Theoretical and computational analysis of sizes of branch-and-bound trees

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Joint work with...

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Georgia Tech

1
Introduction

Integer program

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$$\begin{aligned} \min \quad & c^\top x \\ \text{s.t.} \quad & Ax \leq b \qquad \qquad \text{(IP)} \\ & x \in \mathbb{Z}^n \end{aligned}$$

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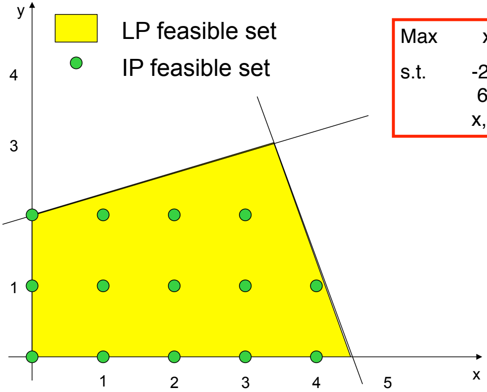
Many applications:

- Decision making with vast economic and societal impact
- Power systems, Sustainibility, IMRT cancer treatment, Circuit design, Healthcare analytics, Network design, Supply chain Design, Urban mobility, Production planning, National security, etc.

Branch-and-Bound

Branch-and-bound is the basic algorithm underlying state-of-art IP solvers.



$$\begin{array}{ll} \text{Max} & x + 2y \\ \text{s.t.} & -2x + 7y \leq 14 \\ & 6x + 2y \leq 27 \\ & x, y \geq 0 \text{ and integer} \end{array}$$

Example/Picture credit: Natashia Boland

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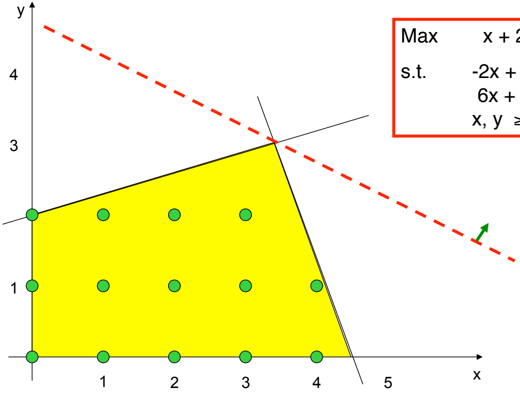
Solving Root Note



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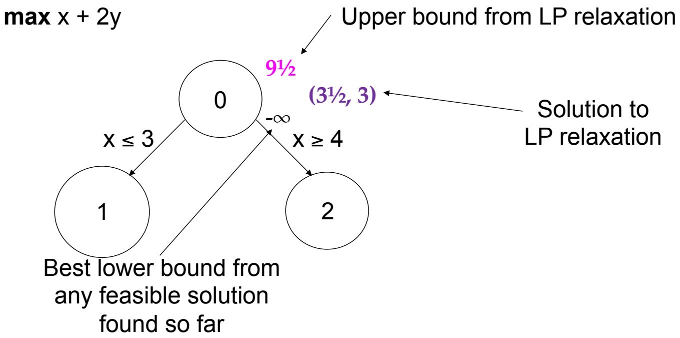

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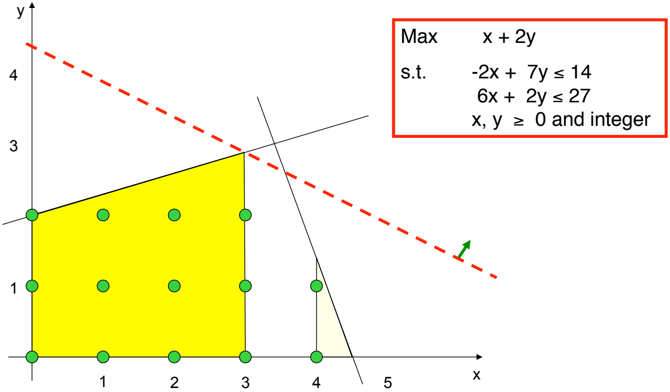
Branching process



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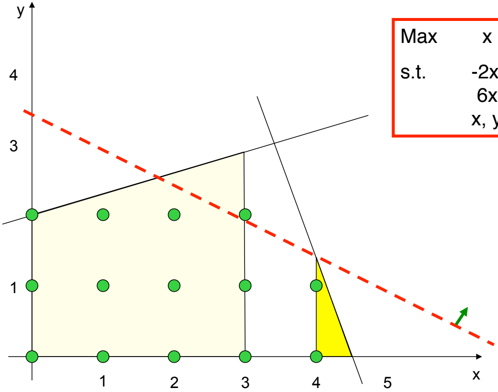

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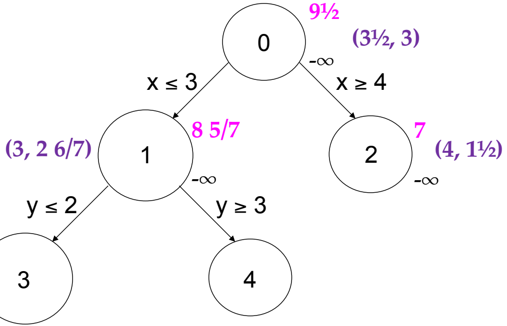

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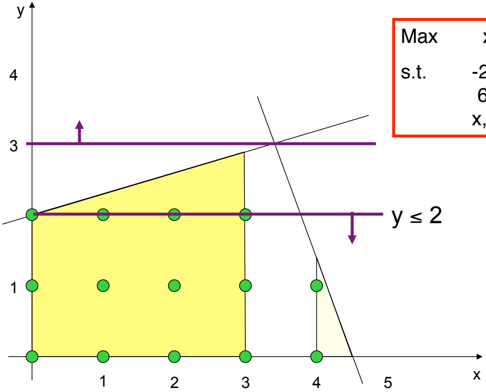

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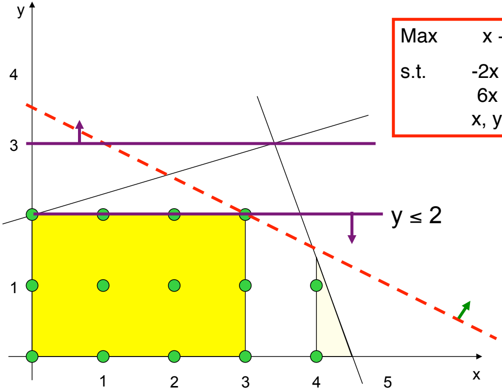

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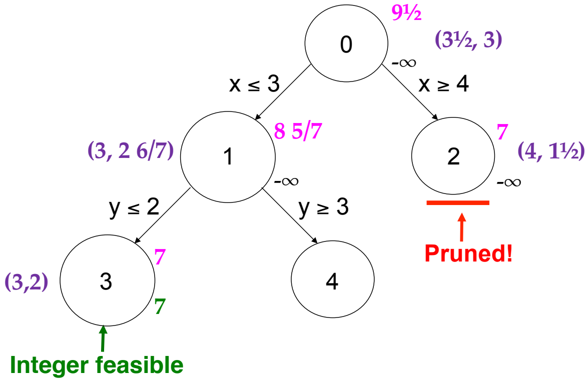

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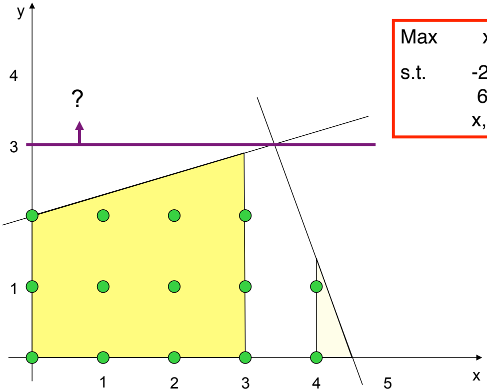

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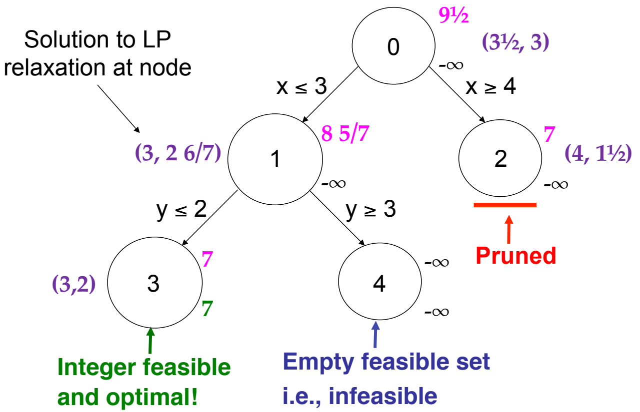

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Well-defined branch-and-bound algorithm

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- Partitioning the feasible region of an LP at a node
  - Simple branch-and-bound: Used in practise by solvers

    $$\begin{aligned} x_j &\leq \lfloor \hat{x}_j \rfloor & --> \text{Added to left node} \\ x_j &\geq \lceil \hat{x}_j \rceil & --> \text{Added to right node} \end{aligned}$$

    Need rule to decide which variable to branch on: *Full strong branching*, *Reliability branching*, *Pseudocost branching*: will discuss some of these later.
  - General branch-and-bound:

    $$\begin{aligned} \pi^\top x &\leq \pi_0 & --> \text{Added to left node} \\ \pi^\top x &\geq \pi_0 + 1 & --> \text{Added to right node} \end{aligned}$$

    where $\pi \in \mathbb{Z}^n$ is an integer vector and $\pi_0 \in \mathbb{Z}$ is an integer.

Branch-and-bound procedure

- The branch and bound algorithm was invented by Land and Doig in 1960.

Ailsa Land

Picture credit: Wikipedia

Alison Doig

Branch-and-bound procedure

- The branch and bound algorithm was invented by Land and Doig in 1960.
- Almost 60 years now, but there is very little theoretical analysis of the branch-and-bound algorithm!

What kind of questions we want to answer

- What is known: There are simple examples (i.e. knapsack IPs) with n variables that require $\mathcal{O}(2^n)$ nodes when using simple branch-and-bound tree. [Jeroslow (1974)], [Chvátal (1980)]

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- The simple examples above can be solved using a polynomial number of nodes using general branch-and-bounds [Yang, Boland, Savelsbergh (2021)]. Can we understand lower bounds for general branch-and-bound. (Preliminary results: [Dadush, Tiwari (2020)])

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- Can we understand and analyse properties of some well-known rules for partitioning mentioned above? Hopefully this will lead to better rules.

2

Main results

2.1
Branch-and-bound solves (a class of) random IPs in polynomial time

Random model of IPs

We consider the following model of random IPs:

$$\begin{array}{ccl} \max & c^\top x & c \sim \text{Uniform}([0,\ 1]^n) \\ \text{s.t.} & Ax \leq b & A \sim \text{Uniform}([0,\ 1]^{m\times n}) \\ & x \in \{0,1\}^n & , \end{array}$$

where $b = \beta \cdot n, \beta \in \left(0, \frac{1}{2}\right)^m$.

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- Analysis of gap and enumerative algorithms: [Lueker (1982)], [Goldberg, Marchetti-Spaccamela (1984)], [Beier, Vocking (2003)], [Dyer, Frieze (1989)]

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- Analysis of gap and enumerative algorithms: [Lueker (1982)], [Goldberg, Marchetti-Spaccamela (1984)], [Beier, Vocking (2003)], [Dyer, Frieze (1989)]
- General branching: [Pataki, Tural, Wong (2010)]

Result for random IPs

Theorem (D., Dubey, Molinaro)

Consider a branch-and-bound algorithm using the following rules:

- *Partitioning rule: Variable branching, where any fractional variable can be used to branch on.*
- *Node selection rule: Worst bound rule (Select a node with largest LP value as the next node to branch on.)*

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Consider $n \geq m + 1$ and a random instance of IP described previously. Then with probability at least $1 - \frac{1}{n} - 2^{-\alpha \bar{a}_2}$, the branch-and-bound algorithm applied to this random instance produces a tree with at most

$$n^{\bar{a}_1 \cdot (m + \alpha \log m)}$$

nodes for all $\alpha \leq \min\{30m, \frac{\log n}{\bar{a}_2}\}$, where $\bar{a}_1$ and $\bar{a}_2$ are constant depending only on m and β.

Result for random IPs

Simplified...

Theorem (D., Dubey, Molinaro)

Any branch-and-bound tree using the worst bound rule for node selection, solving the above problem has no more than $(n^{\mathcal{O}(m)})$ nodes with good probability.

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Nice follow up work [Borst, Dadush, Huiberts, Tiwari (2021)]

2.2
Lower bounds on size of general branch-and-bound tree

Lower bounds

- Remember when using general branch-and-bound, we are allowed to use general disjunctions:

$$\begin{array}{lcll} \pi^\top x & \leq & \pi_0 & - - > \text{Added to left node} \\ \pi^\top x & \geq & \pi_0 + 1 & - - > \text{Added to right node} \end{array}$$

  where π is an integer vector and π_0 is an integer.
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- Very recently, [Dadush,Tiwari (2020)] showed the following:

Theorem (Dadush, Tiwari)

Any (general) branch-and-bound tree that certifies the following instance is integer feasible requires at least $\frac{2^n}{n}$ leaf nodes:

$$C := \left\{ x \in \{0,1\}^n \,|\, \sum_{j\in S} x_j + \sum_{j \in [n]\setminus S} (1 - x_j) \geq \frac{1}{2} \; \forall S \subseteq [n] \right\}$$

Lets consider the cross-polytope again..

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- So $\frac{v+w}{2}$ satisfies all the constraints at the node. Equivalently, the node is non-empty.
- In order to prove integer-infeasiblilty of C, every leaf node should be infeasible. So from above, there must at at least 2^n leaf nodes!

More results –I: Hardness of some combinatorial problems

Theorem (D., Dubey, Molinaro)

Let n be a even positive integer. Any branch-and-bound tree, solving the following instance

$$\begin{aligned} \max \quad & \sum_{j \in [n]} x_j \\ \text{s.t.} \quad & \sum_{k \in S} x_j \leq \frac{n}{2} - 1, \ \forall S \subseteq [n], |S| = \frac{n}{2} \\ & x \in \{0,1\}^n \end{aligned}$$

requires at least $2^{\Omega(n)}$ nodes.

More results –II: Hardness for travelling saleman problem

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Theorem (D., Dubey, Molinaro)

Let P be LP relaxation of the usual travelling saleman problem formulation (with sub tour elimination) with n cities. There exist an objective function c, such that any branch-and-bound tree, solving the following instance

$$\begin{array}{ll} \max & c^\top x \\ \text{s.t.} & x \in P \\ & x \in \{0,1\}^{\frac{(n)(n-1)}{2}} \end{array}$$

requires at least $2^{\Omega(n)}$ nodes.

More results –III: Smoothened analysis not possible

Random family of instances:

$$Q := \sum_{i \in I} \left(1 + N\left(0, \tfrac{1}{20^2}\right)\right) x_i + \sum_{i \notin I} \left(1 - \left(1 + N\left(0, \tfrac{1}{20^2}\right)\right) x_i\right) \geq \frac{1.6n}{20}, \forall I \subseteq [n]$$

$$x \in [0, 1]^n,$$

where each occurrence of $N(0, \frac{1}{20^2})$ is independent.

Theorem (D., Dubey, Molinaro)

With probability at least $1 - \frac{2}{e^{n/2}}$ the polytope Q is integer-infeasible and every branch-and-bound tree proving its infeasibility has at least $2^{\Omega(n)}$ nodes.

2.3

Analysis of full strong branching rule for partitioning

Full strong branching

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- Let $\text{OPT} :=$ the optimal value of the LP at this node.
- Let $\text{OPT}_{j,0} :=$ the optimal value of the LP of the child node where we have the inequality $x_j \leq 0$.
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  Let $\text{OPT}_{j,1} :=$ the optimal value of the LP of the child node where we have the inequality $x_j \geq 1$.
- Let

$$\text{score}_j = \max\{|\text{OPT} - \text{OPT}_{j,1}|, \epsilon\} \cdot \max\{|\text{OPT} - \text{OPT}_{j,0}|, \epsilon\},$$

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- Let $\mathrm{OPT} :=$ the optimal value of the LP at this node.
- Let $\mathrm{OPT}_{j,0} :=$ the optimal value of the LP of the child node where we have the inequality $x_j \leq 0$.
  Let $\mathrm{OPT}_{j,1} :=$ the optimal value of the LP of the child node where we have the inequality $x_j \geq 1$.
- Let

  $$\mathrm{score}_j = \max\{|\mathrm{OPT} - \mathrm{OPT}_{j,1}|, \epsilon\} \cdot \max\{|\mathrm{OPT} - \mathrm{OPT}_{j,0}|, \epsilon\},$$

  where $\epsilon > 0$ is a small number related to machine precision.
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- Let $j^* := \text{argmax}_{j \in F}\,(\text{score}_j)$.
- Branch on j^*.

More on full strong branching

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- However, this rule is not used in practise, because we need to solve $2|F|$ LPs just to decide one branching decision.
- Recently there has been many attempts made to mimic full strong branching using machine learning. [Alvarez, Louveaux, and Wehenkel (2017)], [Gasse, Chetelat, Ferroni, Charlin, Lodi (2019)], [Khalil, Le Bodic, Song, Nemhauser, Dilkina (2016)], [Nair et al. (2020)]

Some questions..

- How large is the tree produced by strong-branching in comparison to the smallest possible branch-and-bound tree for a given instance? Answering this question may lead us to finding better rules.

Introduction

Main results

Random IPs

Lower bounds on size of general branch-and-bound tree

Analysis of full strong branching rule for partitioning

Strong branching applied to specific problems

A computational evaluation of strong branching

Proof Outlines

Some questions..

- How large is the tree produced by strong-branching in comparison to the smallest possible branch-and-bound tree for a given instance? Answering this question may lead us to finding better rules.
- A more refined questions is the following: it would be useful to understand the performance of strong-branching vis-á-vis different classes of instances.

2.3.1
Strong branching applied to specific problems

Vertex cover

Definition (Vertex cover)

The vertex cover problem over a graph $G = (V, E)$ can be expressed as the following integer program (IP)

$$\begin{array}{lll} \min & \sum_{v \in V} x_v & \\ \text{s.t.} & x_u + x_v \geq 1, & uv \in E \\ & x_v \in \{0, 1\}, & v \in V \end{array}$$

Given an instance I of this IP, we let OPT(I) denote optimal objective function value and $\mathrm{OPT}_L(I)$ be the optimal objective function of the LP relaxation (i.e. when the variable constraints are $x_v \in [0, 1]$). Then let

$$\Gamma(I) := \mathrm{OPT}(I) - \mathrm{OPT}_L(I).$$

Strong branching works well for vertex cover

Theorem (D., Dubey. Molinaro, Shah)

Let I be any instance of vertex cover on n nodes. Assume we break ties within the worst-bound rule for node selection rule by selecting a node with the largest depth.

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$$|\mathcal{T}_S(I)| \leq 2^{2\Gamma(I)+1} + \mathcal{O}(n).$$

Strong branching does not work well for other IP models

$$\left\{(x, y) \in \{0,1\}^n \times \{0,1\}^n \,|\, y_i \leq 2x_i, y_i \leq 2 - 2x_i, \forall i \in [n], \sum_{i=1}^{n} y_i = 1\right\}$$

Theorem

The smallest branch-and-bound tree that shows that the above set is integer infeasible requires no more than $4n + 1$ nodes. On the other hand, strong branching requires at least 2^n nodes.

2.3.2

A computational evaluation of strong branching

Optimal branch-and-bound tree

Optimal branch-and-bound tree

- It is not possible to analyse different problems analytically.

Optimal branch-and-bound tree

- It is not possible to analyse different problems analytically.
- So we came up with a Dynamic programming algorithm to compute the optimal branch-and-bound tree.

Theorem (D., Dubey, Molinaro, Shah)

There is a DP algorithm with running time $\mathrm{poly}(data) \cdot 3^{O(n)}$ *time to compute an optimal branch-and-bound tree for any binary MILP instance defined on n binary variables.*

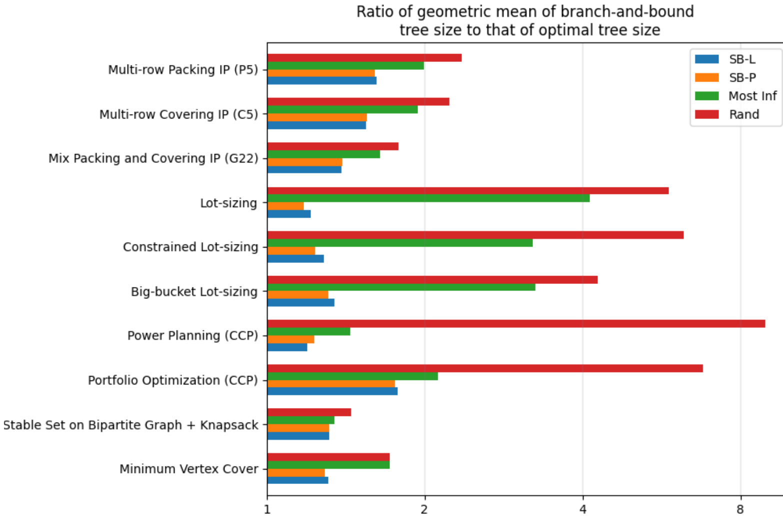

Figure: Ratio of geometric mean of branch-and-bound tree sizes to geometric mean of optimal tree sizes over all instances of a problem for various branching strategies. “Rand" stands for random, “Most Inf" stands for most infeasible, “SB-P" stands for strong-branching with product score function, and “SB-L" stands for strong-branching with linear score function.

3

Proof Outlines

3.1
Random IPs Theorem

Reminder...

$$
\begin{array}{lll}
\max & c^\top x & c \sim \text{Uniform}([0,\ 1]^n) \\
\text{s.t.} & Ax \le b & A \sim \text{Uniform}([0,\ 1]^{m\times n}) \\
 & x \in \{0,1\}^n & ,
\end{array}
$$

where $b = \beta \cdot n, \beta \in \left(0, \frac{1}{2}\right)^m$.

Theorem (D., Dubey, Molinaro)

Any branch-and-bound tree using the worst bound rule for node selection, solving the above problem has no more than $(n^{\mathcal{O}(m)})$ nodes (with good probability).

Proof Sketch

$$\Delta(x) = \sum_{j \in [n]} \underbrace{(c_j - \langle \lambda^*, A^j \rangle)}_{\text{reduced cost}} \cdot (\underbrace{x_j^*}_{\text{LP Opt.}} - x_j),$$

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1. The number of internal nodes in a branch-and-bound tree is at most n times the number of good integer solutions G.
2. The number of good integer solutions is at most $n^{\mathcal{O}(m)}$ (with good probability).

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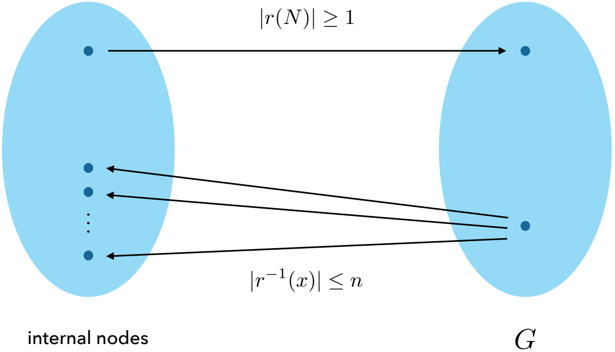

Picture credit: Yatharth Dubey

3.2

Optimal branch-and-bound tree

Dynamic programming algorithm

$$\max_{x \in P \cap \{0,1\}^n} c^\top x$$

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Algorithm 1 Computing Optimal Branch-and-bound Tree

Phase-1: Pruning by Infeasibility or Bound

Solve $\max_{x \in P \cap \{0,1\}^n} \langle c, x \rangle$; let x^* be the solution
Initialise: $\mathcal{S} \leftarrow \mathcal{F}$
for F in $\mathcal{S}$ **do**
  Solve $\max_{x \in F \cap P} \langle c, x \rangle$; let x^*_F be the optimal solution ($x^*_F = \emptyset$ if LP is infeasible)
  if $x^*_F = \emptyset$ **or** $\langle c, x^*_F \rangle \leq \langle c, x^* \rangle$ **then**
    $\overline{\mathrm{OPT}}(F) \leftarrow 0$
    $\mathcal{S} \leftarrow \mathcal{S} \setminus \{F\}$
  end if
end for

Phase-2: Recursive bottom-up computation

Sort $\mathcal{S}$ in order of increasing dimension
for F in $\mathcal{S}$ **do**
  $\overline{\mathrm{OPT}}(F) \leftarrow 1 + \min_j (\overline{\mathrm{OPT}}(F_{j,0}) + \overline{\mathrm{OPT}}(F_{j,1}))$
end for
return $\overline{\mathrm{OPT}}([0,1]^n)$

Thank You.

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