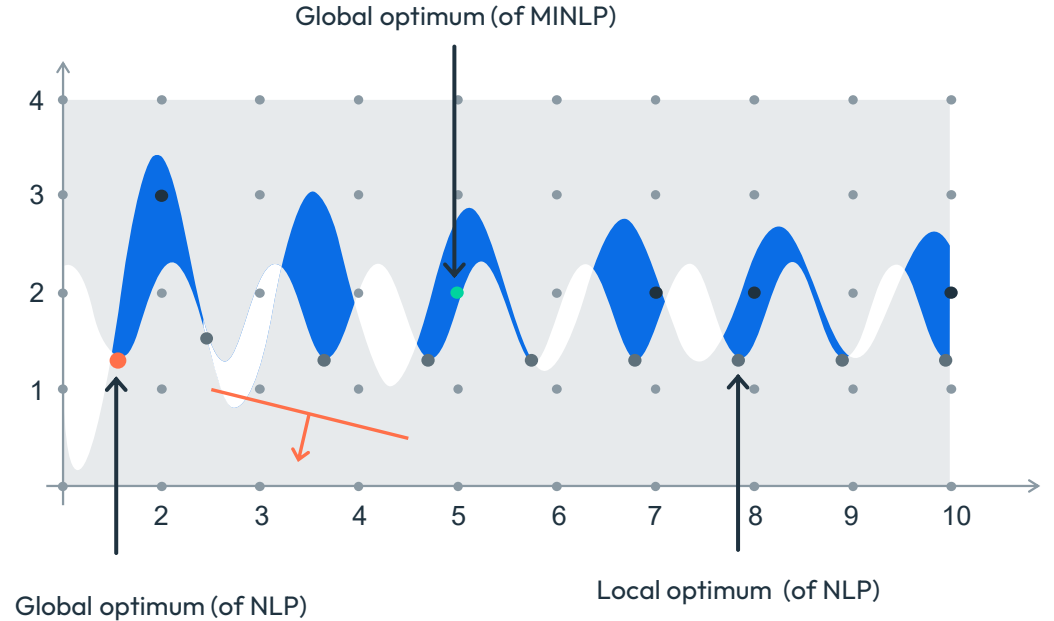
- General MINLP:
 - maximizing a **nonlinear objective** function over a set of **nonlinear constraints**
 - Some or all variables have to take **integral values**
 - $\min f(x)$
s. t. $g_j(x) \leq 0$ for $k = 1, \dots, m$,
 $x \in \mathbb{Z}^I \times \mathbb{R}^{N \setminus I}$
 $\ell \leq x \leq u$
where $f, g_j: \mathbb{R}^n \supseteq [l, u] \rightarrow \mathbb{R}$



- A couple of state-of-the-art **MIP solvers** have recently been **extended to MINLP**
- Solution algorithm: (supercharged) LP-based **branch-and-bound** (on integer **and continuous** variables)
 - Convex MINLP: Once the integer variables take integral value in the LP solution, **cutting planes** can be used to get to ε -feasibility
 - **Nonconvex MINLP**: Might **need to branch on continuous variables** to reach constraint feasibility

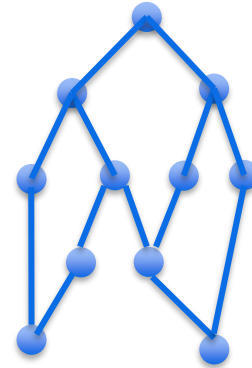
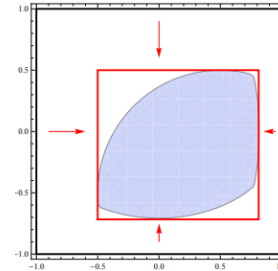
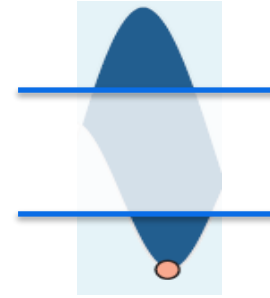
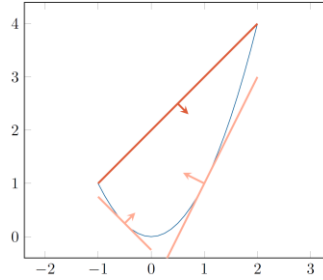
Nonconvex MINLP

- Example: Two nonconvex inequalities
 - six disconnected regions
 - nine local optima
- Rich literature on local optimization
- This talk: [Global Optimization](#)
 - of nonconvex MINLPs
 - using FICO Xpress Global



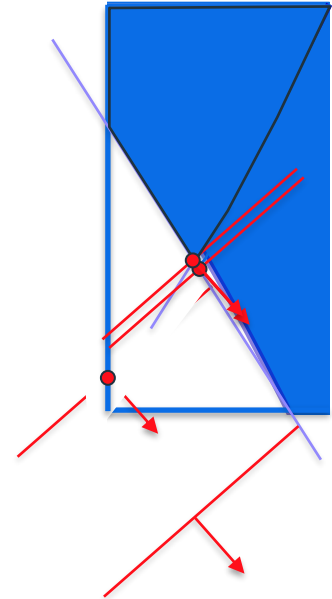
Global Optimizations Techniques

- Nothing to be afraid of 😊
- Cutting Planes
- Branching
- Presolving / bound tightening
- And a (maybe peculiar, but super-useful) representation of the **problem** as a **graph**



Spatial Branching: Why? (example)

- $\min y - x$
s. t. $y \geq x^2$
 $y \geq 8 - x^2$
- Feasible region: “curved, purple W-shape”
- First constraint: Easy to relax linearly
 - Second constraint: No linear relaxation
- Solve LP
 - Violates the second constraint
 - Resolve via spatial branching
 - Now, add linear relaxation of the second constraint
- Solve LP
 - Add cut
 - Solve again
- Are we good?
 - Still on secant, need to branch again



On Which Variable Do We Branch?

- We generally know good rules for branching on integers (in MIP)
 - Strong branching & pseudocost branching
 - Reliability branching
 - Hybrid branching
- We know good rules for branching on spatial branching candidates
 - “What closes the [convexification gap](#) the most?”
 - Plus some history information
- But...[how do we combine](#) those?
 - Integer violations first, then nonconvexities?
 - Or mix?
 - [Different solvers have different answers](#) to that question

⇒ [Machine Learning](#) opportunity

Let's look for good features

- Constraints

- Percentage nonlinear constraints
- Linear nonzeros vs size of the DAG (number of nonlinear expressions)

- Percentage equality constraints

- Variables

- Percentage integer variables

- Branching „situation“ at the root node

- Average number of integer candidates
- Average number of spatial candidates

- Average relative bound change of spatial (integer) strong branches
- Percentage variables fixed by integer/spatial strong branching

- Cost of strong branching

- Average work

- Numerics of convexification cuts

Nonlinearity of
the problem

Combinatorics
of the problem

Where is the
infeasibility?

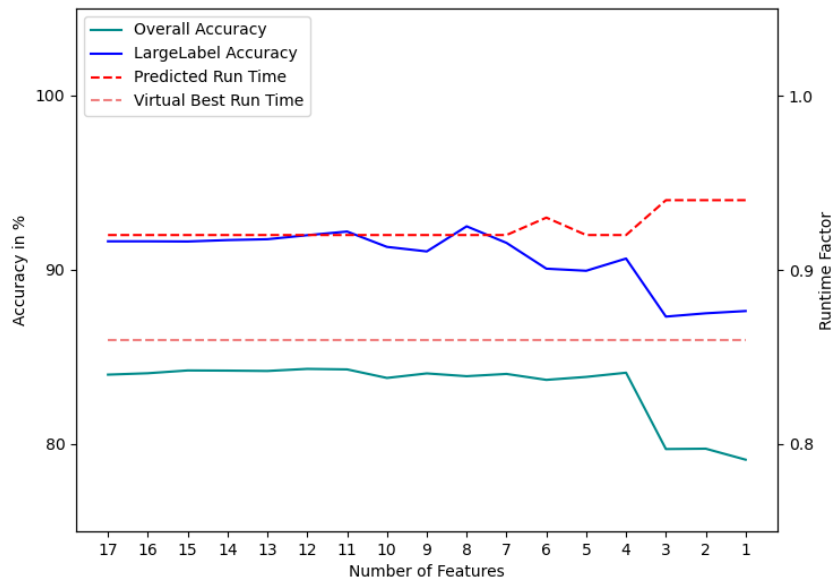
Effect of
branching

Cost/benefit
consideration

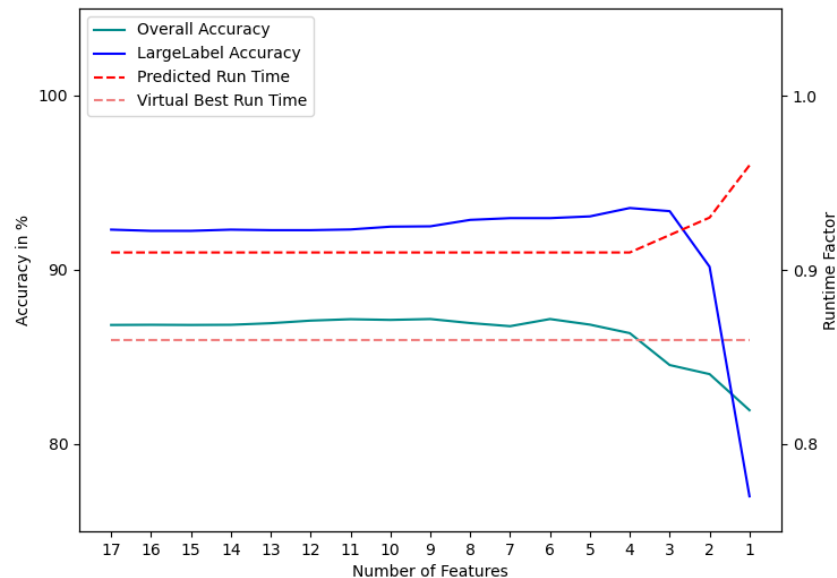
Computational Experiments

- All features get scaled
- Our models map features to **speedup factor**: $y: \mathbb{R}^{17} \rightarrow \mathbb{R}$
- Label $fac(t_{INT}, t_{MIX}) := \begin{cases} t_{INT}/t_{MIX} - 1 & \text{if } t_{INT} \geq t_{MIX} \\ -t_{MIX}/t_{INT} + 1 & \text{else} \end{cases}$
for t_{INT} the runtime with integer-first branching, t_{MIX} the runtime with mixed branching
- Performance Measures:
 - **Accuracy**: $\text{sign}(y(f)) = \text{sign}(fac(t_{INT}, t_{MIX}))$, if $|fac(t_{INT}, t_{MIX})| \geq 1.01$
 - LargeLabel Accuracy: for instances with $|fac(t_{INT}, t_{MIX})| \geq 4$
 - **RunTime** (shifted geometric mean)
 - (virtual best runtime for comparison)
- 683 instances from MINLPLib and FICO customers
- Xpress 9.6, ML models trained with Scikit-learn

Feature Reduction



Linear regression



Random forest regression

- Good: High Accuracy, low runtime
- Performance ~constant when **reducing from 17→4 features**
- Drops with fewer than four features

Final Performance

	Linear		Forest	
Accuracy	Train	Test	Train	Test
Overall	84.2%	84.1%	89.1%	86.4%
LargeLabel	91.9%	90.7%	99.7%	93.6%
Time Factor				
Predicted	0.914	0.919	0.884	0.910
Virtual Best	0.862	0.863	0.862	0.863

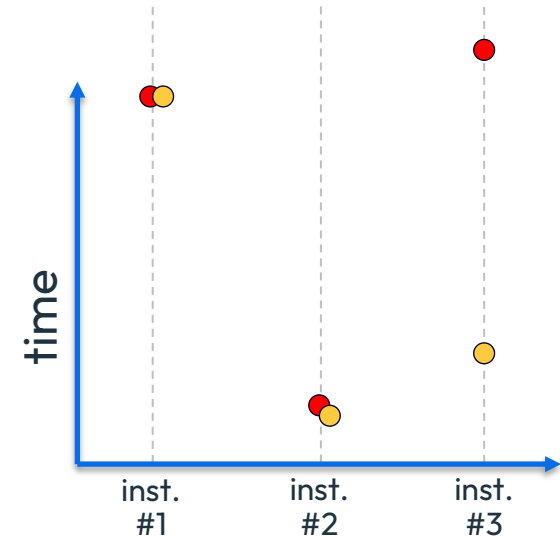
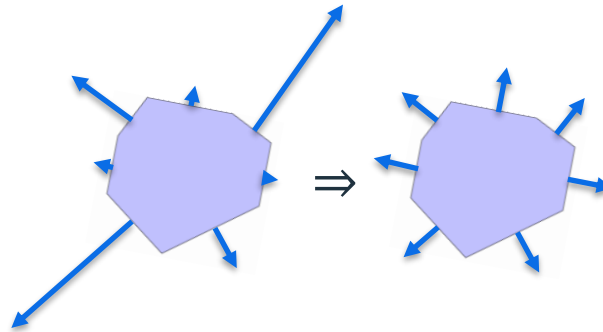
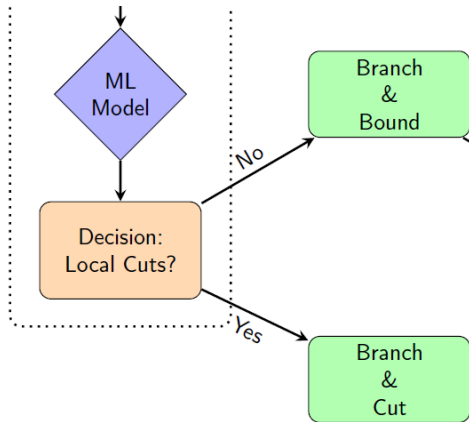
- Both models achieve [significant improvements](#)
- Forest shows clear signs of overfitting, linear model not at all
- Linear model closes more than [half of the gap to virtual best](#)
- [Results transfer](#) to other solver versions
 - 9.6 linear model as good on 9.8 data as model retrained from scratch



Conclusion

Key take-aways

- Modern MIP solvers use (fast, interpretable) [ML models for decision making](#)
- Faster is not the only definition of better
 - [Improving numeric stability](#) or reducing performance variability valuable by itself
- Use regression for „classification“ w.r.t. a continuous measure



Thank You!

PD Dr. Timo Berthold

Private Lecturer @ TU Berlin

Director, Mixed-Integer Optimization @ FICO



Learning To Select Cuts

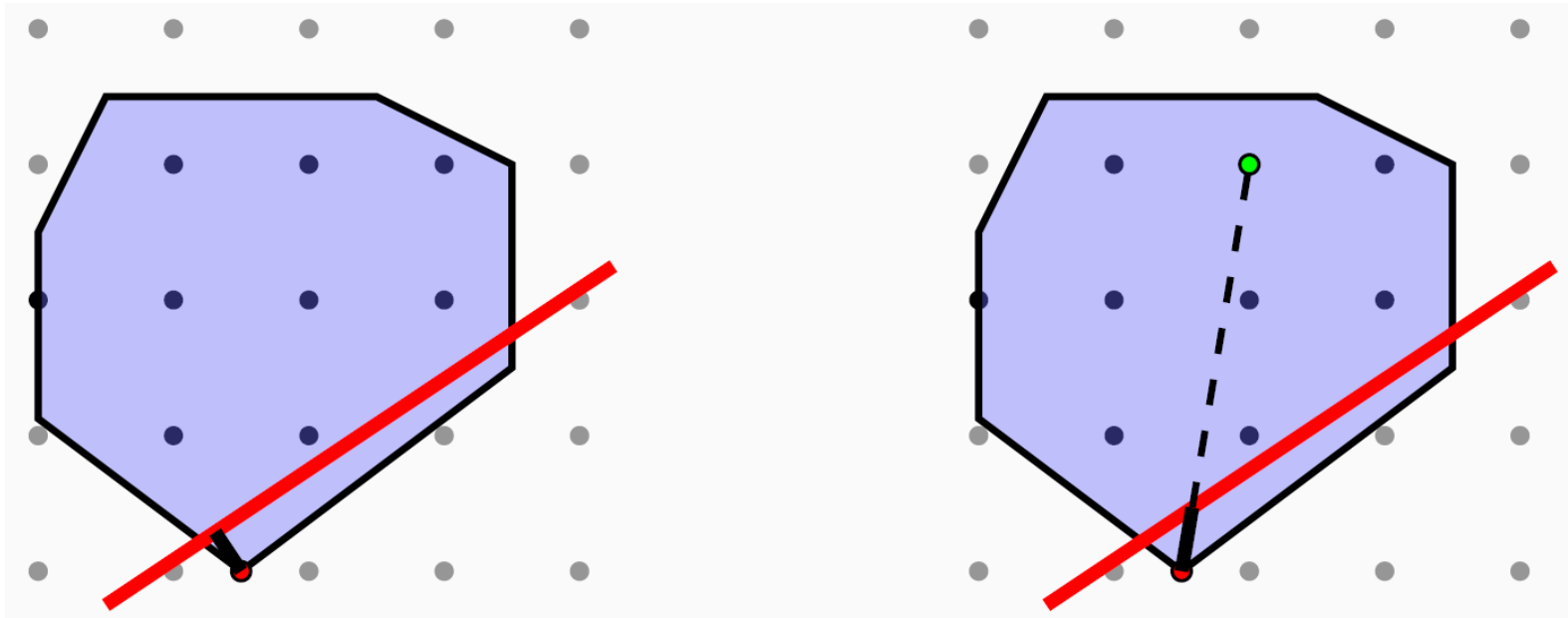
Proceedings of CPAIOR 2023,
joint work with Mathieu Besançon, Mark Turner, Thorsten Koch

Cut Selection

- Cuts generated in rounds: separate, solve LP, rinse and repeat
- Most separation routines cheap (much cheaper than LP solve)
 - $\Rightarrow$ Generate more cuts than needed, select the best ones
- Trade-off:
 - Adding more cuts?
 - Expensive LPs, numerically unstable
 - Adding less cut?
 - More nodes needed to solve
- $\Rightarrow$ Sweet spot in between $\Rightarrow$ How do we select promising cuts?

Cut Selection: state-of-the-art

- Efficacy – Intuition: Chop as much volume of the polyhedron as possible
- Directed cutoff distance (dcd) – Intuition: cut as close to the incumbent as possible

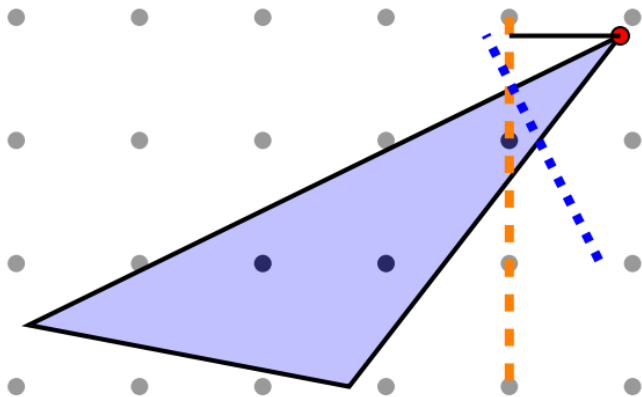


What is wrong with efficacy (and dcd)?

- Distance-based measures: How intuitive and robust are they really?

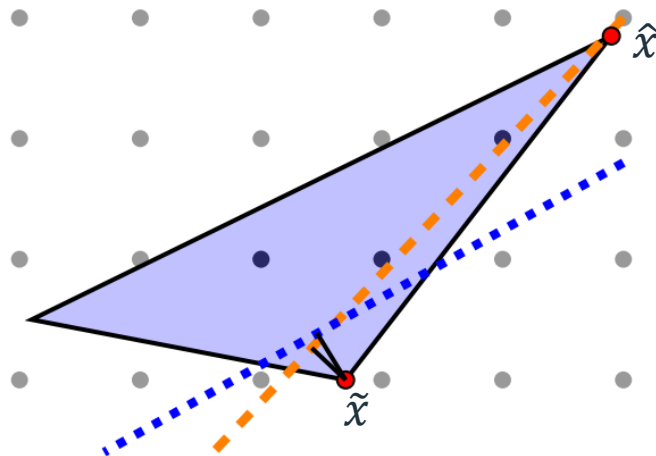
Distances to an infeasible projection

- Blue cut “better”
- But orange cut only “bad” outside polyhedron



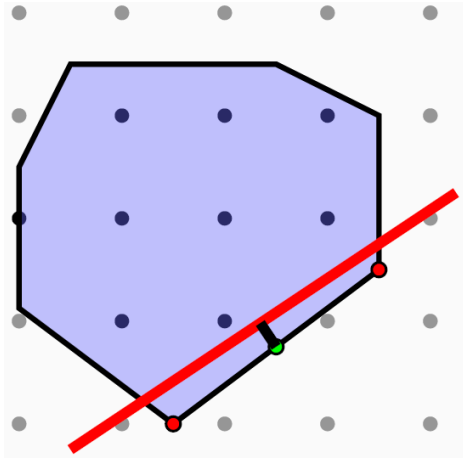
Dual degeneracy (optimal face)

- Blue cut slightly “better” for solution $\tilde{x}$
- But does not cut off solution $\hat{x}$
- Arbitrary solution (similar for dcd – incumbent)



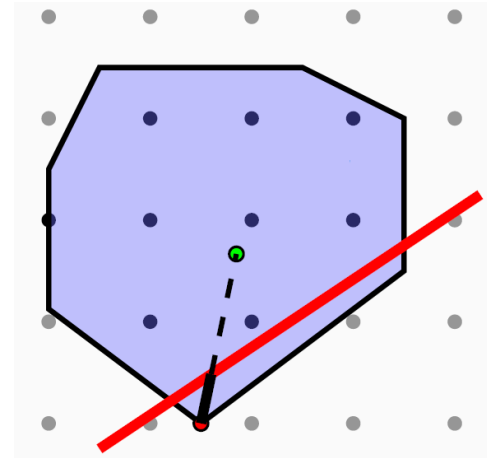
How might we do better?

- Use analytic centers (AC) $\approx$ central point
- Can be computed as LP, side-product of barrier algo



AC of the optimal face (AC-efficacy)

- Counters degeneracy
- Reduces risk to „project outside“



AC of polyhedron (AC-dcd)

- Projection always inside polyhedron
 - Expected to be central
- Constant reference point

Instance features

- Goal: Determine **best selection** criterion (out of eight):
Given instance features, which score will produce the minimum tree size/runtime?
- Features of the transformed problem:
 - Dual **degeneracy**: % non-basic variables with zero-reduced cost
 - Primal degeneracy: % basic variables at bounds
 - Solution **fractionality** at root node
 - **Thinness**: % equality constraints
 - **Density** of the whole constraint matrix
- Test set: MIPLIB2017 Collection, solver: SCIP 8.0

Multiregression model

- Not a binary decision (but 8-fold): Classification?
- No single best for many instances:
 - no cut selected, certain cuts always selected, etc...
 - ties allowed?
- Multi-output regression: $\frac{\text{\#nodes}_{\text{best}}}{\text{\#nodes}}$
- Support vector regression with cubic kernel
 - Several attempted models: regression trees, support vectors, random forests

Results

- **Boxenplots**: More right = better, **olive**: learned model
 - **Nodes**: Median and all percentiles are **better**
 - In particular at the lower end
 - Time: On par with **Analytic DCD**
 - Sh. geom. mean: Better for nodes, worse for time
 - Reduced performance variability

