Computational Integer Optimization

Timo Berthold & Gennesaret K. Tjusila
TU Berlin, ZIB, MODAL, FICO

Who Am I?

Timo Berthold

- Master's (2006) and PhD (2014) at TU Berlin
- Working in Computational Optimization since 2005
  - SCIP developer until 2013
  - FICO Xpress Developer since 2014
  - Leading Mixed-Integer Optimization R&D team since 2023
- Habilitation and private lecturer at TU Berlin since 2022
  - Teaching one course per year
    - This summer: Computational Integer Optimization, Aug 24-28
  - Supervising Bachelor, Master's, and PhD students
  - Also some teaching at HTW and FU Berlin

- Goal: Bring academic research and teaching together with industrial research and practices

Gennesaret Kharistio Tjusila

- PhD student at the IOL Int Group, Zuse Institute Berlin, part of the team developing SCIP!
- Research: GPU acceleration for Mixed Integer Programming (MIP)
- Originally from Jakarta, Indonesia (My favourite Indonesian spot is Nusantara @ Turmstraße)
- Almost a true Berliner: Studienkolleg → Bachelor → Master → PhD in Berlin
- I enjoy programming books, thrillers, and chess!

Weekly Agenda: 15 Lectures (And Five Afternoon Hands-On Sessions)

- High-level review of integer programming
- Modelling
- LP Solving
- Primal heuristics
- Branching
- Optimization on GPU
- Presolving
- Cutting planes
- Symmetries
- Numerics
- How to build & benchmark a solver
- Conflict analysis
- Machine learning in solvers
- Working with industry partners
- Packing problems with nonlinear optimization

Special guests:

Ambros Gleixner

Gennesaret Tjusila

Domenico Salvagnin

Gioni Mexi

Thorsten Koch

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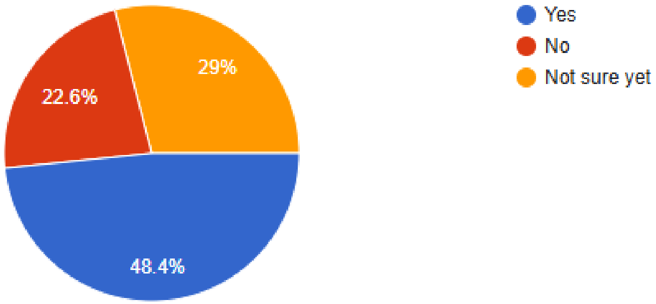
Exams



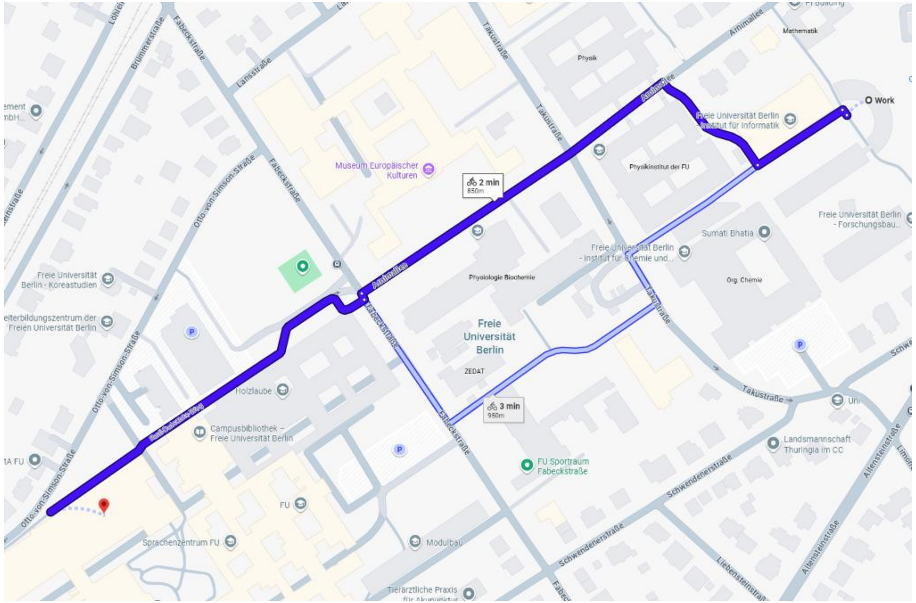
- Originally planned for week Sep 7-11
- Format: Depends on number of participants
  - → survey
- Let's go with the assumption that this will be an oral exam
- Registration via paper form on Friday for TU&FU students

- More details (like actual dates) in the next days…
- Of course, all content from the lectures and basic content from the exercises is relevant
  - You will not have to program during the exam
- Slides will be made available

Daily Agenda

Time	Activity
09.00-10.00	Lecture
10.00-10.30	Coffee Break
10.30-11.30	Lecture
11.30-12.00	Coffee Break
12.00-13.00	Lecture
13.00-14.15	Lunch Break
14.15-15.45	Exercise
15.45-16.15	Flexible Break
16.15-17.45	Exercise

- Coffee Breaks: Vending machine in Pi-Building, gas station, BYO
- Lunch Break: Mensa FU II



- Save the date: Friday evening: Alter Krug

Questions on the Setup?

Let's go!

High-Level Review of Integer Optimization

PD Dr. Timo Berthold
Private Lecturer @ TU Berlin
Director, Mixed-Integer Optimization @ FICO

Computational Mixed Integer Programming

- Bob Bixby (godfather of Computational Optimization): „MIP solvers are a bag of tricks!“
- In 32 years, hardware got a million times faster
- In 32 years, MIP algorithms got six million times faster [Bixby 2024]
  - Those speedups combine!
- In recent years, hardware speedups have gone stale
- MIP solvers are still going strong
  - Xpress: ~15-20% speedup per year
- Goal of this course: taking a look inside the bag…

image source: DALL-E

Trigger Warning for Pure Mathematicians

- This course is not for the faint of heart
- This course will bring us places...
- On Saturday, I found myself typing:

> The largest finite number is 99999999999999983616

- On Thursday, we will learn, why/how
- For now, let‘s start a bit more....conventional...

Agenda for This Lecture

- Some (!) polyhedral fundamentals
- Simplex algorithm
- Cutting plane method
- Branch&Bound

Coarse overview on the „vanilla“ textbook variants that you should be familiar with

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Some (!) Fundamentals

Mathematical Optimization

Optimization Problem

$\rightarrow$ variables $\rightarrow$ solution $\rightarrow$ feasibility
$\rightarrow$ constraints $\rightarrow$ activity $\rightarrow$ feasibility
$\rightarrow$ objective function $\rightarrow$ value $\rightarrow$ quality

$\Rightarrow$ optimal solution $=$ feasible $+$ best possible objective value

Dual bound $\Leftarrow$ **GAP** $\Rightarrow$ **Primal bound**

If the gap is zero, we have a mathematical proof,
that the incumbent solution is optimal.

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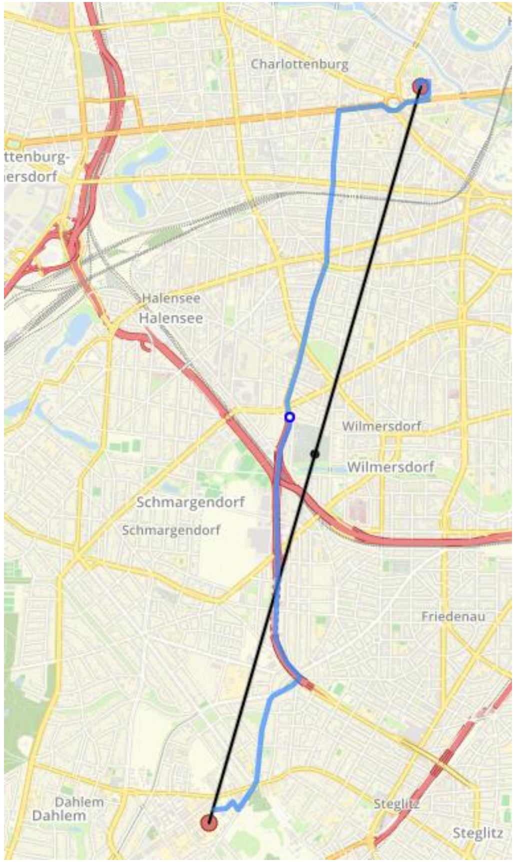
Example: Primal-Dual Gap

- Example: What is the shortest path from
  - Zuse Institute Berlin
    - (where we are right now)
  - TU Berlin
    - (the university hosting this course)
- Primal Bound: 8.07 km driving route
  - Heuristic solution
  - Addressing a different objective
- Dual Bound: Bee line: 6.74 km
    - https://www.distance.to/
- Gap: $\frac{8.07-6.74}{8.07}$ = 16.48%
- Optimization is about driving these bounds towards each other to reach a small gap (ideally, 0%)



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Linear Programming

Linear Program

Objective function:

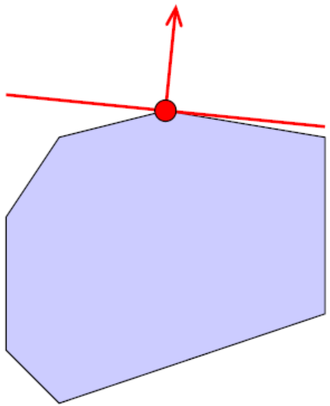
- ▷ linear function

Feasible set:

- ▷ described by linear constraints

Variable domains:

- ▷ real values



$$\begin{aligned} \min \quad & c^T x \\ s.t. \quad & Ax = b \\ & x \in R^n_{\geq 0} \end{aligned}$$

- ▷ convex set
- ▷ “basic” solutions

Mixed-Integer Programming

Definition: MIP

Objective function:

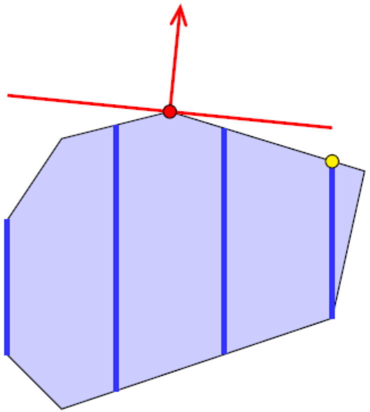
▷ linear function

Feasible set:

▷ described by linear constraints

Variable domains:

▷ integer or real values



$$\begin{aligned} \min \quad & c^T x \\ s.t. \quad & Ax \leq b \\ & x \in \mathbb{Z}^I \times \mathbb{R}^C \end{aligned}$$

▷ not even connected

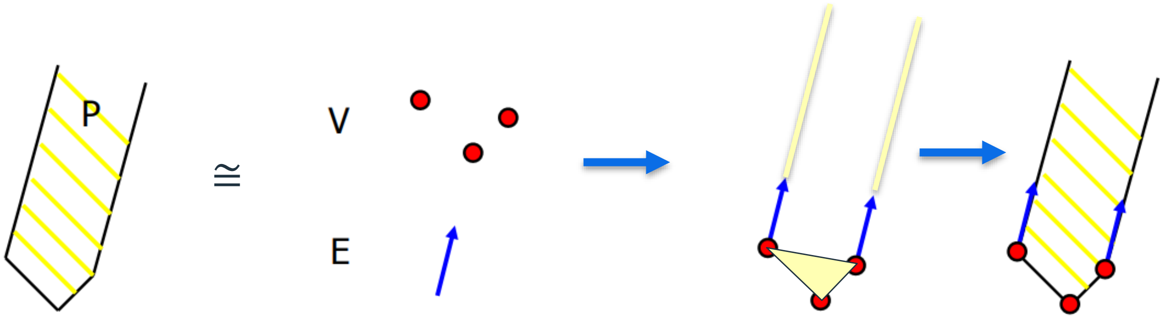
▷ $\mathcal{NP}$-hard problem

LP & Polyhedra

- Linear programming lives (for our purposes) in the n-dimensional real vector space
- polyhedron: intersection of finitely many halfspaces
  - $P = \{x \in \mathbb{R}^n \mid Ax \leq b\}$
- polytope: convex hull of finitely many points
  - $P = conv(V)$, V a finite set in $\mathbb{R}^n$
- convex polyhedral cone: conic combination (i.e., nonnegative linear combination) of finitely many points
  - $K = cone(E)$, E a finite set in $\mathbb{R}^n$

Representation of Polyhedra

- Theorem: For a subset P of $\mathbb{R}^n$ the following are equivalent:
  1. P is a polyhedron: the intersection of finitely many halfspaces, i.e., there exist a matrix A and a vector b with $P = \{x \in \mathbb{R}^n \mid Ax \leq b\}$ (outer representation)
  2. P is the sum of a convex polytope and a finitely generated (polyhedral) cone, i.e., there exist finite sets V and E with $P = conv(V) + cone(E)$ (inner representation)



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How to get a dual bound for an LP?

$$\min\{c^T x \mid Ax \geq b, x \geq 0\}$$

- How do we get a proof of solution quality?
- Easy case: One of our constraints underestimates the objective function
  - E.g., if $c^T x = 2x_1 + x_2$ and one constraint $x_1 + x_2 \geq 3$, then also $\min c^T x \geq 3$
- Observation 1: Constraints are invariant to scaling by positive numbers
- Observation 2: The sum of two valid constraints is a valid constraint
  - Consequence: Conic combinations of constraints are valid
- Task: Find a conic combination of all constraints that is a maximal underestimator for our objective
- This is an LP. The dual LP

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The Dual LP: A bit more formally

$$\min\{c^T x \mid Ax \geq b, x \geq 0\}$$

- Task: Find a conic combination of all constraints that is a maximal underestimator for our objective
- Dual multipliers that yield a conic combination: $y \geq 0$
- Conic combination of all constraints...: $\mathrm{y}^{\mathrm{T}} Ax \geq y^T \mathrm{b}$
- ...that is an (...)underestimator for our objective: $\mathrm{y}^T A \leq c$
- ...and that is a maximal underestimator : $\max \; y^T b$
- This is an LP. The dual LP!

$$\max\{y^T b | \, \mathrm{y}^{\mathrm{T}} A \leq c, y \geq 0\}$$

Dual LP: Scheme

- Each constraint in the primal LP becomes a variable in the dual LP
- Each variable in the primal LP becomes a constraint in the dual LP
- The objective direction is inverted
  - maximize in the primal becomes minimize in the dual and vice-versa
- Inequalties become $\leq$-bounds
- Consequently, equations become free variables

By this scheme: Easy to see that the dual of the dual is the primal

- Side note: All LP/MIP variants ($\{\geq, \leq, =\}$, $\{min, max\}$, {bounded vars, free vars}) can easily be transformed into each other
  - We will always use a variant that is most convenient for our purposes

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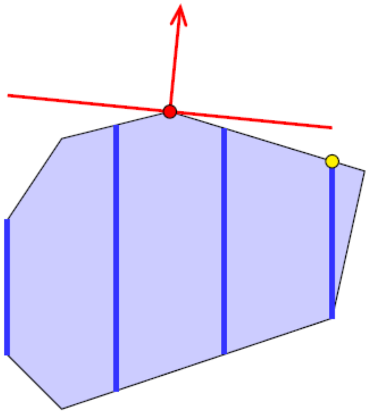
How to get a dual bound for a MIP?

- We solve the LP relaxation

$$\begin{aligned}&\min c^T x\\&Ax \le b\\&x \in \mathbb{Z}^I \times \mathbb{R}^C\end{aligned}$$

$$\Downarrow$$

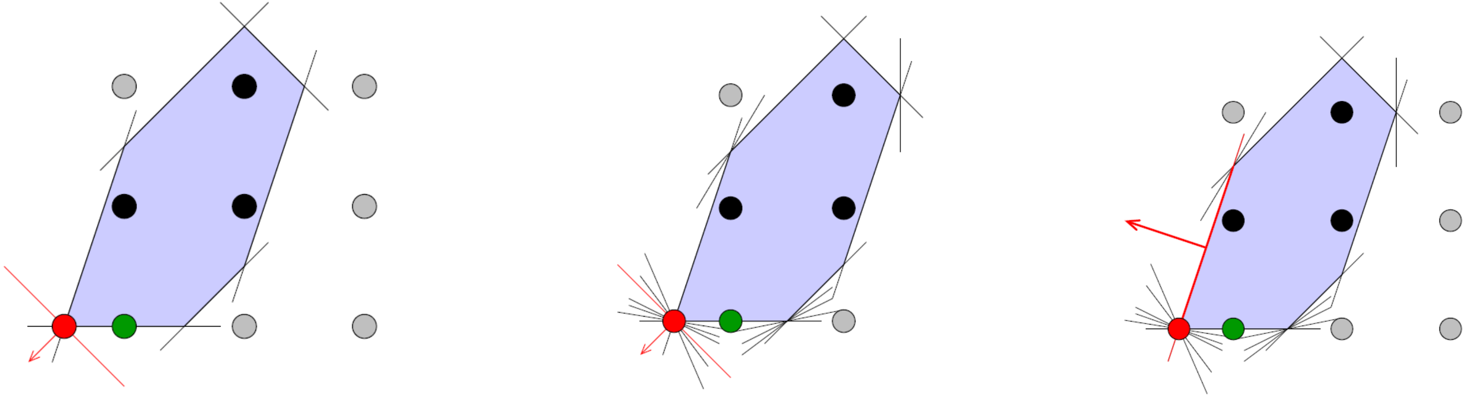
$$\begin{aligned}&\min c^T x\\&Ax \le b\\&x \in \mathbb{R}^n\end{aligned}$$



- This enlarges („relaxes“) the set of feasible solutions
  - Every MIP solution is at least as good as the solution of the LP relaxation

Primal and Dual Degeneracy

- naïvely: one optimal solution, determined by n constraints
- at a second thought: one optimal solution, k > n tight constraints
- but really: an optimal polyhedron
- Can be exploited in some ways. But mostly a burden



Simplex Algorithm

Simplex Idea

- Start at a random vertex
- Among neighboring vertices, choose one which improves the objective, if none: optimal
  - Special case: A ray along which the objective improves
    - Then, the LP is unbounded
- Move along edges towards an optimal vertex
- Why does this work?
  1. Show that an optimal boundary solution exists (convexity)
  2. Narrow down further: an optimal vertex solution exists (linearity)
  3. Local optimality is global optimality (convexity)

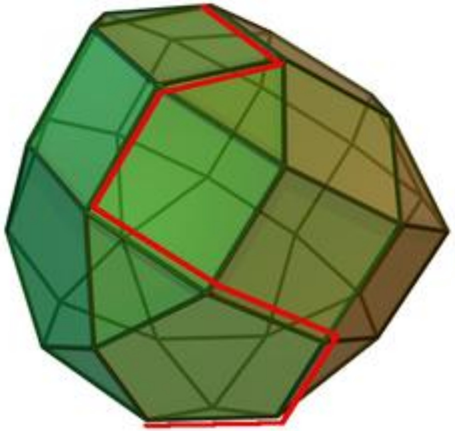


image source: WIkipedia

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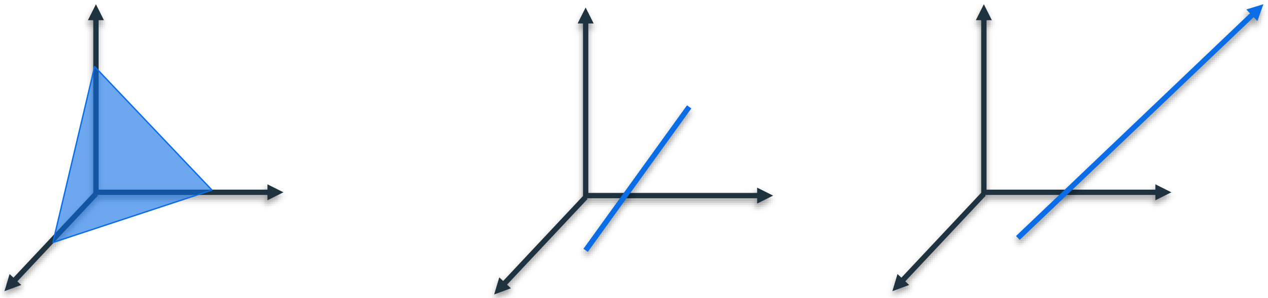
Standard Form

- By adding slack variables etc., every LP can be equivalently transformed to

  $\min \{c^T x \mid Ax = b, x \geq 0\}$

- Nonempty LPs in standard form always have vertices, and are the
  - Intersection of a simplicial cone and an affine subspace, e.g.:



- Further, simplex algo assumes w.l.o.g. $\operatorname{rank}(A) = m < n$, $\{x \mid Ax = b\}$ nonempty

Basic Solution

- W.l.o.g. let $\operatorname{rank} A = m < n$ and consider the computational form

$$\min \{c^T x \mid Ax = b, x \geq 0\}$$

- For every vertex there is a non-singular $m \times m$ sub-matrix B of A

$$A = \boxed{\quad B \quad}\boxed{\qquad N \qquad}$$

- and the corresponding basic solution is given by

$$x_B = B^{-1}b, \qquad x_N = 0$$

- LP is a finite optimization task: $\binom{n}{m}$ possible bases
- Basic solution = vertex solution $\Leftrightarrow$ x primal feasible $\Leftrightarrow$ $x \geq 0 \Leftrightarrow x_B \geq 0$

More in Ambros' lecture

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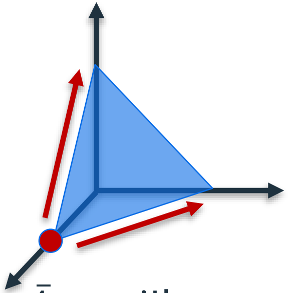
Simplex Idea (Reloaded)

- LP optimal ⇔ there is an optimal vertex solution ⇔ there is an optimal basic solution
  - Just established: There is a finite set of bases
- Idea: Find some feasible basis, exchange one of the columns in the basis („pivoting“), s.t. feasibility is maintained, objective is improved



- $x_i = \bar{b}_i - \bar{A}_i x_N$ with nonzero element $\bar{A}_{ij}$, solve for x_j.
  - Multiply by identity matrix E with jth column: $\frac{-1}{\bar{A}_{ij}} \bar{A}_j$ and (i,j)-th element $\frac{1}{\bar{A}_{ij}}$

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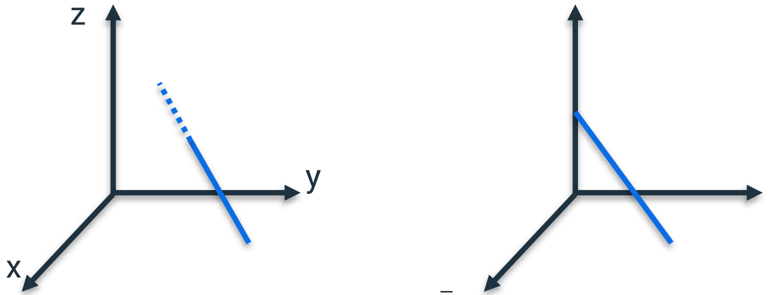
Which Columns to Choose for Pivoting?

- Choose j among all columns for which $\bar{c} = c_N - c_B A_B^{-1} A_N$ is positive
  - Reduced costs, in this direction we can improve
  - If no such j: Done, optimal
- Then, among all i with $\bar{A}_{ij} > 0$ have to choose one with minimal positive $\frac{\bar{b}_i}{\bar{A}_{ij}}$ to stay feasible
  - If no such $(\bar{A}_j \leq 0)$: Done, LP is unbounded



  - Main choice: entering nonbasic column. $\frac{\bar{b}_i}{\bar{A}_{ij}}$ „bottleneck" by how much it can be increased

One Step of the Simplex Algorithm (Dantzig 1947)

1. Check optimality: $\bar{c} \leq 0$?
2. Choose pivot column with $\bar{c}_j > 0$
3. Check unboundedness: $\bar{A}_j \leq 0$?
4. Pick pivot row with minimal $\frac{\bar{b}_i}{\bar{A}_{ij}}$
5. Pivoting: Exchange i,j in N and B, multiply A_B^{-1} by eta matrix
6. Update all data structures $(\bar{A}, \bar{b}, \bar{c})$

Quiz Time

- An LP (in standard form) with 20 constraints over 100 variables
  a) will have at most 20 nonzeros in an optimal basic solution
  b) might have more than 20, but at most 80 nonzeros in an optimal basic solution
  c) might have more than 80, but at most 100 nonzeros in an optimal basic solution
- The set of feasible solutions for a MIP is also called:
  a) a simplex set
  b) a mixed integer set
  c) a linear set
- The dual of $\min\{c^T x \mid Ax \geq b, x \geq 0\}$ is
  a) $\min\{y^T b \mid yA = c, y \leq 0\}$
  b) $\max\{y^T b \mid yA = c, y \geq 0\}$
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Cutting plane method

Gomory Cuts: The First IP Solver

OUTLINE OF AN ALGORITHM FOR INTEGER SOLUTIONS TO LINEAR PROGRAMS

BY RALPH E. GOMORY[1]

Communicated by A. W. Tucker, May 3, 1958

The problem of obtaining the best integer solution to a linear program comes up in several contexts. The connection with combinatorial problems is given by Dantzig in [1], the connection with problems involving economies of scale is given by Markowitz and Manne [3] in a paper which also contains an interesting example of the effect of discrete variables on a scheduling problem. Also Dreyfus [4] has discussed the role played by the requirement of discreteness of variables in limiting the range of problems amenable to linear programming techniques.

It is the purpose of this note to outline a finite algorithm for obtaining integer solutions to linear programs. The algorithm has been programmed successfully on an E101 computer and used to run off the integer solution to small (seven or less variables) linear programs completely automatically.

image source: ralphgomory.com

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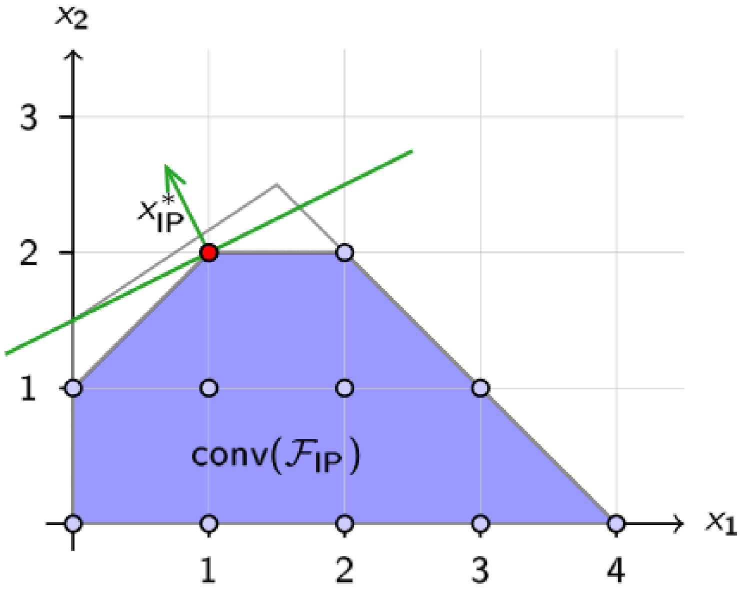
General Cutting Plane Method

- Convex hull of IP-feasible solution $conv(F_{IP})$ is a polyhedron*
- Principally, every IP could be formulated as LP
- Problems:
  - Linear description not known
  - Might require exponentially many rows
- Motivation:
  - For optimal solution, we need at most n rows

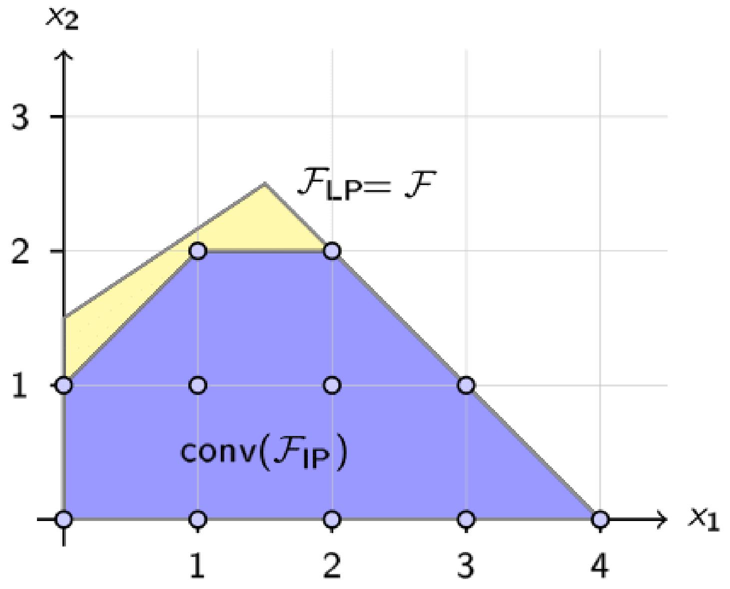


$\min\{c^T x : x \in \text{conv}(\mathcal{F}_{IP})\}$

* = assuming rational data (or bounded domains)

General Cutting Plane Method: Colorful Picture

1. Initialize: $F \leftarrow F_{LP}$
2. Solve $x^* \leftarrow \min\{c^T x \mid x \in F\}$
3. If $x^* \in F_{IP}$:
   Stop!
4. Add inequality to F that is:
   - Valid for $conv(F_{IP})$ and
   - Violated by x^*
5. Goto 2



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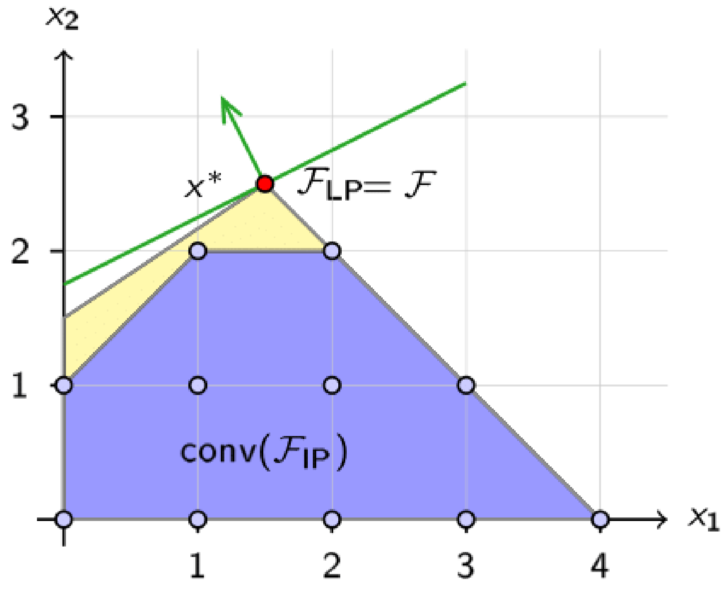

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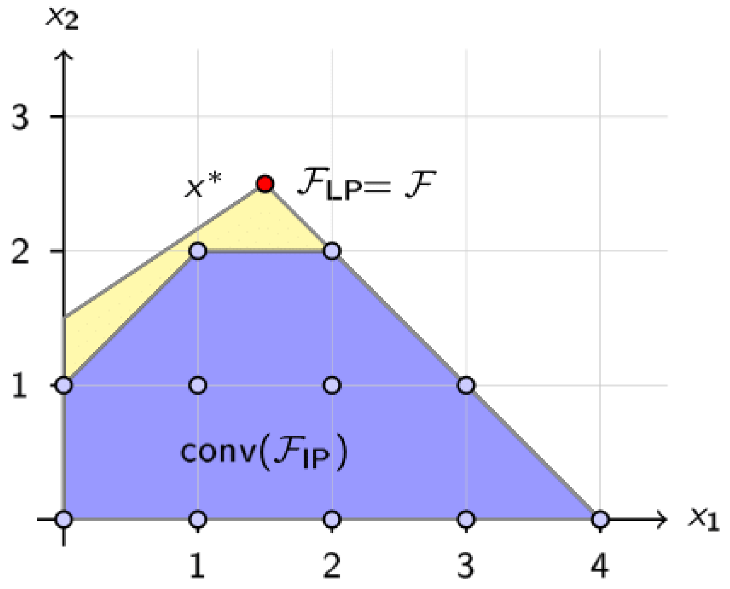

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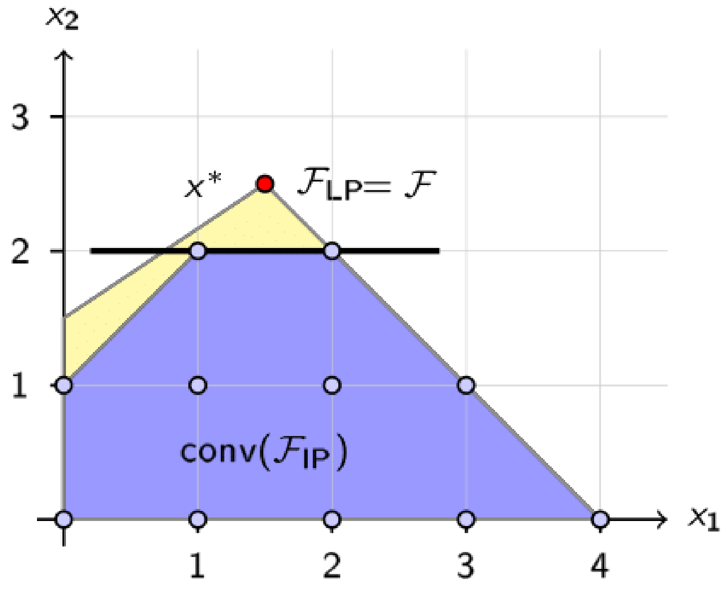

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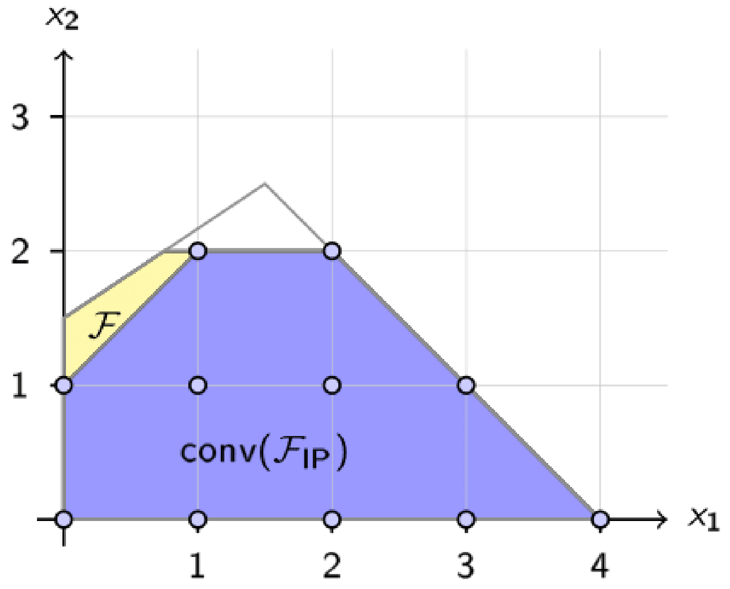

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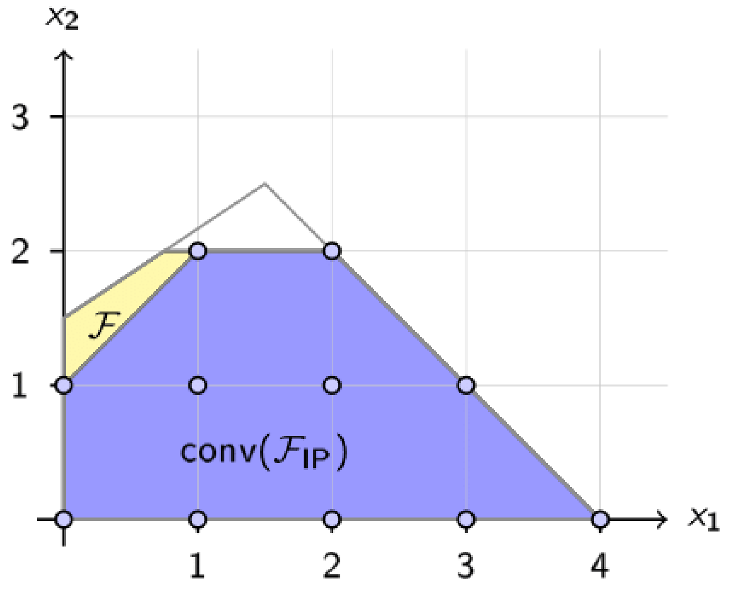

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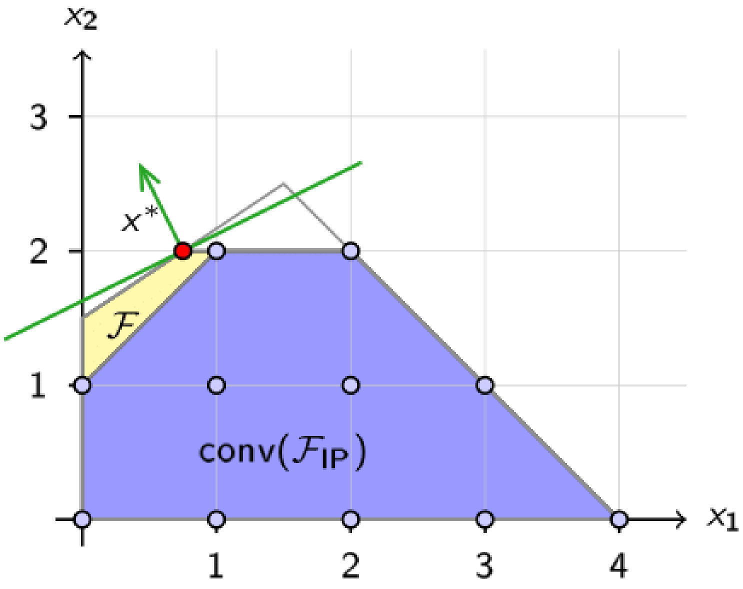

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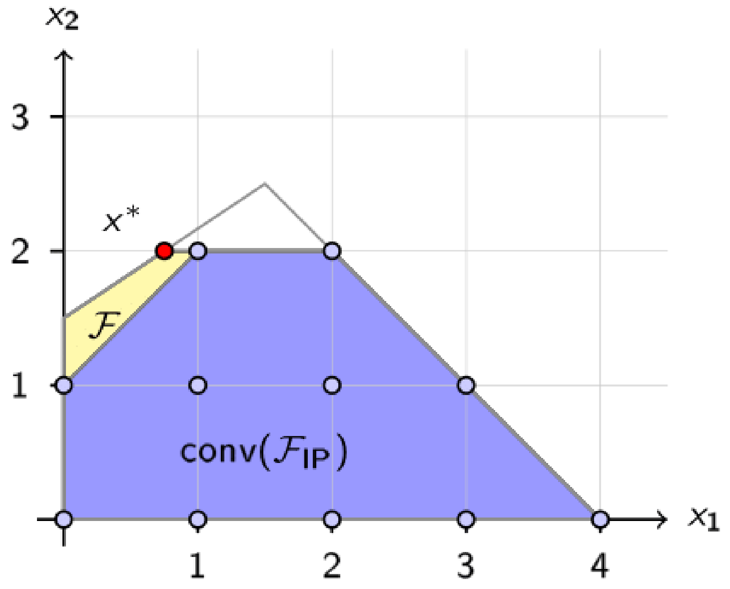

$\min\{c^T x : x \in \text{conv}(\mathcal{F}_{IP})\}$

FICO

General Cutting Plane Method: Colorful Picture

1. Initialize: $F \leftarrow F_{LP}$
2. Solve $x^* \leftarrow \min\{c^T x \mid x \in F\}$
3. If $x^* \in F_{IP}$:
   Stop!
4. Add inequality to F that is:
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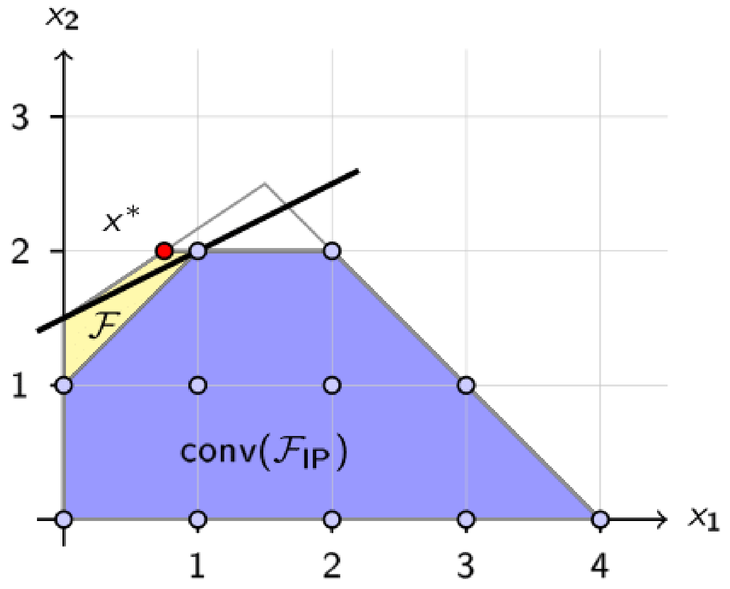

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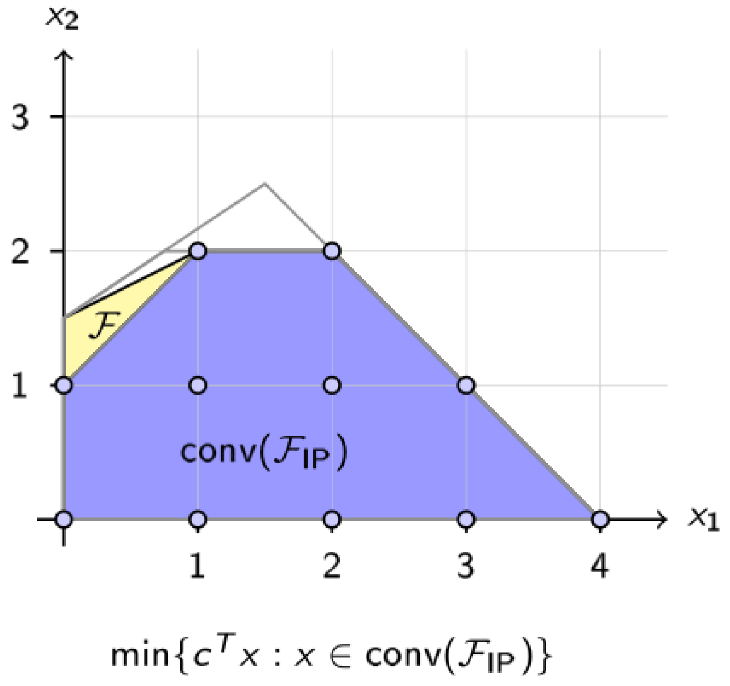

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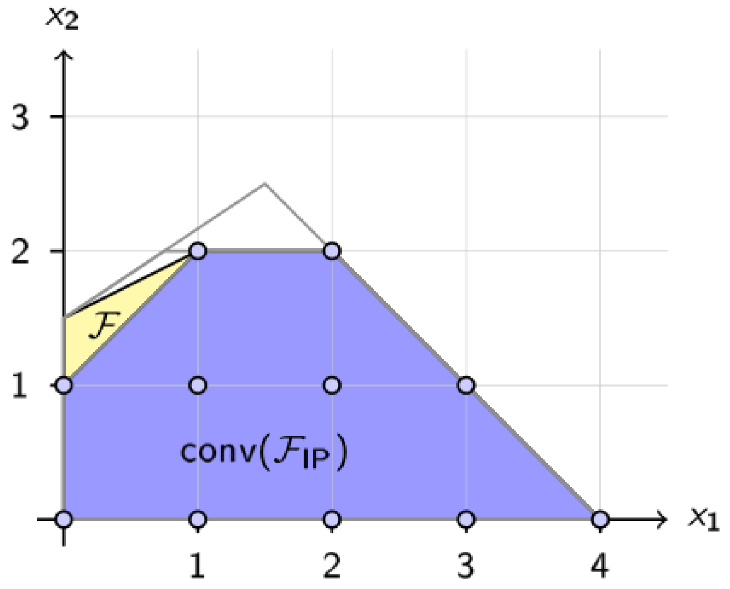

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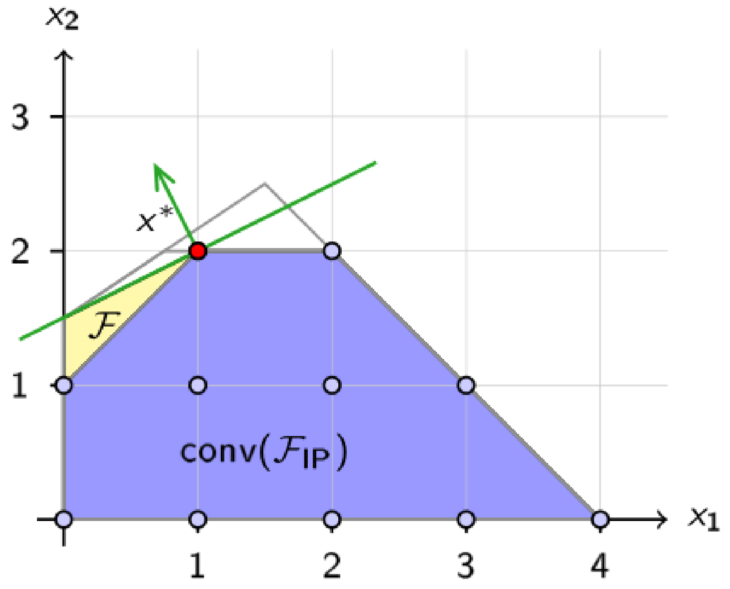

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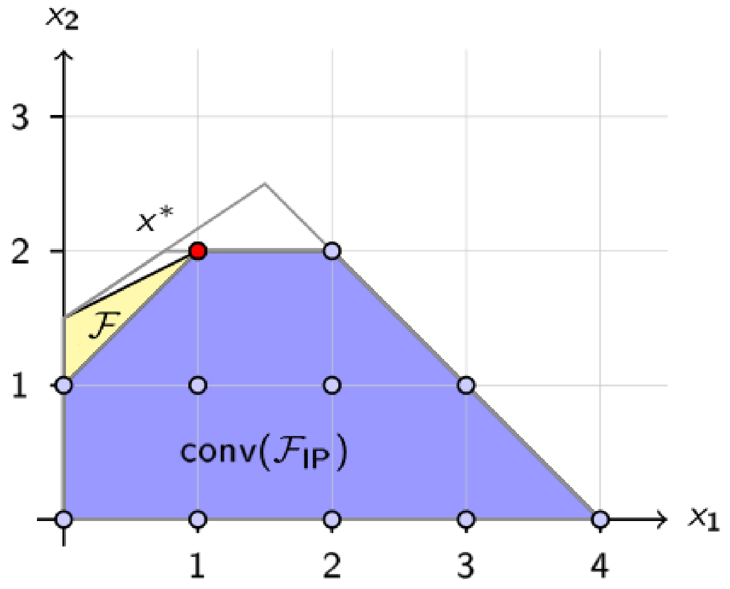

$\min\{c^T x : x \in \text{conv}(\mathcal{F}_{\text{IP}})\}$

FICO

Gomory Cuts (1958)

- Given an arbitrary IP, with an optimal basic solution of its LP relaxation
  - Finds for each fractional variable in the LP solution a hyperplane that separates the LP solution from the set of all feasible solutions of the IP
  - Add one (or all) to the LP relaxation, rinse, repeat
- Can be generalized to MIP

Gamification

- By Gonzalo Muñoz: http://www.columbia.edu/~gm2543/cpgame.html
- Get yourself on the leaderboard!

Branch&Bound

First IFORS Meeting: Kickstart for LP-Based Branch&Bound?

- From Bill Cook's fantastic IFORS distinguished lecture: https://www.youtube.com/watch?v=5VjphFYQKj8

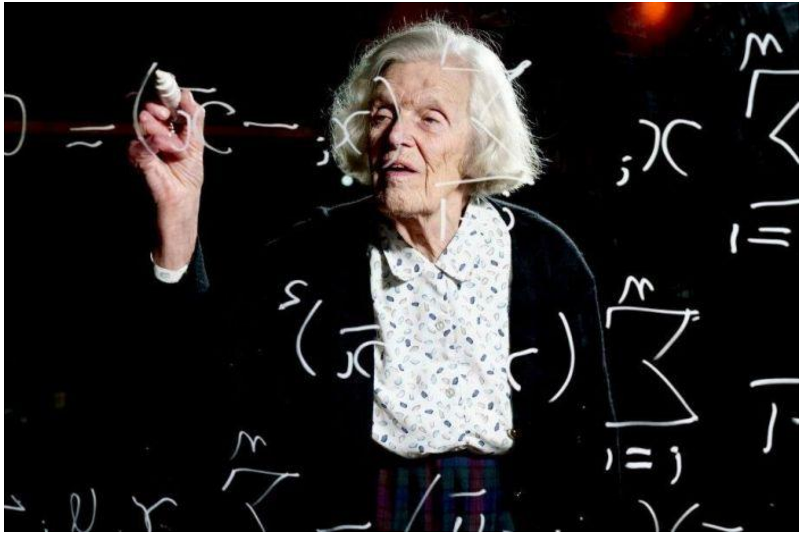

image source: abc.net.au

- Alison Harcourt (née Doig): Victorian Senior Australian of the year 2019

FICO

Branch&Bound [Land&Doig 1960]

- Divide&Conquer
- Split search region into strictly smaller subproblems, hopefully easier to solve, iterate
  - Typically two subproblems, typically disjoint
- Maintain lower and upper bounds, prune subproblems outside of bounds
- General version for discrete problems, already with LP-relaxations, by Land&Doig 1960
- Easier implementation, MIP-specific, by Dakin 1965
  - Dual simplex shines: Warm starts when adding new variable bounds

LP-Based Branch&Bound: Algorithm

Steps

1. Abort criterion
2. Node selection
3. Solve relaxation
4. Bounding
5. Feasibility check
6. Branching

$\mathcal{L} \leftarrow \{P\}, \quad U \leftarrow \infty, \quad x^{\mathrm{IP}} \leftarrow \mathrm{NULL};$

if $\mathcal{L} = \emptyset$ **then return** x^{IP} *and* U;

Select $P_i \in \mathcal{L}, \quad \mathcal{L} \leftarrow \mathcal{L} \setminus \{P_i\}$;

Solve LP relaxation of $P_i, \quad L_{\mathrm{loc}} \leftarrow c(x^{\mathrm{LP}})$ or ∞;

if $L_{loc} \geq U$ **then goto** line 2;

if $x^{LP} \in P$ **then** $x^{\mathrm{IP}} \leftarrow x^{\mathrm{LP}}, \quad U \leftarrow L_{\mathrm{loc}},$ **goto** line 2;

Select $j \in I : x_j^{\mathrm{LP}} \notin \mathbb{Z}$. Split P_i into $P_{2i+1} := P_i \cup \{x_j \leq \lfloor x_j^{\mathrm{LP}} \rfloor\}$, and $P_{2i+2} := P_i \cup \{x_j \geq \lceil x_j^{\mathrm{LP}} \rceil\}, \quad \mathcal{L} \leftarrow \mathcal{L} \cup \{P_{2i+1}, P_{2i+2}\},$ **goto** line 2;

LP-Based Branch&Bound (Colorful Picture)

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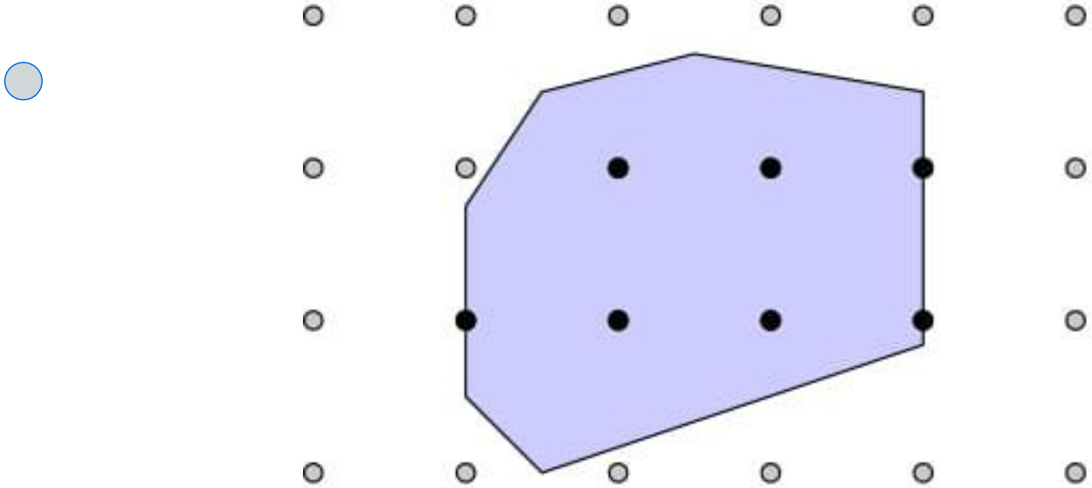

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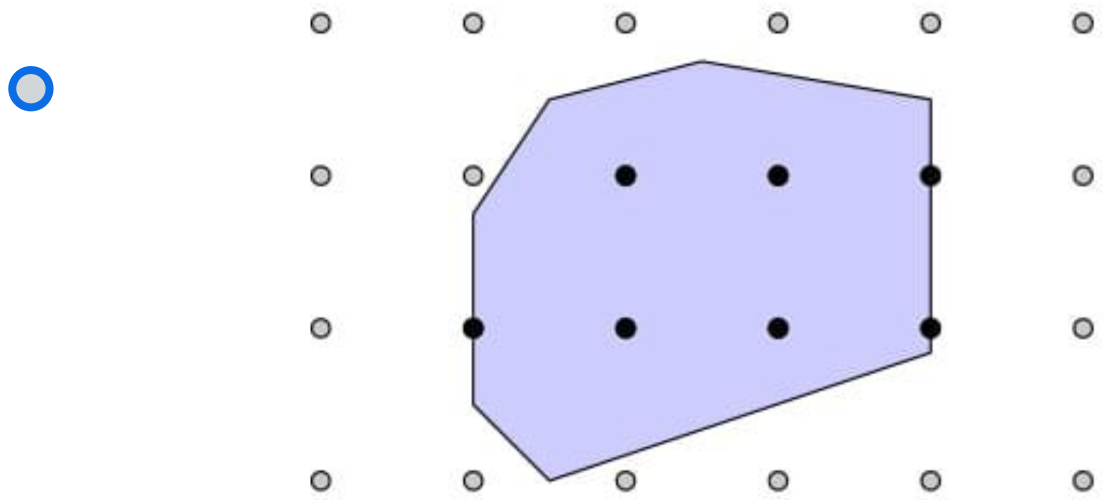

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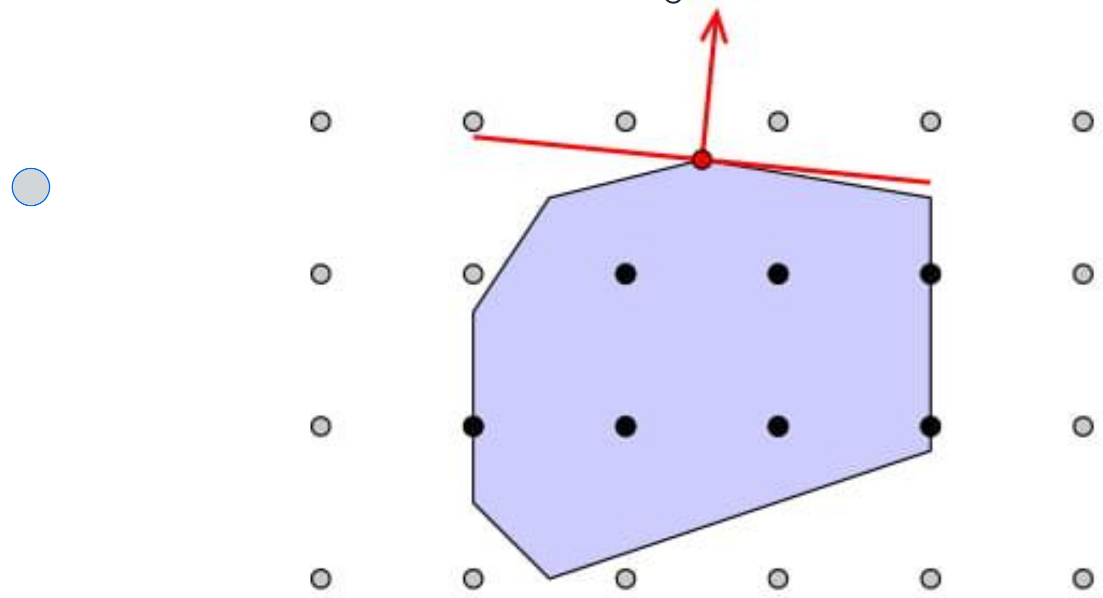

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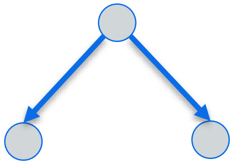

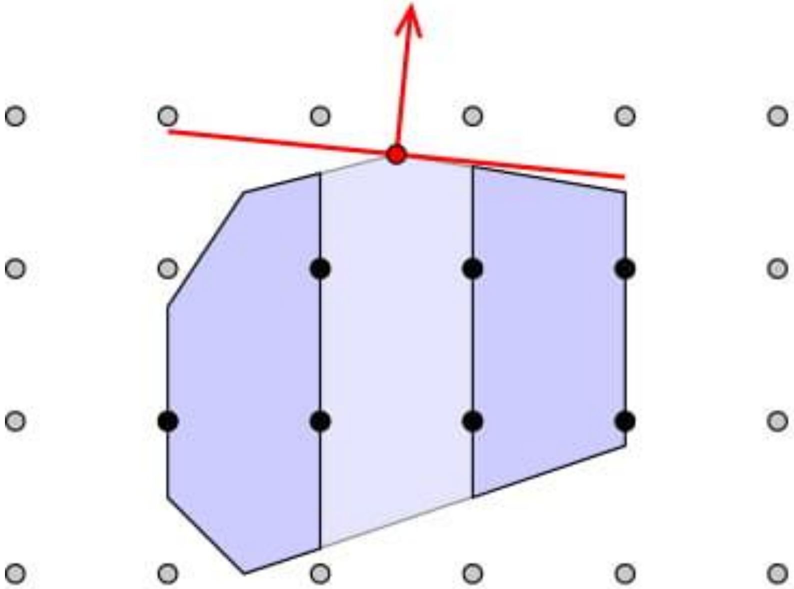

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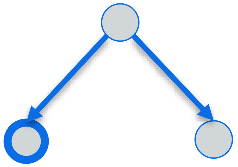

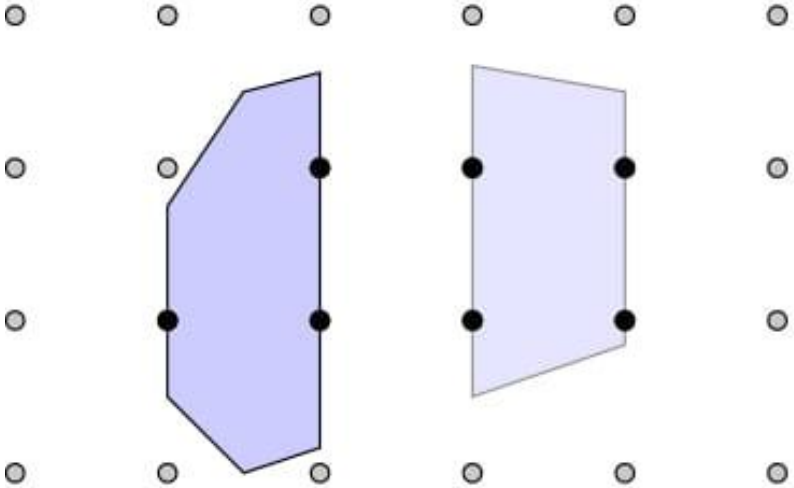

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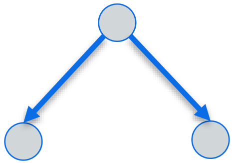

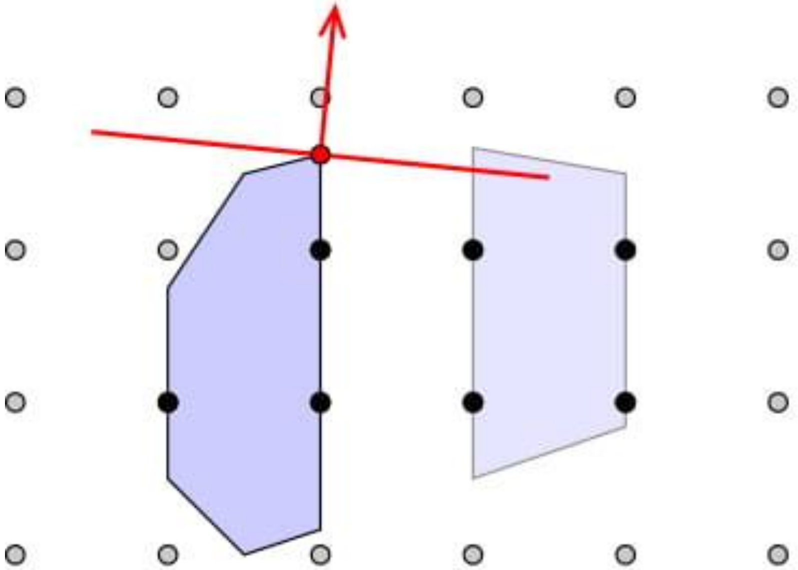

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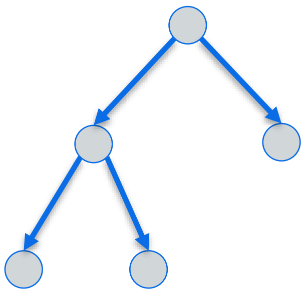

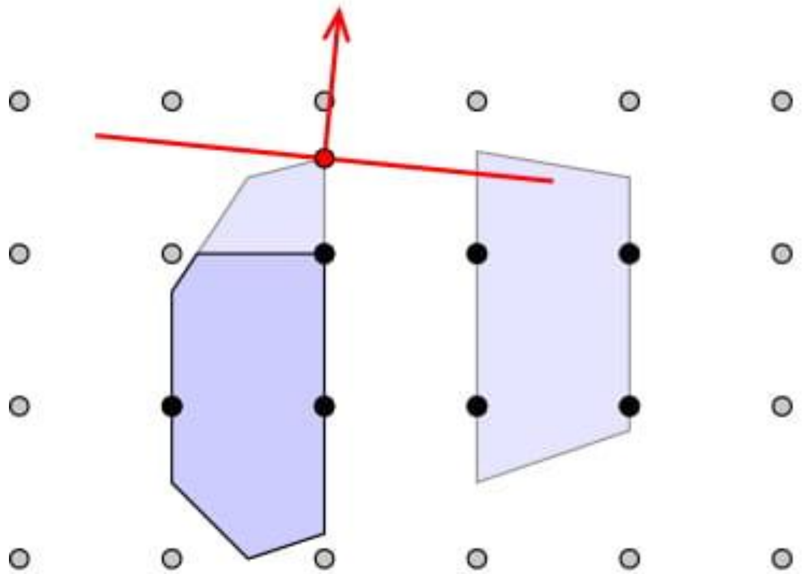

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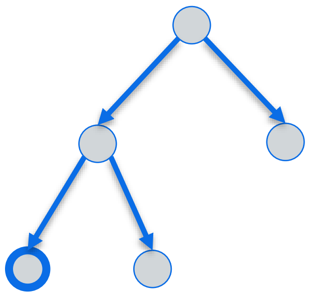

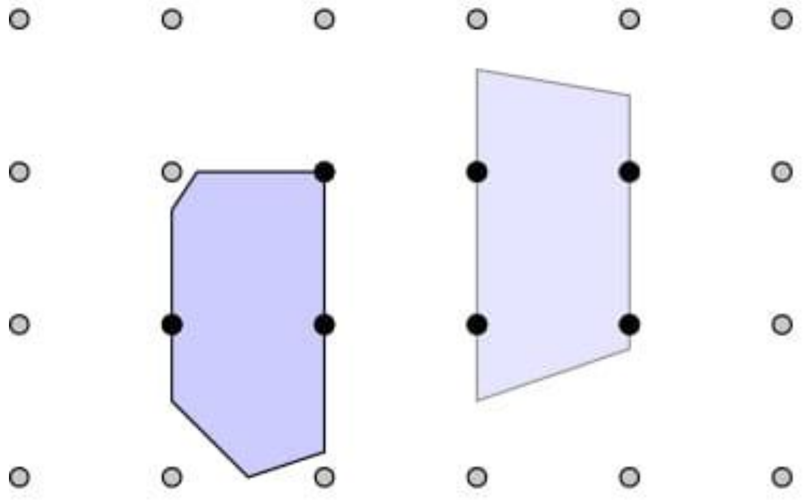

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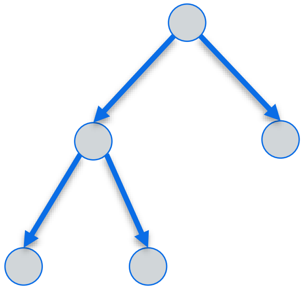

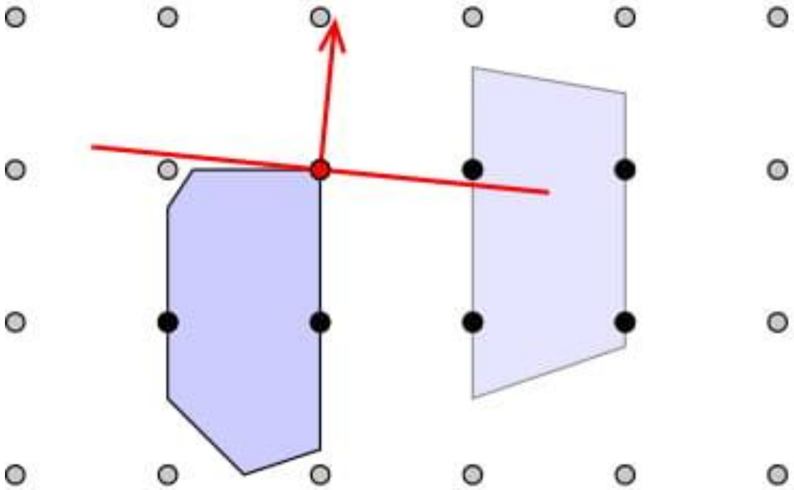

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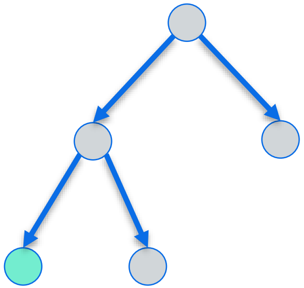

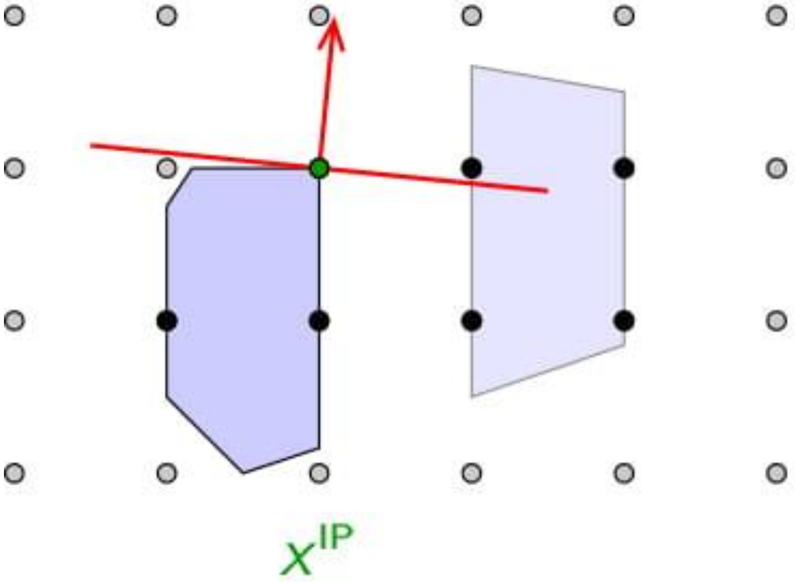

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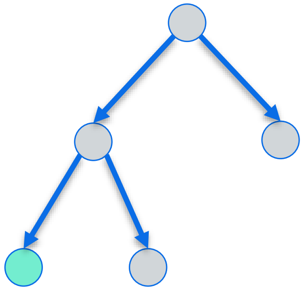

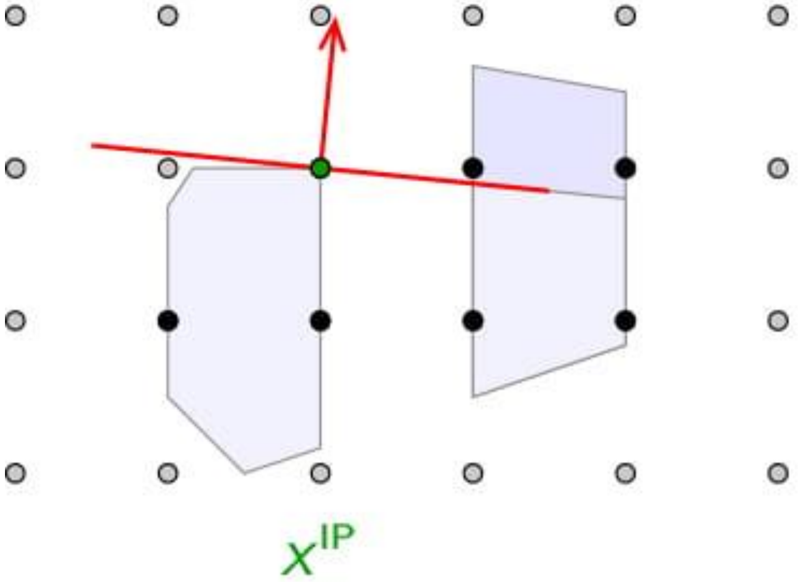

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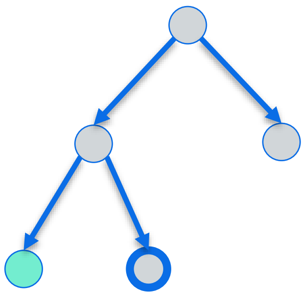

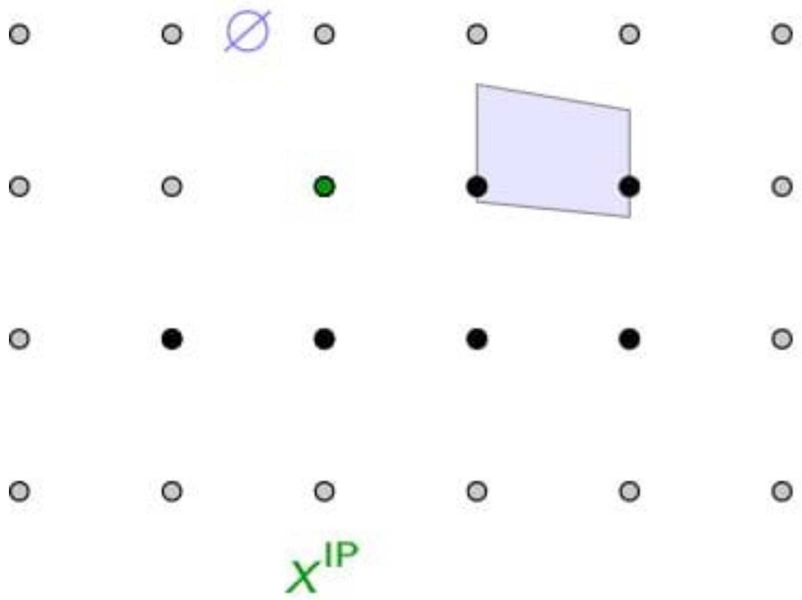

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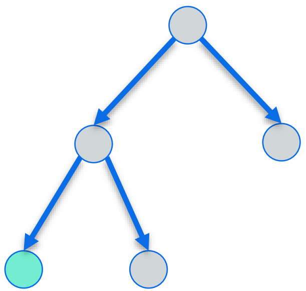

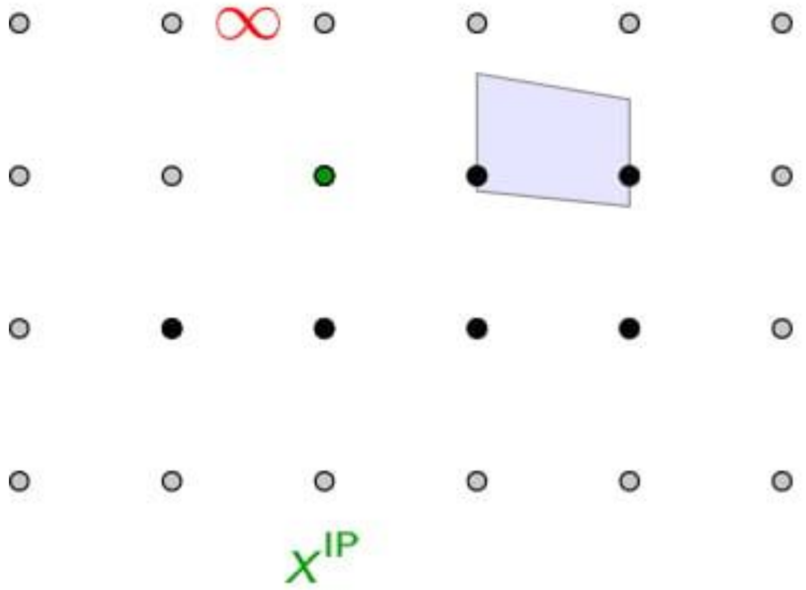

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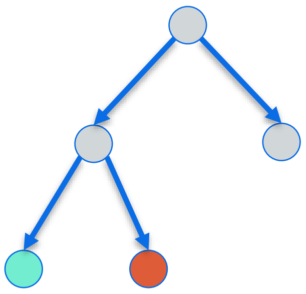

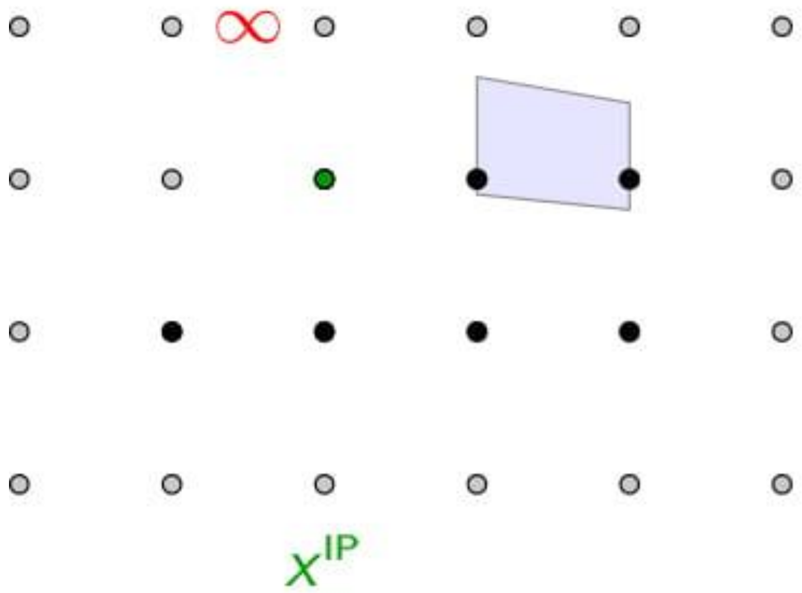

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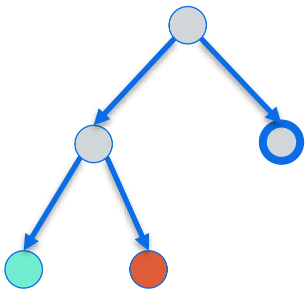

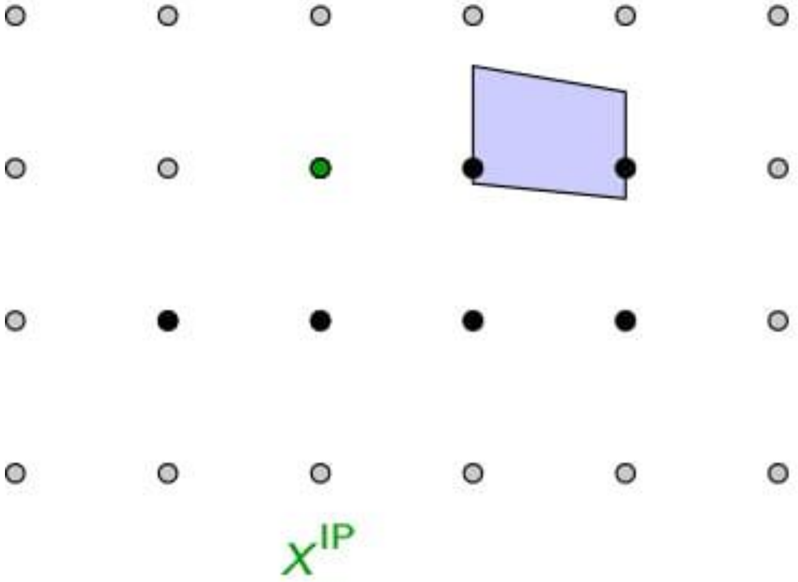

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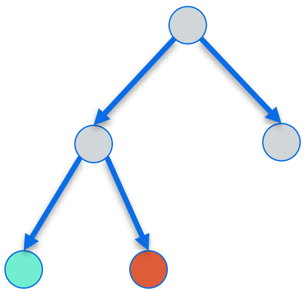

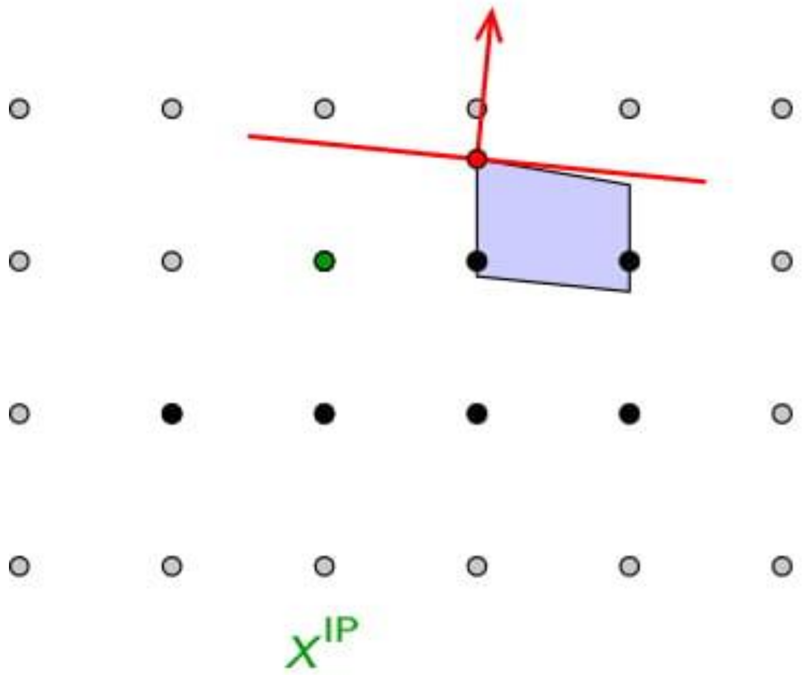

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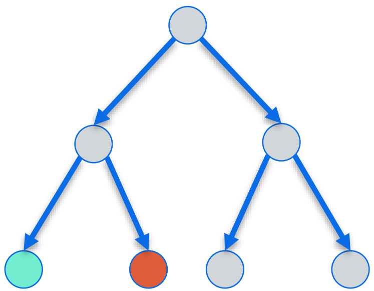

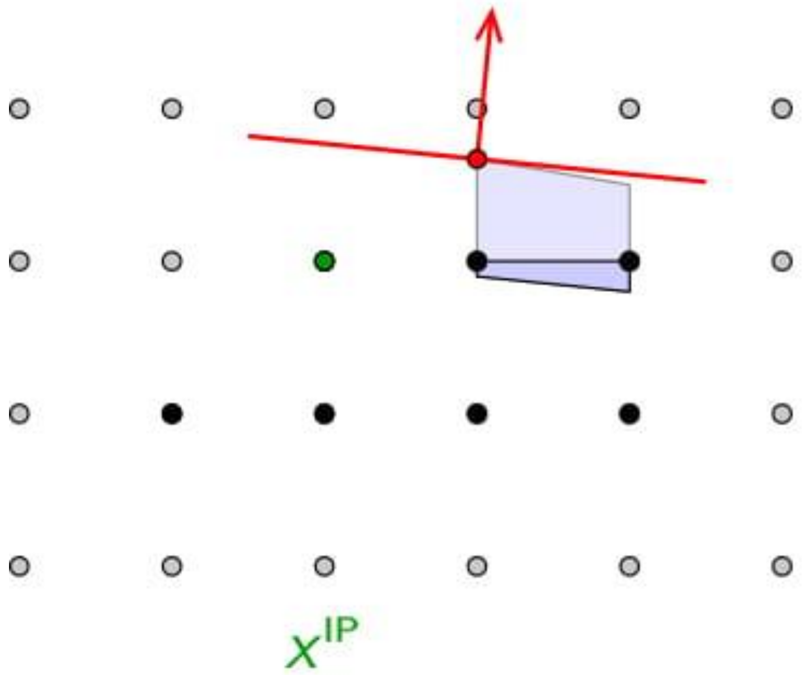

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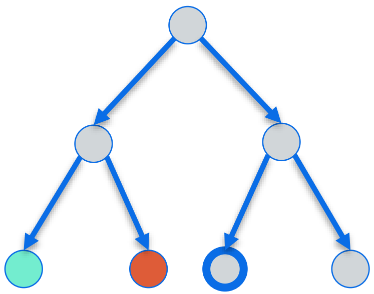

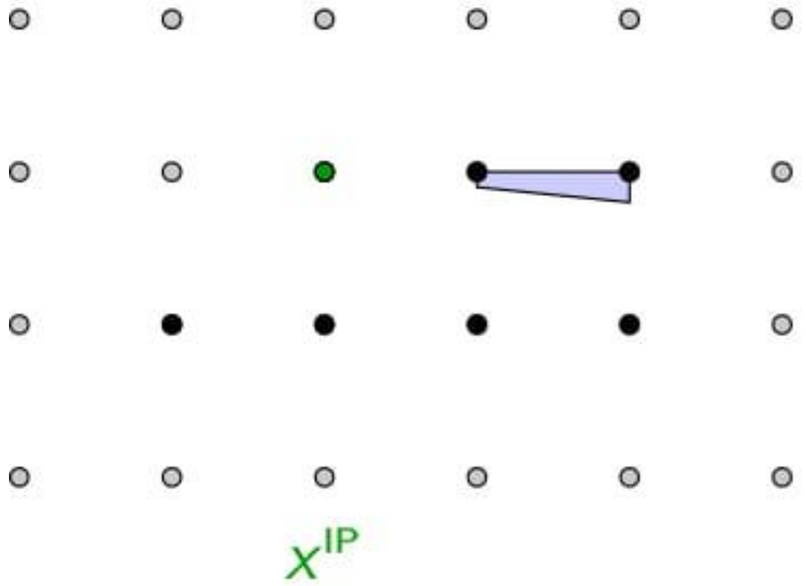

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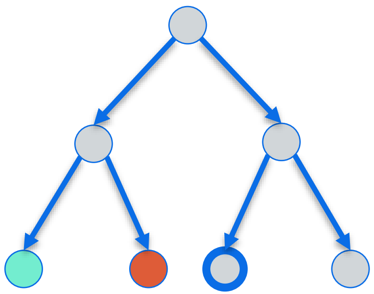

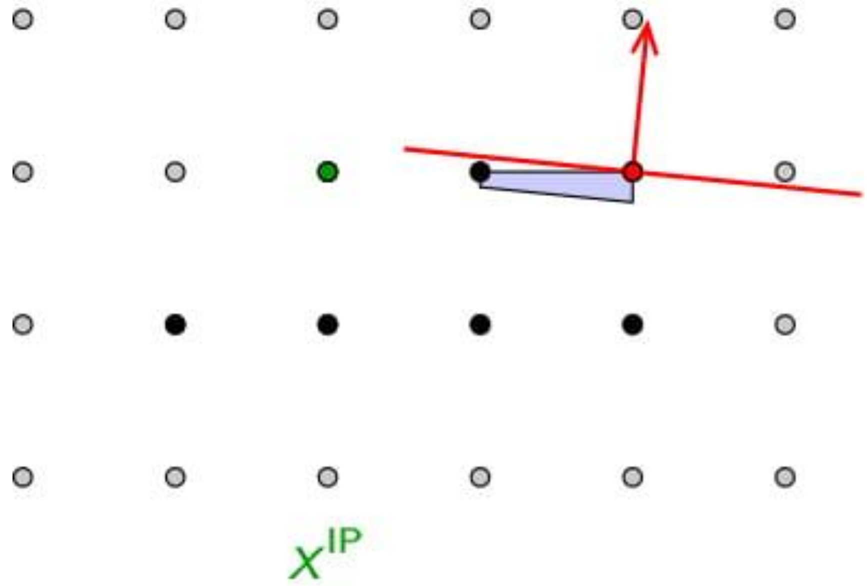

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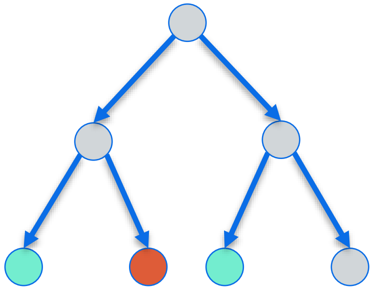

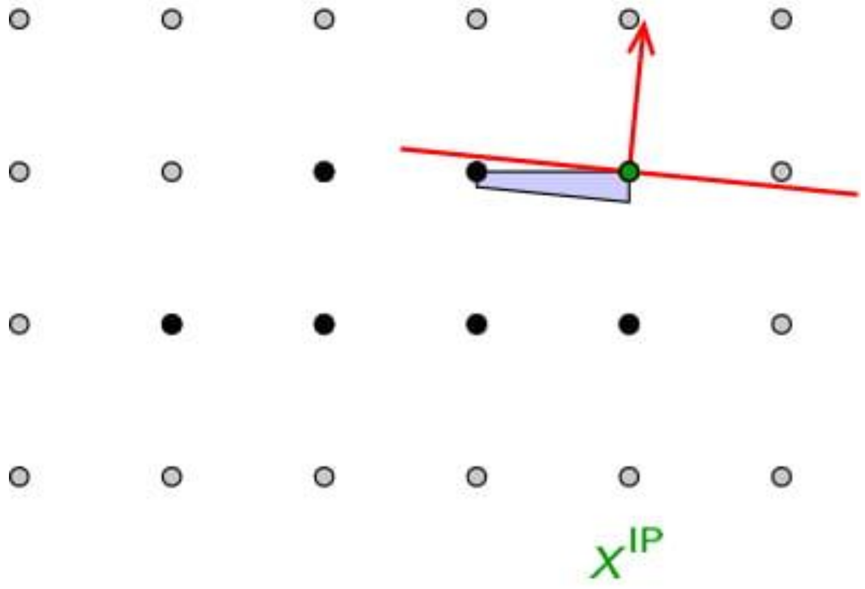

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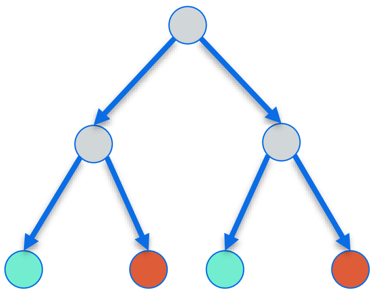

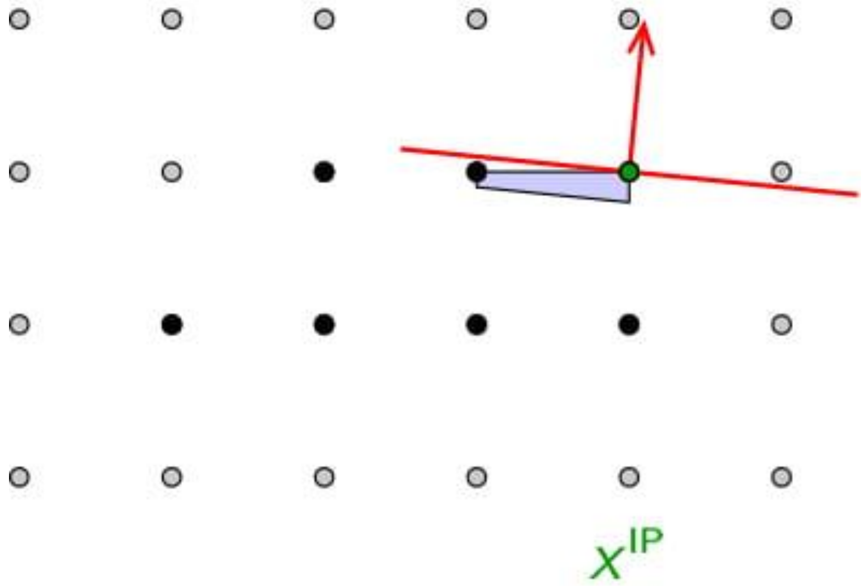

FICO

Quiz Time

- With Gomory's algorithm, the first integer solution found
  a) will be an optimal solution
  b) might be suboptimal, but within a factor 2 of optimality
  c) has a minimum number of nonzero variables
- You get one Gomory cut per
  a) basic solution
  b) basic variable
  c) fractional variable
- The LP algorithm of choice for LP-based branch-and-bound is:
  a) Primal Simplex
  b) Dual Simplex
  c) Barrier

FICO

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Thank You!

PD Dr. Timo Berthold
Private Lecturer @ TU Berlin
Director, Mixed-Integer Optimization @ FICO

Running Time

- Branch&Bound can obviously be exponential, but is it even finite?

```
Minimize
  obj: x3
Subject To
  c1: 12 x1 + 9 x2 - x3 = 0
Bounds
  -inf <= x1
  -inf <= x2
  1 <= x3
General
  x1 x2 x3
End
```

Careful modelling matters!