# ORIE 3310/5310 : Optimization II

1. Linear and Integer Programming

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# Linear Programming Review (22/1/2024)

• A vector  $x \in \mathbb{R}^n$  is an array of real numbers:

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$
 or  $x^T = [x_1, x_2, \dots, x_n].$ 

• The inner (or, "dot") product of two vectors  $x, y \in \mathbb{R}^n$  is:

$$x^T y = \sum_{i=1}^n x_i y_i. \qquad \leftarrow \text{this is a number}$$

• A  $m \times n$  matrix A is an array of real numbers  $a_{ij}$ :

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{bmatrix}$$

We say  $A \in \mathbb{R}^{m \times n}$  (number of rows first, columns second)

• Given a matrix  $A \in \mathbb{R}^{m \times n}$  and a vector  $x \in \mathbb{R}^n$ :

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \dots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{bmatrix}, \qquad x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

• The matrix-vector product of A and x is:

$$Ax = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^n a_{1i} x_i \\ \sum_{i=1}^n a_{2i} x_i \\ \vdots \\ \sum_{i=1}^n a_{mi} x_i \end{bmatrix}$$

- The number of columns of A must equal the number of rows of x.
- ullet The number of rows of Ax equals the number of rows of A

• Given a matrix  $A \in \mathbb{R}^{m \times n}$  and a vector  $x \in \mathbb{R}^n$ :

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \dots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{bmatrix}, \qquad x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

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- The number of columns of A must equal the number of rows of x.
- The number of rows of Ax equals the number of rows of A.

Given two matrices A and B, you can multiply them

only if the number of columns of A is same as the number of rows of B:

$$A \in \mathbb{R}^{m \times k}$$
 and  $B \in \mathbb{R}^{k \times n}$ .

The resulting matrix D = AB has m rows and n columns:  $D \in \mathbb{R}^{m \times n}$ 

Remember matrix multiplication is not commutative:

AB is not same as BA

### A linear programming problem

minimize 
$$2x_1-x_2+4x_3 \qquad \text{objective function}$$
 subject to 
$$x_1+x_2-x_3+x_4\leq 2\\ 3x_2-x_3+x_3=5\\ x_3+x_4\geq 3 \qquad \text{constraints}$$
 
$$x_1,x_2,x_3,x_4\geq 0 \qquad \text{non-negativity}$$

- $x^T = [x_1, x_2, x_3, x_4]$  are the decision variables.
- ullet The objective function is linear and it can be written as  $c^Tx$ , where

$$c^T = [2, -1, 4, 0]$$

- The constraints are linear equations and inequalities They have the form  $a^Tx=b$ , or  $a^Tx\leq b$ , or  $a^Tx\geq b$ 
  - Example: The first constraint is of the form  $a^T x \leq b$ , with

$$a^T = [1, 1, 0, 1]$$
 and  $b = 2$ 

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- The constraints are linear equations and inequalities
   They have the form a<sup>T</sup>x = b, or a<sup>T</sup>x ≤ b, or a<sup>T</sup>x ≥ b.
  - Example: The first constraint is of the form  $a^Tx \leq b$ , with

$$a^T = [1, 1, 0, 1] \qquad \text{and} \qquad b = 2$$

# Writing LPs in " $\geq$ " form

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 constraints 
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 non-negativity

#### Notice that:

• The first constraint can also be rewritten as

$$-x_1 - x_2 - x_4 \ge -2$$

The second constraint is equivalent to the two constraints:

$$3x_2 - x_3 \ge 5$$
 and  $3x_2 - x_3 \le 5$  (i.e.,  $-3x_2 + x_3 \ge -5$ ).

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Therefore any linear programming problem can then be written as:

minimize  $c^T x$  subject to  $Ax \ge b$ ,  $x \ge 0$ .

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 A vector x is feasible to the first LP if and only if it is feasible to the second LP.

• We can write any linear programming problem in " $\geq$ " form.

$$min c^T x$$
s. t.  $Ax \ge b, x \ge 0$ 

where

$$c^T = (2, -1, 4, 0),$$

$$A = \begin{bmatrix} -1 & -1 & 0 & -1 \\ 0 & 3 & -1 & 0 \\ 0 & -3 & 1 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix},$$

and, 
$$b^T = (-2, 5, -5, 3)$$
.

min 
$$2x_1 - x_2 + 4x_3$$
  
s. t.  $-x_1 - x_2 - x_4 \ge -2$   
 $3x_2 - x_3 \ge 5$   
 $-3x_2 + x_3 \ge -5$   
 $x_3 + x_4 \ge 3$   
 $x_1, x_2, x_3, x_4 \ge 0$ 

• We can write any linear programming problem in " $\geq$ " form.

where

$$c^T = (2, -1, 4, 0),$$

$$A = \begin{bmatrix} -1 & -1 & 0 & -1 \\ 0 & 3 & -1 & 0 \\ 0 & -3 & 1 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}, \qquad \begin{array}{c} \text{Data for this LP:} \\ \bullet \ n \ \text{variables,} \ c \in \mathbb{R}^n \\ \bullet \ m \ \text{constraints,} \ b \in \mathbb{R}^n \\ \end{array}$$

and, 
$$b^T = (-2, 5, -5, 3)$$
.

$$\begin{array}{lllll} \min & 2x_1 - x_2 + 4x_3 \\ \text{s. t.} & -x_1 - x_2 - x_4 & \geq & -2 \\ & & 3x_2 - x_3 & \geq & 5 \\ & & -3x_2 + x_3 & \geq & -5 \\ & & x_3 + x_4 & \geq & 3 \\ & & x_1, x_2, x_3, x_4 & \geq & 0 \end{array}$$

- m constraints,  $b \in \mathbb{R}^m$
- $A \in \mathbb{R}^{m \times n}$

• Sometimes it is more natural to write LPs in "≤" form.

min 
$$2x_1 - x_2 + 4x_3$$
  
s. t.  $-x_1 - x_2 - x_4 \ge -2$   
 $3x_2 - x_3 \ge 5$   
 $-3x_2 + x_3 \ge -5$   
 $x_3 + x_4 \ge 3$   
 $x_1, x_2, x_3, x_4 \ge 0$ 

Sometimes it is more natural to write LPs in "≤" form.

$$\begin{array}{lllll} \min & 2x_1 - x_2 + 4x_3 \\ \text{s. t.} & x_1 + x_2 + x_4 & \leq & 2 \\ & -3x_2 + x_3 & \leq & -5 \\ & 3x_2 - x_3 & \leq & 5 \\ & -x_3 - x_4 & \leq & -3 \\ & x_1, x_2, x_3, x_4 & \geq & 0 \end{array}$$

# Example LP in matrix notation cont. again

• We can also write LPs in (standard) "=" form.

min 
$$2x_1 - x_2 + 4x_3$$
  
s.t.  $x_1 + x_2 + x_4 \le 2$   
 $3x_2 - x_3 = 5$   
 $x_3 + x_4 \ge 3$   
 $x_1, x_2, x_3, x_4 \ge 0$ 

$$\begin{array}{ll}
\min & c^T x \\
\text{s. t.} & Ax \le b \\
& x \ge 0
\end{array}$$

min 
$$c^T x$$
  
s. t.  $Ax + Is = b$   
 $x \ge 0, s \ge 0$ 

$$\begin{array}{ll}
\min & c^T x \\
\text{s. t.} & Ax \ge b \\
& x \ge 0
\end{array}$$

min 
$$c^{x}x$$
  
s.t.  $Ax - Is = b$   
 $x \ge 0, s \ge 0$ 

# Example LP in matrix notation cont. again

• We can also write LPs in (standard) "=" form.

min 
$$2x_1 - x_2 + 4x_3$$
 min  $2x_1 - x_2 + 4x_3$   
s. t.  $x_1 + x_2 + x_4 \le 2$  s. t.  $x_1 + x_2 + x_4 + s_1 = 2$   
 $3x_2 - x_3 = 5$   $3x_2 - x_3 = 5$   
 $x_3 + x_4 \ge 3$   $x_3 + x_4 - s_3 = 3$   
 $x_1, x_2, x_3, x_4 \ge 0$   $x_1, x_2, x_3, x_4 \ge 0$   
 $x_1, x_2 \ge 0$ 

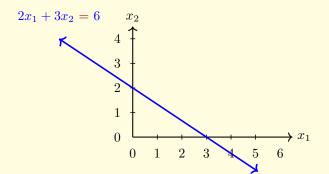
### Halfspaces

• A hyperplane in  $\mathbb{R}^n$  is the set points  $x \in \mathbb{R}^n$  that satisfy the equation

$$a^T x = b \iff a_1 x_1 + a_2 x_2 + \ldots + a_n x_n = b$$

This set of points divide the space  $\mathbb{R}^n$  into two halfspaces.

Example: Consider the line  $2x_1 + 3x_2 = 6$  in  $\mathbb{R}^2$ 



#### Halfspaces

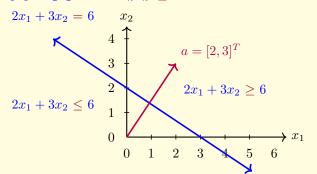
All points in one of the halfspaces satisfy the inequality

$$a_1x_1 + a_2x_2 + \ldots + a_nx_n \ge b$$

Points in the other satisfy

$$a_1x_1 + a_2x_2 + \ldots + a_nx_n \leq b.$$

• The vector  $a = (a_1, a_2, \dots, a_n)^T$  points in the direction where the points satisfying  $a_1x_1 + a_2x_2 + \dots + a_nx_n \ge b$  are.

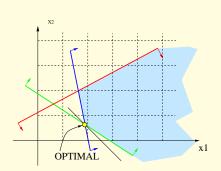


### Geometrically an LP looks like

Intersecting all constraints (halfspaces) gives the feasible set  ${\cal P}$  (polyhedron)

Solving the LP  $\equiv$  find a point  $x \in P$  with minimum  $c^Tx$ .

min 
$$||x_1 + ||x_2||$$
  
 $2x_1 + 3x_2 \ge 6$   
 $-x_1 + 2x_2 \le 2$   
 $5x_1 + ||x_2| \ge 10$ 



If there is an opt. solution, then there is an extreme point opt. solution

$$\underbrace{2x_1 + 3x_2 = 6, \ 5x_1 + x_2 = 10}_{\text{both constraints satisfied at equality (tight)}} \implies x = \left(\frac{24}{13}, \frac{10}{13}\right)$$

### Optimal solutions of LPs

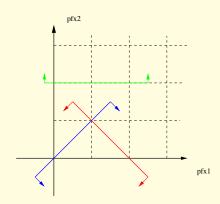
• Given a generic LP with *n* variables:

- There are four possible (mutually exclusive) outcomes:
  - (a) The feasible set P might be empty (problem is infeasible)

$$P = \left\{ x \in \mathbb{R}^n : Ax \ge b, \ x \ge 0 \right\} = \emptyset$$

- (b) There might be a unique optimal solution (one and only one).
- (c) There might be multiple optimal solutions. (all with the same objective value)
- (d) The objective value might be unbounded  $(-\infty)$ : No feasible solution is optimal.

# Example: Infeasible problem



$$P = \{x \in \mathbb{R}^2 : x_1 - x_2 \ge 0, \ x_1 + x_2 \le 2, \ x_2 \ge 2\} = \emptyset$$

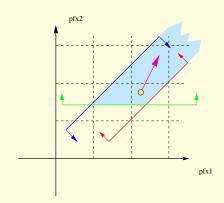
# Example: Unbounded problem

$$\max \quad |x_1 + 2x_2|$$

$$2x_1 - 2x_2 \ge -1$$

$$|x_1 - 2x_2 \le 1|$$

$$2x_1 + 2x_2 \ge 3/2$$

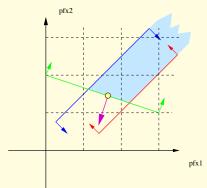


- **1.**  $P = \{x \in \mathbb{R}^2 : 2x_1 2x_2 \ge -1, x_1 x_2 \le 1, x_2 \ge 3/2\} \ne \emptyset$
- 2. For any  $x \in P$ , there exists a  $x' \in P$  such that  $c^T x' \ge c^T x + 1$

Note: If an LP is unbounded, its feasible region must be unbounded.

. But, an LP can be bounded while its feasible region is unbounded.

# Example: Multiple optima

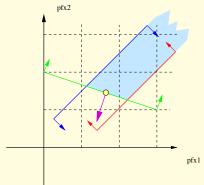


$$P = \{x \in \mathbb{R}^2 : 2x_1 - 2x_2 \ge -1, \ x_1 - x_2 \le 1, \ x_1 + 3x_2 = 6\} \ne \emptyset$$

In conclusion an LP is either

- Feasible or infeasible.
- If feasible, the optimal value is either bounded or unbounded.
- If feasible and bounded, optimial solution may not be unique.

# Example: Multiple optima



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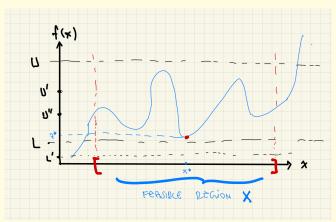
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# Upper/lower bounds and LP duality

### Upper and lower bounds for minimization problems

• Consider an optimization problem:

the optimal value 
$$\longrightarrow \ z^* = \min_{x \in X} \ f(x) \qquad \text{where} \quad X \subseteq \mathbb{R}^n$$



- U is an upper bound for  $z^*$ , (so are U' and U'')
- L is a lower bound for  $z^*$  (L' is a lower bound as well)

### Upper bounds for minimization problems

• Given an optimization problem:

$$z^* = \min_{x \in X} f(x)$$
 where  $X \subseteq \mathbb{R}^n$ 

 $\bullet$  An upper bound  $U \in \mathbb{R}$  is a number that can be certified to be greater than or equal to  $z^*$ 

In other words: 
$$\min_{x \in X} f(x) \le U$$

This does not mean

$$f(x) \le U$$
 for all  $x \in X$ 

It is perfectly OK if there are solutions  $x' \in X$  such that

ullet We only need the condition to hold for the optimal solution  $x^*\in X$ 

$$f(x^*) < U$$

- We can obtain upper bounds without solving the problem to optimality.
  - For example, any feasible point  $\bar{x} \in X$  gives an upper bound

$$U = f(\bar{x})$$

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### Upper bounds for minimization problems: LP example

• Consider the LP with 4 variables:

$$z^* = \min 2x_1 - x_2 + 4x_3$$
s.t. 
$$x_1 + x_2 + x_4 \leq 6$$

$$3x_2 - x_3 = 5$$

$$x_3 + x_4 \geq 2$$

$$x_1, x_2, x_3, x_4 \geq 0$$

• And consider the point (or, solution):

$$\bar{x} = \begin{bmatrix} 0 \\ 2 \\ 1 \\ 2 \end{bmatrix} \quad \begin{array}{l} \leftarrow \bar{x}_1 \\ \leftarrow \bar{x}_2 \\ \leftarrow \bar{x}_3 \\ \leftarrow \bar{x}_4 \end{array}$$

- The point  $\bar{x}$  is feasible as it satisfies all constraints.
- It has an objective function value of : 2(0) 1(2) + 4(1) + 0(2) = 2
- Since we are minimizing, we conclude that  $z^*$  cannot be larger than 2.
- Therefore, U=2 is **an** upper bound for this LP.  $\longleftarrow z^* \leq 2$

### A slight detour

#### The LP:

$$z^* = \min 2x_1 - x_2 + 4x_3$$
s. t. 
$$x_1 + x_2 + x_4 \le 6$$

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$$x_3 + x_4 \ge 2$$

$$x_1, x_2, x_3, x_4 \ge 0$$

#### A feasible solution:

$$\bar{x} \ = \left[ \begin{array}{c} 0 \\ 2 \\ 1 \\ 2 \end{array} \right] \quad \begin{array}{c} \leftarrow \bar{x}_1 \\ \leftarrow \bar{x}_2 \\ \leftarrow \bar{x}_3 \\ \leftarrow \bar{x}_4 \end{array}$$

with

$$c^T \bar{x} = 2 \longleftarrow \text{ an UB on } z^*$$

Question: Is this solution optimal?  $\rightarrow$  Not sure: maybe, maybe not.

Question: Is this an extreme point solution?  $\rightarrow$  NO

- The feasible set lives in  $\mathbb{R}^4$ .
- An ext. pt. must satisfy 4 linearly indep. constraints as equality
- $\bar{x}$  only satisfies two:  $3x_2 x_3 = 5$  and  $x_1 \ge 0$  constraint

Here is an ex. pt:  $\hat{x}^T = [0, 5/3, 0, 2]$  with  $c^T \hat{x} = -5/3 \leftarrow$  a better UB

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with

$$c^T \bar{x} = 2 \longleftrightarrow \text{ an UB on } z^*$$

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#### A feasible solution:

$$\bar{x} \ = \left[ \begin{array}{c} 0 \\ 2 \\ 1 \\ 2 \end{array} \right] \quad \begin{array}{c} \leftarrow \bar{x}_1 \\ \leftarrow \bar{x}_2 \\ \leftarrow \bar{x}_3 \\ \leftarrow \bar{x}_4 \end{array}$$

with

$$c^T\bar{x} = 2 \ \longleftarrow \ \text{an UB on} \ z^*$$

Question: Is this solution optimal?  $\rightarrow$  Not sure: maybe, maybe not.

Question: Is this an extreme point solution?  $\rightarrow$  NO!

- The feasible set lives in  $\mathbb{R}^4$ .
- An ext. pt. must satisfy 4 linearly indep. constraints as equality
- $\bar{x}$  only satisfies two:  $3x_2 x_3 = 5$  and  $x_1 \ge 0$  constraint

Here is an ex. pt:  $\hat{x}^T = [0, 5/3, 0, 2]$  with  $c^T \hat{x} = -5/3 \leftarrow$  a better UB

#### A slight detour

#### The LP:

$$z^* = \min 2x_1 - x_2 + 4x_3$$
s. t. 
$$x_1 + x_2 + x_4 \le 6$$

$$3x_2 - x_3 = 5$$

$$x_3 + x_4 \ge 2$$

$$x_1, x_2, x_3, x_4 \ge 0$$

#### A feasible solution:

$$\bar{x} \ = \left[ \begin{array}{c} 0 \\ 2 \\ 1 \\ 2 \end{array} \right] \quad \begin{array}{c} \leftarrow \bar{x}_1 \\ \leftarrow \bar{x}_2 \\ \leftarrow \bar{x}_3 \\ \leftarrow \bar{x}_4 \end{array}$$

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### Lower bounds for minimization problems

Again consider the optimization problem:

$$z^* = \min_{x \in X} f(x)$$
 where  $X \subseteq \mathbb{R}^n$ 

• A lower bound  $L \in \mathbb{R}$  is a number that can be certified to be less than or equal to  $z^*$ .

In other words: 
$$\min_{x \in X} f(x) \ge L$$

- We have to make sure that the best solution has to have an objective value larger than or equal to L.
- Which means that

$$f(x) \ge L$$
 for all  $x \in X$ 

- Finding lower bounds is usually complicated.
  - For LP problems, remember the weak duality theorem:
     (Feasible solutions to the dual give lower bounds for the primal LP.)

# Lower bounds for minimization problems: LP Example

• Consider the following simple (feasible) LP with 2 variables:

$$z^* = \min 2x_1 + 6x_2$$
  
s. t.  $x_1 + 3x_2 \ge 2$   
 $x_2 \ge 9$ .

- We would like to find a lower bound L for  $z^*$ .
- ullet L must be less than the objective value of **all** feasible solutions.
- ullet Consider an arbitrary feasible point  $ar{x}=[ar{x}_1,ar{x}_2]$
- As  $\bar{x}$  is feasible, we know that  $\bar{x}_1 + 3\bar{x}_2 \geq 2$  and therefore

$$2\bar{x}_1 + 6\bar{x}_2 \ge 4$$

$$z^* > 4$$
  $\leftarrow L = 4$  is a lower bound on  $z^*$ 

### Lower bounds for minimization problems: LP Example

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$$z^* \ge 4 \quad \leftarrow \quad L = 4 \text{ is a lower bound on } z^*$$

### Lower bounds for minimization: Another LP example

• Let's try a different example:

$$z^* = \min x_1 + 3x_2$$
  
s.t.  $x_1 + x_2 \ge 4$   
 $x_2 \ge 1$ .

- How can we express the objective function in terms of the constraints?
- We can do it by summing the constraints as follows:

$$x_1 + x_2 \ge 4$$

$$+ 2 \cdot (x_2 \ge 1)$$

$$= x_1 + 3x_2 \ge 6$$

$$z^* \geq 6 \quad \leftarrow \quad L = 6 \text{ is a lower bound on } z^*$$

### Lower bounds for minimization: Another LP example

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$$x_1 + x_2 \ge 4$$
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=  $x_1 + 3x_2 \ge 6$ 

$$z^* \ge 6 \quad \leftarrow \quad L = 6 \text{ is a lower bound on } z^*$$

#### Lower bounds for minimization: One last LP example

• Here is a more interesting example:

$$z^* = \min x_1 + 3x_2$$
  
s.t.  $x_1 + x_2 \ge 2$   
 $x_2 \ge 1$   
 $x_1 - x_2 \ge 3$ .

- How can we express the objective function in terms of the constraints?
- For any choice of  $p_1, p_2, p_3 \ge 0$  we can write

$$p_1 \cdot (x_1 + x_2 \ge 2) + p_2 \cdot (x_2 \ge 1) + p_3 \cdot (x_1 - x_2 \ge 3)$$

$$\Rightarrow \underbrace{(p_1+p_3)}_{\text{if }=1} x_1 + \underbrace{(p_1+p_2-p_3)}_{\text{and if }=3} x_2 \ \geq \underbrace{2p_1+p_2+3p_3}_{\text{then you obtain } L}$$

- The lower bound L we obtain depends on the choice of p:
  - $-p_1 = 1, p_2 = 2, p_3 = 0$  gives us the lower bound L = 4.
  - $-v_1 = 0, v_2 = 4, v_3 = 1$  gives us the lower bound L = 7.

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#### LP Duality

• A natural question is: how can we obtain the **best** lower bound on  $z^*$ ?

$$z^* = \min x_1 + 3x_2$$
  
s. t.  $x_1 + x_2 \ge 2$   
 $x_2 \ge 1$   
 $x_1 - x_2 \ge 3$ .

• Maximize  $2p_1 + p_2 + 3p_3$  over the constraints that p should satisfy:

$$w^* = \max 2p_1 + p_2 + 3p_3$$
  
s. t.  $p_1 + p_3 = 1$   
 $p_1 + p_2 - p_3 = 3$   
 $p_1, p_2, p_3 \ge 0$ .

ullet This is the dual LP and  $w^*$  gives the best lower bound on  $z^*$ 

#### LP Duality

• A natural question is: how can we obtain the best lower bound on  $z^*$ ?

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s.t.  $x_1 + x_2 \ge 2$   
 $x_2 \ge 1$   
 $x_1 - x_2 \ge 3$ .

• Maximize  $2p_1 + p_2 + 3p_3$  over the constraints that p should satisfy:

$$w^* = \max 2p_1 + p_2 + 3p_3$$
 s. t. 
$$p_1 + p_3 = 1$$
 
$$p_1 + p_2 - p_3 = 3$$
 
$$p_1, p_2, p_3 \ge 0.$$

Dual

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	Deimont		Duai
	Primal		1.T
minimize	_T	maximize	o $p$
minimize	c $x$	1	AT
subject to	Ax > b	subject to	$A^{-}p=c$
subject to	$Ax \geq 0$		m > 0
			$p \geq 0$ .

# Non-negativity constraints

• Example:

$$z^* = \min \quad x_1 + 3x_2$$
  
s.t.  $x_1 + x_2 \ge 2$   
 $x_2 \ge 1$   
 $x_1 - x_2 \ge 3$   
 $x_1 \ge 0$   
 $x_2 \ge 0$ .

• For any choice of  $p_1, p_2, p_3, p_4, p_5 \ge 0$  we can write

$$p_1 \cdot (x_1 + x_2 \ge 2) + p_2 \cdot (x_2 \ge 1) + p_3 \cdot (x_1 - x_2 \ge 3) + p_4 \cdot (x_1 \ge 0) + p_5 \cdot (x_2 \ge 0)$$

$$\Rightarrow \underbrace{(p_1+p_3+p_4)}_{\text{if }=1} x_1 + \underbrace{(p_1+p_2-p_3+p_5)}_{\text{and if }=3} x_2 \ \geq \underbrace{2p_1+p_2+3p_3}_{\text{then you obtain } L}$$

- The lower bound L we obtain depends on the choice of p:
- Find the best p using linear programming

• To find the best lower bound on  $z^*$ :

$$z^* = \min x_1 + 3x_2$$
s. t.  $x_1 + x_2 \ge 2$ 

$$x_2 \ge 1$$

$$x_1 - x_2 \ge 3$$

$$x_1 \ge 0$$

$$x_2 \ge 0.$$

• Maximize  $2p_1 + p_2 + 3p_3$  over the constraints that p should satisfy:

$$\max 2p_1 + p_2 + 3p_3 \qquad \max$$
s. t.  $p_1 + p_3 + p_4 = 1$ 

$$p_1 + p_2 - p_3 + p_5 = 3$$

$$p_1, p_2, p_3, p_4, p_5 \ge 0.$$

$$\begin{aligned} \max & 2p_1 + p_2 + 3p_3 \\ \text{s.t.} & p_1 + p_3 \leq 1 \\ & p_1 + p_2 - p_3 \leq 3 \\ & p_1, p_2, p_3 \geq 0. \end{aligned}$$

# (1/24/2024)

Recap: Upper bounds and lower for minimization problems
Given an optimization problem:

$$z^* = \min_{x \in X} f(x)$$
 where  $X \subseteq \mathbb{R}^n$ 

• An upper bound  $U \in \mathbb{R}$  is a number that satisfies:

$$\min_{x \in X} f(x) \le U$$

It is perfectly OK if there are solutions  $x' \in X$  such that f(x') > U

We only need the condition to hold for the optimal solution  $x^* \in X$ .

Any feasible point  $\bar{x} \in X$  gives an upper bound  $U = f(\bar{x})$ 

• A lower bound  $L \in \mathbb{R}$  is a number that satisfies:

$$\min_{x \in X} f(x) \ge L$$

Which means that

$$f(x) > L$$
 for all  $x \in X$ 

Finding lower bounds is usually complicated

• Small upper bounds and large lower bounds are better.

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# Recap: Lower bounds via duality

• For any LP, there is a corresponding dual LP.

	Primal LP		Its Dual LP
minimize	$4x_1 + 3x_2$	maximize	$2p_1 + 1p_2 + 3p_3$
subject to	$1x_1 + 1x_2 \ge 2$	subject to	$1p_1 + 0p_2 + 1p_3 \le 4$
	$0x_1 + 1x_2 \ge 1$		$1p_1 + 1p_2 - 1p_3 \le 3$
	$1x_1 - 1x_2 \ge 3,$		$p_1, p_2, p_3 \ge 0.$
	$x_1, x_2 > 0$		

• More generally:

	Primal		Dual
minimize	$c^T x$	maximize	$b^T p$
subject to	$Ax \ge b$	subject to	$A^T p \le \epsilon$
	$x \ge 0$		$p \ge 0$

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	Primal LP		Its Dual LP
minimize	$4x_1 + 3x_2$	maximize	$2p_1 + 1p_2 + 3p_3$
subject to	$1x_1 + 1x_2 \ge 2$	subject to	$1p_1 + 0p_2 + 1p_3 \le 4$
	$0x_1 + 1x_2 \ge 1$		$1p_1 + 1p_2 - 1p_3 \le 3$
	$1x_1 - 1x_2 \ge 3,$		$p_1, p_2, p_3 \ge 0.$
	$x_1, x_2 \ge 0.$		

More generally:

Weak Duality Thm: If  $\bar{x}$  is primal feasible and  $\bar{p}$  is dual feasible:

(min. objective)  $c^T \bar{x} \geq b^T \bar{p}$  (max. objective)

# Recap: Lower bounds via duality

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	Primal LP		Its Dual LP
minimize	$4x_1 + 3x_2$	maximize	$2p_1 + 1p_2 + 3p_3$
subject to	$1x_1 + 1x_2 \ge 2$	subject to	$1p_1 + 0p_2 + 1p_3 \le 4$
	$0x_1 + 1x_2 \ge 1$		$1p_1 + 1p_2 - 1p_3 \le 3$
	$1x_1 - 1x_2 \ge 3,$		$p_1, p_2, p_3 \ge 0.$
	$x_1, x_2 \ge 0.$		

More generally:

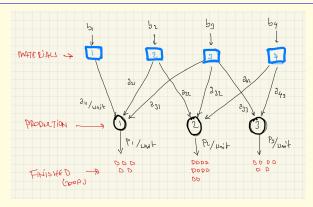
$$\begin{array}{lll} & \text{Primal} & \text{Dual} \\ \\ \text{minimize} & c^T x & \text{maximize} & b^T p \\ \\ \text{subject to} & Ax \geq b & \text{subject to} & A^T p \leq c \\ \\ & x \geq 0 & p \geq 0. \end{array}$$

Strong Duality Thm: If  $x^*$  is primal optimal and  $p^*$  is dual optimal:

(min. objective)  $c^T x^* = b^T p^*$  (max. objective)

- A firm produces n different products using m different materials.
- Let  $b_i \geq 0$ , i = 1, ..., m, be the available amount of the *i*th material.
- The jth product,  $j=1,\ldots,n$ , requires  $a_{ij}\geq 0$  units of the ith material and results in a revenue of  $p_j\geq 0$  per unit produced.
- Decide how much of each product to produce to maximize revenue.

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- Decide how much of each product to produce to maximize revenue.
- The decision variables  $x_j$ , denote how much jth product is produced.
- The problem can now be formulated as follows:

maximize 
$$p_1x_1 + p_2x_2 + \dots + p_nx_n$$
  
subject to  $a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n \le b_1$   
 $a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n \le b_2$   
 $\vdots$   $\vdots$   $\vdots$   $\vdots$   $a_{m1}x_1 + a_{m2}x_2 + \dots + a_{mn}x_n \le b_m$   
 $x_1, x_2, \dots, x_n, > 0$ 

- A firm produces n different products using m different raw materials.
- The decision variables  $x_j$ , denote how much jth product is produced.

maximize 
$$p_1x_1 + \cdots + p_nx_n$$
  
subject to  $a_{i1}x_1 + \cdots + a_{in}x_n \le b_i$   $i = 1, \dots, m$   
 $x_j \ge 0$   $j = 1, \dots, n$ .

#### LP problem using summations:

$$\max \sum_{j=1}^{n} p_j x_j$$
  
s. t. 
$$\sum_{j=1}^{n} a_{ij} x_j \le b_i \quad i = 1, \dots m$$
  
$$x_j \ge 0 \quad j = 1, \dots, n.$$

#### Written in matrix form:

$$\max p^{T}x$$
s.t.  $Ax \leq b$ ,
$$x \geq 0$$

$$p^{T} = [p_{1}, p_{2}, \dots, p_{n}]$$

$$\begin{bmatrix} \frac{a_{11}}{a_{21}} & \frac{a_{12}}{a_{22}} & \dots & \frac{a_{1n}}{a_{2n}} \\ \vdots & \vdots & \ddots & \vdots \end{bmatrix}, b = \begin{bmatrix} \frac{b_{1}}{b_{2}} \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}$$

(In this example we allow x variables to take fractional value, ex:  $x_3 = 2.7$ )

- A firm produces n different products using m different raw materials.
- The decision variables  $x_j$ , denote how much jth product is produced.

maximize 
$$p_1x_1+\cdots+p_nx_n$$
  
subject to  $a_{i1}x_1+\cdots+a_{in}x_n\leq b_i$   $i=1,\ldots,m$   
 $x_j\geq 0$   $j=1,\ldots,n.$ 

#### LP problem using summations:

# $\max \sum_{j=1}^{n} p_{j} x_{j}$ s.t. $\sum_{j=1}^{n} a_{ij} x_{j} \leq b_{i} \quad i = 1, \dots m$ $x_{j} \geq 0 \quad j = 1, \dots, n.$

#### Written in matrix form:

$$\max \quad p^T x$$

$$\text{s.t.} \quad Ax \le b,$$

$$x \ge 0$$

$$p^T = [p_1, p_2, \dots, p_n]$$

$$\begin{bmatrix} \frac{a_{11}}{a_{21}} & \frac{a_{12}}{a_{22}} & \dots & \frac{a_{1n}}{a_{2n}} \\ \vdots & \vdots & \ddots & \vdots \end{bmatrix}, b = \begin{bmatrix} \frac{b_1}{b_2} \\ \vdots \\ \vdots \\ \vdots \end{bmatrix}$$

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$$x_j \ge 0 \quad j = 1, \dots, n.$$

#### Written in matrix form:

$$\max \quad p^T x$$
s.t.  $Ax \le b$ ,
$$x \ge 0$$

$$p^T = [p_1, p_2, \dots, p_n]$$

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ a_{n+1} & a_{n+2} & a_{n+2} & a_{n+2} \end{bmatrix}, b = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ \vdots \\ \vdots \\ b_n \end{bmatrix}$$

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$$x_{j} \geq 0 \quad j = 1, \dots, n.$$

#### Written in matrix form:

$$\max p^{T} x$$
s.t.  $Ax \le b$ ,
$$x \ge 0$$

$$p^{T} = [p_{1}, p_{2}, \dots, p_{n}]$$

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{bmatrix}, b = \begin{bmatrix} b_{1} \\ b_{2} \\ \vdots \\ b_{m} \end{bmatrix}$$

(In this example we allow x variables to take fractional value, ex:  $x_3=2.7$  )

# Integer Programming

- A hospital wants to make a weekly night shift (10pm-6am) schedule for its nurses.
- The demand for nurses for the night shift on day j is an integer  $d_j$ , for all  $j \in \{Su, Mo, Tu, We, Th, Fr, Sa\}$ .
- Every nurse works 5 consecutive days and takes the next 2 days off.
- Find the minimum number of nurses the hospital needs to hire.

Question: What are the decision variables?

#### What are the decision variables?

- We could try using a decision variable y<sub>j</sub> equal to the number of nurses that work on day j.
- However, with this definition we would not be able to capture the constraint that every nurse works 5 days in a row.
- We need to know the starting day of a nurse to model the problem correctly.
- We define  $x_j$  as the number of nurses starting their week on day  $j \in \{Mo, Tu, We, Th, Fr, Sa, Su\}$ .
- We can now write a constraint for every day of the week to make sure that the demand is satisfied.

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- We can now write a constraint for every day of the week to make sure that the demand is satisfied.

We then have the following problem formulation:

$$\begin{array}{llll} \text{minimize} & x_{Su} & +x_{Mo} + x_{Tu} & +x_{We} + x_{Th} & +x_{Fr} + x_{Sa} \\ & & & & +x_{We} + x_{Th} & +x_{Fr} + x_{Sa} & \geq d_{Su} \\ & & & & & +x_{Th} & +x_{Fr} + x_{Sa} & \geq d_{Mo} \\ & & & & & +x_{Th} & +x_{Fr} + x_{Sa} & \geq d_{Mo} \\ & & & & & +x_{Mo} + x_{Tu} & +x_{We} & +x_{Fr} + x_{Sa} & \geq d_{Tu} \\ & & & & & & +x_{Mo} + x_{Tu} & +x_{We} & +x_{Th} & \geq d_{Tu} \\ & & & & & & & & \geq d_{We} \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\$$

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#### Question:

#### What symbols do we use for numbers?

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- Q Fractional numbers (Quotients)
- N Natural numbers
- $\mathbb{Z}$  Integers

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Answer: The use of the letter Z to denote the set of integers comes from the German word Zahlen ("numbers") and has been attributed to David Hilbert. [from Wikipedia]

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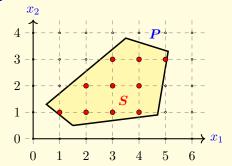
# What is an Integer (Linear) Program?

A pure integer program (IP):

$$\begin{aligned} & \min \quad c^T x \\ & \text{s. t.} \quad Ax \geq b \\ & \quad x \geq 0 \\ & \quad x \quad \text{integral (i.e., } x \in \mathbb{Z}^n). \end{aligned}$$

 $\textbf{Feasible} \ \ \text{set:} \quad S \ = \ \left\{ x \in \mathbb{Z}^n : Ax \geq b, x \geq 0 \right\} = \ \textit{Polyhedron} \cap \mathbb{Z}^n \ .$ 

When n=2



#### Remember the labor scheduling problem

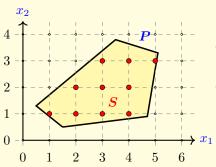
 If we ignore ("relax") the integrality constraints, we obtain the so-called LP relaxation of this problem.

minimize 
$$x_{Su}$$
 + $x_{Mo}$  +  $x_{Tu}$  +  $x_{We}$  +  $x_{Th}$  +  $x_{Fr}$  +  $x_{Sa}$  subject to  $x_{Su}$  +  $x_{We}$  +  $x_{Th}$  +  $x_{Fr}$  +  $x_{Sa}$   $\geq d_{Su}$  +  $x_{Su}$  +  $x_{Mo}$  +  $x_{Th}$  +  $x_{Fr}$  +  $x_{Sa}$   $\geq d_{Mo}$  +  $x_{Su}$  +  $x_{Mo}$  +  $x_{Tu}$  +  $x_{We}$  +  $x_{Fr}$  +  $x_{Sa}$   $\geq d_{We}$  +  $x_{Su}$  +  $x_{Mo}$  +  $x_{Tu}$  +  $x_{We}$  +  $x_{Th}$  +  $x_{Fr}$  +  $x_{$ 

$$x_j \geq 0 \ \ \text{and} \ \ x_j \in \mathbb{Z}, \qquad \quad j \in \{Su, Mo, Tu, We, Th, Fr, Sa\}.$$

 All feasible solutions to the integer program are also feasible to the LP relaxation.

#### LP relaxations - minimization objective



- P is the feasible set for the LP relaxation (ignore integrality)
- ullet S is the feasible set for the integer program:

$$S = P \cap \mathbb{Z}^n$$

Question: How would

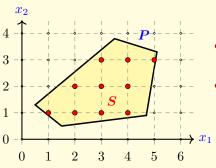
$$z_{IP} = \min c^T x$$
 s. t.  $x \in S$ 

compare to

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Answer:  $z_{IP} \geq z_{LP} \leftarrow \text{because } S \subseteq P \text{ and we are minimizing.}$ 

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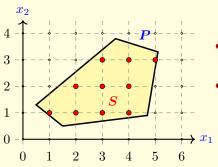
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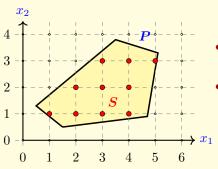
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### Relaxations - lower bounds (minimization objective)

• More generally, consider the following 2 optimization problems:

$$z_S = \min f(x)$$
 s. t.  $x \in S$  (small set)  
 $z_B = \min f(x)$  s. t.  $x \in B$  (big set)

where we optimize the same objective function over 2 different feasible sets  ${\cal S}$  and  ${\cal B}$  such that

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(B is called a **relaxation** of S as it contains more solutions.)

Assume that both problems are feasible and have an optimal solution.

Claim:  $z_S \geq z_B$ .

**Proof.** Let  $x^S \in S$  be an optimal solution for the first problem.

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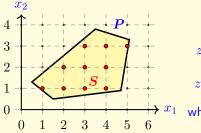
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Integer program v.s. its linear programming relaxation:



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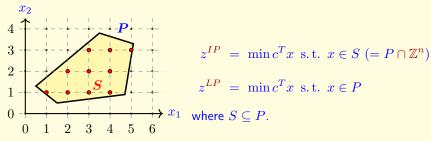
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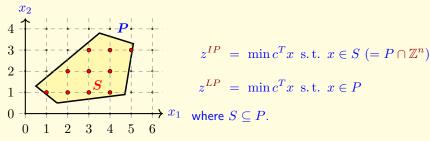


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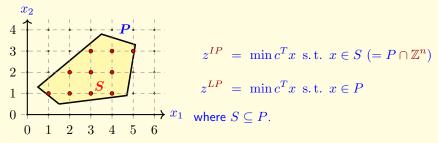
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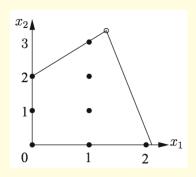
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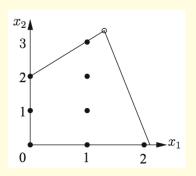
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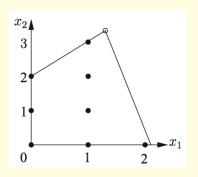
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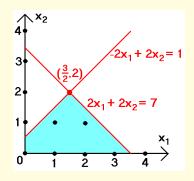
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- It also looks like we can round (1.3, 3.3) to the optimum solution (1,3), but...

#### Another example: Rounding LP solutions

$$\begin{array}{ll} \max & 15x_2 \\ \text{s. t.} & -2x_1+2x_2 \leq 1 \\ & 2x_1+2x_2 \leq 7 \\ & x_1,x_2 \geq 0 \\ & x_1,x_2 \text{ integer} \end{array}$$

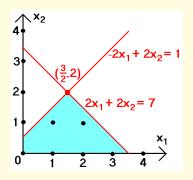


- Optimal IP solutions ares (1,1) and (2,1) with obj. value 15.
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- We cannot always round the solution of the LP relaxation to the optimal solution of the IP:
  - 1. Rounding to it a feasible integer solution might be impossible
  - 2. Moreover, the IP can be infeasible even though the LP is feasible Example:  $P = \{x \in \mathbb{R}^2 : 0.6 \ge x_1 \ge 0.2, 0.75 \ge x_2 \ge 0.41\}$
  - 3. Even if rounding to an integer solution is possible, the opt. IP sol. can be arbitrarily far (different) from the opt. LP sol.
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# Solving IPs: Branch and Bound

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$$z^{IP} = \min c^T x \text{ s.t. } Ax \ge b, \ x \ge 0, \ x \in \mathbb{Z}^n$$
 (IP)

- Relaxing integrality gives an LP problem (easy to solve)
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$$\mathsf{IP}_1: x_1 \le \lfloor x_1^{LP} \rfloor = 3$$
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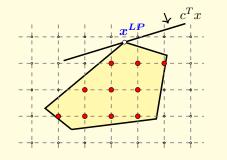
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$$\mathsf{IP}_1: x_1 \le \lfloor x_1^{LP} \rfloor = 3 \qquad \qquad \mathsf{IP}_2: x_1 \ge \lceil x_1^{LP} \rceil = 4$$

Instead of solving IP, we not solve both  $IP_1$  and  $IP_2$ .

Note: **Any** feasible (optimal) solution of IP is either in IP $_1$  or in IP $_2$ Note: **No** feasible solution of LP $_1$  or LP $_2$  can have  $x_1=3.31$ 

# Partitioning step for integer programs



$$(\mathsf{IP}_1) \quad \min \ c^T x \text{ s.t. } x \in P_1 \cap \mathbb{Z}^n$$



(IP)  
min 
$$c^T x$$
  
s. t.  $\underbrace{Ax \ge b, \ x \ge 0}_{P = \{x \in \mathbb{R}^n : Ax > b, x > 0\}} x \in \mathbb{Z}^n$ 

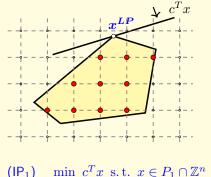
Let x<sup>LP</sup> be the opt. sol. to the LP relaxation.

$$(\mathsf{IP}_2) \quad \min \ c^T x \text{ s.t. } x \in P_2 \cap \mathbb{Z}^n$$



$$P_2 = \{x : Ax \ge b, x_1 \ge \lceil x_1^{LP} \rceil, x \ge 0\}$$

# Partitioning step for integer programs



(IP)  
min 
$$c^T x$$
  
s. t.  $\underbrace{Ax \ge b, \ x \ge 0}_{P = \{x \in \mathbb{R}^n : Ax \ge b, x \ge 0\}} x \in \mathbb{Z}^n$ 

Let x<sup>LP</sup> be the opt. sol. to the LP relaxation.

(IP<sub>2</sub>) min  $c^T x$  s.t.  $x \in P_2 \cap \mathbb{Z}^n$ 

$$P_{2} = \{x : Ax \geq b, x_{1} \geq \lceil x_{1}^{LP} \rceil, x \geq 0\}$$

# Partitioning an IP problem into 2 subproblems

• Solve the LP relaxation:

$$z^{LP} = \min\{c^T x : x \in P\} = c^T x^{LP}$$

• Divide:

$$P_1 = P \cap \{x_1 \le \left\lfloor x_1^{LP} \right\rfloor \}$$
 and  $P_2 = P \cap \{x_1 \ge \left\lceil x_1^{LP} \right\rceil \}$ 

• We have:

$$P \cap \mathbb{Z}^n = (P_1 \cap \mathbb{Z}^n) \cup (P_2 \cap \mathbb{Z}^n) \leftarrow \text{integer points}$$

• Whereas:

$$P \supseteq P_1 \cup P_2 \quad \longleftarrow \text{ fractional points}$$

 $\begin{array}{lll} \mbox{Integer program (IP):} & \mbox{LP relaxation of IP:} \\ \\ z^{IP} &= \min\{c^Tx: x \in P \cap \mathbb{Z}^n\} & \geq & z^{LP} &= \min\{c^Tx: x \in P\} \\ \\ z^{IP1} &= \min\{c^Tx: x \in P_1 \cap \mathbb{Z}^n\} & \geq & z^{LP1} &= \min\{c^Tx: x \in P_1\} \\ \\ z^{IP2} &= \min\{c^Tx: x \in P_2 \cap \mathbb{Z}^n\} & \geq & z^{LP2} &= \min\{c^Tx: x \in P_2\} \\ \\ z^{IP} &= \min\{z^{IP1}, z^{IP2}\} & \geq & \min\{z^{LP1}, z^{LP2}\} \geq z^{LP2} \\ \end{array}$ 

# Partitioning an IP problem into 2 subproblems

Solve the LP relaxation:

$$z^{LP} = \min\{c^T x : x \in P\} = c^T x^{LP}$$

• Divide:

$$P_1 = P \cap \{x_1 \le |x_1^{LP}|\}$$
 and  $P_2 = P \cap \{x_1 \ge \lceil x_1^{LP} \rceil\}$ 

• We have:

$$P \cap \mathbb{Z}^n = (P_1 \cap \mathbb{Z}^n) \cup (P_2 \cap \mathbb{Z}^n) \leftarrow \text{integer points}$$

Whereas:

$$P \supseteq P_1 \cup P_2 \quad \longleftarrow \text{ fractional points}$$

Integer program (IP): LP relaxation of IP:  $z^{IP} = \min\{c^T x : x \in P \cap \mathbb{Z}^n\} \qquad \geq \qquad z^{LP} = \min\{c^T x : x \in P\}$   $z^{IP1} = \min\{c^T x : x \in P_1 \cap \mathbb{Z}^n\} \qquad \geq \qquad z^{LP1} = \min\{c^T x : x \in P_1\}$   $z^{IP2} = \min\{c^T x : x \in P_2 \cap \mathbb{Z}^n\} \qquad \geq \qquad z^{LP2} = \min\{c^T x : x \in P_2\}$   $z^{IP} = \min\{z^{IP1}, z^{IP2}\} \qquad \geq \qquad \min\{z^{LP1}, z^{LP2}\} \geq z^{LP}$ 

#### More generally: Divide and conquer principle

Consider

$$z^* = \min \left\{ f(x) : x \in S \right\}$$

If a collection of disjoint sets  $\{S_1, S_2, \dots, S_k\}$  satisfy

$$S = S_1 \cup S_2 \cup \ldots \cup S_k$$

then  $\{S_1, S_2, \dots, S_k\}$  is called a partition of S

Let 
$$z^i = \min\{f(x) : x \in S_i\}$$
, and  $z^i \geq z^i_{LR} \leftarrow$  a lower bound

Observation 1:

$$z^* = \min\{z^1, z^2, z^3, \dots, z^k\}$$

Observation 2:

$$z^* \le \min\{z^1, z^3, z^8, \ldots\} \quad \longleftarrow \text{ some } z^i \text{s are missing here}$$

Observation 3

$$z^* \geq \min\{z_{LB}^1, z_{LB}^2, \dots, z_{LB}^k\}$$

(In branch and bound, we dynamically decide how to partition of S.)

#### More generally: Divide and conquer principle

Consider

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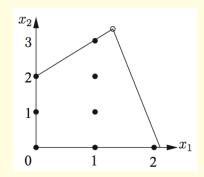
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(In branch and bound, we dynamically decide how to partition of S.)

# Example

$$\begin{array}{ll} \text{(IP)} & \min & x_1 - 2x_2 \\ & \text{s. t.} & -x_1 + x_2 \leq 2 \\ & 8x_1 + 2x_2 \leq 17 \\ & x_1, x_2 \geq 0 \\ & x_1, x_2 \text{ integer} \end{array}$$



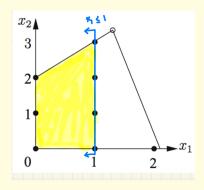
- Optimal solution to LP is  $x^{LP} = (1.3, 3.3)^T$  with objective  $z^{LP} = -5.3$
- We now have a lower bound for the IP: L=-5.3
- We can branch on either  $x_1$  or  $x_2$
- Choose  $x_1 \Rightarrow$  Create 2 subproblems by adding the constraints:

(i) 
$$x_1 \le 1$$
 and (ii)  $x_1 \ge 2$ 

to the IP.

# Example

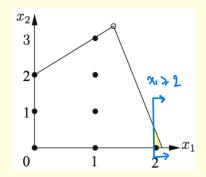
$$\begin{array}{lll} \text{(IP1)} & \min & x_1 - 2x_2 \\ & \text{s. t.} & -x_1 + x_2 \leq 2 \\ & & 8x_1 + 2x_2 \leq 17 \\ & & x_1 \leq 1 \\ & & x_1, x_2 \geq 0 \\ & & x_1, x_2 \text{ integer} \end{array}$$



- Optimal solution to LP1 is  $x^{\mathrm{LP1}} = (1,3)^T$  with  $z^{\mathrm{LP1}} = -5$
- As the LP solution is integral, we solved IP1 to optimality:  $z^{\rm IP1}=-5$  (We do not need to explore this subproblem anymore.)
- We now have an upper bound for the IP:  $oldsymbol{U} = -5$
- Let's go back to the other subproblem IP2.

## Example

$$\begin{array}{lll} \text{(IP2)} & \min & x_1 - 2x_2 \\ & \text{s. t.} & -x_1 + x_2 \leq 2 \\ & 8x_1 + 2x_2 \leq 17 \\ & x_1 \geq 2 \\ & x_1, x_2 \geq 0 \\ & x_1, x_2 \text{ integer} \end{array}$$



- Optimal solution to LP2 is  $x^{LP2} = (2, 0.5)^T$  with  $z^{LP2} = 1$
- Notice that

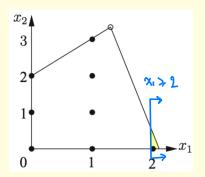
$$z^{{\sf IP2}} \, \geq \, z^{{\sf LP2}} \, = \, 1 \, > \, -5 \, = \, U$$

- There cannot be better integer solutions in this subproblem.
- We are done:

$$z^{\mathsf{IP}} = -5$$

# Example

$$\begin{array}{ll} \text{(IP2)} & \min & x_1 - 2x_2 \\ & \text{s. t.} & -x_1 + x_2 \leq 2 \\ & 8x_1 + 2x_2 \leq 17 \\ & x_1 \geq 2 \\ & x_1, x_2 \geq 0 \\ & x_1, x_2 \text{ integer} \end{array}$$



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- There cannot be better integer solutions in this subproblem.
- We are done:

$$z^{\mathsf{IP}} = -5$$

# 1/29/2024

# Recap: Divide and conquer principle

Consider

$$z^* = \min \left\{ f(x) : x \in S \right\}$$

If a collection of disjoint sets  $\{S_1, S_2, \dots, S_k\}$  satisfy

$$S = S_1 \cup S_2 \cup \ldots \cup S_k$$

then  $\{S_1, S_2, \dots, S_k\}$  is called a partition of S

Let 
$$z^i = \min\{f(x) : x \in S_i\}$$
, and  $z^i \geq z^i_{LB} \leftarrow$  a lower bound

Observation 1:

$$z^* = \min\{z^1, z^2, z^3, \dots, z^k\}$$

Observation 2:

$$z^* \leq \min\{z^1, z^3, z^8, \ldots\} \quad \longleftarrow \text{ some } z^i \text{s are missing here}$$

Observation 3:

$$z^* \geq \min\{z_{LB}^1, z_{LB}^2, \dots, z_{LB}^k\}.$$

(In branch and bound, we dynamically decide how to partition of S.)

# Consider a generic IP: $z^* = \min \{c^T x : x \in S\}$ where $S = P \cap \mathbb{Z}^n$ Partitioning S:

$$[0]$$
  $S$ 

$$[1] \quad S = S_1 \cup S_2$$

$$S_1 = S_3 \cup S_4$$

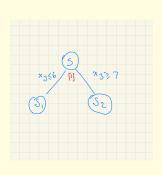
$$[2] \quad S = S_3 \cup S_4 \cup S_5$$

$$S_2 = S_5 \cup S_6$$

$$[3] \quad S = S_3 \cup S_4 \cup S_5 \cup S_6$$

$$S_5 = S_7 \cup S_8$$

$$[4] \quad S = S_3 \cup S_4 \cup S_7 \cup S_8 \cup S_6$$



Consider a generic IP:  $z^* = \min \left\{ c^T x : x \in S \right\}$  where  $S = P \cap \mathbb{Z}^n$  Partitioning S:

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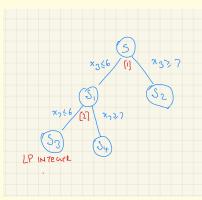
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# Consider a generic IP: $z^* = \min \{c^T x : x \in S\}$ where $S = P \cap \mathbb{Z}^n$

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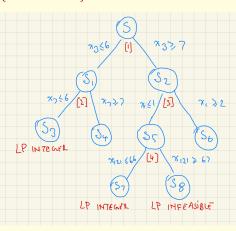
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Partitioning *S*:

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[2] 
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 $S_2 = S_5 \cup S_6$ 

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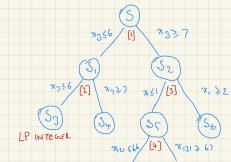
$$S_5 = S_7 \cup S_8$$

$$[1] \quad z^* = \min\{z^1, z^2\}$$

[4]  $S = S_3 \cup S_4 \cup S_7 \cup S_8 \cup S_6$ 

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[3] 
$$z^* = \min\{z^3, z^4, z^5, z^6\}$$



LP IMFEASIBLE

60 / 179

$$\{z,z^4\}$$
  $\longleftarrow$   $z^* \leq U = z^3$  (IP $^3$  solved)

$$z^* = \min\{z^2, z^3, z^4\} \qquad \qquad z \leq U = z^5 \qquad \text{(IPS solved)}$$
 $z^* = \min\{z^3, z^4, z^5, z^6\}$ 
 $z^* = \min\{z^3, z^4, z^6, z^7, z^8\} \qquad \longleftarrow \quad z^* \leq U = \min\{z^3, z^7\}$ 

LP INTEGER

Consider a generic IP:  $z^* = \min \{c^T x : x \in S\}$  where  $S = P \cap \mathbb{Z}^n$ 

#### Partitioning S:

$$[0]$$
  $S$ 

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$$S_5 = S_7 \cup S_8$$

[4] 
$$S = S_3 \cup S_4 \cup S_7 \cup S_8 \cup S_6$$

$$z^* \; \geq \; \boldsymbol{L} \; = \; \min\{z_{LB}^3 \; , z_{LB}^4 , \; z_{LB}^6 , \; z_{LB}^7 , \; z_{LB}^8 \}$$

$$z^* \leq U = \min\{z^3, z^7\} \leftarrow$$
 because we solved  $\mathsf{IP}^3$  and  $\mathsf{IP}^7$ 

When L = U we have solved the IP.

# When we solve the LP relaxation of a subproblem

- When we solve the LP relaxation of IP<sub>1</sub> (call it LP<sub>1</sub>)
  - If LP<sub>1</sub> is infeasible, then IP<sub>1</sub> is also infeasible.
  - If the optimal solution to LP $_1$  is integral then IP $_1$  is solved to optimality and  $z^{\rm IP}{_1}=z^{\rm LP}{_1}$ 
    - [As we have a feasible integer solution at hand,  $z^{\rm IP_1}$  is an upper bound on IP (minimization)]
  - If the LP solution is **not** integral, then we can again divide IP<sub>1</sub> into two new subproblems IP<sub>3</sub> and IP<sub>4</sub>.
- Repeating this process, we create subproblems  $\mathsf{IP}_k$  for  $k=1,\ldots$
- We have to further divide any subproblem IP<sub>k</sub> unless its LP relaxation LP<sub>k</sub> returns an integral solution or it is infeasible.
- Notice that at each step we might replace one IP/LP with two!
- This might lead to exponential blow up!
   (However, this is still the best way to solve general IPs.)

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   (However, this is still the best way to solve general IPs.)

# Pruning subprobems

- After solving its LP relaxation, we do not partition a subproblem IP<sub>k</sub> into 2 new subproblems in one of these cases:
  - If its LP relaxation is infeasible.
  - If the LP solution is integral (in this case we solved  ${\sf IP}_k$  to optimality and found a new lower bound  ${\pmb L}=z^{{\sf IP}_k}$  for  ${\sf IP})$

- ullet Let's now assume that we have already found an integral solution earlier, giving us an upper bound U.
  - What happens if  $z^{\mathsf{LP}_k} \geq U$  ?
  - IP<sub>k</sub> cannot contain a better solution to the IP

$$z^{\text{IP}_k} \ge z^{\text{LP}_k}$$
  $\ge U \ge z^*$ 

I herefore, we do care about IP<sub>k</sub> and we prune it
 (it cannot contain a better solution so we do not explore it further)

## Pruning subprobems

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$$z^{\mathsf{IP}_k} \geq z^{\mathsf{LP}_k}$$
  $\geq U \geq z^*$ 

Therefore, we do care about IP<sub>k</sub> and we prune it
 (it cannot contain a better solution so we do not explore it further)

# Branch&Bound for minimization problems

$$(\mathsf{IP}) \ z^* = \min \left\{ c^T x : x \in P \cap \mathbb{Z}^n \right\}$$

- Set the list of problems to solve to  $\mathcal{L} \leftarrow \{\mathsf{IP}\}$  and set  $U = +\infty$ .
- While  $\mathcal{L} \neq \emptyset$ 
  - Pick a subproblem  $\mathsf{IP}'$  from  $\mathcal{L}$  and set  $\mathcal{L} = \mathcal{L} \setminus \{\mathsf{IP}'\}$
  - Relax IP'  $\rightarrow$  solve LP'  $\rightarrow$  obtain solution  $x^{\text{LP'}}$  with obj.  $z^{\text{LP'}}$
  - If LP' is infeasible, break
  - If  $x^{\mathsf{LP}'}$  is integral, update  $U \leftarrow \min\{U, z^{\mathsf{LP}'}\}$ , break
  - If the optimal value  $z^{\mathsf{LP}'} \geq \boldsymbol{U}$ , break
  - Choose a fractional  $x_j$  i.e.,  $x_j^{\mathsf{LP}'} \notin \mathbb{Z}$ 
    - Create IP" with additional constraint:  $x_j \leq \lfloor x_j^{\mathsf{LP}'} \rfloor$
    - Create IP''' with additional constraint:  $x_j \geq \lceil x_j^{\mathsf{LP'}} \rceil$

$$\mathcal{L} \leftarrow \mathcal{L} \cup \{\mathsf{IP''}, \mathsf{IP'''}\}$$

# Branch&Bound for maximization problems

(IP) 
$$z^* = \max \left\{ c^T x : x \in P \cap \mathbb{Z}^n \right\}$$

- Set the list of problems to solve to  $\mathcal{L} \leftarrow \{\mathsf{IP}\}$  and set  $L = -\infty$ .
- While  $\mathcal{L} \neq \emptyset$ 
  - Pick a subproblem  $\mathsf{IP}'$  from  $\mathcal L$  and set  $\mathcal L = \mathcal L \setminus \{\mathsf{IP}'\}$
  - Relax IP'  $\rightarrow$  solve LP'  $\rightarrow$  obtain solution  $x^{\text{LP'}}$  with obj.  $z^{\text{LP'}}$
  - If LP' is infeasible, break
  - If  $x^{\mathsf{LP}'}$  is integral, update  $\mathbf{L} \leftarrow \max\{\mathbf{L}, z^{\mathsf{LP}'}\}$ , break
  - If the optimal value  $z^{\mathsf{LP}'} \leq L$ , break
  - Choose a fractional component  $x_j^{\mathsf{LP}'} \notin \mathbb{Z}$

Create IP" with additional constraint  $x_j \leq \lfloor x_j^{\mathsf{LP'}} \rfloor$ 

Create IP''' with additional constraint  $x_j \geq \lceil x_j^{\mathsf{LP'}} \rceil$ 

$$\mathcal{L} \leftarrow \mathcal{L} \cup \{\mathsf{IP''}, \mathsf{IP'''}\}$$

# For maximization problems

$$(\mathsf{IP}) \ z^* = \max \left\{ c^T x : x \in P \cap \mathbb{Z}^n \right\}$$

#### B&B summary:

- $\mathcal{L} = \{IP^2, IP^5, IP^7, IP^8, IP^9, ...\}$  contains the subproblems that have the potential to contain the optimal solution to the IP.
- $\bullet$  The best LP objective value of the subproblems in  $\mathcal L$  give an upper bound on  $z^*$

$$z^* \leq \max\{z^{LP^2}, z^{LP^5}, z^{LP^7}, z^{LP^8}, z^{LP^9}, \ldots\} \leftarrow U$$

• Whenever we encounter an integer solution we update

$$\boldsymbol{L} \leftarrow \max\{\boldsymbol{L}, z^{\mathsf{LP}'}\}$$

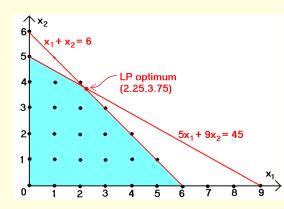
(we also remember the best integral solution so far and call it the incumbent)

- We stop when  $\mathcal{L} = \emptyset$ . The incumbent is the optimal solution to IP with value L.
- If we terminate early (i.e.  $\mathcal{L} \neq \emptyset$ ) then we know:  $U \geq z^* \geq L$ .

# One last example

# Example (maximization)

 $x_1, x_2 \ge 0$ , and integer



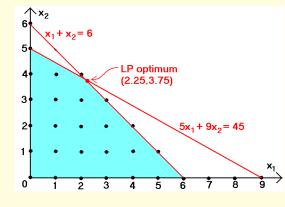
- The optimal solution of the LP relaxation is  $x^* = [2.25, 3.75]^T$ ,
- The optimal LP objective value is  $z^{LP}=41.25$ .
- $\bullet$  Therefore we know that optimal IP value is at most U=41.25

(Note: This actually means that  $U=41=\lfloor 41.25 \rfloor$ , why?)

• We branch on  $x_2: x_2 \leq 3$  or  $x_2 \geq 4$ 

# Example (maximization)

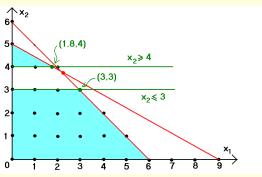
 $x_1, x_2 \geq 0$ , and integer



- The optimal solution of the LP relaxation is  $x^* = [2.25, 3.75]^T$ ,
- The optimal LP objective value is  $z^{LP} = 41.25$ .
- Therefore we know that optimal IP value is at most U=41.25 (Note: This actually means that  $U=41=\lfloor 41.25 \rfloor$ , why?)
- We branch on  $x_2$ :  $x_2 \le 3$  or  $x_2 \ge 4$

# Create 2 subproblems

 $x_1, x_2 \geq 0$ , and integer



68 / 179

 $x_1, x_2 \geq 0$ , and integer

# Solve the LP relaxation of the subproblems

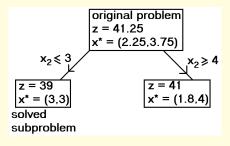
LP optimal solution:

$$\boldsymbol{x}^{LP1} = [3, 3]^T$$
 , with  $\boldsymbol{z}^{LP1} = 39$ 

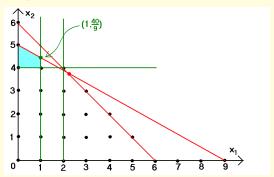
LP optimal solution:

$$x^{LP1} = [3,3]^T \text{, with } z^{LP1} = 39 \\ \qquad \qquad x^{LP2} = [1.8,4]^T \text{, with } z^{LP2} = 41$$

- $IP_1$  is solved to optimality. We have now a lower bound of L=39.
- We need to explore (divide)  $IP_2$  further: branch on  $x_1$ .



# Create 2 more subproblems



$$\begin{array}{ll} (\mathsf{IP}_3) & \max & 5x_1+8x_2\\ & \text{s. t.} & x\in P,\ x_2\geq 4 \ x_1\leq 1\\ & x_1,x_2 \ \text{integer} \end{array}$$

LP optimal solution:

$$x^{LP3}=[1,4\frac{4}{9}]^T$$
 with  $z^{LP1}=40\frac{5}{9}$ 

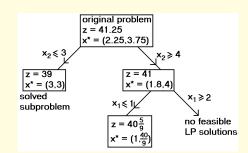
$$\begin{array}{ll} \mathsf{(IP_4)} & \max & 5x_1+8x_2\\ & \mathrm{s.\,t.} & x\in P,\ x_2\geq 4 \ x_1\geq 2\\ & x_1,x_2 \ \mathsf{integer} \end{array}$$

LP infeasible:

Subproblem  ${\sf IP}_4$  is also infeasible.

# After solving $x^{LP3}$ and $x^{LP4}$ , this is the current B&B tree $\rightarrow$ .

- We have a lower bound of  ${m L}=39$  for the IP
- We have improved the IP upper bound to  ${\pmb U}=40\frac{5}{9} \ \to 40$



After solving  $x^{LP3}$  and  $x^{LP4}$ , this is the current B&B tree  $\rightarrow$ .

- We have a lower bound of  ${m L}=39$  for the IP
- We have improved the IP upper bound to  $U=40\frac{5}{9} \to 40$

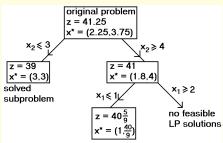
Exploring IP $_3$  further we create 2 new subproblems branching on  $x_2$ 

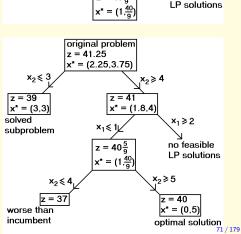
• IP<sub>5</sub> has an additional constraint

$$x_2 \leq 4$$

• IP<sub>6</sub> has an additional constraint

$$x_2 \ge 5$$





# Solving the knapsack problem

## The 0-1 Knapsack problem



- You are going on a camping trip
- You have a knapsack that can carry a maximum weight b > 0.
- There are n different items that you could take.
- Each item of type i has weight  $a_i > 0$ .
- Each item of type i has value  $c_i > 0$ .
- You want to load the knapsack with some of these items
- Which items should you pack? (Without exceeding the knapsack capacity)

## The 0-1 knapsack problem

- As we can pack only one unit of each item we will use binary variables.
- The 0,1 knapsack set K is:

$$K := \left\{ x \in \{0,1\}^n : \sum_{i=1}^n a_i x_i \le b \right\}.$$

• The 0,1 knapsack problem:

$$\max\{c^T x : x \in K\}.$$

In other words,

$$\max \sum_{i=1}^n c_i x_i$$
 s.t. 
$$\sum_{i=1}^n a_i x_i \le b$$
 
$$x_i \in \{0,1\} \text{ for all } i=1,\dots,n.$$

# Why don't we just enumerate possible solutions?

- In the 0-1 Knapsack Problem, what we want is to :
  - Choose a subset  $S \subseteq I$  of possible items  $I = \{1, \dots, n\}$
  - Make sure they fit:  $\sum_{i \in S} a_i \leq b$
  - Maximize: reward =  $\sum_{i \in S} c_i$

Why don't we simply numerate all possible subsets of I, consider the ones that weigh at most b, pick the best among them.

How long will it take to do this using the fastest supercomputer:

	Solutions to check	Time
10	1024	
		2 sec
110		

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50	$2^{50}$	2 sec
110	$2^{110}$	Take a guess

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$\overline{n}$	Solutions to check	Time
3	8	0
10	1024	0
50	$2^{50}$	2 sec
110	$2^{110}$	69 billion years*

<sup>\*</sup>That's four times the age of the universe as we know it!

(remember, I has  $2^n$  distinct subsets.)

# Solving The Knapsack Problem

We will solve the following knapsack problem using branch-and-bound:

$$\begin{split} z^{\mathsf{IP}} &= \max \quad 2x_1 &+ 1x_2 &+ 4x_3 &+ 5x_4 &+ 10x_5 \\ &\text{s. t.} & 8x_1 &+ 2x_2 &+ 5x_3 &+ 4x_4 &+ 2x_5 &\leq 9 \\ &x_1, &x_2, &x_3, &x_4, &x_5 &\in \{0,1\} \end{split}$$

• We start with solving its LP relaxation

$$\max \sum_{i=1}^{n} c_i x_i$$
s. t. 
$$\sum_{i=1}^{n} a_i x_i \le b$$

$$1 \ge x_i \ge 0 \quad x_i \in \{0,1\} \text{ for all } i = 1, \dots, n.$$

• The LP relaxation is solved using the greedy algorithm:

$$z^{\mathsf{LP}} = \max \quad 2x_1 \quad +1x_2 \quad +4x_3 \quad +5x_4 \quad +10x_5$$
 s. t.  $8x_1 \quad +2x_2 \quad +5x_3 \quad +4x_4 \quad +2x_5 \quad \leq 9, \quad \ 1 \geq x_i \geq 0 \ \forall i$ 

- We will next look at properties of an optimal solution of this LP.
- Let  $\bar{x}=(\bar{x}_1,\bar{x}_2,\bar{x}_3,\bar{x}_4,\bar{x}_5)$  be the optimal solution to LP
- Can we have  $\bar{x}_4 > \bar{x}_5$ ?
  - Notice that  $x_5$  gives more bang for the buck.

$$\frac{c_5}{a_5} = \frac{10}{2} > \frac{c_4}{a_4} = \frac{5}{4}$$

- If  $\bar{x}_4 > \bar{x}_5$ , using  $1 \geq x_i \geq 0$  for all  $x_i$ , we know that

$$1 \ge \bar{x}_4 > \bar{x}_5 \ge 0 \implies (i) \ 1 > \bar{x}_5, \quad \text{and} \qquad (ii) \ \bar{x}_4 > 0$$

- Now consider a new solution x' obtained by by decreasing  $\bar{x}_4$  by a tiny number  $\delta > 0$  and increasing  $\bar{x}_5$  twice as much:

$$x' = (\bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4 - \delta, \bar{x}_5 + 2\delta)$$

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• If  $\bar{x}_4 > \bar{x}_5$ , then for some small  $\delta > 0$ , consider

$$x' = (\bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4 - \delta, \bar{x}_5 + 2\delta)$$

• As  $a_4/a_5 = 4/2 = 2$ , the constraint is still satisfied:

$$\sum a_i x_i' = \sum a_i \bar{x}_i - 4\delta + 2 \cdot 2\delta = \sum a_i \bar{x}_i \le b$$

• The new solution x' has a strictly better objective value for any  $\delta > 0$ :

$$\sum c_i x_i' = \sum c_i \bar{x}_i - 5\delta + 20\delta = \sum c_i \bar{x}_i + 15\delta > \sum c_i \bar{x}_i$$

• We also need to make sure that  $1 \ge x' \ge 0$ : How large can  $\delta$  be?

$$-x'_4 = \bar{x}_4 - \delta \in [0, 1] \implies \bar{x}_4 \ge \delta$$
$$-x'_5 = \bar{x}_5 + 2\delta \in [0, 1] \implies \bar{x}_5 + 2\delta \le$$

 $\implies$  Pick  $\delta = \min\left\{\bar{x}_4, \frac{1}{2}(1-\bar{x}_5)\right\} > 0$  to obtain a better LP solution

$$z^{\mathsf{LP}} = \max \quad 2x_1 \quad +1x_2 \quad +4x_3 \quad +5x_4 \quad +10x_5$$
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$$\implies$$
 Pick  $\delta = \min \left\{ \bar{x}_4, \frac{1}{2} (1 - \bar{x}_5) \right\} > 0$  to obtain a better LP solution.

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• We therefore established that if

$$\bar{x} = (\bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4, \bar{x}_5)$$

is an optimal solution to LP then we cannot have  $\bar{x}_4 > \bar{x}_5$ .

- Then, in any optimal solution we must have  $\bar{x}_5 \geq \bar{x}_4$ . [because 10/2 > 5/4 meaning that  $x_5$  gives more bang for the buck]
- How about  $\bar{x}_4$  and  $\bar{x}_3$ ?
- With the same reasoning optimal solution must have  $\bar{x}_4 \geq \bar{x}_3.$  [because 5/4 > 4/5]
- And  $\bar{x}_3 \geq \bar{x}_2$ , and  $\bar{x}_2 \geq \bar{x}_1$ .

You will always prefer items that give more bang for the buck for the LP.

$$z^{\mathsf{LP}} = \max \quad 2x_1 \quad +1x_2 \quad +4x_3 \quad +5x_4 \quad +10x_5$$
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You will always prefer items that give more bang for the buck for the LP.

# Solving the 0-1 knapsack problem with branch and bound

• To solve the LP relaxation of the Knapsack problem:

• Look at the reward/weight ratio  $(c_i/a_i)$  of each item and sort the items:

least desirable 
$$\rightarrow \frac{2}{8} \leq \frac{1}{2} \leq \frac{4}{5} \leq \frac{5}{4} \leq \frac{10}{2} \leftarrow \text{most desirable}$$

• Therefore, in the optimal solution to LP, we have:

$$1 \; \geq \; x_5^{LP} \; \geq \; x_4^{LP} \; \geq \; x_3^{LP} \; \geq \; x_2^{LP} \; \geq \; x_1^{LP} \geq 0$$

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- Moreover if  $x_4^{LP}=x_5^{LP}$  then they must either both 0, or 1.
  - [otherwise, you can again decrease  $x_4$  by  $\delta$  and increase  $x_5$  by  $2\delta$  to improve the objective.]
- Therefore, you will fill your knapsack (fractionally) with more profitable (meaning, larger  $c_i/a_i$ ) items first.

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$$1 \ge x_5^{LP} \ge x_4^{LP} \ge x_3^{LP} \ge x_2^{LP} \ge x_1^{LP} \ge 0$$

- The LP relaxation is solved using the greedy algorithm:
  - Set the remaining budget  $B \leftarrow 9$
  - For j=5,4,3,2,1 (Sorted from best to worst reward/weight ratio.)

if 
$$a_i \leq B$$
, then set  $x_i^{LP} \leftarrow 1$  and  $B \leftarrow B - a_i$ 

if  $a_i \leq B$ , else set  $x_i^{LP} \leftarrow B/a_i$ ; stop

#### Solve the LP relaxation

Solve the LP relaxation using the greedy algorithm:

• Sort the items in decreasing order of reward/weight ratio:

- Set the current budget B=9
- for i = 5, 4, 3, 2, 1 (In order of best to worst reward/weight ratio.)

$$[i = 5]$$
  $2 = a_5 \le B = 9$ , therefore we set  $x_5^{LP} = 1$  and  $B = 9 - 2 = 7$ 

$$[i=4]$$
  $4=a_4 \leq B=7$ , therefore we set  $x_4^{LP}=1$  and  $B=7-4=3$ 

$$[i = 3]$$
 5 =  $a_3 \le B = 3$ , therefore we set  $x_3^{LP} = B/a_3 = 3/5$ ; **stop**

$$x^{\mathsf{LP}} = (0, 0, 3/5, 1, 1)$$

#### Solve the LP relaxation

• Solve the LP relaxation using the greedy algorithm:

- $\bullet \ \, {\rm Solution:} \ \, x^{\rm LP} = (0,0,3/5,1,1) \quad z^{\rm LP} = 17\tfrac{2}{5}$
- $z^{\text{LP}}$  gives an upper bound for IP:  $U = 17\frac{2}{5}$ .
- We do not have a lower bound (need an integral solution) (do we have one?)
- Split the problem into two sub-problems:
- $x_3^{\text{LP}} = 3/5$  is the only fractional variable

- IP<sub>1</sub>: 
$$x_3 \le 0 \implies x_3 = 0$$
 (because  $1 \ge x_3 \ge 0$ )

- 
$$IP_2$$
:  $x_3 \ge 1 \implies x_3 = 1$  (because  $1 \ge x_3 \ge 0$ )

#### Solve the LP relaxation

• Solve the LP relaxation using the greedy algorithm:

- $\bullet \ \, {\rm Solution:} \ \, x^{\rm LP} = (0,0,3/5,1,1) \quad z^{\rm LP} = 17\tfrac{2}{5}$
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- $x_3^{\rm LP}=3/5$  is the only fractional variable
  - IP<sub>1</sub>:  $x_3 \le 0 \implies x_3 = 0$  (because  $1 \ge x_3 \ge 0$ )
  - $IP_2$ :  $x_3 \ge 1 \implies x_3 = 1$  (because  $1 \ge x_3 \ge 0$ )

# Consider subproblem IP<sub>1</sub>

Solve  $LP_1$  with  $x_3 = 0$  (we will consider  $IP_2$  later)

- Solve LP<sub>1</sub> using the greedy algorithm.
- Solution:  $x^{\text{LP1}} = (1/8, 1, 0, 1, 1)$   $z^{\text{LP1}} = 16\frac{1}{4}$
- $x_1^{\mathsf{LP1}}$  is fractional
- We will need to split the problem IP<sub>1</sub> into two sub-problems:
  - IP<sub>3</sub> would have an additional constraint  $x_1 = 0$
  - IP<sub>4</sub> would have an additional constraint:  $x_1 = 1$

# Consider subproblem IP<sub>1</sub>

Solve  $LP_1$  with  $x_3 = 0$  (we will consider  $IP_2$  later)

$$z^{\mathsf{LP1}} = \max_{\substack{s. \, \mathsf{t.}}} 2x_1 + 1x_2 + 0 + 5x_4 + 10x_5 \\ \text{s. \, t.} \quad 8x_1 + 2x_2 + 0 + 4x_4 + 2x_5 \leq 9 \\ x_1, \quad x_2, \quad x_4, \quad x_5 \in [0, 1]$$

- Solve LP<sub>1</sub> using the greedy algorithm.
- Solution:  $x^{LP1} = (1/8, 1, 0, 1, 1)$   $z^{LP1} = 16\frac{1}{4}$
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# Consider subproblem IP2

Solve LP<sub>2</sub> problem with  $x_3 = 1$ 

- Solve LP<sub>2</sub> (with budget 9 5 = 4) using the greedy algorithm.
- Solution:  $x^{\text{LP2}} = (0, 0, 1, 1/2, 1)$   $z^{\text{LP2}} = 16\frac{1}{2}$
- $x_4^{\mathsf{LP2}}$  is fractional
- We need to split the problem IP<sub>2</sub> into two sub-problems:
  - $\text{ IP}_5$ :  $x_4 = 0$
  - $\mathsf{IP}_6$ :  $x_4 = 1$

# Consider subproblem IP2

Solve LP<sub>2</sub> problem with  $x_3 = 1$ 

- Solve LP<sub>2</sub> (with budget 9 5 = 4) using the greedy algorithm.
- $\bullet \ \, {\rm Solution:} \ \, x^{\rm LP2} = (0,0,1,1/2,1) \quad z^{\rm LP2} = 16\tfrac{1}{2}$
- $x_4^{\mathsf{LP2}}$  is fractional
- We need to split the problem IP<sub>2</sub> into two sub-problems:
  - IP<sub>5</sub>:  $x_4 = 0$
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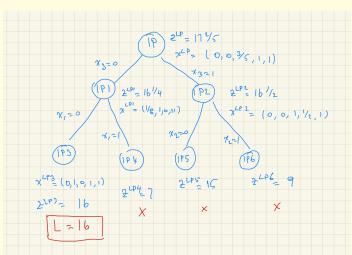
#### Knapsack B&B

(IP) 
$$z^{\text{IP}} = \max_{\mathbf{x}} 2x_1 + 1x_2 + 4x_3 + 5x_4 + 10x_5$$
  
s. t.  $8x_1 + 2x_2 + 5x_3 + 4x_4 + 2x_5 \le 9$   
 $x_1, x_2, x_3, x_4, x_5 \in \{0, 1\}$   
LP solution:  $x^{\text{LP}} = (0, 0, 3/5, 1, 1), z^{\text{LP}} = 17\frac{2}{5}$ 

$$\begin{split} \text{(IP$_1$)} \ \ [x_3 = 0] \qquad & x^{\text{LP1}} = (1/8, 1, 0, 1, 1) \quad z^{\text{LP1}} = 16\frac{1}{4} \\ \text{(IP$_3$)} \ \ [x_3 = 0, x_1 = 0] \quad & x^{\text{LP3}} = (0, 1, 0, 1, 1), \ z^{\text{LP3}} = z^{\text{IP3}} = 16 \ \leftarrow \ \textbf{\textit{L}} \\ \text{(IP$_4$)} \ \ [x_3 = 0, x_1 = 1] \quad & x^{\text{LP4}} = (1, 0, 0, 0, 1/2), \quad z^{\text{LP4}} = 7 < \textbf{\textit{L}} \\ \text{(IP$_2$)} \ \ & x_3 = 1 \qquad x^{\text{LP2}} = (0, 0, 1, 1/2, 1) \quad & w^2 = 16\frac{1}{2} \\ \text{(IP$_5$)} \ \ [x_3 = 1, x_4 = 0] \quad & x^{\text{LP5}} = (0, 1, 1, 0, 1), \quad z^{\text{LP5}} = z^{\text{IP5}} = 15 < \textbf{\textit{L}} \\ \text{(IP$_6$)} \ \ & [x_3 = 1, x_4 = 1] \quad & x^{\text{LP6}} = (0, 0, 1, 1, 0), \quad z^{\text{LP6}} = z^{\text{IP6}} = 9 < \textbf{\textit{L}} \end{split}$$

#### The B&B tree

(IP) 
$$z^{\text{IP}} = \max_{\mathbf{x}} 2x_1 + 1x_2 + 4x_3 + 5x_4 + 10x_5$$
  
s.t.  $8x_1 + 2x_2 + 5x_3 + 4x_4 + 2x_5 \le 9$   
 $x_1, x_2, x_3, x_4, x_5 \in \{0, 1\}$ 



### A small detour: What is the "knap" in knapsack?

- In English knap means
  - Crest of a hill (summit), if it is a noun
  - To break with a quick blow, if it is a verb.
- But then, why do we call a knapsack a knapsack?
- Possible answers from different languages: (this part is not completely factual)
  - It comes from Arabic, where it means treasure.
  - It comes from German, where it means to bite
  - It comes from Dutch, where it means laundry.

Question: Which one is it?

### A small detour: What is the "knap" in knapsack?

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  - It comes from Arabic, where it means treasure.
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  - It comes from Dutch, where it means laundry.

Question: Which one is it?

Answer: Knapsack comes from the German *knappen*, "to bite," and some experts believe that the name evolved from the fact that soldiers carried food in their knapsacks.

# Integer Knapsack

(1/31/2024)

#### The integer knapsack problem



- You are going on a camping trip
- You have a knapsack that can carry a maximum weight b > 0.
- There are *n* different items that you could take.
- Each item of type i has weight  $a_i > 0$ .
- Each item of type i has value  $c_i > 0$ .
- You can pack up to  $u_i$  copies of item of type i.
- You want to load the knapsack with items (possibly several items of the same type).
- Which how many copies of each item should you pack?
   (Without exceeding the knapsack capacity)

# IP formulation of the 0-1 integer knapsack problem

- Now we can pack multiple copies of the same item in the *knap*sack,
- Let variable  $x_i \in \mathbb{Z}$  represent the number of items of type i that you pack.
- The **knapsack set** S contains all feasible loads:

$$S := \left\{ x \in \mathbb{Z}^n : \sum_{i=1}^n a_i x_i \le b, \ u \ge x \ge 0 \right\}.$$

• The integer knapsack problem is:

$$\max\Big\{\sum_{i=1}^n c_i x_i : x \in S\Big\}.$$

In other words,

$$\max \sum_{i=1}^{n} c_i x_i$$
s. t. 
$$\sum_{i=1}^{n} a_i x_i \le b$$

 $u_i \ge x_i \ge 0$  and integer for all  $i = 1, \dots, n$ 

To solve the LP relaxation of the Knapsack problem:

• Look at the reward/weight ratio  $(c_i/a_i)$  of each item and sort the items:

least desirable 
$$\rightarrow \frac{1}{4} \leq \frac{5}{10} \leq \frac{4}{5} \leq \frac{5}{4} \leftarrow \text{most desirable}$$

 In the optimal LP solution more desirable items would be picked first (up to their upper bounds) before less desirable items.

• To solve the LP relaxation of the Knapsack problem:

$$\begin{split} z^{\mathsf{IP}} &= \max \quad 1x_1 \quad + 5x_2 \quad + 4x_3 \quad + 5x_4 \\ &\qquad \text{s. t.} \quad 4x_1 \quad + 10x_2 \quad + 5x_3 \quad + 4x_4 \quad \leq \ 29 \\ \\ &\qquad 3 \geq x_1 \geq 0, \ 2 \geq x_2 \geq 0, \ 1 \geq x_3 \geq 0, \ 2 \geq x_4 \geq 0 \text{ and integer} \end{split}$$

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- In the optimal LP solution more desirable items would be picked first (up to their upper bounds) before less desirable items.
- Meaning
  - If  $x_4 < 2$ , then  $x_3 = 0$
  - If  $x_3 < 1$ , then  $x_2 = 0$
  - If  $x_2 < 2$ , then  $x_1 = 0$

• To solve the LP relaxation of the Knapsack problem:

$$\begin{split} z^{\mathsf{IP}} &= \max \quad 1x_1 \quad + 5x_2 \quad + 4x_3 \quad + 5x_4 \\ &\quad \text{s. t.} \quad 4x_1 \quad + 10x_2 \quad + 5x_3 \quad + 4x_4 \quad \leq \ 29 \\ \\ &\quad 3 \geq x_1 \geq 0, \ 2 \geq x_2 \geq 0, \ 1 \geq x_3 \geq 0, \ 2 \geq x_4 \geq 0 \text{ and integer} \end{split}$$

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- The LP relaxation is solved using the greedy algorithm:
  - Set the remaining budget  $B \leftarrow 29$
  - for i = 4, 3, 2, 1 (Sorted from best to worst reward/weight ratio.)

if 
$$a_i u_i \leq B$$
, then set  $x_i^* \leftarrow u_i$  and  $B \leftarrow B - a_i u_i$   
if  $a_i u_i \leq B$ , else set  $x_i^* \leftarrow B/a_i$ ; stop

• To solve the LP relaxation of the Knapsack problem:

• Look at the reward/weight ratio  $(c_i/a_i)$  of each item and sort the items:

least desirable 
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• For i = 4, 3, 2, 1 (In order of best to worst reward/weight ratio.)

$$\begin{split} [j=4] \quad &8 = a_4 u_4 \leq B = 29, \ \, \Rightarrow \text{set} \,\, x_4^{LP} = 2 \,\, \text{and} \,\, B = 29 - 8 = 21 \\ [j=3] \quad &5 = a_3 u_3 \leq B = 21, \ \, \Rightarrow \text{set} \,\, x_3^{LP} = 1; \,\, \text{and} \,\, B = 21 - 5 = 16 \\ [j=3] \quad &20 = a_2 u_2 \not \leq B = 16, \ \, \Rightarrow \text{set} \,\, x_2^{LP} = B/a_2 = 16/10; \quad \textbf{Stop} \\ x^{\text{LP}} = (0, \ 1.6, \ 1, \ 2) \quad \text{and} \quad z^{\text{LP}} = 5(1.4) + 4(1) + 5(2) = 14.8 \leftarrow \textbf{\textit{U}} \end{split}$$

(rest will be in next homework)

What can you say about the following 3 sets:

$$K^{1} = \left\{ x \in \{0, 1\}^{3} : 3x_{1} + 4x_{2} + 5x_{3} \leq 6 \right\}$$

$$K^{2} = \left\{ x \in \{0, 1\}^{3} : \begin{array}{c} x_{1} + x_{2} \leq 1 \\ x_{1} + x_{3} \leq 1 \end{array} \right\}$$

$$K^{3} = \left\{ x \in \{0, 1\}^{3} : x_{1} + x_{2} + x_{3} \leq 1 \right\}$$

Are they the same or are they different?

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Are they the same or are they different?

They are the same:

$$K^1 = K^2 = K^3 = \Big\{(0,0,0), (1,0,0), (0,1,0), (0,0,1)\Big\}$$

Now lets look at the polyhedra (relaxations) defining them:

$$P^{1} = \left\{ x \in \mathbb{R}^{3} : 3x_{1} + 4x_{2} + 5x_{3} \leq 6, \ 1 \geq x_{i} \geq 0 \ \forall i \right\}$$

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$$P^{3} = \left\{ x \in \mathbb{R}^{3} : x_{1} + x_{2} + x_{3} \leq 1, \ 1 \geq x_{i} \geq 0 \ \forall i \right\}$$

Claim 1: 
$$P^1 \supseteq P^2$$
:

*Proof.* If  $\bar{x} \in P^2$  then

$$\begin{vmatrix} \bar{x}_1 + \bar{x}_2 & \leq & 1 \\ 2\bar{x}_1 + 2\bar{x}_3 & \leq & 2 \\ 3\bar{x}_2 + 3\bar{x}_3 & \leq & 3 \end{vmatrix} \Longrightarrow 3\bar{x}_1 + 4\bar{x}_2 + 5\bar{x}_3 \leq 6 \Longrightarrow \bar{x} \in P$$

Did we prove the claim? No. We also need to argue that  $P^1 \neq P^2$ 

We have  $x' = (1, 3/4, 0) \in P^1$  but  $x' \notin P^2$ 

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\end{vmatrix} \implies 3\bar{x}_1 + 4\bar{x}_2 + 5\bar{x}_3 \leq 6 \implies \bar{x} \in P^1$$

Did we prove the claim? No. We also need to argue that  $P^1 \neq P^2$ 

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$$P^{3} = \left\{ x \in \mathbb{R}^{3} : x_{1} + x_{2} + x_{3} \leq 1, \ 1 \geq x_{i} \geq 0 \ \forall i \right\}$$

Claim 2:  $P^2 \supseteq P^3$ .

**Proof.** If  $\bar{x} \in P^3$  then  $\bar{x}_i \ge 0 \ \forall i$  and

$$\bar{x}_1 + \bar{x}_2 + \bar{x}_3 \le 1 \implies \bar{x}_i + \bar{x}_j \le 1 \ \forall i, j \implies \bar{x} \in P^2$$

To complete the proof:

Also notice that 
$$x'' = (1/2, 1/2, 1/2) \in P^2$$
 but  $x'' \notin P^3$ 

Now lets look at the polyhedra (relaxations) defining them:

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To complete the proof:

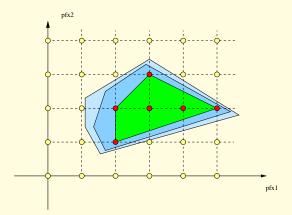
Also notice that 
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 but  $x'' \notin P^3$ 

#### Geometrically

They are different ways to formulate the same integer program:

$$P^1 \supsetneqq P^2 \supsetneqq P^3 \ \ \text{where as} \ \ K^1 = K^2 = K^3$$

where  $K^i = P^i \cap \mathbb{Z}^n$  for i = 1, 2, 3



#### Two formulations of the same IP problem

$$(IP_1)$$

$$z^{IP1} = \max \quad 7x_1 + 8x_2 + 9x_3$$
s.t.  $x_1 + x_2 \le 1$ 

$$x_1 + x_3 \le 1$$

$$x_2 + x_3 \le 1$$

$$x_1, x_2, x_3 \in \{0, 1\}$$

$$(IP_2)$$

$$z^{IP2} = \max \quad 7x_1 + 8x_2 + 9x_3$$
s.t.  $x_1 + x_2 + x_3 \le 1$ 

$$x_1, x_2, x_3 \in \{0, 1\}$$

#### Optimal solutions to LP relaxations:

$$\begin{split} \mathsf{LP_1} \colon \, x^{\mathsf{LP1}} &= (\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}), \quad z^{\mathsf{LP1}} = 12 \implies \quad 12 \geq z^{\mathsf{IP_1}} = z^{\mathsf{IP2}} \\ \mathsf{LP_2} \colon \, x^{\mathsf{LP2}} &= (0, 0, 1), \quad z^{\mathsf{LP2}} = \quad 9 \implies \quad 9 \geq z^{\mathsf{IP1}} = z^{\mathsf{IP2}} \\ x^{\mathsf{LP2}} \text{ is feasible for } \mathsf{IP_1} \text{ and } \mathsf{IP_2}! \implies \quad z^{\mathsf{IP1}} = z^{\mathsf{IP2}} \geq 1 \end{split}$$

Two formulations of the same IP problem

$$z^{\mathsf{IP1}} = \max \quad 7x_1 + 8x_2 + 9x_3$$
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$$x_1 + x_3 \le 1$$

$$x_2 + x_3 \le 1$$

$$x_1, x_2, x_3 \in \{0, 1\}$$

$$z^{\mathsf{IP2}} = \max \quad 7x_1 + 8x_2 + 9x_3$$
s.t.  $x_1 + x_2 + x_3 \le 1$ 

$$x_1, x_2, x_3 \in \{0, 1\}$$

Optimal solutions to LP relaxations:

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## Modeling with Binary Variables

## Binary variables

- Help model yes/no decisions:  $x_i \in \{0, 1\}$ 
  - $-x_i=0$  if the decision is "no",
  - $-x_i=1$  if it is "yes"
- They can also model logical operators. When 3 cousins go out to have ice cream, if their grandma says:
  - Mario or Luigi can have ice cream, but **not both**:

$$x_{\text{Mario}} + x_{\text{Luigi}} \le 1$$

— At least one among Mario and Luigi will have ice cream:

$$x_{\mathrm{Mario}} + x_{\mathrm{Luigi}} \ge 1$$

— If Mario has ice cream, then Giovanni will have one too:

$$x_{\text{Mario}} \le x_{\text{Giovanni}}$$

Luigi gets ice cream if and only if Giovanni does not get any:

$$x_{\text{Luigi}} = 1 - x_{\text{Giovanni}}$$

## Facility Location Problem

- A set J of retailers has to be served by a set of plants, yet to be built.
- ullet There is a set I of potential sites for plants, and there is
  - a cost  $f_i$  for building plant  $i \in I$
  - a (transportation) cost  $c_{ij}$  from plant  $i \in I$  to retailer  $j \in J$
- Each retailer  $j \in J$  will be served by exactly one plant  $i \in I$ .
- Choose a subset S of I such that the total cost is minimized.

#### Variables:

 $-x_i \in \{0,1\}$  for  $i \in I$  indicates if plant is built

$$x_i = \begin{cases} 1 & \text{if plant } i \text{ is built} \\ 0 & \text{otherwise} \end{cases}$$

 $-y_{ij} \in \{0,1\}$  indicates if retailer  $j \in J$  is assigned to  $i \in I$ :

$$y_{ij} = \left\{ egin{array}{ll} 1 & ext{if } i ext{ serves retailer } j \ 0 & ext{otherwise} \end{array} 
ight.$$

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#### **Objective function:**

$$\sum_{i \in I} f_i x_i + \sum_{i \in I} \sum_{j \in J} c_{ij} y_{ij}$$

#### **Constraints:**

• Each retailer  $j \in J$ , should be assigned to one plant:

$$\sum_{i \in I} y_{ij} = 1 \qquad \forall j \in J$$

• A retailer  $j \in J$  can be assigned to plant  $i \in I$  only if it is built:

$$y_{ij} \le x_i \quad \forall i \in I, j \in J$$

or, alternatively:

$$\sum_{j \in J} y_{ij} \le |J| x_i \qquad \forall i \in I$$

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## Two correct formulations for the facility location problem

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- Which one to use?
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$$\bar{y}_{ij} \le \bar{x}_i, \ \forall j \in J \implies \sum_{j \in J} \bar{y}_{ij} \le |J|\bar{x}_i$$

Implying that,  $(\bar{x}, \bar{y})$  is a feasible solution to LP<sub>2</sub>. Therefore  $P_1 \subset P_2$ 

• When |I| = 150, |J| = 50,  $|P_2|$  takes an hour,  $|P_1|$  takes seconds to solve.

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## Size of formulations: Counting non-zero entries of constraint matrix

#### $IP_1$

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s. t. 
$$\sum_{i \in I} y_{ij} = 1 \quad \forall j \in J$$
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$$x_i, y_{ij} \in \{0, 1\} \ \forall i \in I, j \in J$$

#### Non-zeroes:

- $\leftarrow$  objective has  $|I| + |I| \cdot |J|$  nonzeroes (not important)
- $\leftarrow \quad \text{Each one has } 2 \text{ nonzeroes} \\ \implies 2|I|\cdot|J|$
- When |I|=150, |J|=50, the nonzero entries of the constraint matrix is  $3|I|\cdot |J|=3\cdot 150\cdot 50=22,500$
- It has  $|I| + |I| \cdot |J| = 150 + 150 \cdot 50 = 7600$  binary variables
- Generally, formulations with fewer nonzeroes and fewer integer variables solve faster but the strength of the LP formulation matters most.

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#### IP₁

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$$\sum_{i \in I} y_{ij} = 1 \quad \forall j \in J$$
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- $\leftarrow \quad \text{Each one has } |I| \text{ nonzeroes} \\ \Longrightarrow \quad |I| \cdot |J|$
- $\leftarrow \quad \text{Each one has } 2 \text{ nonzeroes} \\ \implies 2|I|\cdot|J|$
- $\leftarrow$  There are |I| many x variables and  $|I| \cdot |J|$  many y variables.
- When |I|=150, |J|=50, the nonzero entries of the constraint matrix is  $3|I|\cdot|J|=3\cdot150\cdot50=22,500$
- It has  $|I| + |I| \cdot |J| = 150 + 150 \cdot 50 = 7600$  binary variables
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# A Brief Detour to Machine Learning and a Clustering Problem

## Supervised vs. unsupervised learning tasks

• In supervised ML each data point  $x=[x_1,x_2,\ldots]$  has a label(s) y and the ML task is to guess y correctly. i.e. Find a function f such that

$$f(x) \approx y$$

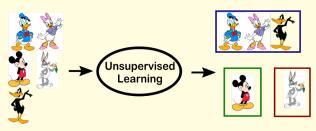
- Classification: if y takes discrete values i.e.  $y \in \{good, bad, ugly\}$
- **Regression**: if y takes continuous values i.e.  $y \in [0,8]$  (height)
- In unsupervised ML there are no labels and goal is to infer a structure present within the data points. Example:

## Supervised vs. unsupervised learning tasks

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## An unsupervised ML task: Clustering

- Clustering is an ML problem that involves the grouping of data points.
  - Data points in the same cluster should be "similar"
  - Data points in different clusters should be "dissimilar".
- ullet Each data point is represented by its features  $x \in \mathbb{R}^n$
- Given points  $x^i, x^j \in \mathbb{R}^n$ , how to measure similarity?
  - For example we can use the Euclidean distance between the points

$$d(i,j) = \|x^i - x^j\|_2 = \sqrt{\sum_{k=1}^n (x_k^i - x_k^j)^2}$$

- Points with smaller distance can be considered more similar.
- Depending on the application there might be different ways to measure similarity (distance).
- Given a collection of points and distances between them we can now define the clustering problem formally.

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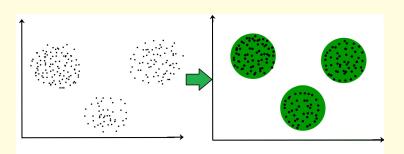
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- Depending on the application there might be different ways to measure similarity (distance).
- Given a collection of points and distances between them we can now define the clustering problem formally.

Given an integer k>1 and a collection of points  $X=\{x^1,x^2,\ldots\}$  together with distances between pairs of these points. Partition the points in X into k clusters  $C_1,\ldots,C_k$ , such that minimum distance between pairs of points in different clusters:

$$\min_{i \in C_p, \ j \in C_q, \ p \neq q} d(i, j)$$

is maximized.



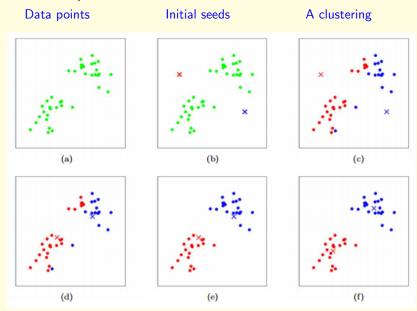
## Lloyd's algorithm: K-Means clustering

Clustering problem: Partition X into clusters  $C_1, \ldots, C_k$  so as to maximize minimum distance between clusters :

$$d^* = \max_{C_1 \dots, C_k \text{ is a partition }} \left( \min_{i \in C_p, j \in C_q, \, p \neq q} d(i, j) \right)$$

- K-Means is the most popular clustering algorithm (it is a heuristic).
  - 1. Randomly pick k seed points (one for each cluster).
  - 2. Assign points to the closest seed to form the clusters.
  - 3. Change the seed points to a "central" point in each cluster
  - 4. Repeat until clusters do not change much.
  - 5. Return the best solution found during the search
- Easy to understand and implement.
- It is a good heuristic for the clustering problem (practical performance).

## K-Means example



## Clustering when $d(i, j) \in \{0, 1\}$

(points are either similar or dissimilar)

#### Consider the following clustering problem:

- There are n objects  $N = \{1, \ldots, n\}$ .
- Any pair of objects  $i,j \in N$  is either similar (d(i,j)=0) or dissimilar (d(i,j)=1)
- We are given a set D that contains pairs of dissimilar objects (the other pairs are similar)
- We want to cluster the objects in exactly k clusters so that each cluster  $C_1, \ldots, C_k$  consists of items that are mostly similar to each other.  $K = \{1, \ldots, k\}$
- Each cluster must contain at least ℓ objects.
- Model this as an IP where we the objective is to minimizing the total number of pairs of dissimilar objects put in the same cluster.

#### Input:

- n objects numbered  $1, 2, \ldots, n$
- Desired number of clusters k, and a lower bound  $\ell$  on the number of objects in a cluster
- A set D of pairs of dissimilar objects

#### Output:

- ullet A partitioning of the objects into cluster  $C_1, C_2, \dots, C_k$ 
  - Partitioning means:
  - (i)  $C_1 \cup C_2 \cup \cdots \cup C_k = \{1, 2, \dots, n\}$ , and
  - (ii)  $C_s \cap C_t = \emptyset$  for all  $s \neq t$ .

#### Goal:

• Minimize the total number of pairs  $\{i,j\}$  where i and j are clustered in the same cluster, but are dissimilar (meaning,  $\{i,j\} \in D$ )

#### Decision variables

$$y_{is} \stackrel{\text{interpretation}}{=} \begin{cases} 1 & \text{if object } i \text{ is put in cluster } C_s \\ 0 & \text{otherwise.} \end{cases}$$
 
$$x_{ijs} \stackrel{\text{interpretation}}{=} \begin{cases} 1 & \text{if both objects } i \text{ and } j \text{ are put in cluster } C_s \\ 0 & \text{otherwise.} \end{cases}$$
 (only for  $i < j$ )

$$x_{ijs} \in \{0, 1\}$$
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$$\begin{array}{lll} \min & \sum_{\{i,j\} \in D} \sum_{s \in K} x_{ijs} & \longleftarrow & \text{dissimilar pairs in the same cluster} \\ \text{s.t.} & \sum_{s \in K} y_{is} = 1 & \forall i \in N & \longleftarrow & \text{objects} \\ & \sum_{i \in N} y_{is} \geq \ell & \forall s \in K & \longleftarrow & \text{clusters} \\ & \text{How do we say:} & x_{ijs} = & \begin{cases} 1 & \text{if } y_{is} = 1 \text{ and } y_{js} = 1 \\ 0 & \text{otherwise.} \end{cases} \\ & x_{ijs} \in \{0,1\} & \forall i < j \in N \;, \forall s \in K \end{cases}$$

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$$x_{ijs} = \begin{cases} 1 & \text{if } y_{is} = 1 \text{ and } y_{js} = 1 \\ 0 & \text{otherwise.} \end{cases}$$

using the fact that x and y take  $\{0,1\}$  values?

• First idea: We can write

$$x_{ijs} \ge y_{is} + y_{js} - 1$$

and

$$x_{ijs} \le \frac{1}{2}(y_{is} + y_{js})$$

- When both  $y_{is} = 1$  and  $y_{js} = 1$  the we have

$$x_{ijs} \ge 1 + 1 - 1 = 1$$
 and  $x_{ijs} \le \frac{1}{2}(1+1) = 1 \implies x_{ijs} = 1$ 

- If not, then we must have  $y_{is}+y_{js}\leq 1$  and

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- It works! (because  $x_{ijs} \in \{0,1\}\}$ )

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## Clustering Problem: Formulation 0

Decision variables

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 (only for  $i < j$ )

$$\begin{array}{lll} & \min & \sum_{\{i,j\} \in D} \sum_{s \in K} x_{ijs} \\ & \text{s.t.} & \sum_{s \in K} y_{is} = 1 & \forall i \in N & \longleftarrow \text{ objects} \\ & \sum_{i \in N} y_{is} \geq \ell & \forall s \in K & \longleftarrow \text{ clusters} \\ & x_{ijs} \geq y_{is} + y_{js} - 1 & \forall i < j \in N \;, s \in K \\ & x_{ijs} \leq \frac{1}{2} (y_{is} + y_{js}) & \forall i < j \in N \;, s \in K \\ & x_{ijs} \in \{0,1\} & \forall i < j \in N \;, \forall s \in K \\ & y_{is} \in \{0,1\} & \forall i \in N \;, \forall s \in K \end{array}$$

• We want to say:

$$x_{ijs} = \begin{cases} 1 & \text{if } y_{is} = 1 \text{ and } y_{js} = 1 \\ 0 & \text{otherwise.} \end{cases}$$

using the fact that x and y take  $\{0,1\}$  values?

• This is same as

$$x_{ijs} = y_{is}y_{js}$$

- But we cannot write this in a linear integer program.
- So instead we wrote 2 linear inequalities

$$x_{ijs} \ge y_{is} + y_{js} - 1$$

and

$$x_{ijs} \le \frac{1}{2}(y_{is} + y_{js})$$

Question: Can we do better?

## Taking a step back: Multiplying binary variables

- Let  $y_1 \in \{0,1\}$  and  $y_2 \in \{0,1\}$  be two binary variables.
- Assume we are interested in their product  $y_1 \cdot y_2$ .
- How can we express their product  $x = y_1y_2$  using linear inequalities?

$$x = \begin{cases} 1 & \text{if } y_1 = 1 \text{ and } y_2 = 1 \\ 0 & \text{otherwise.} \end{cases}$$

Consider the following inequalities:

$$\begin{aligned} x &\leq y_1 \\ x &\leq y_2 \\ x &\geq 0 \\ x &\geq y_1 + y_2 - 1 \end{aligned}$$

#### Claim

If  $y_1, y_2 \in \{0, 1\}$  and x satisfies the constraints above, then

$$x = y_1 y_2$$

#### Claim

If  $x, y_1, y_2$  satisfy the McCormick constraints

$$x \le y_1,$$
  
 $x \le y_2,$   
 $x \ge y_1 + y_2 - 1,$   
 $x \ge 0,$ 

and

$$y_1, y_2 \in \{0, 1\}$$

then  $x = y_1 y_2$ .

#### **Proof**:

$oldsymbol{y}_1$	$oldsymbol{y}_2$	constraints		
0	0	$x \leq y_1$ ,	$x \ge 0$	0
0	1	$x \leq y_1$ ,	$x \ge 0$	0
1	0	$x \leq y_2$ ,	$x \ge 0$	0
1	1	$x \ge y_1 + y_2 - 1,$	$x \le y_1$	1

## Back to Formulation 0 for the Clustering Problem

Decision variables

$$y_{is} = \begin{cases} 1 & \text{if } i \text{ in } C_s \\ 0 & \text{otherwise.} \end{cases} \qquad x_{ijs} = \begin{cases} 1 & \text{if both } i \text{ and } j \text{ are in } C_s \\ 0 & \text{otherwise.} \end{cases}$$

(Notice that we want  $x_{ijs}$  variable to be equal to  $y_{is} \cdot y_{js}$ )

$$\begin{array}{lll} \min & \sum_{\{i,j\} \in D} \sum_{s \in K} x_{ijs} \\ \\ \text{s.t.} & \sum_{s \in K} y_{is} = 1 \qquad \forall i \in N \qquad \longleftarrow \quad \text{objects} \\ & \sum_{i \in N} y_{is} \geq \ell \qquad \forall s \in K \qquad \longleftarrow \quad \text{clusters} \\ & x_{ijs} \geq y_{is} + y_{js} - 1 \qquad \forall i < j \in N \;, s \in K \\ & x_{ijs} \leq \frac{1}{2} (y_{is} + y_{js}) \qquad \forall i < j \in N \;, s \in K \\ & x_{ijs} \in \{0,1\} \qquad \forall i < j \in N \;, \forall s \in K \\ & y_{is} \in \{0,1\} \qquad \forall i \in N \;, \forall s \in K \end{array}$$

## Clustering Problem: Formulation 1

Decision variables

$$y_{is} = \begin{cases} 1 & \text{if } i \text{ in } C_s \\ 0 & \text{otherwise.} \end{cases} \qquad x_{ijs} = \begin{cases} 1 & \text{if both } i \text{ and } j \text{ are in } C_s \\ 0 & \text{otherwise.} \end{cases}$$

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## Comparing formulations 0 and 1

• Size of the formulation for n=40 objects and k=3 clusters:

	variables	constraints	nonzeros
Formulation 0	2,460	4,723	14,280
Formulation 1	2,460	7,063	16,620

 $-y_{is}$  variables:  $40 \times 3 = 120$ 

 $- x_{ijs}$  variables:  $\binom{40}{2} \times 3 = 780 \times 3 = 2340$ 

Solution time

	B& B nodes	Simplex iterations	Solution time
Formulation 0		11,210,558	
Formulation 1	23,050	4,033,965	159.24 seconds

- Formulation 1 is  $\approx$  20% faster per B&B node and much fewer nodes are needed. (Remember, at each node we solve an LP)
- In both formulations x variables are declared binary
- Form.0 has 2 constraints for each  $x_{ijs}$  variable, Form.1 has 3.

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 $-y_{is}$  variables:  $40 \times 3 = 120$ 

 $-x_{ijs}$  variables:  $\binom{40}{2} \times 3 = 780 \times 3 = 2340$ 

#### Solution time:

	B& B nodes	Simplex iterations	Solution time
Formulation 0	40,560	11,210,558	327.78 seconds
Formulation 1	23,050	4,033,965	159.24 seconds

- Formulation 1 is  $\approx$  20% faster per B&B node and much fewer nodes are needed. (Remember, at each node we solve an LP)
- In both formulations x variables are declared binary
- Form.0 has 2 constraints for each  $x_{ijs}$  variable, Form.1 has 3.

## Optional Weekend Homework:)

- Winnie the Pooh has 9 pots with honey whose weights are 1, 2, ..., 9 lbs.
- Each pot has its weight written on it.
- In addition, someone put a small (1 oz) piece of cheese into one of the pots.

Question: How can Winnie, in two weighings on a balance scale (with no additional weights), find out which pot contains the cheese?





# next time

Observation 0: If  $x, y_1, y_2$  satisfy the constraints

$$\begin{split} x &\geq y_1 + y_2 - 1 \\ x &\leq \frac{1}{2}(y_1 + y_2) \\ y_1, y_2 &\in \{0,1\} \text{ and } x \in \{0,1\} \end{split}$$

then  $x = y_1y_2$ . (i.e., x = 1 only when both  $y_1 = 1$  and  $y_2 = 1$ )

Without  $x \in \{0,1\}$ , the point  $\underbrace{(1,0,\frac{1}{2})}_{(y_1,y_2,x)}$  is feasible to the system above.

Observation 1: If  $x, y_1, y_2$  satisfy the constraints

$$x \le y_1, \quad x \le y_2,$$
  
 $x \ge 0, \quad x \ge y_1 + y_2 - 1,$   
 $y_1, y_2 \in \{0, 1\}$ 

then  $x = y_1y_2$ . Notice that x variable is not declared to be binary

Observation 0: If  $x, y_1, y_2$  satisfy the constraints

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$$x \leq \frac{1}{2}(y_1 + y_2)$$
 
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## Clustering Problem: Formulation 1<sup>+</sup>

#### Decision variables

$$y_{is} = \begin{cases} 1 & \text{if } i \text{ in } C_s \\ 0 & \text{otherwise.} \end{cases} \qquad x_{ijs} = \begin{cases} 1 & \text{if both } i \text{ and } j \text{ are in } C_s \\ 0 & \text{otherwise.} \end{cases}$$

$$\begin{array}{llll} & \min & \sum_{\{i,j\} \in D} \sum_{s \in K} x_{ijs} \\ & \text{s.t.} & \sum_{s \in K} y_{is} = 1 & \forall i \in N & \longleftarrow & \text{objects} \\ & \sum_{i \in N} y_{is} \geq \ell & \forall s \in K & \longleftarrow & \text{clusters} \\ & x_{ijs} \geq y_{is} + y_{js} - 1 & \forall i < j \in N \;, s \in K \\ & x_{ijs} \leq y_{is}, \; x_{ijs} \leq y_{js} & \forall i < j \in N \;, s \in K \\ & \underbrace{x_{ijs} \in \{0,1\}} \; x_{ijs} \geq 0 & \forall i < j \in N \;, s \in K \\ & y_{is} \in \{0,1\} & \forall i \in N \;, s \in K \end{array}$$

# Comparing formulations 0, 1 and $1^+$

• Size of the formulation for n=40 objects and k=3 clusters:

	variables	constraints	nonzeros
Formulation 0	2,460	4,723	14,280
Formulation 1	2,460	7,063	16,620
Formulation $1^+$	2,460	7,063	16,620

- $-y_{is}$  variables:  $40 \times 3 = 120$  ← binary
- $-x_{ijs}$  variables:  $\binom{40}{2} \times 3 = 780 \times 3 = 2340 \leftarrow \text{continuous in F } 1^+$

Solution time

			Solution time
Formulation 0		11,210,558	
Formulation 1	23,050	4,033,965	159.24 seconds
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 $-\,$  Formulation  $1^+$  is 5 imes faster than Formulation 1

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	B& B nodes	Simplex iterations	Solution time
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Clustering Problem: Formulation 1<sup>++</sup>

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$$y_{is} = \begin{cases} 1 & \text{if } i \text{ in } C_s \\ 0 & \text{otherwise.} \end{cases} \qquad x_{ijs} = \begin{cases} 1 & \text{if both } i \text{ and } j \text{ are in } C_s \\ 0 & \text{otherwise.} \end{cases}$$

IP Formulation:

$$\begin{array}{lll} & \min & \sum_{\{i,j\} \in D} \sum_{s \in K} x_{ijs} \\ & \text{s.t.} & \sum_{s \in K} y_{is} = 1 & \forall i \in N & \longleftarrow \text{ objects} \\ & \sum_{i \in N} y_{is} \geq \ell & \forall s \in K & \longleftarrow \text{ clusters} \\ & x_{ijs} \geq y_{is} + y_{js} - 1 & \forall i < j \in N \;, s \in K \\ & x_{ijs} \leq y_{is} \;, \; x_{ijs} \leq y_{js} & \forall i < j \in N \;, s \in K \\ & x_{ijs} \geq 0 & \forall i < j \in N \;, s \in K \\ & y_{is} \in \{0,1\} & \forall i \in N \;, s \in K \end{array}$$

Question: In an optimal sol., would  $x_{ijs} = 1$  if either  $y_{is} = 0$  or  $y_{js} = 0$ ?

## Comparing the Formulations 0, 1, $1^+$ and $1^{++}$

• Size of the formulation:

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- Form.  $1^{++}$  enumerates more nodes but the speed up is 6x.
- LPs are now much easier to solve (fewer constraints and non-zeroes)

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# Clustering Problem: Formulation 2

Decision variables

$$y_{is} \overset{\text{interpretation}}{=} \begin{cases} 1 & \text{if object } i \text{ is put in cluster } C_s \\ 0 & \text{otherwise.} \end{cases}$$
 
$$z_{ij} \overset{\text{interpretation}}{=} \begin{cases} 1 & \text{if objects } i \text{ and } j \text{ are put in the same cluster} \\ 0 & \text{otherwise.} \end{cases}$$
 (only for  $i < j$ )

$$\begin{array}{lll} \min & \sum_{\{i,j\}\in D} z_{ij} \\ \text{s.t.} & \sum_{s\in K} y_{is} = 1 & \forall i\in N & \longleftarrow \text{ objects} \\ & \sum_{i\in N} y_{is} \geq \ell & \forall s\in K & \longleftarrow \text{ clusters} \\ & \text{How to say } z_{ij} = 1 & \text{when both } y_{is}, y_{js} = 1 \text{ for some } s\in K \\ & z_{ij} \geq 0 & \forall i< j\in N \\ & y_{is} \in \{0,1\} & \forall i\in N \ , s\in K \end{array}$$

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(Formulation 2 is 35% faster than Formulation  $1^{++}$ )

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#### Non-zeroes of a formulation

Consider the following LP formulation

$$\label{eq:continuous} \begin{array}{ll} \text{minimize} & c^T x \\ \text{subject to} & A^1 x \geq b^1, \\ & A^2 x = b^2, \\ & x > 0 \end{array}$$

- The non-zeroes of this formulation is the number of nonzero entries in the matrices A<sup>1</sup> and A<sup>2</sup>.
- In practice LPs are solved using either the simplex method or interior point algorithms,
- In both cases one has to solve (many, many) linear equations
- ullet The computational burden grows with the number of non-zero entries of the constraint matrices  $A^1$  and  $A^2$
- It also grows with the number of rows of  $A^1$  and  $A^2$ .
- LP formulations with more non-zeroes typically take longer to solve.

# Gurobi Output for Formulation 2

```
Gurobi log file for last model:
```

Objective range [1e+00, 1e+00] Bounds range [1e+00, 1e+00] RHS range [1e+00, 1e+01]

900 variables, all binary 2383 constraints, all linear; 7260 nonzeros 40 equality constraints 2343 inequality constraints 1 linear objective; 226 nonzeros.

Gurobi 9.1.1: outlev=1
threads=4
Gurobi Optimizer version 9.1.1 build v9.1.1rc0 (linux64)
Thread count: 32 physical cores, 64 logical processors, using up Optimize a model with 2383 rows, 900 columns and 7260 nonzeros
Model fingerprint: Oxae721739
Variable types: 0 continuous, 900 integer (900 binary)
Coefficient statistics:
Matrix range [1e+00, 1e+00]

```
(continued....)
```

Found heuristic solution: objective 81.0000000 Presolve removed 1662 rows and 554 columns

Presolve time: 0.00s

Presolved: 721 rows, 346 columns, 2274 nonzeros

Variable types: 0 continuous, 346 integer (346 binary)

Root relaxation: objective 0.000000e+00, 161 iterations, 0.00 se

Nodes|Current Node|Obj. Bounds|Work |Expl Unexpl | Obj | Depth IntInf | Incumbent BestBd|Gap | It/Node Time

0	0	0.0	0	58	81.00	0.00	100%	_	0s
Н	0	0			34.00	0.00	100%	-	0s
0	0	0.0	0	85	34.00	0.00	100%	-	0s
0	0	1.5	0	127	34.00	1.50	95.6%	-	0s
0	0	1.5	0	124	34.00	1.50	95.6%	-	0s
0	2	1.5	0	121	34.00	1.50	95.6%	-	0s
*	271	239		17	32.00	9.04	71.7%	103	0s
Н	494	297			29.00	10.35	64.3%	93.5	0s

```
H 630 351 28.00 11.21 59.9% 94.5 0s
* 633 335 18 27.00 11.21 58.5% 94.3 0s
H 691 316 25.00 12.30 50.8% 95.0 0s
```

Explored 4392 nodes (369175 simplex iterations) in 3.98 seconds

24.00 13.91 42.0% 95.5 1s

Optimal solution found (tolerance 1.00e-04)
Best objective 2.400e+01, best bound 2.400e+01, gap 0.0000%

369175 simplex iterations 4392 branch-and-cut nodes

#### Cutting planes:

(continued....)

H 974 354

Gomory: 3

MIR: 7

Zero half: 26

RLT: 128 BQP: 60

# Clustering recap, QAP, SVM (2/8/2023)

### Recap: A clustering problem

#### Input:

- n objects numbered  $1, 2, \ldots, n$
- Desired number of clusters k, and a lower bound  $\ell$  on the number of objects in a cluster
- A set D of pairs of dissimilar objects

### Output:

- ullet A partitioning of the objects into cluster  $C_1, C_2, \dots, C_k$ 
  - Partitioning means:
  - (i)  $C_1 \cup C_2 \cup \cdots \cup C_k = \{1, 2, \ldots, n\}$ , and
  - (ii)  $C_s \cap C_t = \emptyset$  for all  $s \neq t$ .

#### Goal:

• Minimize the total number of pairs  $\{i,j\}$  where i and j are clustered in the same cluster, but are dissimilar (meaning,  $\{i,j\} \in D$ )

#### Decision variables

$$y_{is} \stackrel{\text{interpretation}}{=} \begin{cases} 1 & \text{if object } i \text{ is put in cluster } C_s \\ 0 & \text{otherwise.} \end{cases}$$
 
$$x_{ijs} \stackrel{\text{interpretation}}{=} \begin{cases} 1 & \text{if both objects } i \text{ and } j \text{ are put in cluster } C_s \\ 0 & \text{otherwise.} \end{cases}$$
 (only for  $i < j$ )

#### IP Formulation:

$$\begin{array}{lll} \min & \sum_{\{i,j\} \in D} \sum_{s \in K} x_{ijs} & \longleftarrow & \text{dissimilar pairs in the same cluster} \\ \text{s.t.} & \sum_{s \in K} y_{is} = 1 & \forall i \in N & \longleftarrow & \text{objects} \\ & \sum_{i \in N} y_{is} \geq \ell & \forall s \in K & \longleftarrow & \text{clusters} \\ & \text{How do we say: } x_{ijs} = & \begin{cases} 1 & \text{if } y_{is} = 1 \text{ and } y_{js} = 1 \\ 0 & \text{otherwise.} \end{cases} \end{array}$$

i.e. We want  $x_{ijs} = y_{is}y_{js}$ 

$$x_{ijs} \in \{0, 1\}$$
  $\forall i < j \in N , \forall s \in K$   
 $y_{is} \in \{0, 1\}$   $\forall i \in N , \forall s \in K$ 

Observation 0: If  $x, y_1, y_2$  satisfy the constraints

$$x \geq y_1 + y_2 - 1$$
 
$$x \leq \frac{1}{2}(y_1 + y_2)$$
 
$$y_1, y_2 \in \{0, 1\} \text{ and } x \in \{0, 1\}$$

then  $x = y_1y_2$ . (i.e., x = 1 only when both  $y_1 = 1$  and  $y_2 = 1$ )

Without  $x \in \{0,1\}$ , the point  $\underbrace{(1,0,\frac{1}{2})}_{(y_1,y_2,x)}$  is feasible to the system above.

Observation 1: If  $x, y_1, y_2$  satisfy the constraints

$$x \le y_1, \quad x \le y_2,$$
  
 $x \ge 0, \quad x \ge y_1 + y_2 - 1,$   
 $y_1, y_2 \in \{0, 1\}$ 

then  $x = y_1y_2$ . Notice that x variable is not declared to be binary

#### Remember this:

#### Claim

If  $x, y_1, y_2$  satisfy the McCormick constraints

$$x \le y_1,$$
  
 $x \le y_2,$   
 $x \ge 0,$   
 $x \ge y_1 + y_2 - 1,$   
 $y_1, y_2 \in \{0, 1\}$ 

then  $x = y_1y_2$ . Note: x is not declared to be binary

**Proof**: Any point satisfying the above constraints has  $y_1, y_2 \in \{0, 1\}$ .

- If either  $y_1$  or  $y_2$  is 0, then the first 3 constraints imply that x=0.
- the only remaining case is when both  $y_1$  or  $y_2$  is 1. In this case, the first constraint and the last one imply that x=1.

### Formulation 0 for the Clustering Problem

Decision variables

$$y_{is} = \begin{cases} 1 & \text{if } i \text{ in } C_s \\ 0 & \text{otherwise.} \end{cases} \qquad x_{ijs} = \begin{cases} 1 & \text{if both } i \text{ and } j \text{ are in } C_s \\ 0 & \text{otherwise.} \end{cases}$$

(Notice that we want  $x_{ijs}$  variable to be equal to  $y_{is} \cdot y_{js}$ )

$$\begin{array}{lll} & \min & \sum_{\{i,j\} \in D} \sum_{s \in K} x_{ijs} \\ & \text{s.t.} & \sum_{s \in K} y_{is} = 1 & \forall i \in N & \longleftarrow \text{ objects} \\ & \sum_{i \in N} y_{is} \geq \ell & \forall s \in K & \longleftarrow \text{ clusters} \\ & x_{ijs} \geq y_{is} + y_{js} - 1 & \forall i < j \in N \;, s \in K \\ & x_{ijs} \leq \frac{1}{2} (y_{is} + y_{js}) & \forall i < j \in N \;, s \in K \\ & x_{ijs} \in \{0,1\} & \forall i < j \in N \;, \forall s \in K \\ & y_{is} \in \{0,1\} & \forall i \in N \;, \forall s \in K \end{array}$$

# Clustering Problem: Formulation 1

Decision variables

$$y_{is} = \begin{cases} 1 & \text{if } i \text{ in } C_s \\ 0 & \text{otherwise.} \end{cases} \qquad x_{ijs} = \begin{cases} 1 & \text{if both } i \text{ and } j \text{ are in } C_s \\ 0 & \text{otherwise.} \end{cases}$$

$$\begin{array}{lll} & \min & \sum_{\{i,j\} \in D} \sum_{s \in K} x_{ijs} \\ & \text{s.t.} & \sum_{s \in K} y_{is} = 1 & \forall i \in N & \longleftarrow \text{ objects} \\ & \sum_{i \in N} y_{is} \geq \ell & \forall s \in K & \longleftarrow \text{ clusters} \\ & x_{ijs} \geq y_{is} + y_{js} - 1 & \forall i < j \in N \;, s \in K \\ & x_{ijs} \leq y_{is} & \forall i < j \in N \;, s \in K \\ & x_{ijs} \leq y_{js} & \forall i < j \in N \;, s \in K \\ & x_{ijs} \in \{0,1\} & \forall i < j \in N \;, s \in K \\ & y_{is} \in \{0,1\} & \forall i \in N \;, s \in K \end{array}$$

### Clustering Problem: Formulation 1<sup>+</sup>

#### Decision variables

$$y_{is} = \begin{cases} 1 & \text{if } i \text{ in } C_s \\ 0 & \text{otherwise.} \end{cases} \qquad x_{ijs} = \begin{cases} 1 & \text{if both } i \text{ and } j \text{ are in } C_s \\ 0 & \text{otherwise.} \end{cases}$$

$$\begin{array}{llll} & \min & \sum_{\{i,j\} \in D} \sum_{s \in K} x_{ijs} \\ & \text{s.t.} & \sum_{s \in K} y_{is} = 1 & \forall i \in N & \longleftarrow & \text{objects} \\ & \sum_{i \in N} y_{is} \geq \ell & \forall s \in K & \longleftarrow & \text{clusters} \\ & x_{ijs} \geq y_{is} + y_{js} - 1 & \forall i < j \in N \;, s \in K \\ & x_{ijs} \leq y_{is}, \; x_{ijs} \leq y_{js} & \forall i < j \in N \;, s \in K \\ & \underbrace{x_{ijs} \in \{0,1\}} \; x_{ijs} \geq 0 & \forall i < j \in N \;, s \in K \\ & y_{is} \in \{0,1\} & \forall i \in N \;, s \in K \end{array}$$

Clustering Problem: Formulation 1<sup>++</sup>

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IP Formulation:

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Observation: In an optimal sol.,  $x_{ijs}$  would not be 1 for  $\{i,j\} \in D$  if either  $y_{is} = 0$  or  $y_{is} = 0$ .

# Clustering Problem: Formulation 2

Decision variables

$$y_{is} \stackrel{\text{interpretation}}{=} \begin{cases} 1 & \text{if object } i \text{ is put in cluster } C_s \\ 0 & \text{otherwise.} \end{cases}$$
 
$$z_{ij} \stackrel{\text{interpretation}}{=} \begin{cases} 1 & \text{if objects } i \text{ and } j \text{ are put in the same cluster} \\ 0 & \text{otherwise.} \end{cases}$$
 (only for  $i < j$ )

$$\begin{array}{lll} & & \sum_{\{i,j\}\in D} z_{ij} \\ & \text{s.t.} & & \sum_{s\in K} y_{is} = 1 & \forall i\in N & \longleftarrow & \text{objects} \\ & & & \sum_{i\in N} y_{is} \geq \ell & \forall s\in K & \longleftarrow & \text{clusters} \\ & & z_{ij} \geq y_{is} + y_{js} - 1 & \forall i< j\in N \;, s\in K \\ & & z_{ij} \geq 0 & \forall i< j\in N \\ & & y_{is} \in \{0,1\} & \forall i\in N \;, s\in K \end{array}$$

# Comparing the formulations

• Size of the formulation:

	variables	constraints	nonzeros
Formulation 0	2,460	4,723	14,280
Formulation 1	2,460	7,063	16,620
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Formulation 2	4,392	369,175	3.98 seconds

### Solving IPs: computation time

Consider the following LP formulation

$$\label{eq:continuous} \begin{array}{ll} \text{minimize} & c^T x \\ \text{subject to} & A^1 x \geq b^1, \\ & A^2 x = b^2, \\ & x \geq 0 \end{array}$$

- The non-zeroes of this formulation is the number of nonzero entries in the matrices A<sup>1</sup> and A<sup>2</sup>.
- In practice LPs are solved using either the simplex method or interior point algorithms,
- In both cases one has to solve (many, many) linear equations
- The computational burden grows with the number of non-zero entries of the constraint matrices  $A^1$  and  $A^2$
- It also grows with the number of rows of  $A^1$  and  $A^2$ .
- IP solution time depends on the number of B&B nodes and the LP solution time at each node.

# The Quadratic Assignment Problem (QAP)

### The Quadratic Assignment Problem

- Place *n* facilities in *n* locations (one in each location).
- $d_{kl}$  denotes volume of goods to be sent from facility k to facility l, for  $k,l\in\{1,\ldots,n\}$
- $c_{ij}$  denotes the **unit** transportation cost between location i and j, for  $i, j \in \{1, ..., n\}$
- Place the facilities to minimize the total transportation cost.

Let variable  $x_{k,i}$  to indicate that facility k is assigned to location i.

Constraints are easy:

s.t. 
$$\sum_{i=1}^n x_{k,i}=1$$
  $k\in\underbrace{\{1,\ldots,n\}}_{\text{Facilities}}$   $\sum_{k=1}^n x_{k,i}=1$   $i\in\underbrace{\{1,\ldots,n\}}_{\text{Locations}}$   $x_{k,i}\in\{0,1\}$   $i,k\in\{1,\ldots,n\}$ 

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$$\begin{aligned} \text{s.t.} \quad & \sum_{i=1}^n x_{k,i} = 1 \\ & \sum_{k=1}^n x_{k,i} = 1 \\ & x_{k,i} \in \{0,1\} \end{aligned} \qquad \begin{aligned} k \in \underbrace{\{1,\ldots,n\}}_{\text{Facilities}} \\ & i \in \underbrace{\{1,\ldots,n\}}_{\text{Locations}} \\ & i,k \in \{1,\ldots,n\} \end{aligned}$$

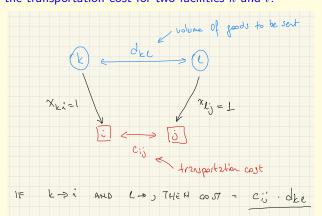
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If facility k is assigned to i and facility l is assigned to j, you pay
 dkl cij for that pair:

$$d_{kl} \cdot \sum_{i=1}^{n} \sum_{j=1}^{n} \underbrace{c_{ij} \ x_{ki} x_{l,j}}_{=0 \text{ unless } x_{ki} = x_{l,j} = 1}$$

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The objective minimizes total transportation cost:

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$$\sum_{k=1}^{n} \sum_{l=1}^{n} \sum_{i=1}^{n} \sum_{i=1}^{n} d_{kl} c_{ij} x_{ki} x_{l,j}$$

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$$\begin{split} & \min & \sum_{k=1}^{n} \sum_{l=1}^{n} \sum_{i=1}^{n} \sum_{j=1}^{n} & c_{ij} \ d_{kl} \underbrace{x_{ki} \, x_{l,j}}_{\text{quadratic}} \\ & \text{s.t.} & \sum_{i=1}^{n} x_{k,i} = 1 & k \in \{1,\dots,n\} \\ & \sum_{k=1}^{n} x_{k,i} = 1 & i \in \{1,\dots,n\} \\ & x_{k,i} \in \{0,1\} & i,k \in \{1,\dots,n\} \end{split}$$

### Remember: Multiplying binary variables

- Let  $x \in \{0,1\}$  and  $y \in \{0,1\}$  be two binary variables.
- Assume we are interested in their product  $x \cdot y$ .
- How can we express their product w = xy using linear inequalities?

$$w = \begin{cases} 1 & \text{if } x = 1 \text{ and } y = 1 \\ 0 & \text{otherwise.} \end{cases}$$

Consider the following McCormick inequalities:

$$\begin{aligned} & w \leq x \\ & w \leq y \\ & w \geq 0 \\ & w \geq x + y - 1 \end{aligned}$$

#### Claim

If  $x, y \in \{0, 1\}$  and w satisfies the constraints above, then w = xy.

### The Quadratic Assignment Problem: IP formulation

ullet We have to place n facilities in n locations.

# Supervised binary classification

### Another ML Example: Supervised binary classification

- ullet We are given m objects and a description of their features.
- For the jth object let  $a^j \in \mathbb{R}^n$  denote the associated feature vector.

Example:  $a^j \in \mathbb{R}^3$  could be: (measured in some scale)

- $-a_1^j$  indicates the ellipticity of the object,
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- Each objects belong to one of two classes.

For example: It is the image of an apple or an orange

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- Given an object with feature vector  $a \in \mathbb{R}^n$ , the classifier declares it to be an apple if

$$\sum_{i=1}^{n} w_i a_i \ge w_0,$$

and an orange if

$$\sum_{i=1}^{n} w_i a_i < w_0.$$

- In words, a linear classifier makes decisions on the basis of a linear combination of the features of the object.
- Our objective is to use known objects to design a "good" linear classifier

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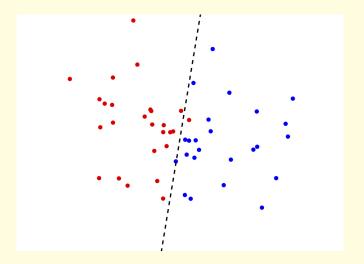
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A linear classifier in  $\mathbb{R}^2$ :



• The coordinates of a point corresponds to its features.

- How to pick  $w \in \mathbb{R}^n$  and  $w_0 \in \mathbb{R}$ ?
- A reasonable approach would be to pick w and w<sub>0</sub> so that the classifier gives correct answer for all known objects (samples).
- Let  $S = S^1 \cup S^2$  be the set of known samples with  $S^2 = S \setminus S^1$ 
  - Let  $S^1$  be the set of objects of type 1 (apples), and,
  - Let  $S^2$  be the set of objects of type 2 (oranges)
- We are then looking for some  $w \in \mathbb{R}^n$  and  $w_0 \in \mathbb{R}$  that will satisfy:

$$w^T a^j \geq w_0, \quad \forall j \in S^1$$
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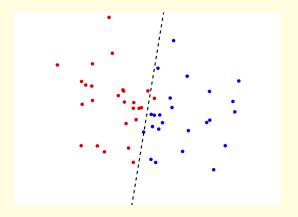
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# SVM Recap, Big Ms, Subset Sum (2/10/2023)

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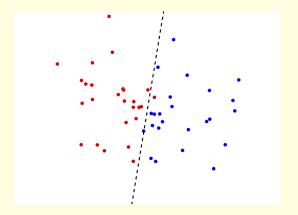
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(remember, the variables are: w,  $\delta_1$  and  $w_0$ )

• The number of nonzeroes coming from this constraint is:

(the nonzero entries of 
$$a^1$$
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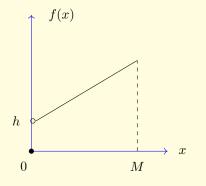
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## Using Big Ms: Lot-sizing Problem

#### **Fixed Charges**

- Economic activities frequently involve fixed and variable costs.
- Example: A production facility.
  - Fixed cost: if anything is produced at all (e.g., cost of starting up machines).
  - Variable cost: linear in the amount produced (e.g., cost of operating machines).



In this case, the cost is

$$f(x) = \begin{cases} 0 & \text{if } x = 0\\ h + cx & \text{if } x > 0 \end{cases}$$

(with h, c > 0).

- This is not a linear function.
- Not even a continuous function.

#### Modeling Fixed Charges

• This can easily be modeled using a binary variable  $y \in \{0,1\}$ 

$$y \stackrel{\text{interpretation}}{=} \begin{cases} 1 & \text{if } x > 0 \text{ (some production)} \\ 0 & \text{if } x = 0 \text{ (no production)}. \end{cases}$$

Then the total cost of production can now be written as

$$hy + cx$$
.

• Let M be some upper bound on the value of variable x.

$$x \le My$$
$$y \in \{0, 1\}$$
$$x > 0$$

Note: y = 1, x = 0 is feasible but if minimizing with h > 0, it is fine!

- Linear programming relaxations of "big M" formulations tend to produce bad LP relaxations.
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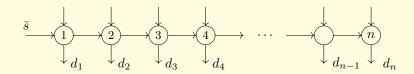
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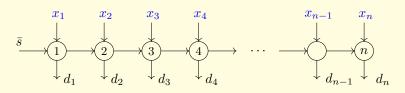
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#### Example: Uncapacitated lot-sizing problem

Production planning for a single item for an n-period horizon:

- Demand for the item is  $d_t$  for t = 1, ..., n.
- There is a fixed cost  $f_t$  of production in period t
- There is a production cost  $p_t$  per unit produced in period t
- There is a starting inventory of  $\bar{s}$  units available at the beginning.
- There is a storage cost of  $h_t$  per unit in period t
- Find the minimum cost production plan to satisfy demand.





#### Decision variables:

- $x_t \ge 0$  to denote the quantity produced in period t
- $y_t \in \{0,1\}$  to denote if production occurs in period t
- $s_t \ge 0$  to denote the stock at the end of period t

#### Formulation:

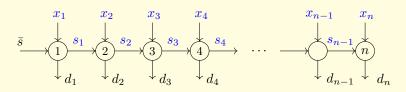
$$\min \sum_{t=1}^{n} p_{t}x_{t} + \sum_{t=1}^{n} f_{t}y_{t} + \sum_{t=1}^{n} h_{t}s_{t}$$
s.t.  $s_{t} = s_{t-1} + x_{t} - d_{t}$   $t \in \{1, \dots, n\}$ 

$$x_{t} \leq My_{t}$$
  $t \in \{1, \dots, n\}$ 

$$s_{0} = \bar{s},$$

$$s_{t}, x_{t}, y_{t} \geq 0, y_{t} \in \{0, 1\}, x_{t} \in \mathbb{Z}$$
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Question: How big should M be?



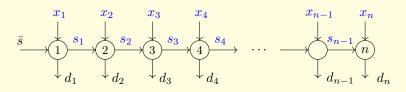
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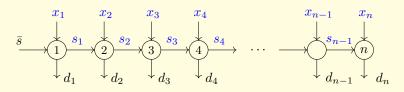
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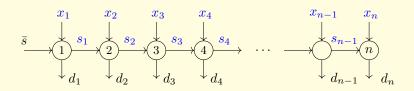
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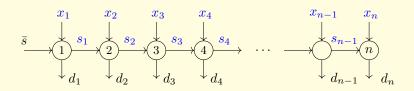
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• The big Ms can be different for different t:

$$x_t \le M^t y_t \qquad t \in \{1, \dots, n\}$$

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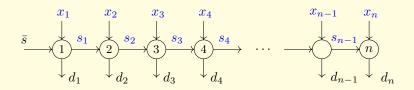
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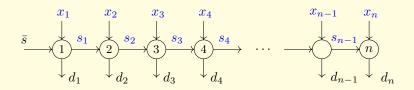
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# A variant: Capacitated lot sizing

- ullet Consider the same set up: Given demands for the next n periods,
- ullet You need to decide on how much to produce in each period  $t=1,\dots,n$
- But now, you produce in batches of size *B*.
- If you produce up to B items, you pay  $f_t$ , then you pay another  $f_t$  if you produce B+1 up to 2B items, etc.

#### Decision variables:

- $x_t$  is the production quantity and  $s_t$  is the stock level as before
- But now  $y_t \in \mathbb{Z}$  denotes how many batches you start in period t

#### Formulation:

$$\min \quad \sum_{t=1}^{n} p_{t}x_{t} + \sum_{t=1}^{n} h_{t}s_{t} + \sum_{t=1}^{n} f_{t}y_{t}$$
s.t.  $s_{t-1} + x_{t} - s_{t} = d_{t}$   $t \in \{1, \dots, n\}$ 

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# Subset Sum Problem

# Example: Subset Sum

Two brothers, Ludwig and Johann, inherit from their dear uncle a set  ${\cal S}$  of antique objects.

- ullet each worth a lot of money,  $c_i$  for all  $i \in S$
- Ludwig and Johann want to share these objects in a balanced manner
- ⇒ minimize the difference between total values of objects each one gets
  - Let  $S_L \subset S$  be the set of objects that Ludwig will get,
  - While  $S_J = A \setminus S_L$  are the remaining objects (Johann gets)
- ⇒ minimize

$$\left| \begin{array}{ccc} \sum_{i \in S_L} c_i & - \sum_{i \in S_J} c_i \\ \text{Ludwig's pile} & \text{Johann's pile} \end{array} \right| \qquad \longleftarrow \quad \text{absolute value}$$

How to model this with IP?

## Example: Subset Sum (cont'd)

$$x_i = \left\{ egin{array}{ll} 1 & ext{if Ludwig gets the $i$-th object} \\ 0 & ext{if Johann gets the $i$-th object} \end{array} 
ight.$$

Then the integer model is:

$$\begin{array}{ccc} \min & \left| \sum_{i \in S} c_i x_i - \sum_{i \in S} c_i (1-x_i) \right| & \longleftarrow & \text{absolute value} \\ & x_i \in \{0,1\} & \forall i \in S \end{array} \right.$$

where the objective in not linear. But we can make it linear, by adding a new variable  $\delta$  that stands for the difference between their inheritance

$$\min \quad \delta$$

$$\sum_{i \in S} c_i x_i - \sum_{i \in S} c_i (1 - x_i) \le \delta$$

$$\sum_{i \in S} c_i (1 - x_i) - \sum_{i \in S} c_i x_i \le \delta$$

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- Now the objective is to minimize the largest difference between brothers
- What are the variables

$$m{x_i} = \left\{ egin{array}{ll} 1 & \mbox{if L gets } i \\ 0 & \mbox{if not} \end{array} 
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where variable  $\delta$  denotes the largest difference between brothers' assets.

Question: Is this formulation correct?

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where variable  $\delta$  denotes the largest difference between brothers' assets.

• We can again make this model linear by replacing each absolute value with 2 linear inequalities. (i.e.  $|\alpha| \le \delta \iff \alpha \le \delta, \ -\alpha \le \delta$ )

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Notice that the number of fairness constraints increase quadratically with the number of brothers: one for each pair:  $\binom{n}{2}$ 

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