

Operations Research II: Algorithms

Branch & Bound and Heuristic Algorithms

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Introduction

- ▶ In some cases, variables must only take **integer values**.
- ▶ The subject of formulating and solving models with integer variables is **Integer Programming** (IP).
 - ▶ An IP is typically a linear IP (LIP).
 - ▶ If the objective function or any functional constraint is nonlinear, it is a nonlinear IP (NLIP).
 - ▶ We will focus on linear IP in this course.

Introduction

- ▶ The **branch-and-bound algorithm** finds an **optimal** solution for any IP.
 - ▶ It “decomposes” an IP to multiple LPs, solve all the LPs, and compares those outcomes to reach a conclusion.
 - ▶ Each LP is solved separately (with the simplex method or other ways).
 - ▶ In general, the process may take a very long time.
- ▶ As finding an optimal solution for an IP may be too time-consuming, we often look for a **near-optimal** feasible solution instead in practice.
 - ▶ An algorithm that generates a **feasible** solution in a **short time** is called a **heuristic algorithm**.
 - ▶ **Hopefully** it is **near-optimal**.
 - ▶ A good heuristic algorithm does not always work, but it works for most of the time.

Road map

- ▶ **Linear relaxation.**
- ▶ The branch-and-bound algorithm.
- ▶ Solving the knapsack problem.
- ▶ Heuristic algorithms.

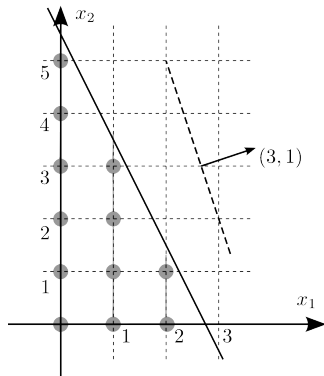
Solving an IP

- ▶ Suppose we are given an IP, how may we solve it?
- ▶ The simplex method does not work!
 - ▶ The feasible region is not “a region”.
 - ▶ It is **discrete**.
 - ▶ There is no way to “move along edges”.
- ▶ But all we know is how to solve LPs. How about solving a **linear relaxation** first?

Definition 1 (Linear relaxation)

For a given IP, its linear relaxation is the resulting LP after removing all the integer constraints.

$$\begin{array}{ll}\max & 3x_1 + x_2 \\ \text{s.t.} & 4x_1 + 2x_2 \leq 11 \\ & x_i \in \mathbb{Z}_+ \quad \forall i = 1, 2.\end{array}$$



Linear relaxation

- What is the linear relaxation of

$$\begin{array}{llll} \max & x_1 & + & x_2 \\ \text{s.t.} & x_1 & + & 3x_2 \leq 10 \\ & 2x_1 & - & x_2 \geq 5 \\ & x_i \in \mathbb{Z}_+ & \forall i = 1, 2? \end{array}$$

- \mathbb{Z} is the set of all integers. \mathbb{Z}_+ is the set of all nonnegative integers.
- The linear relaxation is

$$\begin{array}{llll} \max & x_1 & + & x_2 \\ \text{s.t.} & x_1 & + & 3x_2 \leq 10 \\ & 2x_1 & - & x_2 \geq 5 \\ & x_i \geq 0 & \forall i = 1, 2. \end{array}$$

Linear relaxation

- For the knapsack problem

$$\begin{array}{ll} \max & 16x_1 + 22x_2 + 12x_3 + 8x_4 \\ \text{s.t.} & 5x_1 + 7x_2 + 4x_3 + 3x_4 \leq 10 \\ & x_i \in \{0, 1\} \quad \forall i = 1, \dots, 4, \end{array}$$

the linear relaxation is

$$\begin{array}{ll} \max & 16x_1 + 22x_2 + 12x_3 + 8x_4 \\ \text{s.t.} & 5x_1 + 7x_2 + 4x_3 + 3x_4 \leq 10 \\ & x_i \in [0, 1] \quad \forall i = 1, \dots, 4, \end{array}$$

- $x_i \in [0, 1]$ is equivalent to $x_i \geq 0$ and $x_i \leq 1$.

Linear relaxation provides a bound

- ▶ For a **minimization** IP, its linear relaxation provides a **lower bound**.

Proposition 1

Let z^ and z' be the objective values associated to optimal solutions of a minimization IP and its linear relaxation, respectively, then $z' \leq z^*$.*

Proof. They have the same objective function. However, the linear relaxation's feasible region is (weakly) larger than that of the IP. □

- ▶ For a **maximization** IP, linear relaxation provides an **upper bound**.

Linear relaxation may solve the IP

- ▶ If we are lucky, the linear relaxation may be infeasible or unbounded.
 - ▶ The IP is then infeasible or unbounded.
- ▶ If we are lucky, an optimal solution to the linear relaxation may be **feasible** to the original IP. When this happens, the IP is solved:

Proposition 2

Let x' be an optimal solutions to the linear relaxation of an IP. If x' is feasible to the IP, it is optimal to the IP.

Proof. Suppose x' is not optimal to the IP, there must be another feasible solution x'' that is better. However, as x'' is feasible to the IP, it is also feasible to the linear relaxation, which implies that x' cannot be optimal to the linear relaxation. □

- ▶ What if we are **unlucky**?

Rounding a fractional solution

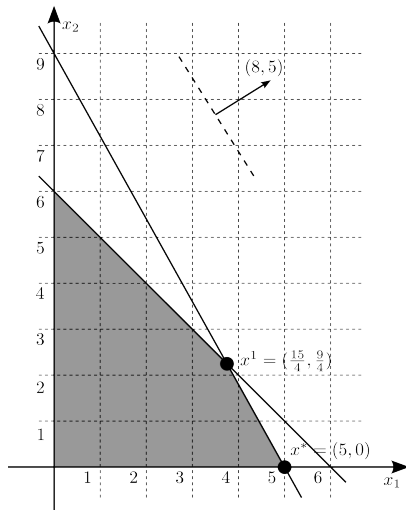
- ▶ Suppose we solve a linear relaxation with an LR-optimal solution x' .
 - ▶ “LR-optimal” means x' is optimal to the linear relaxation.
- ▶ x' , however, has at least one variable violating the integer constraint in the original IP.
- ▶ We may choose to **round** the variable.
 - ▶ Round up or down?
 - ▶ Is the resulting solution always feasible?
 - ▶ Will the resulting solution be close to an IP-optimal solution x^* ?

Rounding a fractional solution

- Consider the following IP

$$\begin{array}{ll}\max & 8x_1 + 5x_2 \\ \text{s.t.} & x_1 + x_2 \leq 6 \\ & 9x_1 + 5x_2 \leq 45 \\ & x_i \in \mathbb{Z}_+ \quad \forall i = 1, 2.\end{array}$$

- $x^* = (5, 0)$ is IP-optimal.
- But $x^1 = (\frac{15}{4}, \frac{9}{4})$ is LR-optimal!
 - Rounding up any variable results in infeasible solutions.
 - None of the four grid points around x^1 is optimal.
- We need a way that guarantees to find an optimal solution.

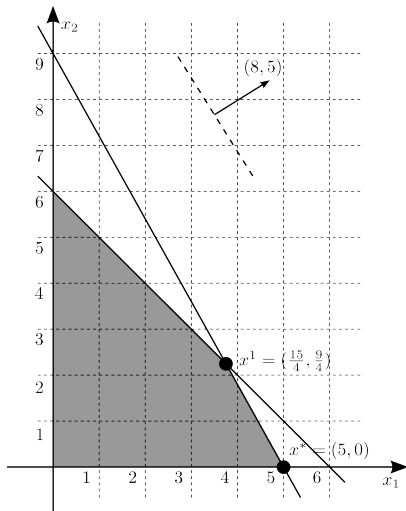


Road map

- ▶ Linear relaxation.
- ▶ **The branch-and-bound algorithm.**
- ▶ Solving the knapsack problem.
- ▶ Heuristic algorithms.

Rounding a fractional solution

- ▶ $x^1 = (\frac{15}{4}, \frac{9}{4})$ is LR-optimal.
 - ▶ Rounding up or down x_1 (i.e., adding $x_1 = 4$ or $x_1 = 3$ into the program) both **fail** to find the optimal solution.
 - ▶ Because we eliminate too many feasible points!
 - ▶ Instead of adding equalities, we should add **inequalities**.
- ▶ What will happen if we add $x_1 \geq 4$ or $x_1 \leq 3$ into the program?
- ▶ We will **branch** this problem into two problems, one with an additional constraint.



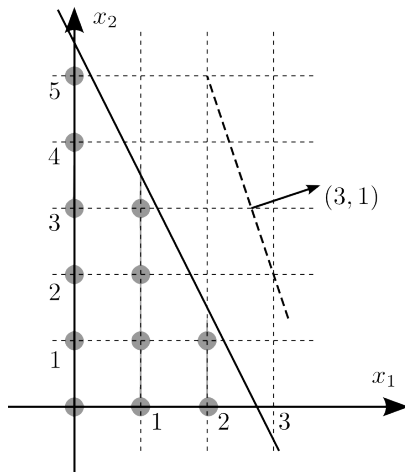
Rounding a fractional solution

- ▶ So when we solve the linear relaxation and find any variable violating an integer constraint, we will **branch** this problem into two problems, one with an additional constraint.
- ▶ The two new programs are still linear programs.
- ▶ Once we solved them:
 - ▶ If their LR-optimal solutions are both IP-feasible, compare them and choose the better one.
 - ▶ If any of them results in a variable violating the integer constraint, **branch** on that variable **recursively**.
 - ▶ Eventually compare all the IP-feasible solutions we obtain.

Example

- Let's illustrate the branch-and-bound algorithm with the following example:

$$\begin{array}{ll}\max & 3x_1 + x_2 \\(P_0) \quad \text{s.t.} & 4x_1 + 2x_2 \leq 11 \\ & x_i \in \mathbb{Z}_+ \quad \forall i = 1, 2.\end{array}$$

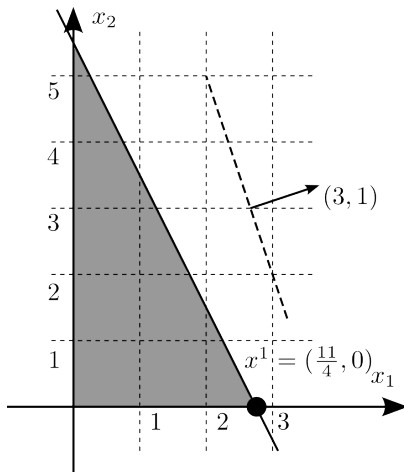


Subproblem 1

- First we solve the linear relaxation:

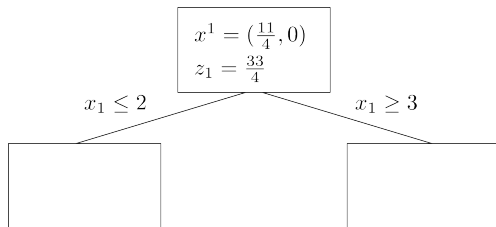
$$\begin{array}{ll}\max & 3x_1 + x_2 \\(P_1) \quad \text{s.t.} & 4x_1 + 2x_2 \leq 11 \\ & x_i \geq 0 \quad \forall i = 1, 2.\end{array}$$

- The optimal solution is $x^1 = (\frac{11}{4}, 0)$.
- So we need to branch on x_1 .



Branching tree

- ▶ The branch and bound algorithm produces a **branching tree**.
 - ▶ Each node represents a subproblem (which is an LP).
 - ▶ Each time we branch on a variable, we create two child nodes.

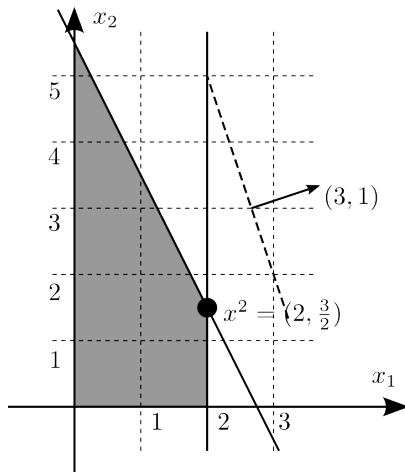


Subproblem 2

- ▶ When we add $x_1 \leq 2$:

$$\begin{array}{llllll} \max & 3x_1 & + & x_2 & & \\ (P_2) \quad \text{s.t.} & 4x_1 & + & 2x_2 & \leq & 11 \\ & x_1 & & & \leq & 2 \\ & x_i & \geq 0 & \forall i = 1, 2. & & \end{array}$$

- ▶ An (P_2) -optimal solution is $x^2 = (2, \frac{3}{2})$.
 - ▶ So later we need to branch on x_2 .
- ▶ Before that, let's solve (P_3) .

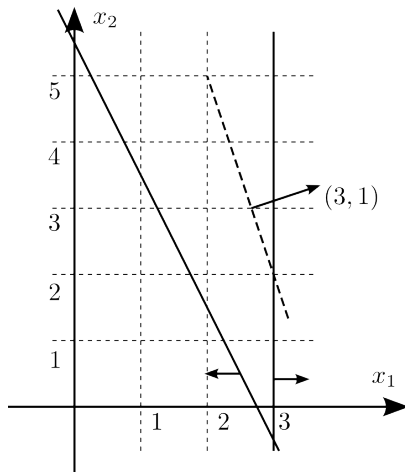


Subproblem 3

- When we add $x_1 \geq 3$:

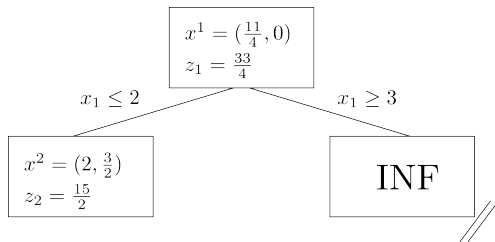
$$(P_3) \quad \begin{array}{llll} \max & 3x_1 & + & x_2 \\ \text{s.t.} & 4x_1 & + & 2x_2 \leq 11 \\ & x_1 & & \geq 3 \\ & x_i \geq 0 & \forall i = 1, 2. \end{array}$$

- The problem is infeasible!
- This node is “dead” and does not produce any candidate solution.



Branching tree

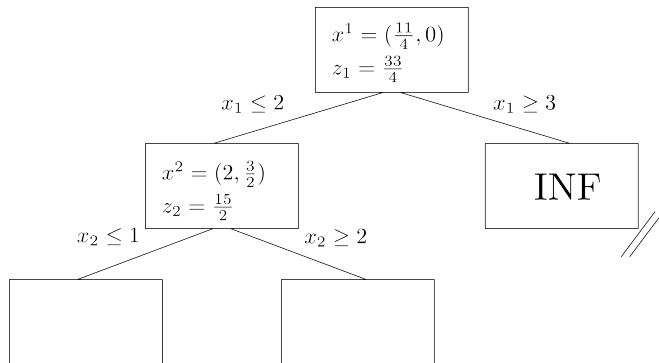
- ▶ The current progress can be summarized in the branching tree.



- ▶ Note that $z_2 = 7.5 < 8.25 = z_1$.
- ▶ In general, when we branch to the next level, the objective value associated with a subproblem-optimal solution will **always** be weakly **lower** (for a maximization problem). Why?

Branching tree

- As $x_2 = \frac{3}{2}$ in x^2 , we will branch subproblem 2 on x_2 .

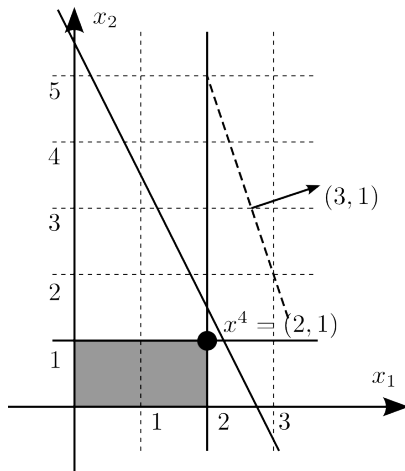


Subproblem 4

- When we add $x_2 \leq 1$:

$$\begin{array}{llllll} \max & 3x_1 & + & x_2 & & \\ \text{s.t.} & 4x_1 & + & 2x_2 & \leq & 11 \\ (P_4) & x_1 & & & \leq & 2 \\ & & & x_2 & \leq & 1 \\ & x_i \geq 0 & \forall i = 1, 2. \end{array}$$

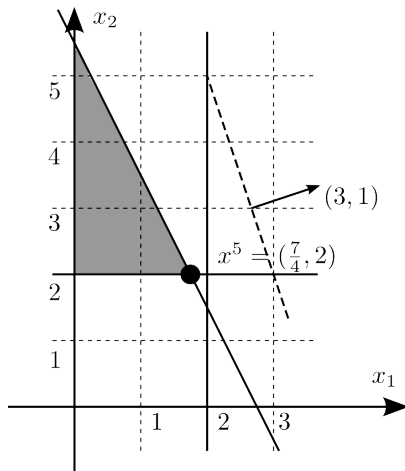
- Note that we add $x_2 \leq 1$ into subproblem 2, so $x_1 \leq 2$ is still there.



Subproblem 5

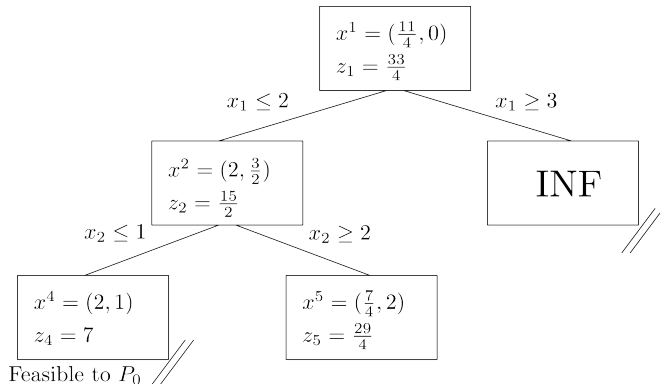
► When we add $x_2 \geq 2$:

$$\begin{array}{llllll} \max & 3x_1 & + & x_2 & & \\ \text{s.t.} & 4x_1 & + & 2x_2 & \leq & 11 \\ (P_5) & x_1 & & & \leq & 2 \\ & & & x_2 & \geq & 2 \\ & x_i & \geq & 0 & \forall i = & 1, 2. \end{array}$$



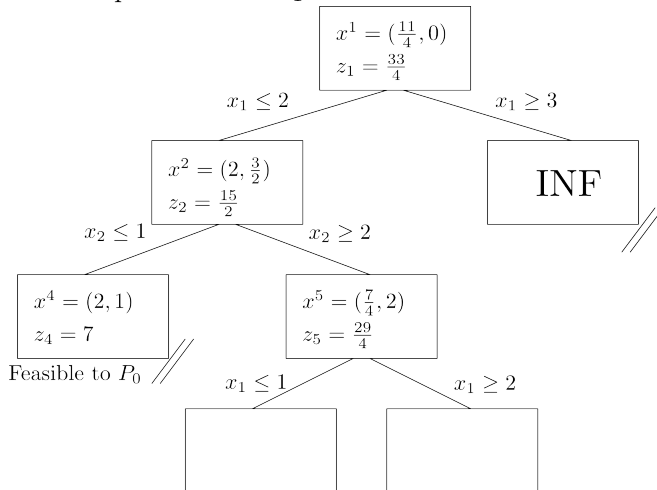
Branching tree

- ▶ x^4 satisfies all the integer constraints.
- ▶ It is IP-feasible and thus a **candidate solution** to the original IP.
- ▶ But branching subproblem 5 may result in a better solution.



Branching tree

- Let's branch subproblem 5 on x_1 .

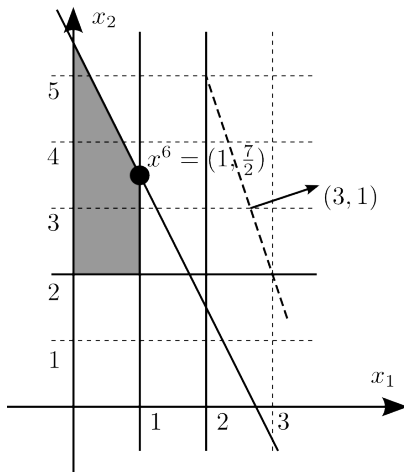


Subproblem 6

- When we add $x_1 \leq 1$:

$$\begin{array}{llll} \max & 3x_1 & + & x_2 \\ \text{s.t.} & 4x_1 & + & 2x_2 \leq 11 \\ (P_6) & x_1 & & \leq 2 \\ & & x_2 & \geq 2 \\ & x_1 & & \leq 1 \\ & x_i \geq 0 & \forall i = 1, 2. \end{array}$$

- $x^6 = (1, \frac{7}{2})$. We may need to branch on x_2 again. However, let's solve subproblem 7 first.

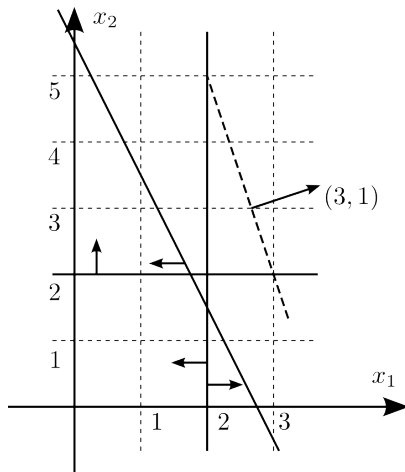


Subproblem 7

- When we add $x_1 \geq 2$:

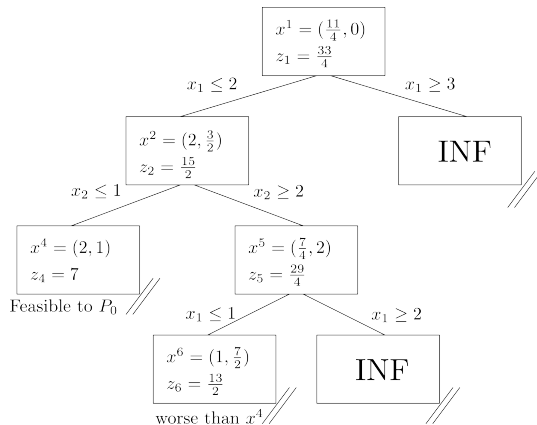
$$\begin{array}{llllll} \max & 3x_1 & + & x_2 & & \\ \text{s.t.} & 4x_1 & + & 2x_2 & \leq & 11 \\ (P_7) & x_1 & & & \leq & 2 \\ & & & x_2 & \geq & 2 \\ & x_1 & & & \geq & 2 \\ & x_i \geq 0 & \forall i = 1, 2. & & & \end{array}$$

- The problem is infeasible.
► The node is “dead”.



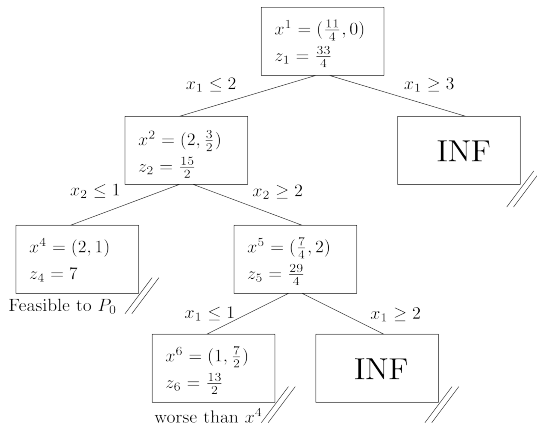
Branching tree

- ▶ The only “alive” node is subproblem 6, with x_2 fractional.
- ▶ Before we branch subproblem 6, consider the following:



Bounding

- ▶ $z_6 = \frac{13}{2}$. If we branch (P_6) , all the candidate solutions (if any) under it will be (weakly) **worse** than $\frac{13}{2}$.
- ▶ However, $\frac{13}{2} < 7 = z_4$, and x_4 is already a candidate!
- ▶ So there is no need to branch (P_6) . This is the “**bounding**” situation in the branch-and-bound algorithm.
 - ▶ This allows us to solve fewer subproblems.



Summary

- ▶ In running the branch-and-bound algorithm, we maintain a tree.
- ▶ If a subproblem-optimal solution is IP-feasible, set it to the candidate solution if it is currently the best among all IP-feasible solutions. Stop branching this node.
- ▶ If a subproblem is infeasible, stop branching this node.
- ▶ If a subproblem-optimal solution is not IP-feasible:
 - ▶ If it is better than the current candidate solution, branch.
 - ▶ Otherwise, stop branching.

Another example

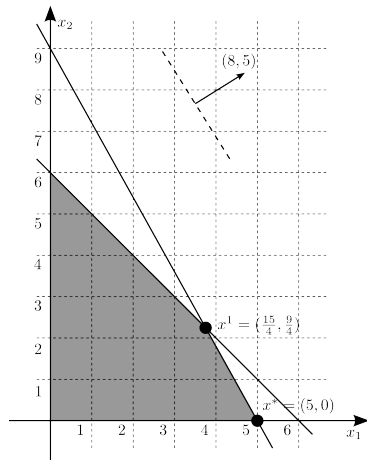
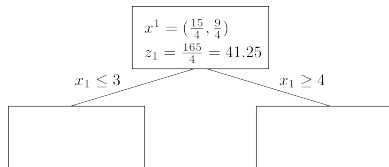
- Now let's go back to our motivating example:

$$\begin{array}{ll} \max & 8x_1 + 5x_2 \\ \text{s.t.} & x_1 + x_2 \leq 6 \\ & 9x_1 + 5x_2 \leq 45 \\ & x_i \in \mathbb{Z}_+ \quad \forall i = 1, 2. \end{array} \quad (Q_0)$$

- Let's solve it with the branch-and-bound algorithm.

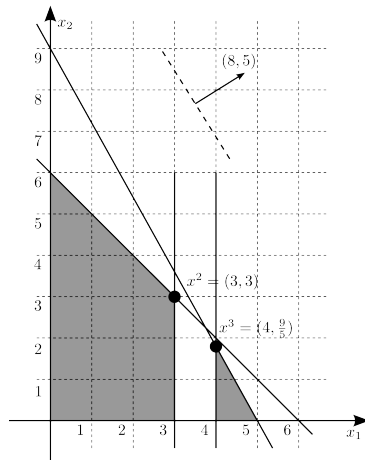
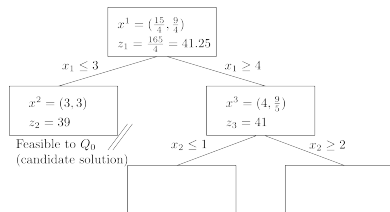
Subproblem 1

- ▶ $x^1 = (\frac{15}{4}, \frac{9}{4})$.
- ▶ We may branch on either variable. Let's branch on x_1 .



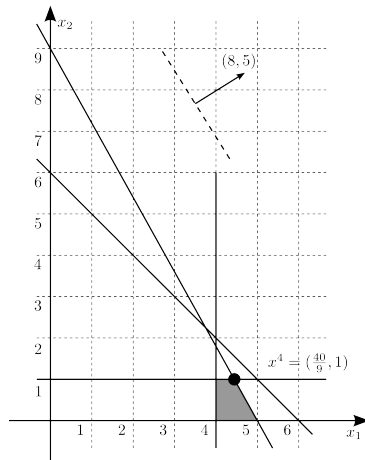
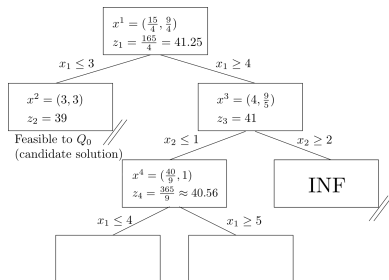
Subproblems 2 and 3

- ▶ Subproblem 2 generates a candidate solution.
- ▶ $x^3 = (4, \frac{9}{5})$. As $z_3 = 41 > z_2 = 39$, we should branch subproblem 3.



Subproblems 4 and 5

- ▶ $x^4 = (\frac{40}{9}, 1)$. As $z_4 = 40.56 > z_2 = 39$, we should branch subproblem 4.
- ▶ Subproblem 5 is infeasible.

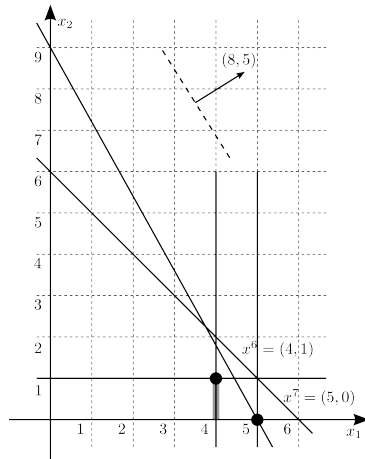
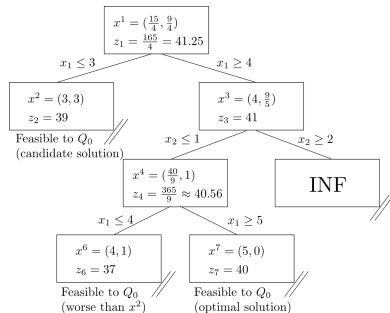


Subproblems 6 and 7

► $x^6 = (4, 1)$ but $z_6 = 37 < 39 = z_2$.

► $x^7 = (5, 0)$ and $z_7 = 40 > 39 = z_2$.

As it is also the last node, x^7 is an optimal solution.



Remarks

- ▶ To select a node to branch:
 - ▶ Among all alive nodes, there are many different ways of selecting a node to branch.
 - ▶ One common approach is to branch the node with the highest objective value (for a maximization problem). Why?
 - ▶ Another popular approach is “once a node is branched, all its descendants are branched before any nondescendant. Why?
- ▶ Choosing a variable to branch on is also a challenging task.
- ▶ The branch-and-bound algorithm guarantees to find an optimal solution, if one exists.
- ▶ However, it is an **exponential-time** algorithm.
 - ▶ Roughly speaking, with n integer variables, the number of subproblems solved is approximately proportional to 2^n .

Road map

- ▶ Linear relaxation.
- ▶ The branch-and-bound algorithm.
- ▶ **Solving the knapsack problem.**
- ▶ Heuristic algorithms.

The knapsack problem

- ▶ We start our illustration with the classic **knapsack** problem.
- ▶ There are five items to select:

Item	1	2	3	4	5
Value (\$)	2	3	4	1	3
Weight (kg)	4	5	3	1	4

- ▶ The knapsack capacity is 11 kg.
- ▶ We maximize the total value without exceeding the knapsack capacity.

The knapsack problem

- ▶ The complete formulation:

$$\begin{array}{ll}\max & 2x_1 + 3x_2 + 4x_3 + x_4 + 3x_5 \\ \text{s.t.} & 4x_1 + 5x_2 + 3x_3 + x_4 + 4x_5 \leq 11 \\ & x_i \in \{0, 1\} \quad \forall i = 1, \dots, 5.\end{array}$$

- ▶ Let's solve the knapsack problem with the branch-and-bound algorithm.

Solving the linear relaxation

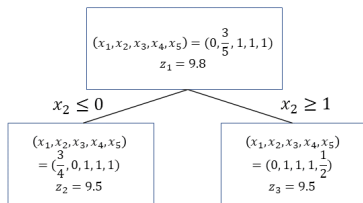
- ▶ The first step is always to solve the linear relaxation:

$$\begin{array}{ll}\max & 2x_1 + 3x_2 + 4x_3 + x_4 + 3x_5 \\ \text{s.t.} & 4x_1 + 5x_2 + 3x_3 + x_4 + 4x_5 \leq 11 \\ & x_i \in [0, 1] \quad \forall i = 1, \dots, 5.\end{array}$$

- ▶ A very intuitive way works:
 - ▶ Sort all items in the **descending order of** $\frac{v_i}{w_i}$, where v_i and w_i are the value and weight of item i , respectively.
 - ▶ Select items one by one according to the order until the knapsack is full. Note that the last item may be **partially** selected.
- ▶ The five ratios are $\frac{2}{4}$, $\frac{3}{5}$, $\frac{4}{3}$, $\frac{1}{1}$, and $\frac{3}{4}$. The order is item 3, item 4, item 5, item 2, and lastly item 1.
 - ▶ An optimal solution to the linear relaxation is $(0, \frac{3}{5}, 1, 1, 1)$.

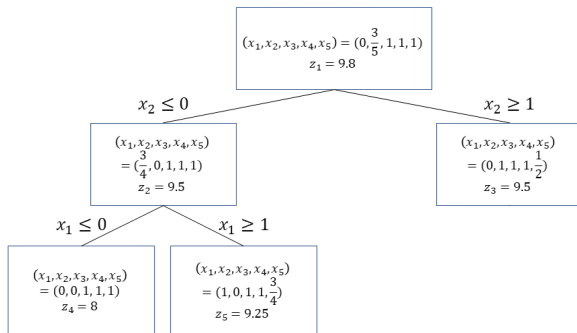
Subproblems 1, 2, and 3

- ▶ We solve the linear relaxation and get $x^1 = (0, 0.6, 1, 1, 1)$ with objective value 9.8.
- ▶ We branch on x_2 .
- ▶ With $x_2 \leq 0$: $x^2 = (0.75, 0, 1, 1, 1)$ and $z_2 = 9.5$.
 - ▶ We set $x_2 = 0$ and then apply the sorting idea on the remaining.
- ▶ With $x_2 \geq 1$: $x^3 = (0, 1, 1, 1, 0.5)$ and $z_3 = 9.5$.
 - ▶ We set $x_2 = 1$ and then apply the sorting idea on the remaining four variables and **residual capacity** 6.



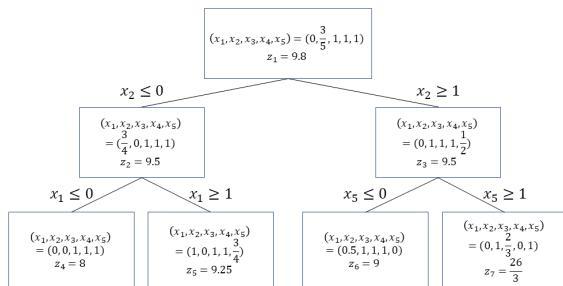
Subproblems 4 and 5

- ▶ We branch the node for x^2 .
- ▶ With $x_2 \leq 0$ and $x_1 \leq 0$:
 $x^4 = (0, 0, 1, 1, 1)$
and $z_4 = 8$. x^4 is the first candidate solution.
- ▶ With $x_2 \leq 0$ and $x_1 \geq 1$:
 $x^5 = (1, 0, 1, 1, \frac{3}{4})$
with $z_5 = 9.25$.



Subproblems 6 and 7

- ▶ We branch the node for x^3 .
- ▶ With $x_2 \geq 1$ and $x_5 \leq 0$:
 $x^6 = (0.5, 1, 1, 1, 0)$
 and $z_6 = 9$.
- ▶ With $x_2 \geq 1$ and $x_5 \geq 1$:
 $x^7 = (0, 1, \frac{2}{3}, 0, 1)$
 and $z_7 = \frac{26}{3}$.



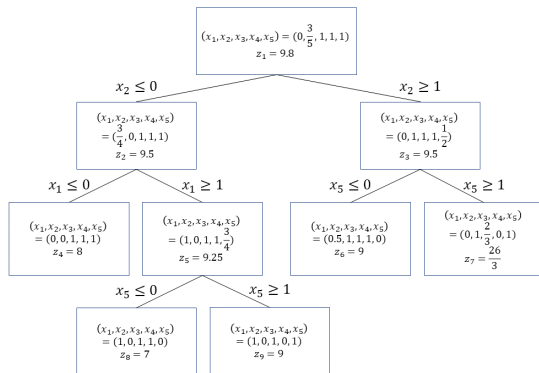
Subproblems 8 and 9

- ▶ With $x_2 \leq 0$,
 $x_1 \geq 1$, $x_5 \leq 0$:
 $x^8 = (1, 0, 1, 1, 0)$
and $z_8 = 7$.

- ▶ With $x_2 \leq 0$,
 $x_1 \geq 1$, $x_5 \geq 1$:
 $x^9 = (1, 0, 1, 0, 1)$
and $z_9 = 9$. x^9
becomes the
currently best
candidate.

- ▶ No need to branch
the nodes for x^6
and x^7 (why?).

- ▶ x^9 is optimal.



Remarks

- ▶ The major process is still branch and bound.
- ▶ The only unique thing is that we have a **special way** to solve the linear relaxation of the knapsack problem.
- ▶ In other words, we may **customize** the branch-and-bound algorithm for each specific type of IP.

Road map

- ▶ Linear relaxation.
- ▶ The branch-and-bound algorithm.
- ▶ Solving the knapsack problem.
- ▶ **Heuristic algorithms.**

The knapsack problem

- ▶ Recall our knapsack example with five items to select and a knapsack with capacity 11 kg:

Item	1	2	3	4	5
Value (\$)	2	3	4	1	3
Weight (kg)	4	5	3	1	4

- ▶ The formulation is

$$\begin{array}{ll}\max & 2x_1 + 3x_2 + 4x_3 + x_4 + 3x_5 \\ \text{s.t.} & 4x_1 + 5x_2 + 3x_3 + x_4 + 4x_5 \leq 11 \\ & x_i \in \{0, 1\} \quad \forall i = 1, \dots, 5.\end{array}$$

- ▶ An optimal solution $x^* = (1, 0, 1, 0, 1)$ may be found by branch and bound. The associated objective value is $z^* = 9$.

Exact and heuristic algorithms

- ▶ Unfortunately, the knapsack problem is **NP-hard**.
 - ▶ Roughly speaking, most researchers in the world believe that there is no efficient (i.e., polynomial-time) **exact algorithm** that finds an optimal solution.
 - ▶ Branch and bound may need too much time to solve an instance of a knapsack problem with thousands of variables.
- ▶ In this case, people look for good **heuristic algorithms**.
 - ▶ The algorithm reports a solution in a short (i.e., **polynomial**) time.
 - ▶ The reported solution is **near-optimal**.

A greedy algorithm

- ▶ Our intuitive **greedy** algorithm may serve as a good one.
 - ▶ First, we sort all items by their value-to-weight ratios from large to small.
 - ▶ Along the order, we then try to put each item into the knapsack. If possible, do it; otherwise, throw it away.
 - ▶ We stop when all items are tried once.
- ▶ Recall our example:

Item	1	2	3	4	5
Value (\$)	2	3	4	1	3
Weight (kg)	4	5	3	1	4

- ▶ The order: items 3, 4, 5, 2, and 1.
- ▶ Items 3, 4, and 5 are okay. Items 2 and 1 are not.
- ▶ The reported solution is $x^{\text{ALG}} = (0, 0, 1, 1, 1)$. The associated objective value is $z^{\text{ALG}} = 8$.

Optimality gap

- ▶ The reported solution is $x^{\text{ALG}} = (0, 0, 1, 1, 1)$ with $z^{\text{ALG}} = 8$.
- ▶ An optimal solution is $x^* = (1, 0, 1, 0, 1)$ with $z^* = 9$.
- ▶ A natural measurement of the quality/performance of a reported solution is the **optimality gap**:

- ▶ The **absolute error** is

$$z^* - z^{\text{ALG}} = 1.$$

- ▶ The **percentage error** is

$$\frac{z^* - z^{\text{ALG}}}{z^*} = 11.1\%.$$

Performance evaluation

- ▶ To test the **average-case performance** of a heuristic algorithm:
 - ▶ **Small-scale random instances** are generated.
 - ▶ Each instance is solved by the algorithm and an exact one.
 - ▶ All the **percentage errors** are averaged.
 - ▶ The smaller the average percentage error, the better the algorithm.
- ▶ Moreover:
 - ▶ **Large-scale** random instances are generated.
 - ▶ Each instance is solved by the algorithm.
 - ▶ An **upper bound** of the objective value of an optimal solution (for a maximization problem) is obtained (e.g., by linear relaxation).
 - ▶ The smaller the average percentage error (which is an **upper bound** for that calculated with an optimal solution), the better the algorithm.
- ▶ In the above example:
 - ▶ Linear relaxation gives $x^{\text{LR}} = (0, 0.6, 1, 1, 1)$ with $z^{\text{LR}} = 9.8$.
 - ▶ The errors are $z^{\text{LR}} - z^{\text{ALG}} = 1.8$ and $\frac{z^{\text{LR}} - z^{\text{ALG}}}{z^{\text{LR}}} = 18.4\%$.

Remarks

- ▶ Some people refer to the gap between a reported solution and an upper bound (rather than an optimal solution) as the optimality gap.
- ▶ Some people analyze the problem and heuristic algorithm to prove a **worst-case performance guarantee**.
 - ▶ Fascinating but difficult.
- ▶ Designing (or proposing) a heuristic algorithm is simple. **Evaluation** and **analysis** are hard.
- ▶ Thanks to integer programming, branch and bound, and linear relaxation:
 - ▶ We may generate an **optimal solution**.
 - ▶ We may use an optimal solution or its **upper/lower bound** as a **benchmark** to evaluate a feasible solution.
 - ▶ We may thus evaluate a heuristic algorithm.