



# Exact Methods of Optimization

Nuno Antunes Ribeiro

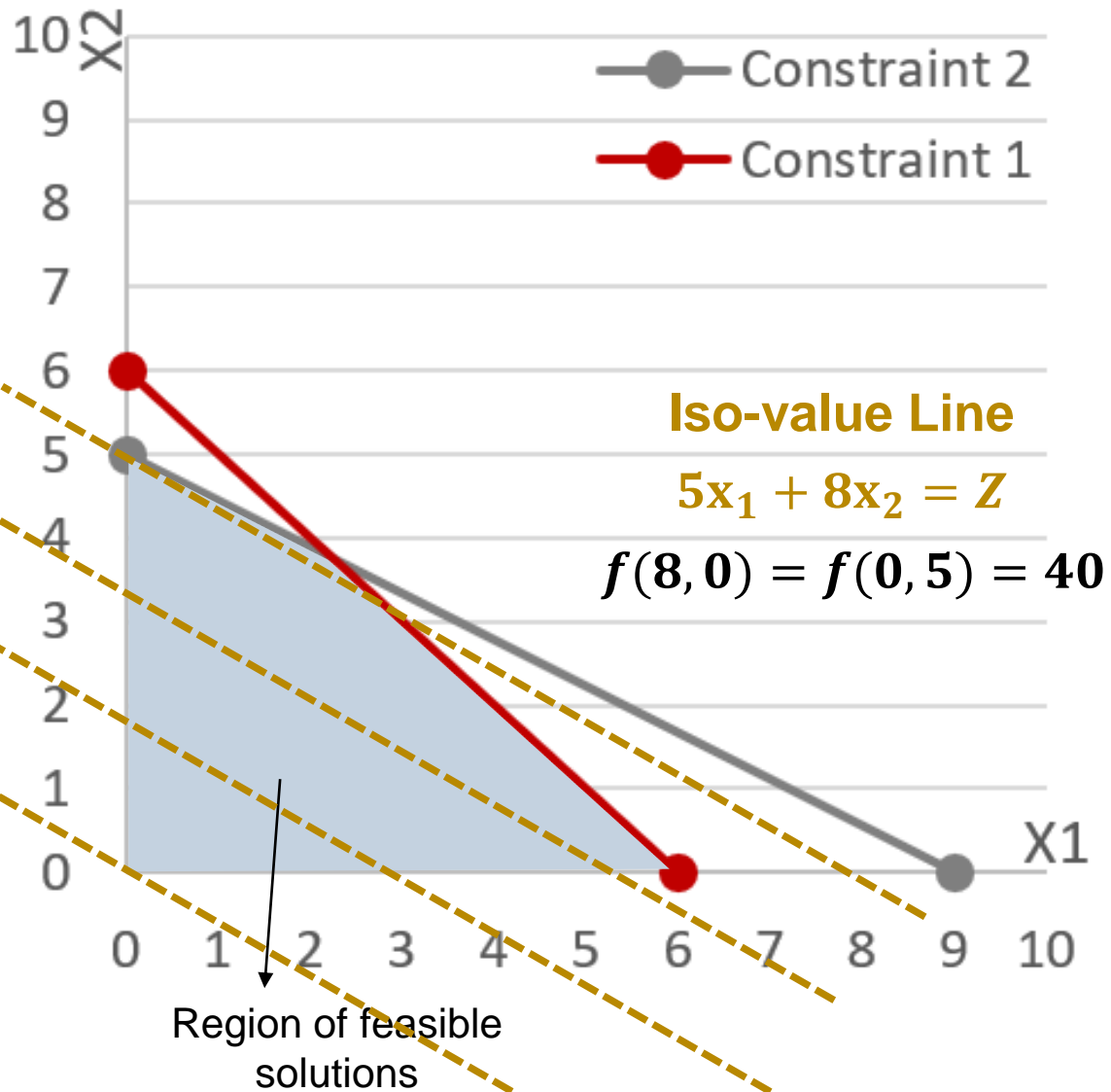
Assistant Professor

# Optimization Problem

- **Optimize:**  $\max(f(x_1, x_2) = 5x_1 + 8x_2)$
- **Constraints:**  $x_1 + x_2 \leq 6$   
 $5x_1 + 9x_2 \leq 45$   
 $x_1, x_2 \geq 0$
- **The Carpenter Problem**
  - A carpenter can either make chairs or tables
  - Chairs take 5 units of lumber, 1 day of labour, and the carpenter makes \$500
  - Tables take 9 units of lumber, 1 day of labour, and the carpenter makes \$800
  - 45 units of lumber available
  - 6 days of labour available per week

**How many chairs and tables to produce per week**

# Linear Programming Model



$$\max(f(x_1, x_2) = 5x_1 + 8x_2)$$

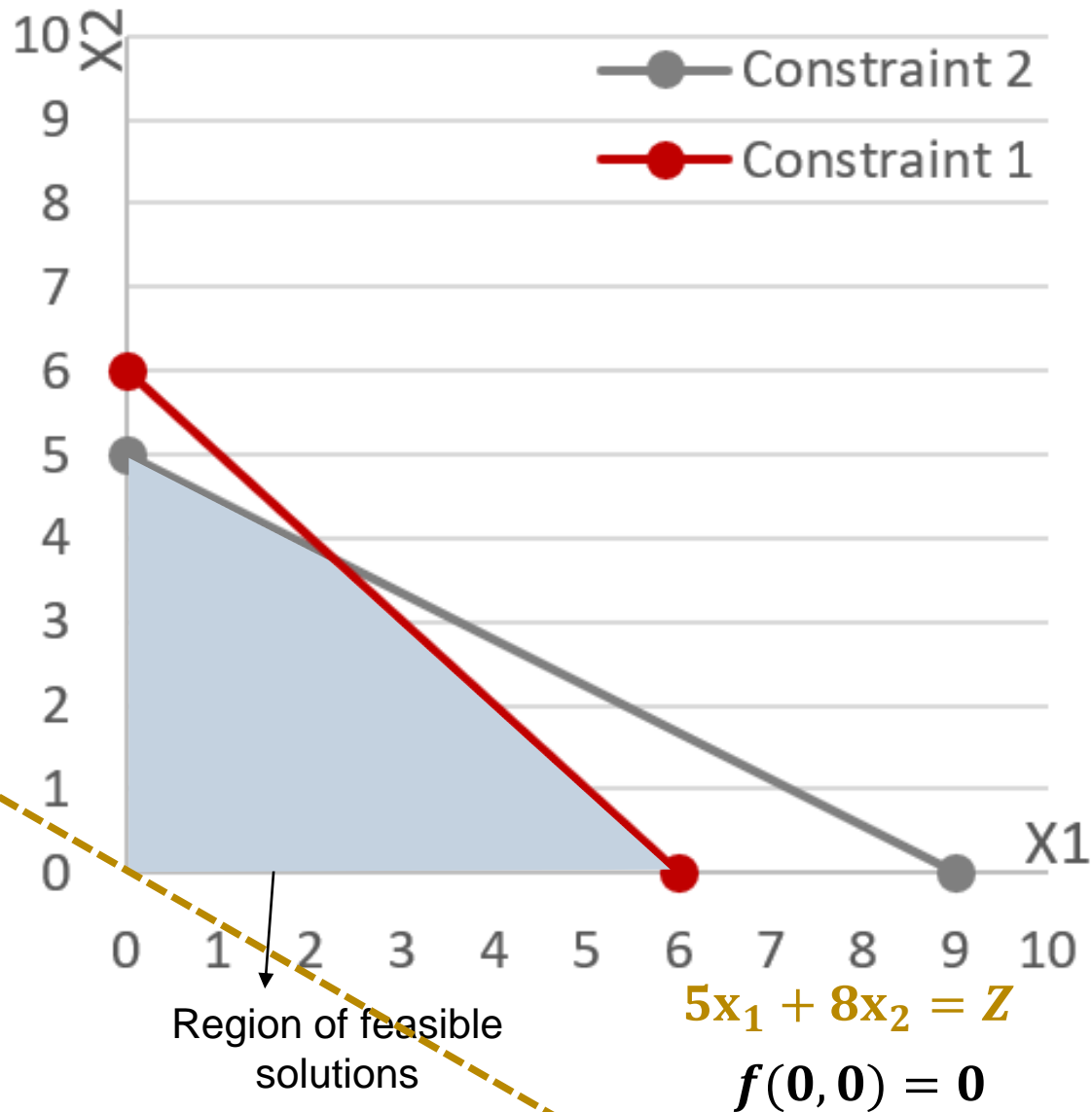
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$$x_1, x_2 \geq 0$$

Constraint 1		Constraint 2	
x1	x2	x1	x2
0	6	9	0
6	0	0	5

# Linear Programming Model



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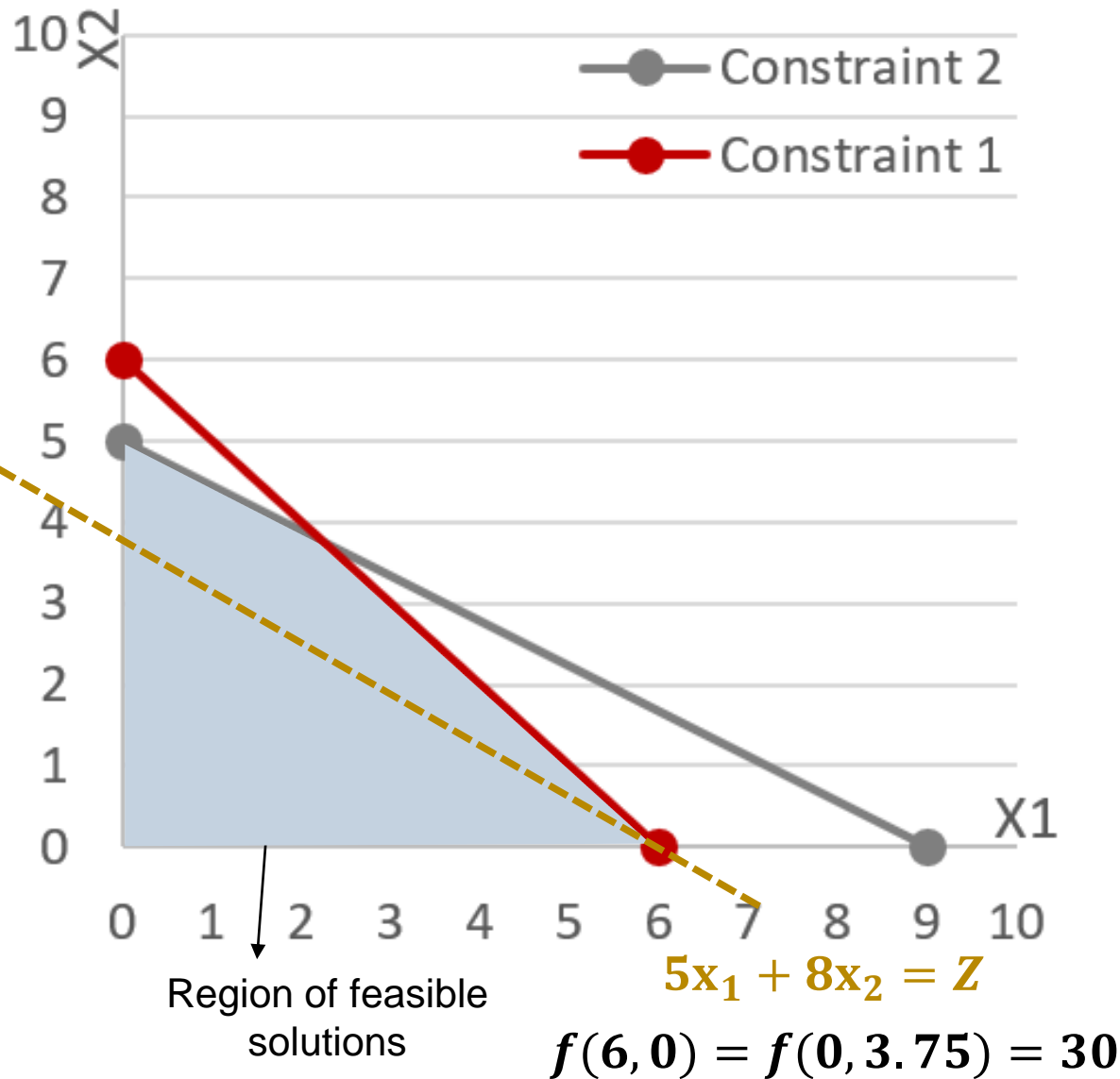
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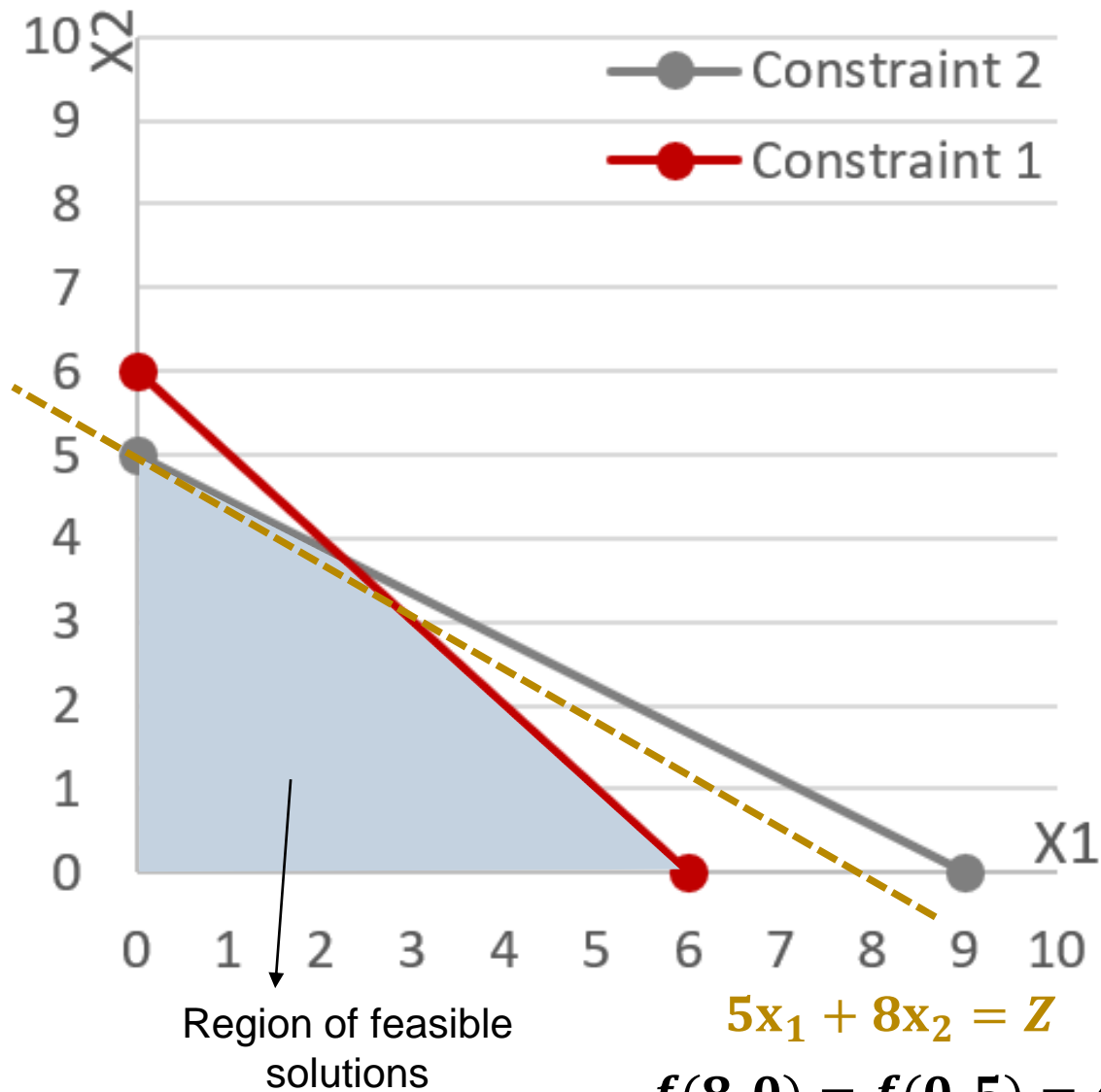
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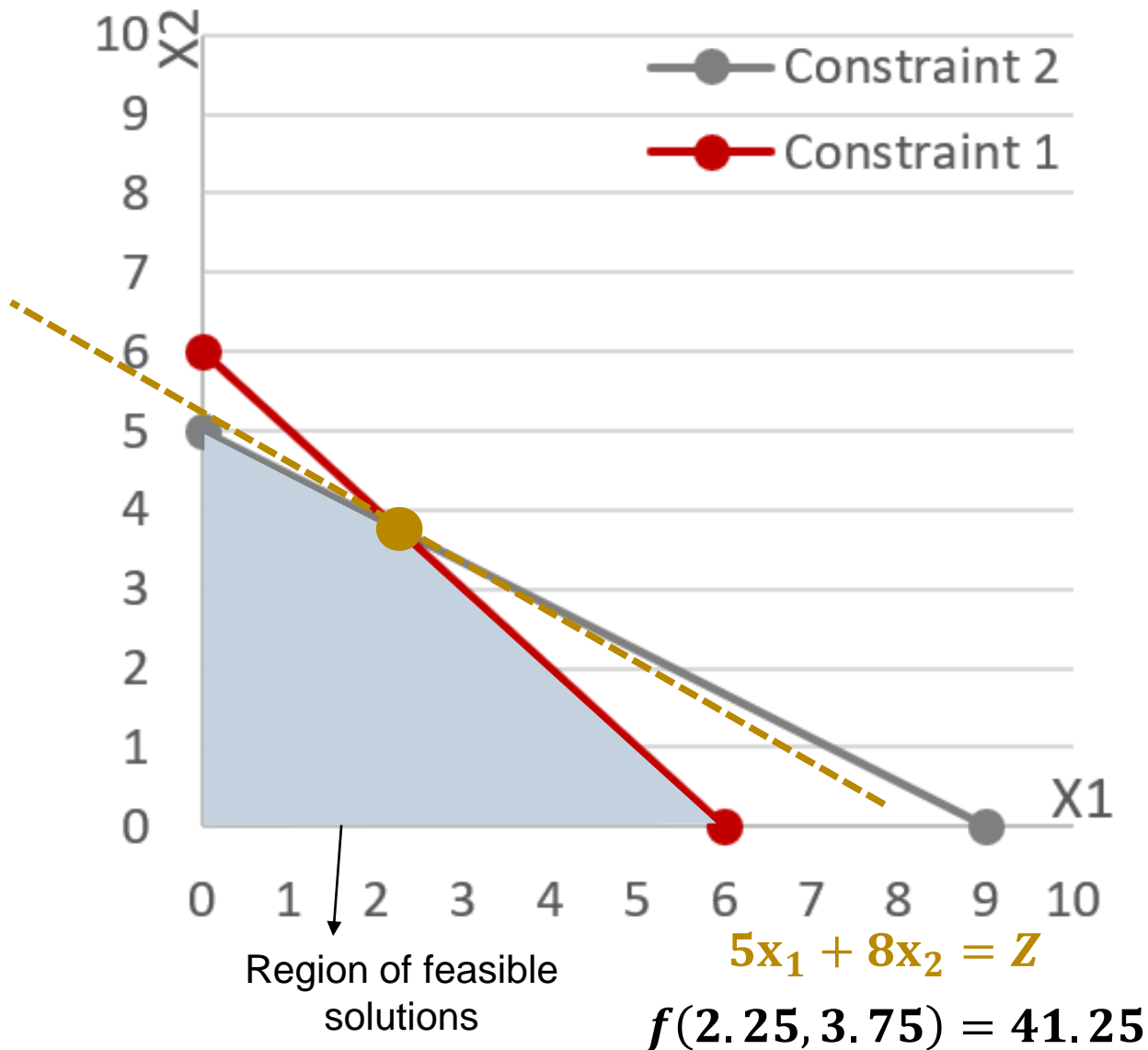
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# Linear Programming Model



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Constraint 1		Constraint 2	
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0	6	9	0
6	0	0	5

from constraint 1;  $x_2 = 6 - x_1$

from constraint 2;  $x_2 = \frac{45 - 9x_1}{5}$

$$6 - x_1 = \frac{45 - 9x_1}{5} \Leftrightarrow x_2 = 3.75; x_1 = 2.25$$

# Standard Linear Programming Model

$$\max z = p_1x_1 + p_2x_2 + \dots + p_ix_i$$

profit

$$s. t. \quad c_{11}x_1 + c_{21}x_2 + \dots + c_{i1}x_n \leq b_1$$

budget

$$c_{12}x_1 + c_{22}x_2 + \dots + c_{i2}x_n \leq b_2$$

cost

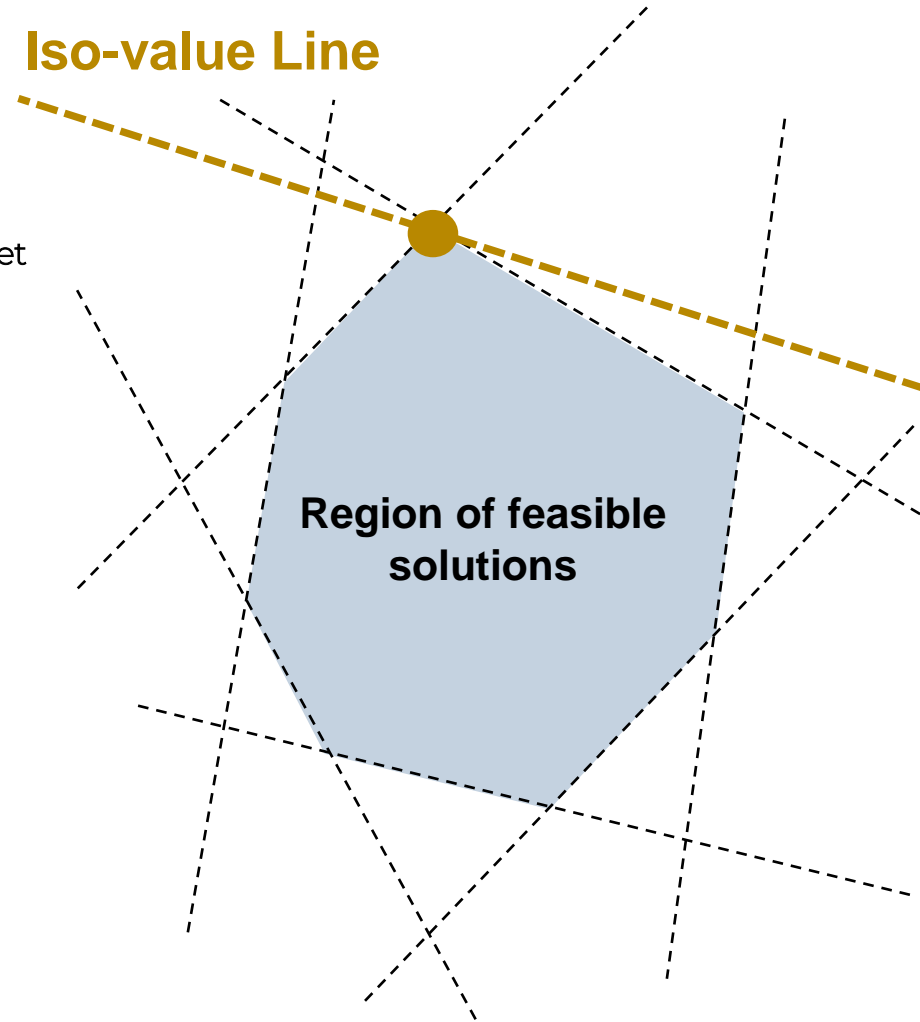
...

$$c_{1j}x_1 + c_{2j}x_2 + \dots + c_{ij}x_i \leq b_j$$

$$x_1, x_2, \dots, x_i \geq 0$$

Jobs

Iso-value Line

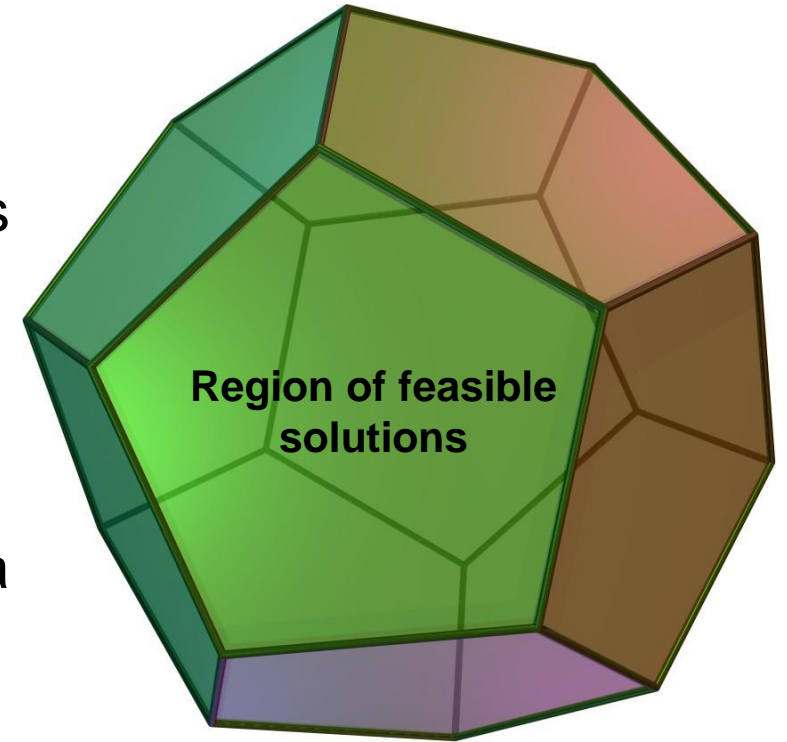




# Idea of Simplex Algorithm

- The *simplex algorithm*, created by the American mathematician George Dantzig in 1947, is a very popular algorithm for solving linear programs.
- The *Simplex method* uses row operations on matrices in Linear Algebra to find the optimal solution of an LP
  - Start at a corner of the feasible region
  - While there is an adjacent corner that is a better solution, move to that corner.
  - For “most” instances, the algorithm terminates (in a finite number of steps) at an optimal solution.

<https://sites.google.com/view/40-510/home>



- Other more sophisticated methods have also been proposed to solve LP problems, such as the *ellipsoid method* or the *barrier method*

# Standard LP Model Formulation

## □ Sets

*Set of Jobs:  $i = 1, 2, \dots, i$*

*Set of Constraints:  $j = 1, 2, \dots, j$*

## □ Parameters

*$p_i$  = unit of profit of working on job  $i$  (profit per unit of time)*

*$c_{ij}$  = cost of job  $i$  under constraint  $j$  (e.g. manpower, resources, inventory, etc.)*

*$b_j$  = budget available under constraint  $j$  (e.g. no. labours, amount of resources, inv. capacity, etc.)*

## □ Decision Variables

*$x_i$  = amount of time working on job  $i$*

# Standard LP Model Formulation

$$\max z = \sum_{i \in N} p_i x_i$$

Sum over all jobs

**Maximize profits**

s. t.

$$\sum_{i \in N} c_{ij} x_i \leq b_j, \quad \forall j \in M$$

Sum over all jobs      For all constraints

**Subject to budget constraints**

$$x_i \geq 0, \quad \forall i \in N$$

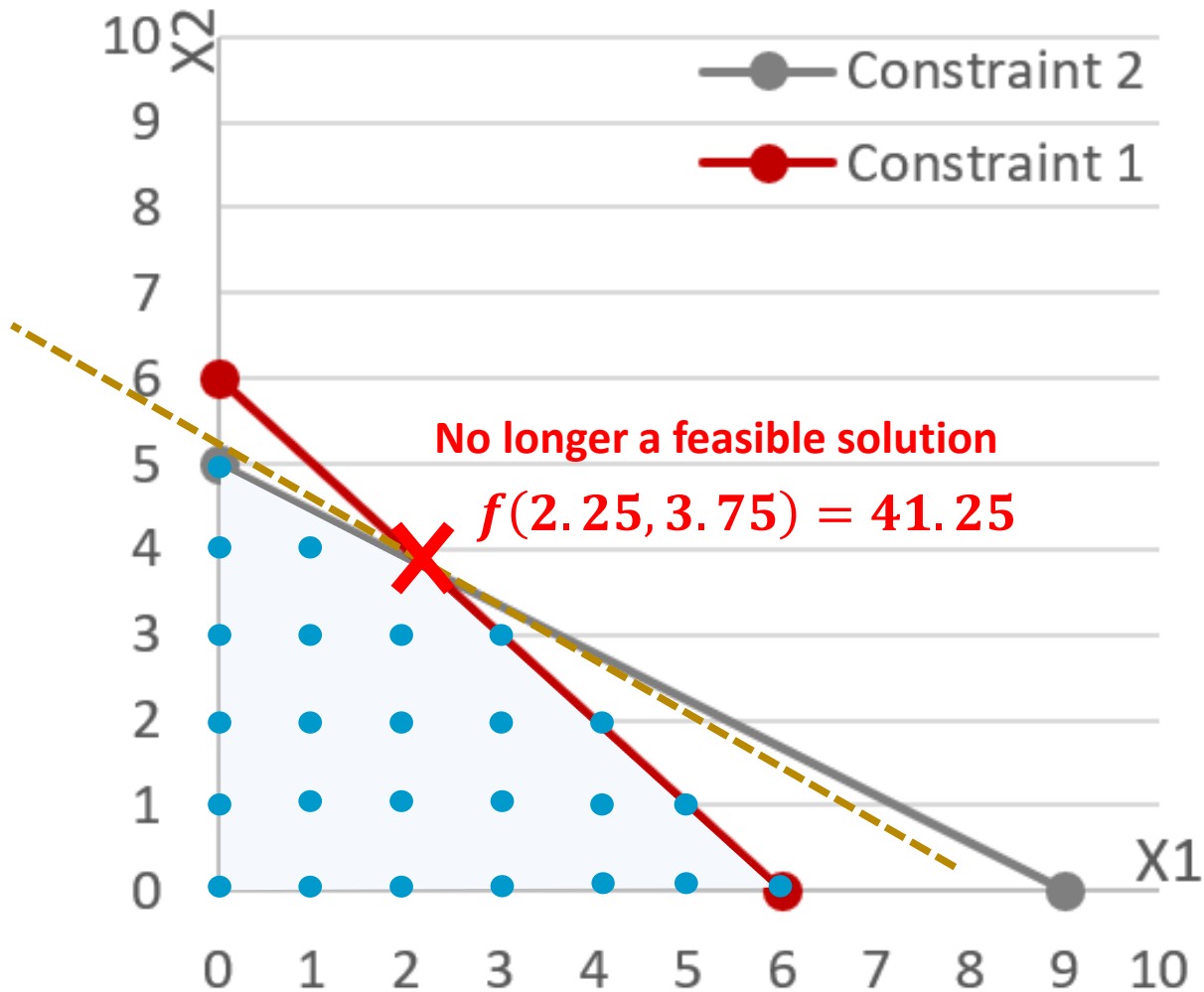
For all jobs

**I cannot spend negative time working on job  $i$**

**What if  $x_i$  needs to be integer**

i.e.  $x_i$  is the number of job  $i$  completions (e.g. number of chairs or tables?)

# Integer Programming Model



$$\max(f(x_1, x_2) = 5x_1 + 8x_2)$$

$$\text{s. t.} \quad x_1 + x_2 \leq 6$$

$$5x_1 + 9x_2 \leq 45$$

$$x_1, x_2 \geq 0, \text{ integer}$$

# Solving Discrete Optimization Problems

Today's class!

Exact Methods

Exhaustive Search

Branch and X

Other Methods

Backtracking

Dynamic Programming

All the other classes!

Approximate Methods

Heuristics

Meta-Heuristics

Single Solution

Population of Solution

Local Search

Simulated Annealing

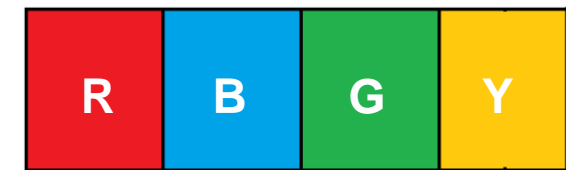
Tabu Search

Evolutionary Algorithms

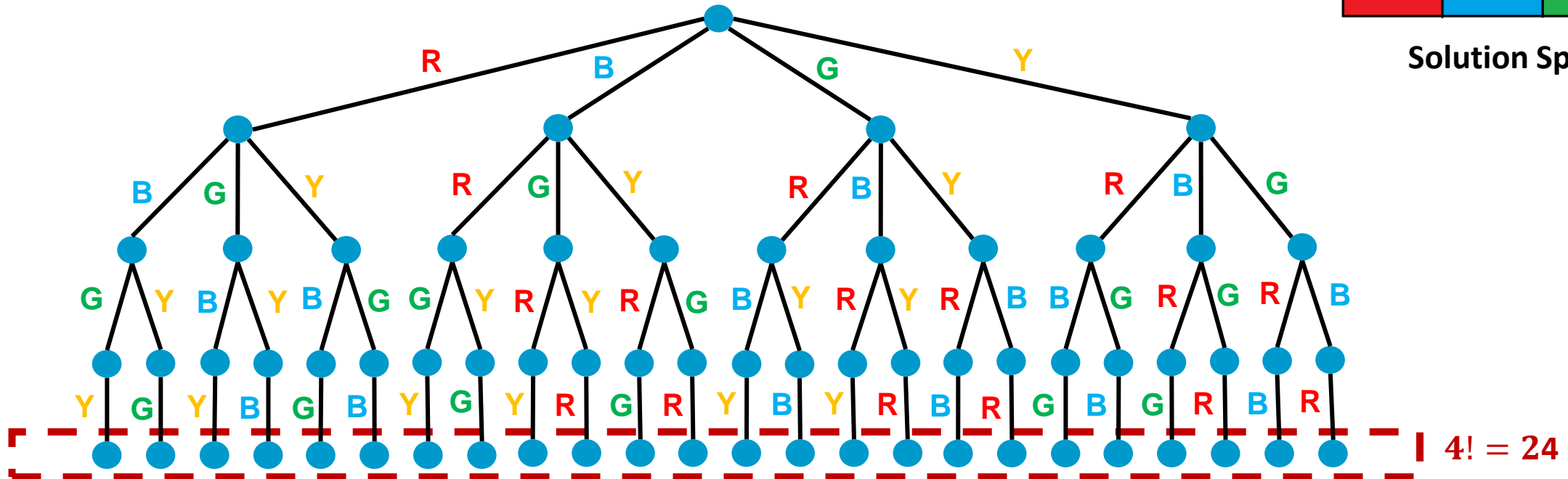
Swarm Search

# Exhaustive Search

- Exhaustive Search is the simplest of the algorithms. It examines every possible combination of permitted levels of all attributes.
- Exhaustive Search is very ineffective and mostly unusable for a real-world problem due to time limitations
- Solutions are generally represented in a **search space tree**

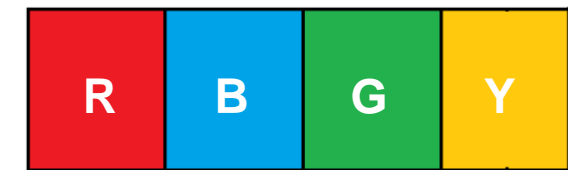


Solution Space =  $n!$



# Backtracking

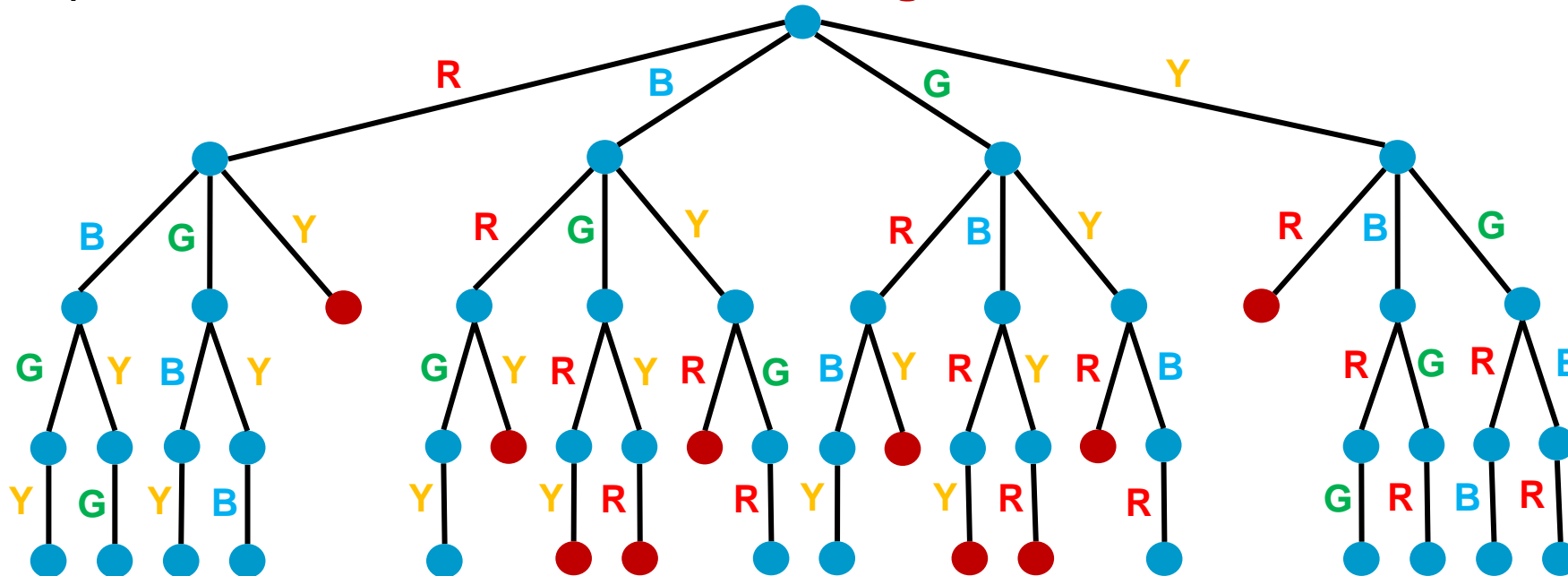
- Backtracking is an algorithmic technique where the goal is to get **one or multiple solutions** to a problem.
- Backtracking **depth-searches** for solutions and then backtracks to the most recent valid path as soon as an end node is reached (i.e., we can proceed no further).
- It is eventually faster than exhaustive search since the search space tree is cut whenever a **bounding constraint** is violated



Solution Space =  $n!$

**Bounding Constraint**  
Yellow and red cannot be adjacent colours

**12 feasible solutions**



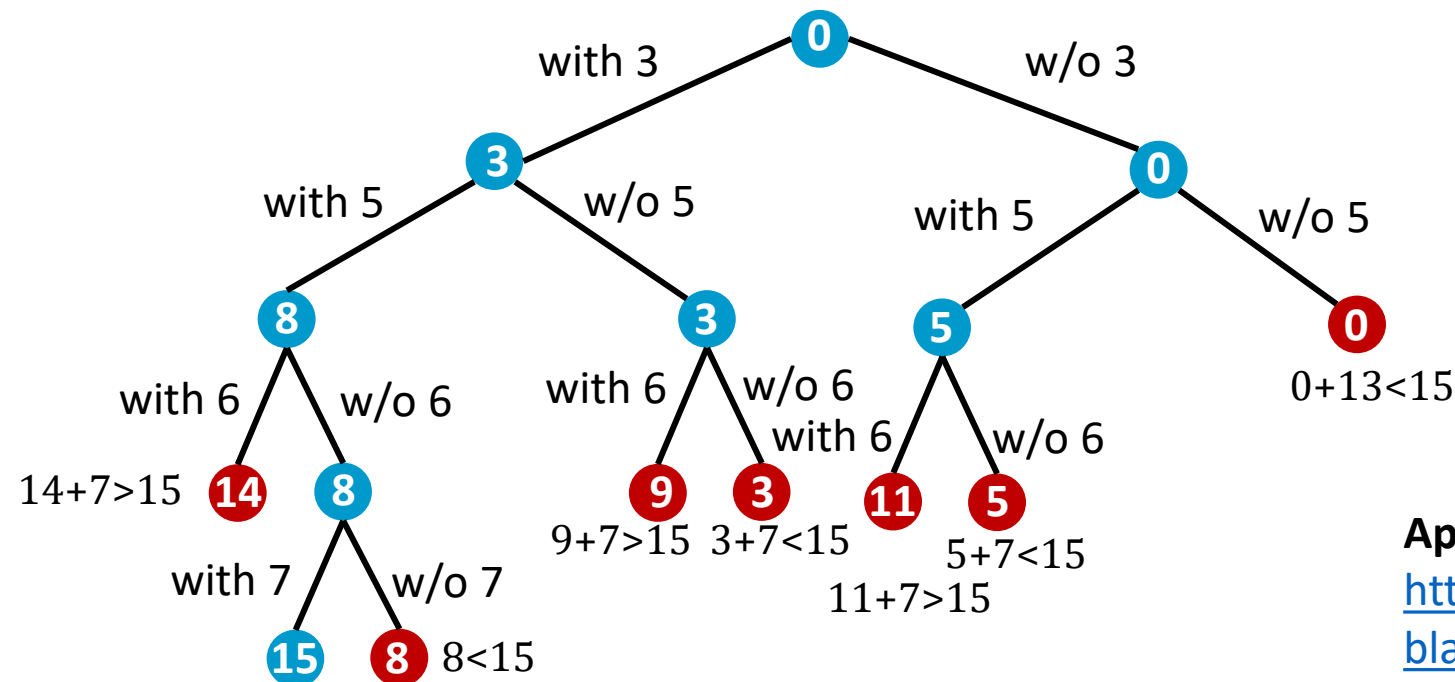
# Example: Sum of Subsets Problem

- Subset sum problem is to find subset of elements that are selected from a given set with  $n$  elements whose sum adds up to a given number  $m$ .
- We are considering the set contains non-negative values. It is assumed that the input set is unique (no duplicates are presented).

$$W[1:n] = \{3,5,6,7\}$$

$$m = 15$$

$$\text{Solution Space} = 2^n = 16$$



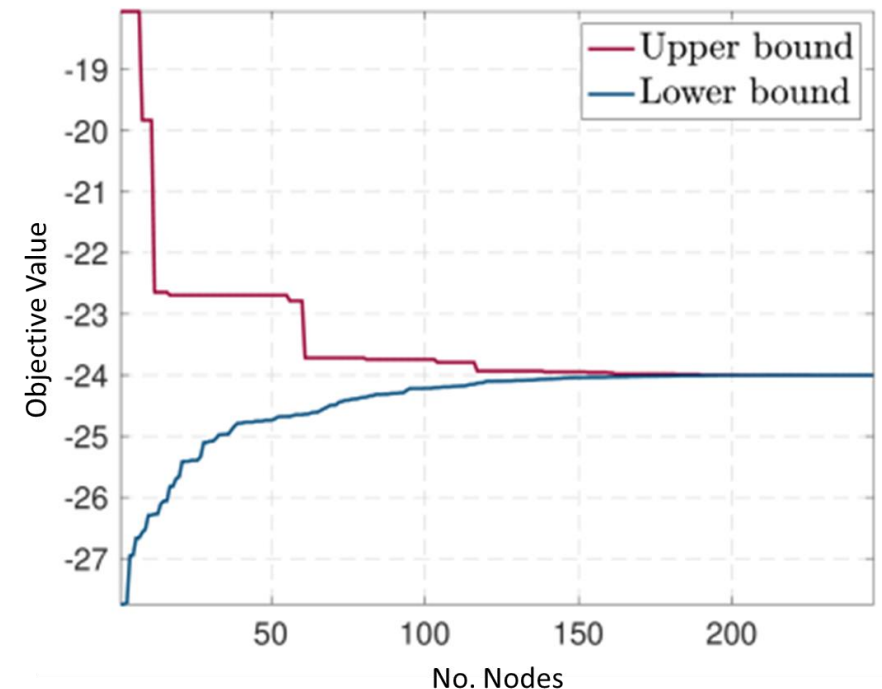
**1 feasible solutions**

**Applications (e.g. computer passwords):**  
[http://www.math.stonybrook.edu/~scott/blair/Other\\_uses\\_subset\\_sum.html](http://www.math.stonybrook.edu/~scott/blair/Other_uses_subset_sum.html)

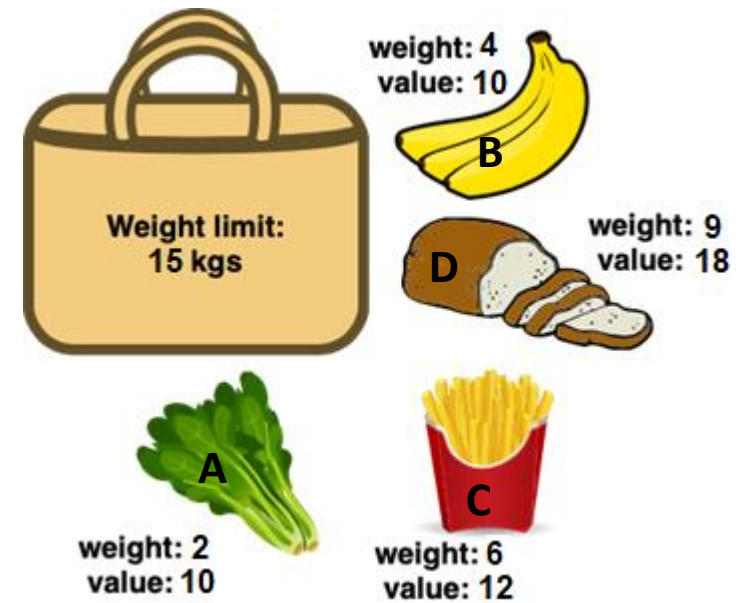


# Branch and Bound

- Rely on two subroutines that (efficiently) compute a lower and an upper bound on the optimal value
  - upper bound can be found by choosing any point in the region, or by a local optimization method
  - lower bound can be found from by applying some relaxation techniques (e.g. LP relaxation)
- Definitions
  - **Upper bound:** a feasible solution
  - **Lower bound:** a solution to an “easier” problem
  - **Node elimination:** (fathom nodes): when lower bound  $\geq$  upper bound
- Branch and Bound assumes we are solving minimization problems



# Example: Knapsack Problem



Item	A	B	C	D
Value	-10	-10	-12	-18
Weight	2	4	6	9

# Example: Knapsack Problem

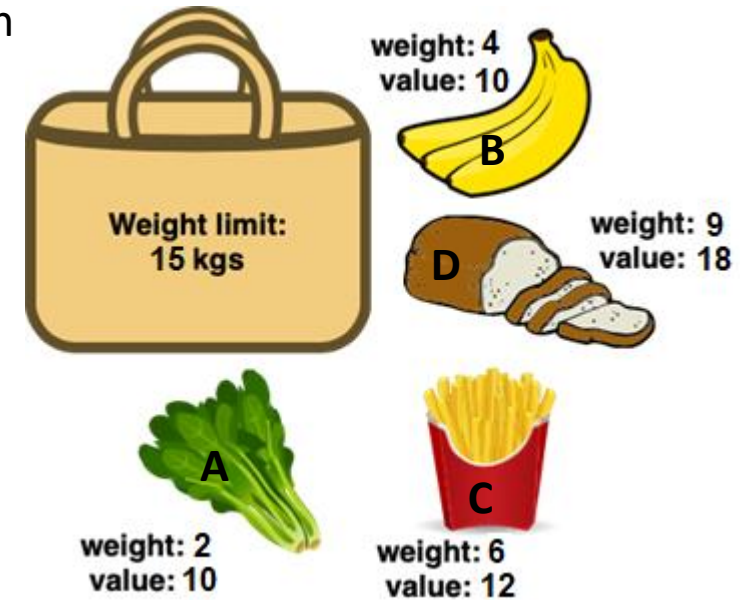
- Pick a random initial **feasible** solution **ABC**

$$\text{Value} = 10 + 10 + 12 = 32$$

$$\text{Weight} = 2 + 4 + 6 = 12$$

Upper Bound =  $10 + 10 + 12 = 32$   
(best you could achieve so far)

Lower Bound = ?  
(best you could achieve in theory)



Let's imagine you could bring a portion of item **D**. What would be the portion to add to solution **ABC**

$$\text{Weight} = 2 + 4 + 6 = 12 + 3 = 15$$

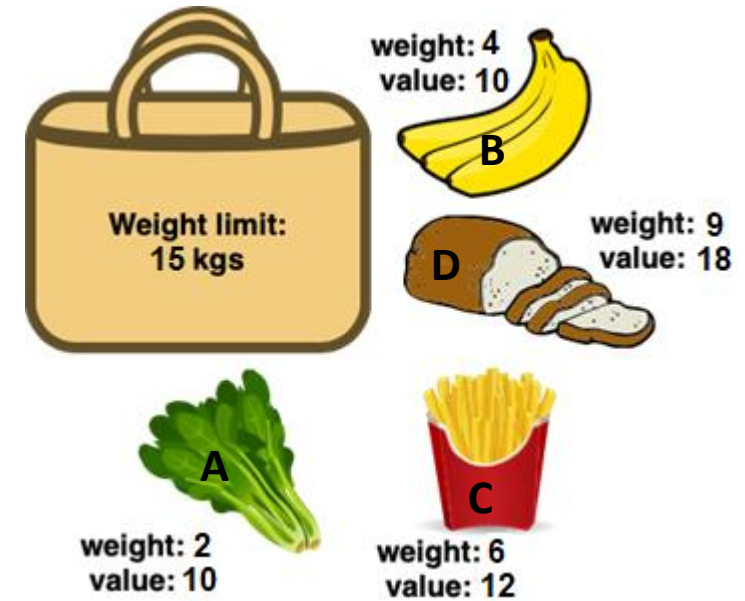
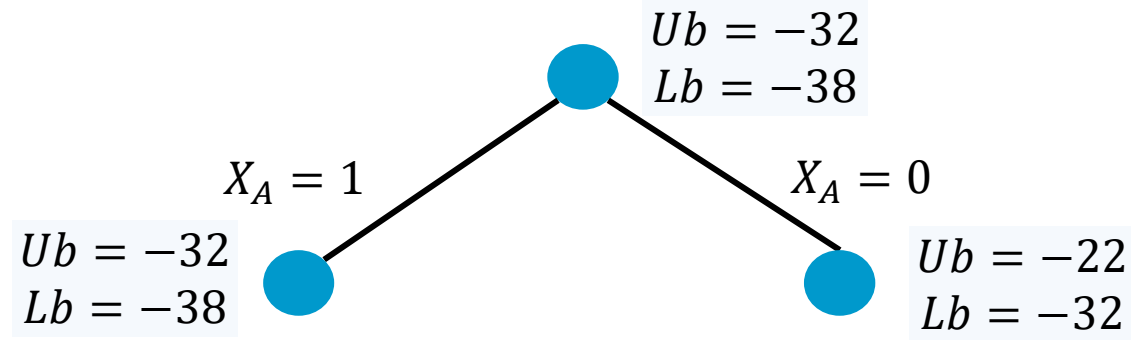
$$\text{Portion} = 3 \div 9$$

$$\text{Value} = 10 + 10 + 12 + 18 \times 3 \div 9 = 38$$

Item	A	B	C	D
Value	-10	-10	-12	-18
Weight	2	4	6	9

# Example: Knapsack Problem

Upper = -32  
Lower = -38



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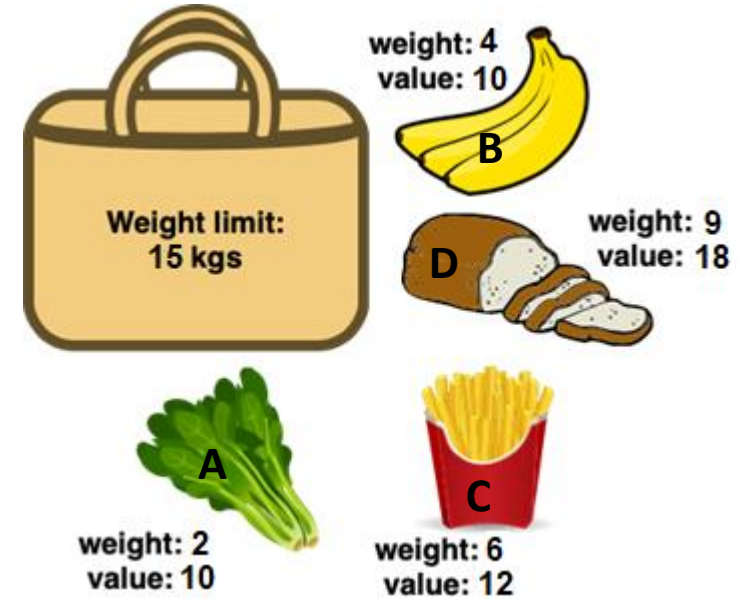
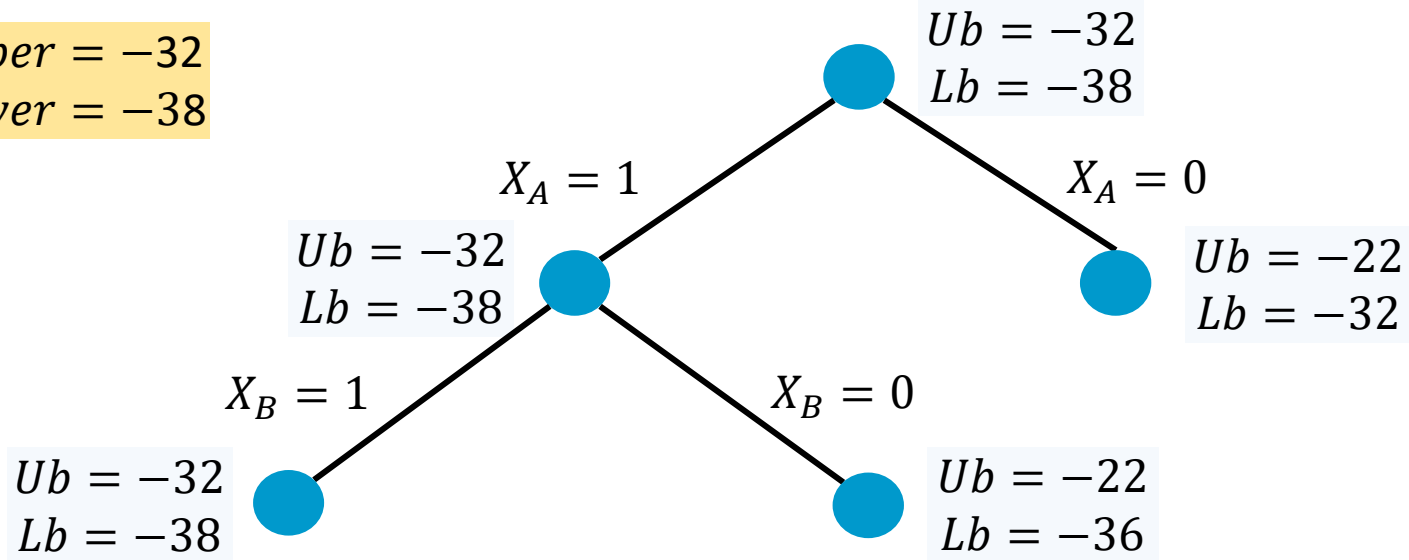
Weight = 4 + 6 = 10 ; Weight = 15 - 10 = 5

Upper Bound = 10 + 12 = **22**

Lower Bound = 10 + 12 +  $\frac{18 \times 5}{9}$  = **32**

# Example: Knapsack Problem

Upper = -32  
Lower = -38



Item	A	B	C	D
Value	10	10	12	18
Weight	2	4	6	9

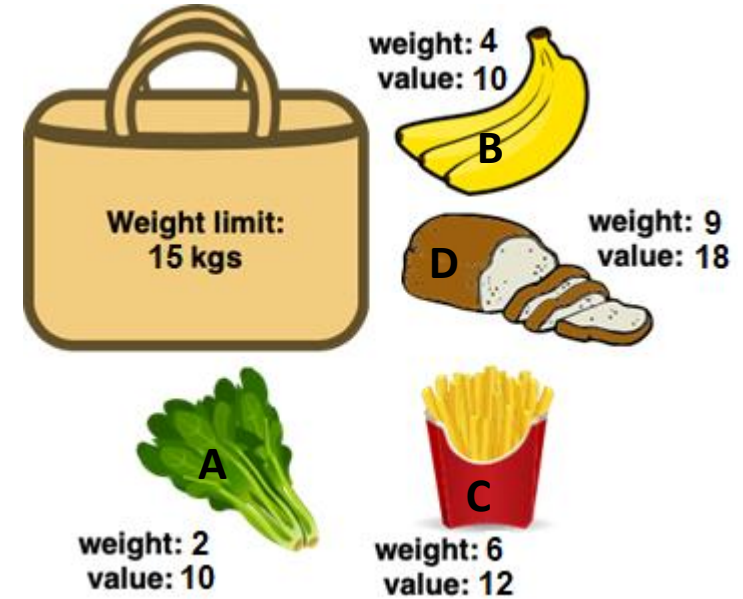
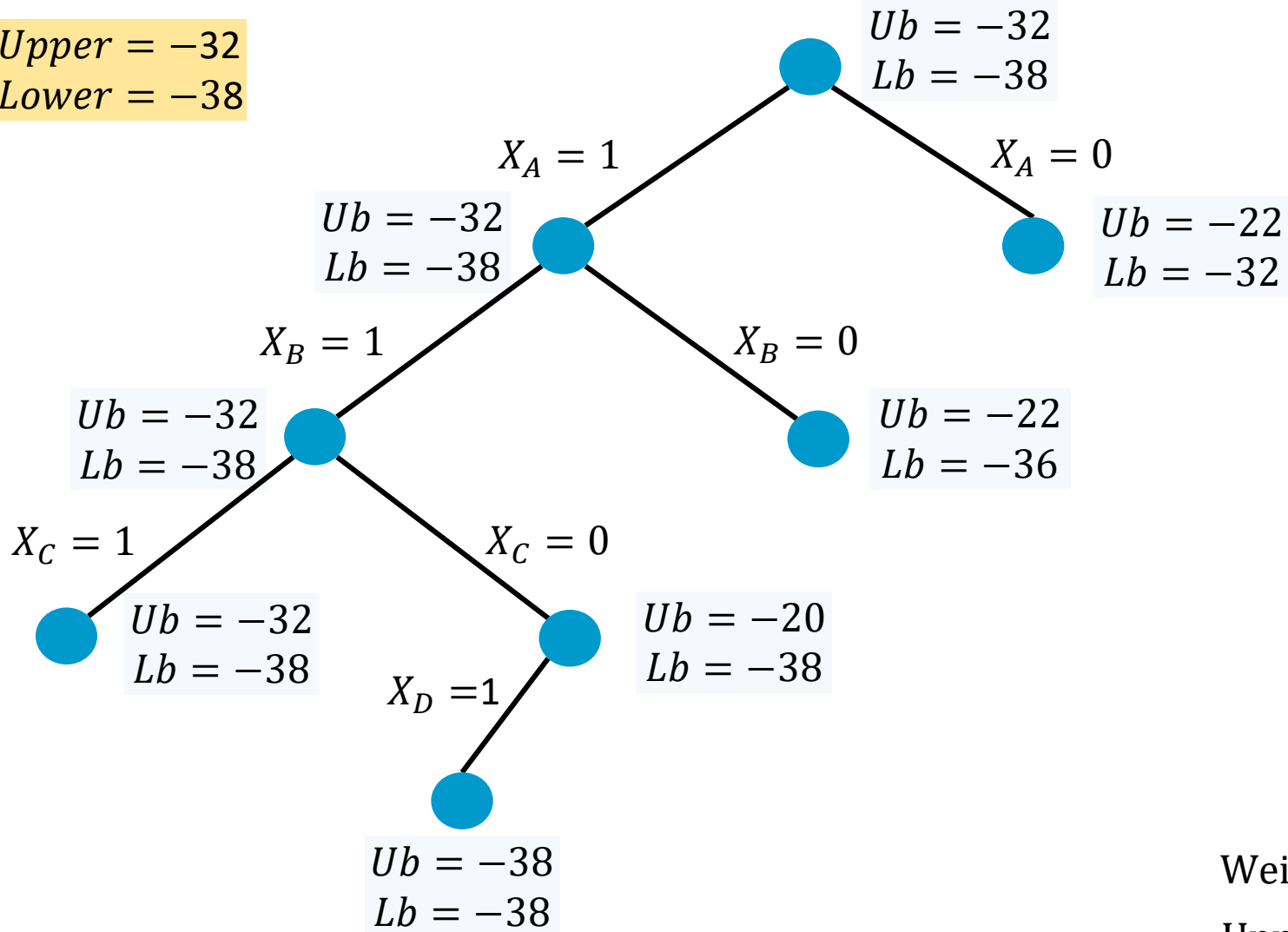
Weight = 2 + 6 = 8 ; Weight = 15 - 8 = 7

Upper Bound = 10 + 12 = **22**

Lower Bound = 10 + 12 +  $\frac{18 \times 7}{9}$  = **36**

# Example: Knapsack Problem

Upper = -32  
Lower = -38



Item	A	B	C	D
Value	-10	-10	-12	-18
Weight	2	4	6	9

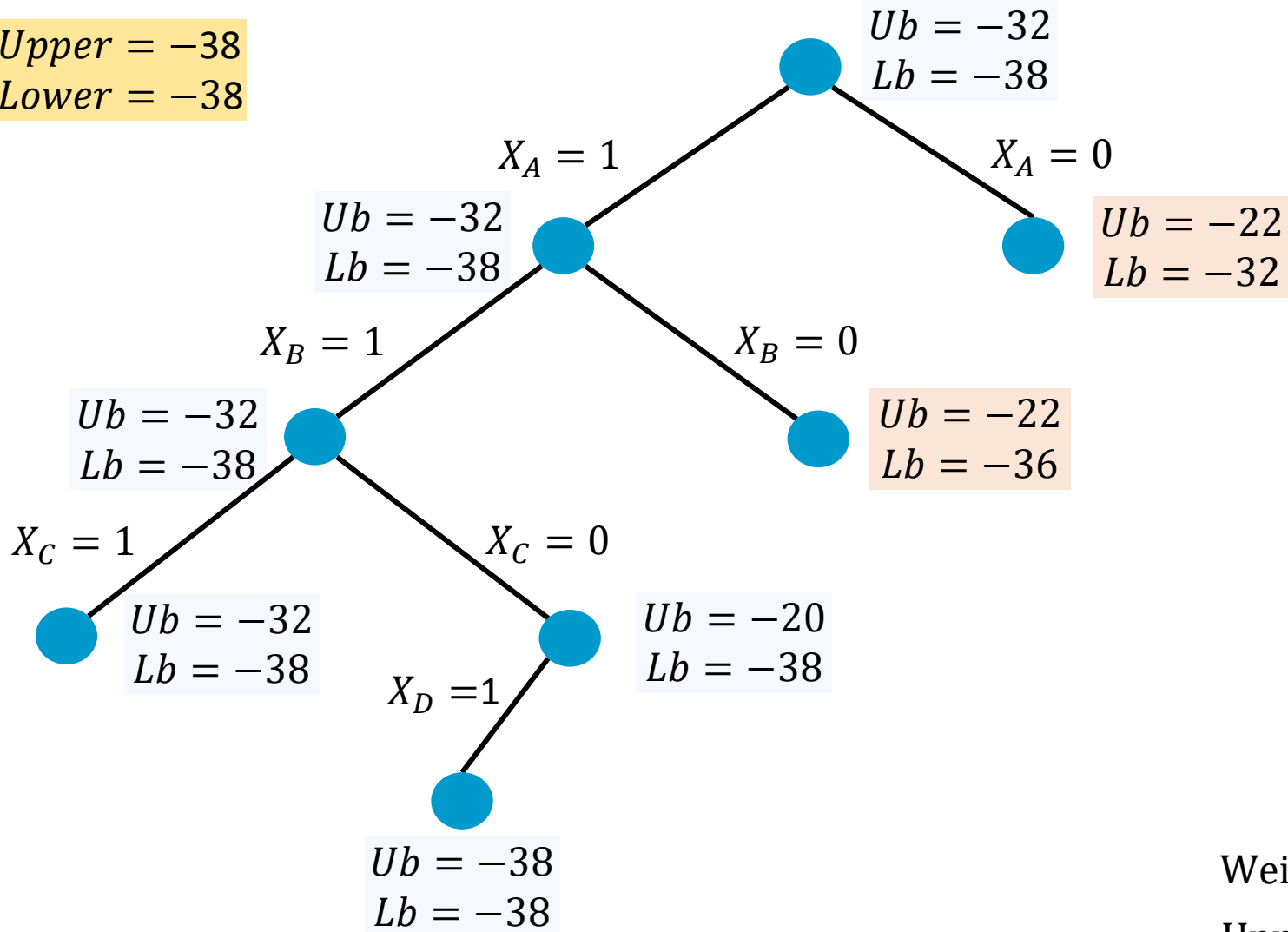
Weight = 2 + 4 = 6 ; Weight = 15 - 6 = 9

Upper Bound = 10 + 10 = **20**

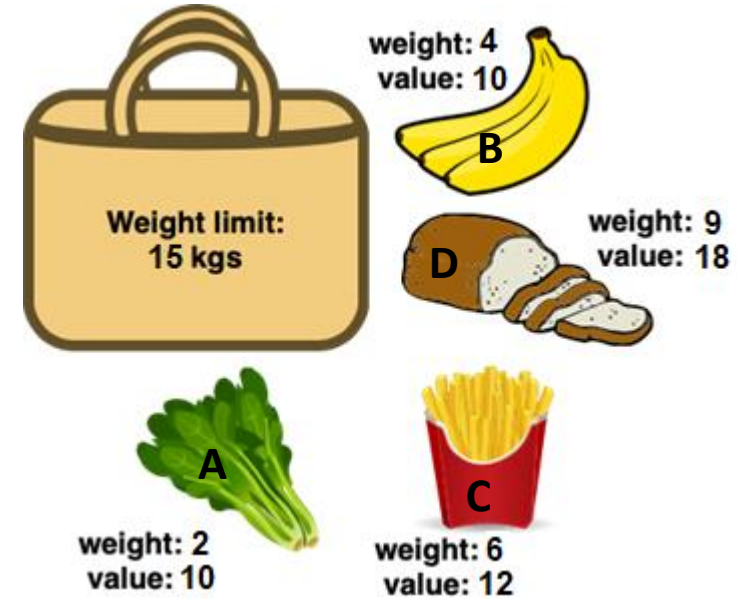
Lower Bound = 10 + 10 +  $\frac{18 \times 9}{9}$  = **38**

# Example: Knapsack Problem

Upper = -38  
Lower = -38



**Optimal Solution**



Item	A	B	C	D
Value	-10	-10	-12	-18
Weight	2	4	6	9

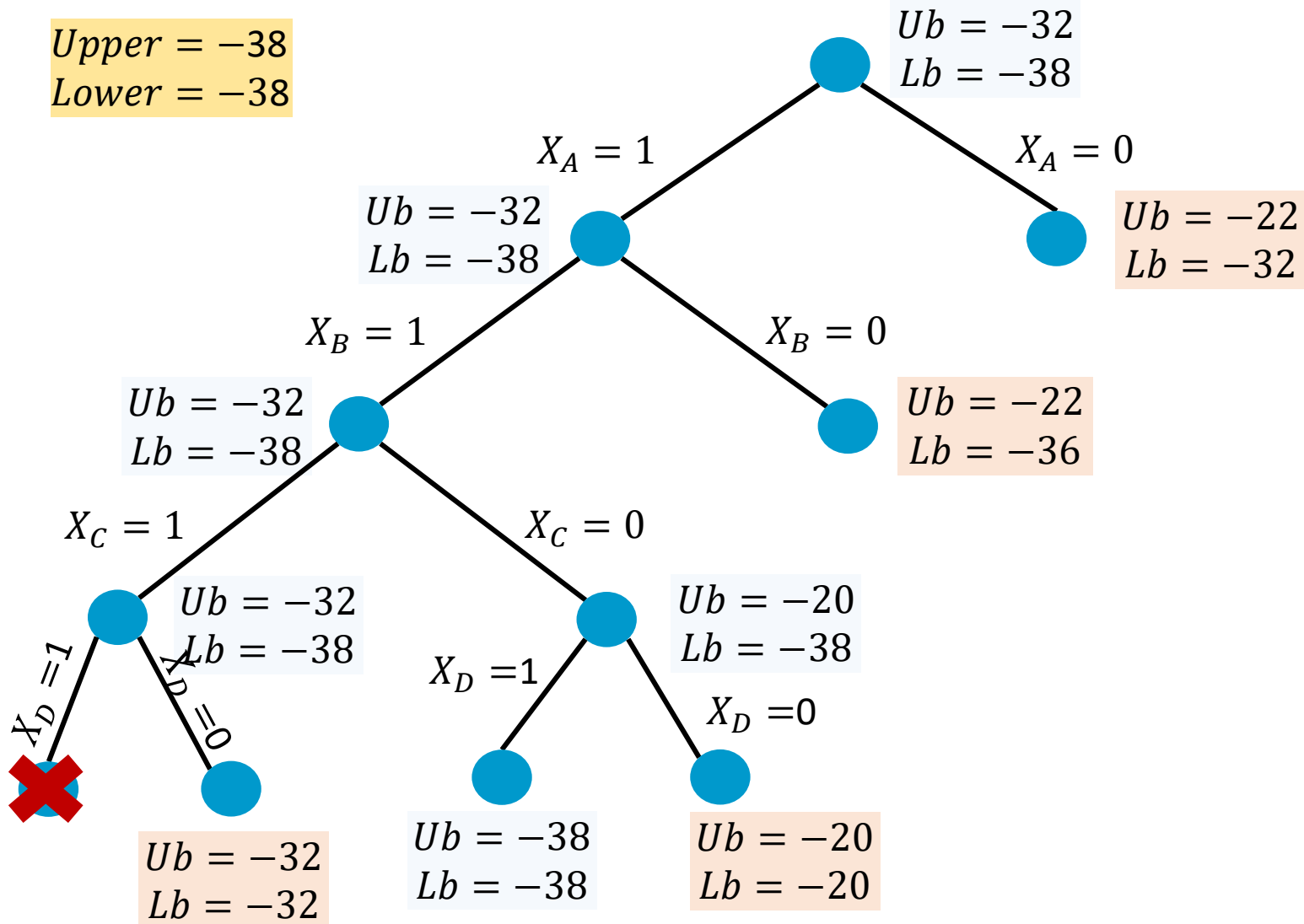
$$\text{Weight} = 2 + 4 + 9 = 15 ; \text{Weight} = 15 - 15 = 0$$

$$\text{Upper Bound} = 10 + 10 + 18 = \mathbf{38}$$

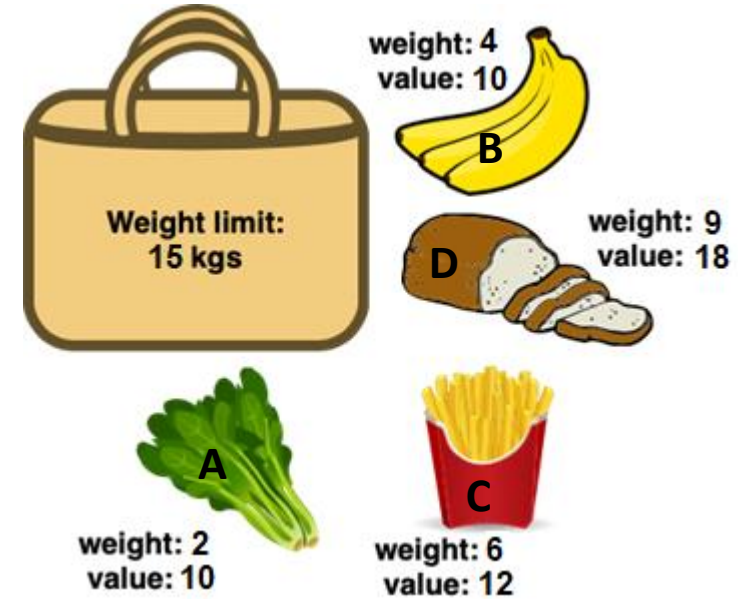
$$\text{Lower Bound} = 10 + 10 + \frac{18 \times 9}{9} = \mathbf{38}$$

# Example: Knapsack Problem

Upper = -38  
Lower = -38



**Optimal Solution**



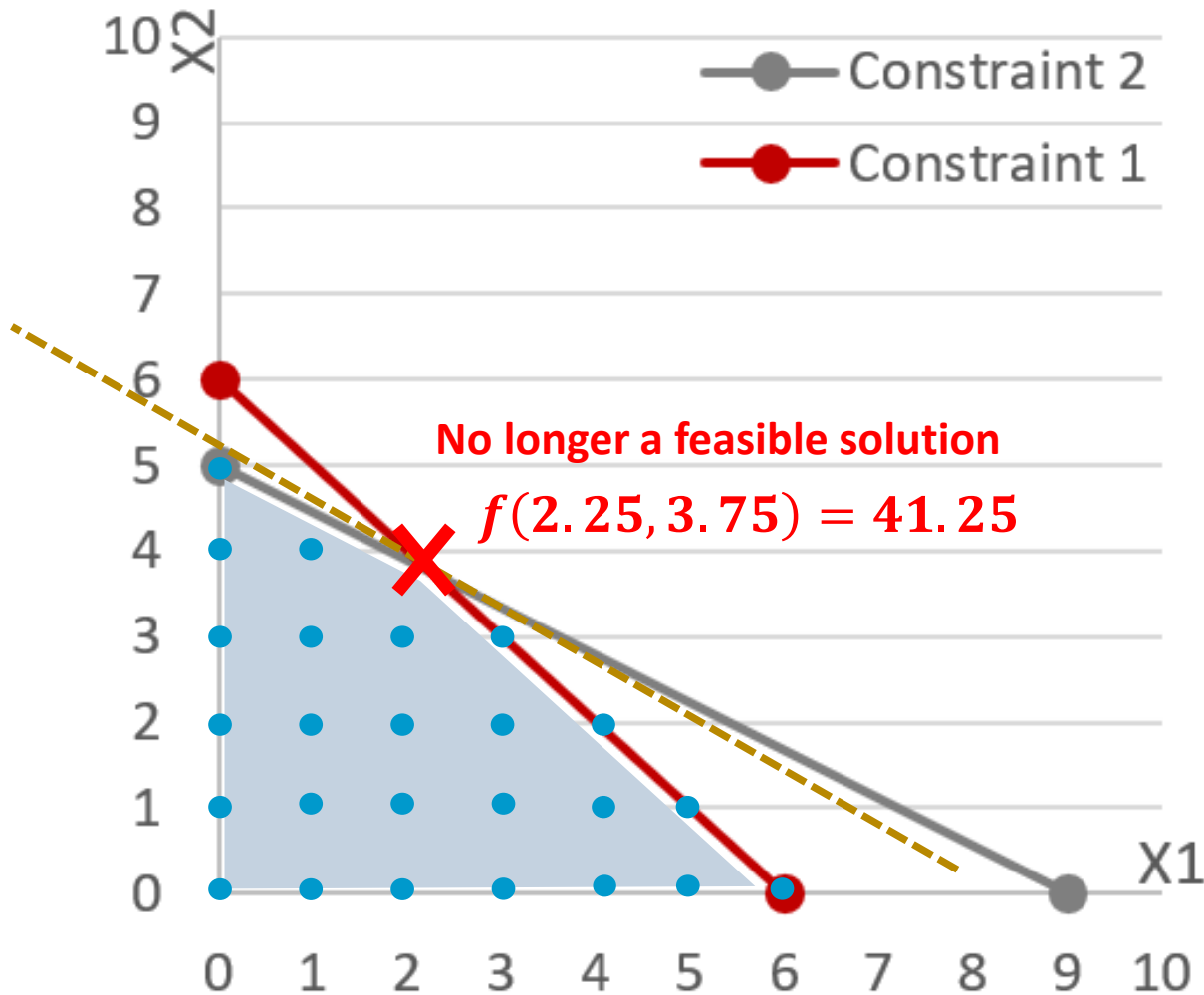
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# Branch and Bound + Simplex

- **Branch and bound builds on the top of LP methods**
  - If the LP is infeasible (i.e., has no solution), then the IP is also infeasible
  - If the LP problem has an integer-valued optimal solution, then the solution is equal to the optimal solution for the IP problem.
  - If the LP problem has a non-integer-value, then the problem needs to be decomposed
- **Branch and bound uses 2 heuristics:**
  - **The branch heuristic:**
    - Used to force the Simplex Method away from a non-integer valued solution - Many different LP problems are generated in the process
  - **The bound heuristic:**
    - Used to limit the number of LP problems generated by the branch heuristic

# Branch and Bound + Simplex



$$\max(f(x_1, x_2) = 5x_1 + 8x_2)$$

$$\text{s. t.} \quad x_1 + x_2 \leq 6$$

$$5x_1 + 9x_2 \leq 45$$

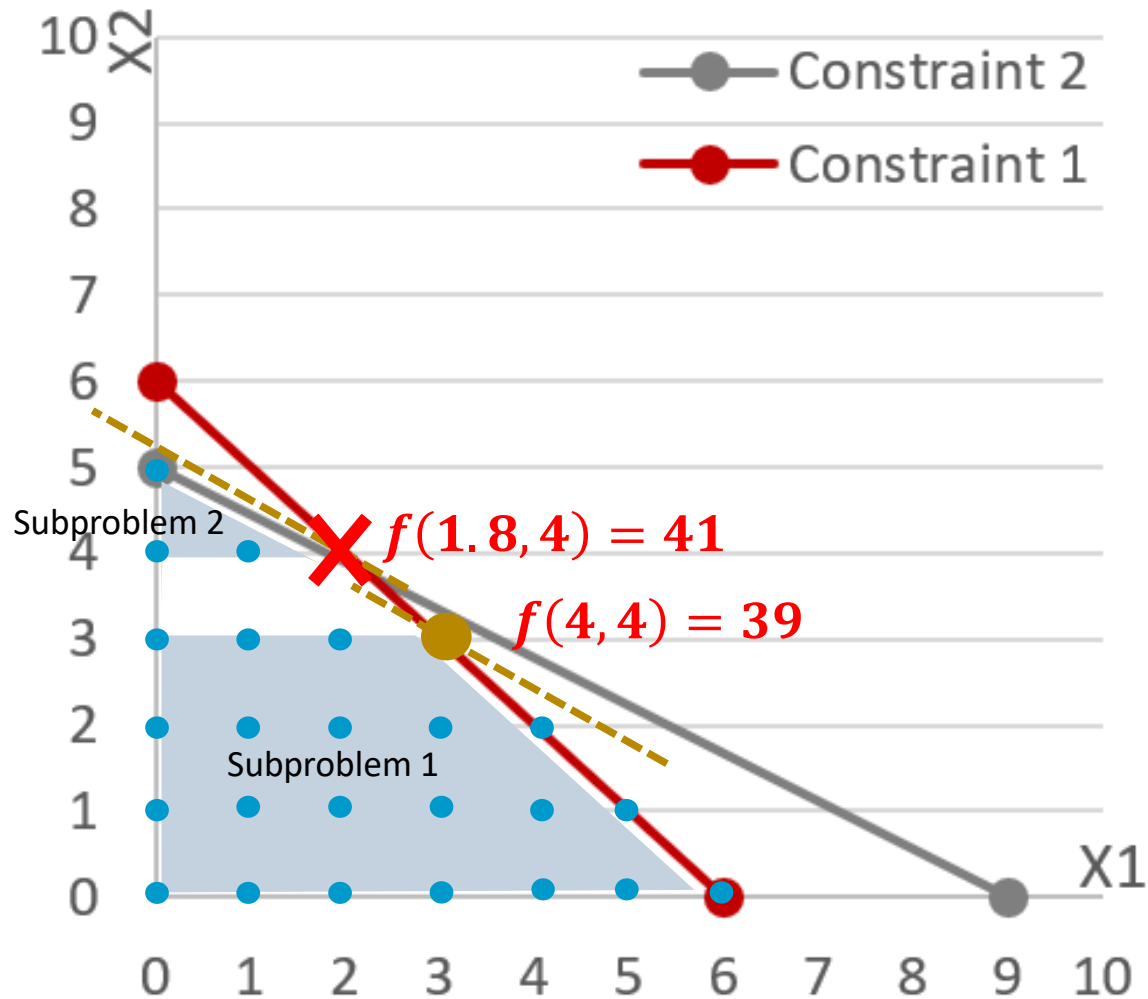
$$x_1, x_2 \geq 0, \text{ integer}$$

- We can force Simplex Method to avoid using  $x_2=3.75$
- The optimal integer solution have be **one of the following:**

$$x_2, \leq 3$$

$$x_2 \geq 4$$

# Branch and Bound + Simplex



$$\max(f(x_1, x_2) = 5x_1 + 8x_2)$$

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# Branch and Bound + Simplex

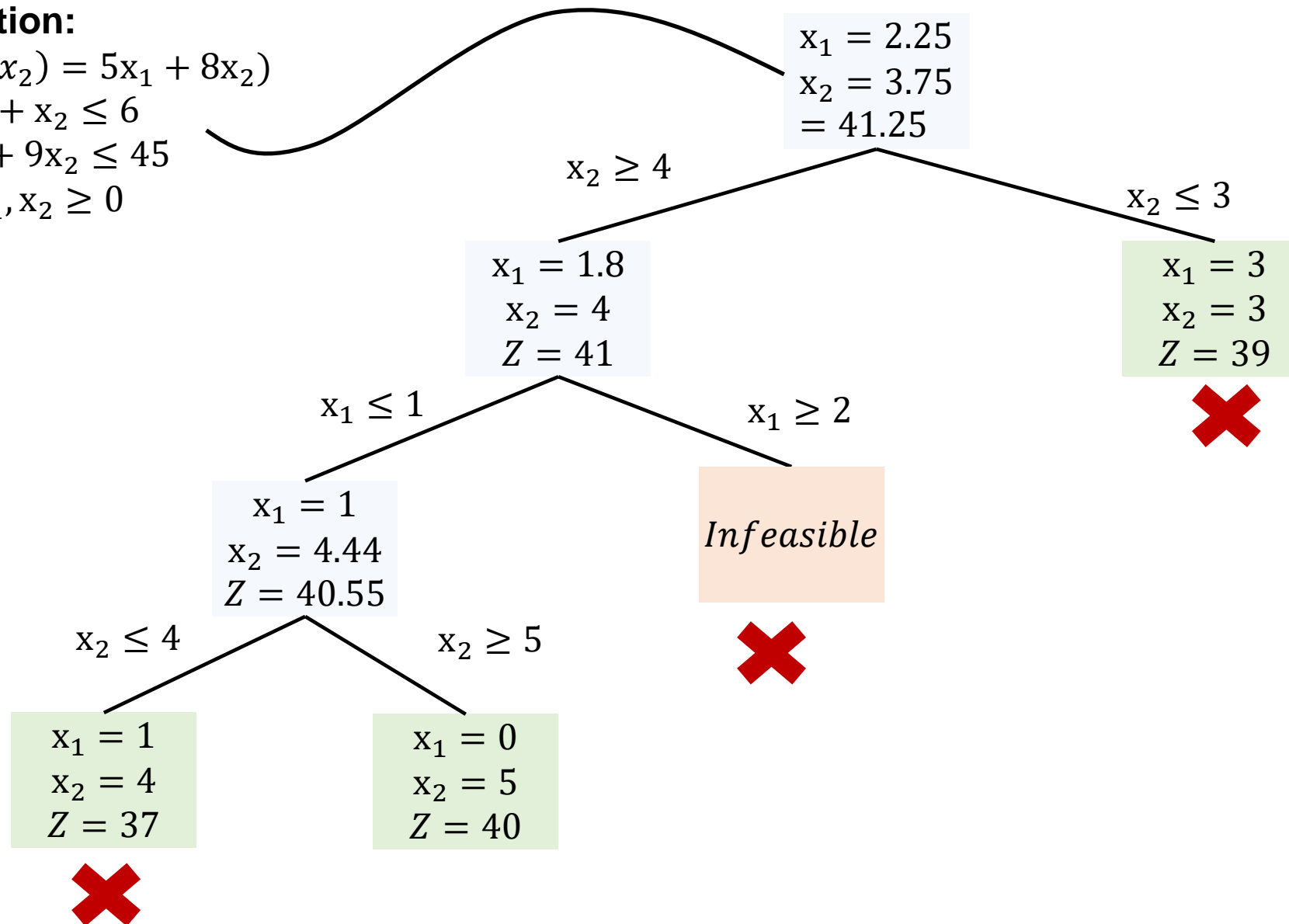
## LP Relaxation:

$$\max(f(x_1, x_2) = 5x_1 + 8x_2)$$

$$x_1 + x_2 \leq 6$$

$$5x_1 + 9x_2 \leq 45$$

$$x_1, x_2 \geq 0$$



Upper =  $inf$   
Lower =  $-41.25$

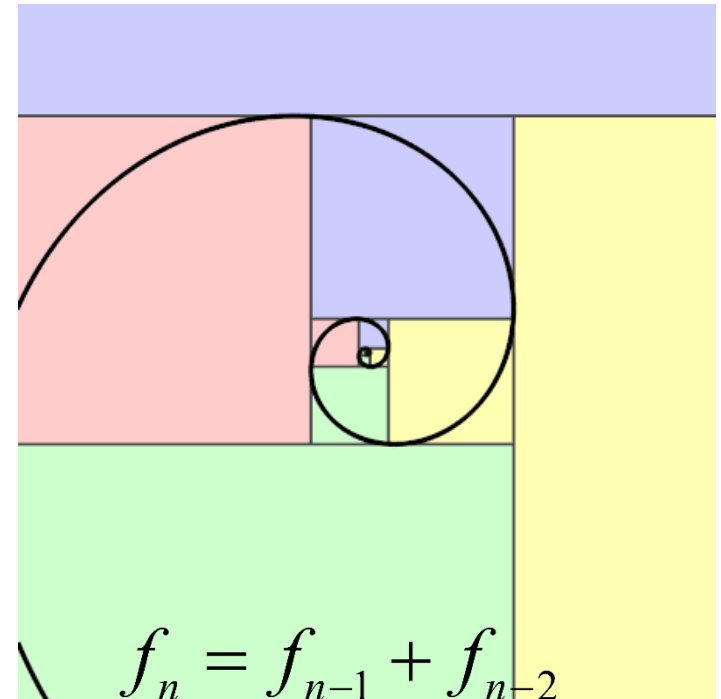
Upper =  $-39$   
Lower =  $-41$

Upper =  $-39$   
Lower =  $-40.55$

Upper =  $-40$   
Lower =  $-40$

# Dynamic Programming

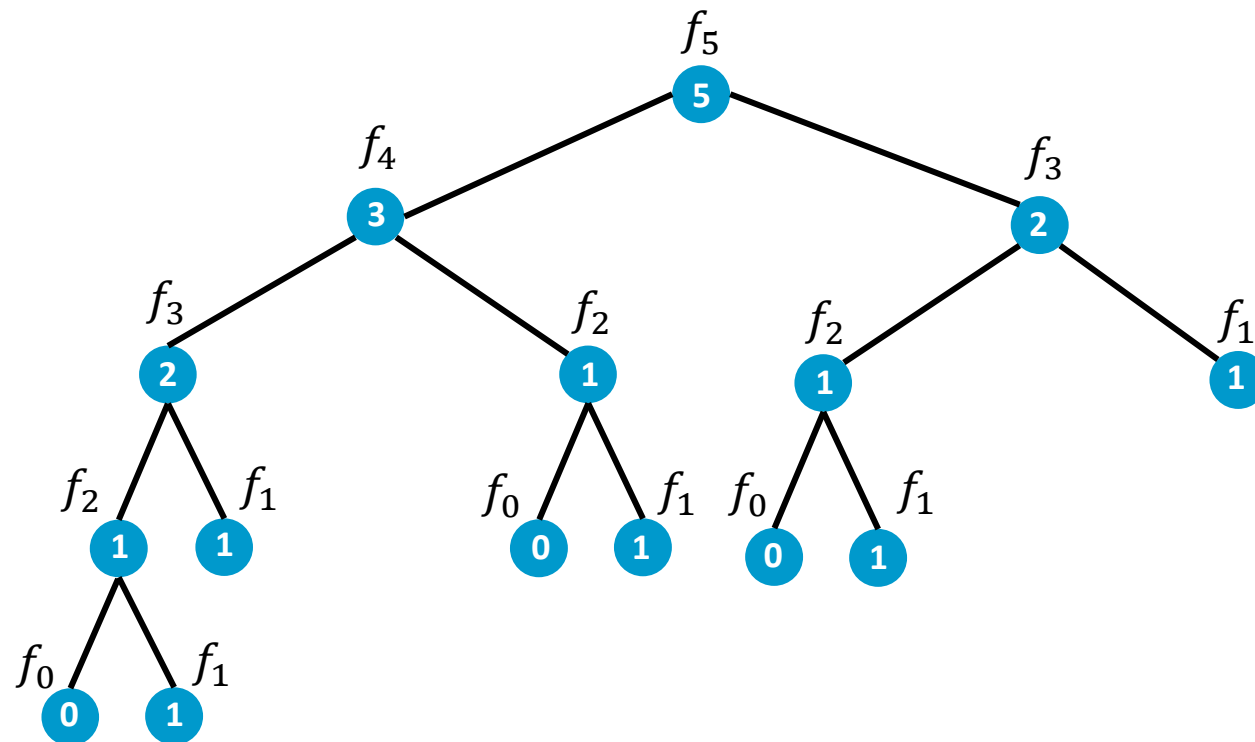
- Dynamic Programming (DP) is an algorithmic technique for solving an optimization problem by breaking it down into simpler **subproblems** and utilizing the fact that the optimal solution to the overall problem depends upon the optimal solution to its subproblems.
- DP relies on **memoization** (not memorization!) by storing past results and reusing it so as to not repeat expensive computation
- Let us compute Fibonacci of 5 using DP



<https://stemettes.org/zine/articles/fibonacci-in-nature/>

# Example: Computing Fibonacci Sequence

- In mathematics, the Fibonacci numbers, commonly denoted  $f_n$ , form a sequence, called the Fibonacci sequence, such that each number is the sum of the two preceding ones, starting from 0 and 1.



$$f_n = f_{n-1} + f_{n-2}$$

$f_0$	$f_1$	$f_2$	$f_3$	$f_4$	$f_5$
0	1	1	2	3	5

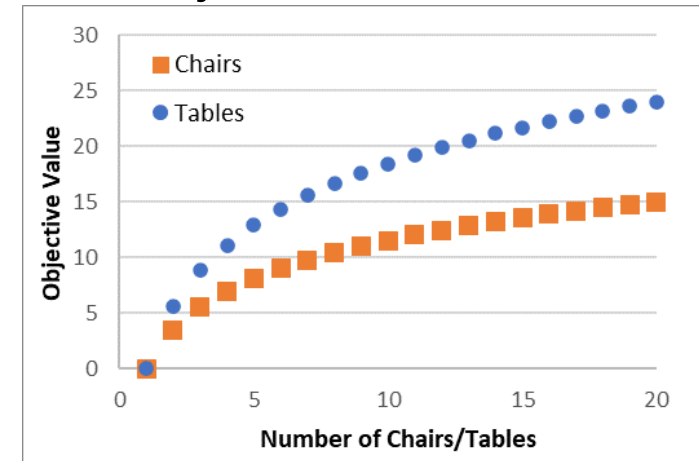
# Non-Linear Optimization

- A **non-linear program** can have a linear or nonlinear objective function with linear and/or nonlinear constraints

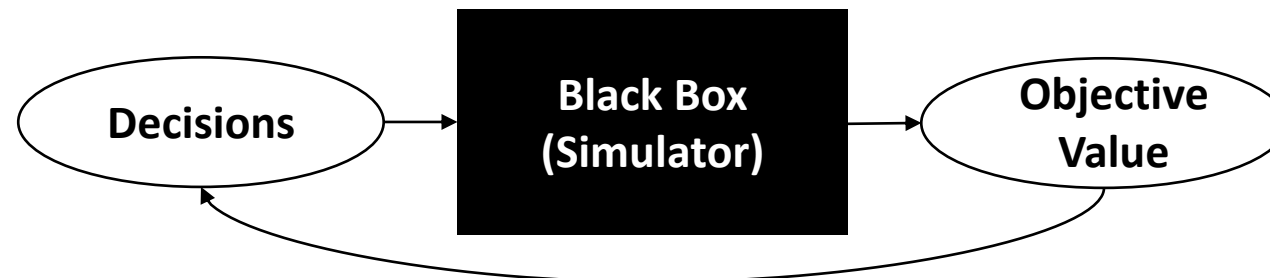
**Optimize:**  $\max(f(x_1, x_2) = 5 \ln(x_1) + 8 \ln(x_2))$

**Constraints:**  $x_1 + x_2 \leq 6$   
 $5x_1 + 9x_2 \leq 45$   
 $x_1, x_2 \geq 0, \text{ integer}$

*Example: Non-linear behaviour due to economies of scale*



- **"Black Box" optimization** refers to a problem setup in which an optimization algorithm is supposed to optimize (e.g., minimize) an objective function through a so-called black-box interface (simulation ; machine learning ; etc.)





# Optimization Software

Nuno Antunes Ribeiro

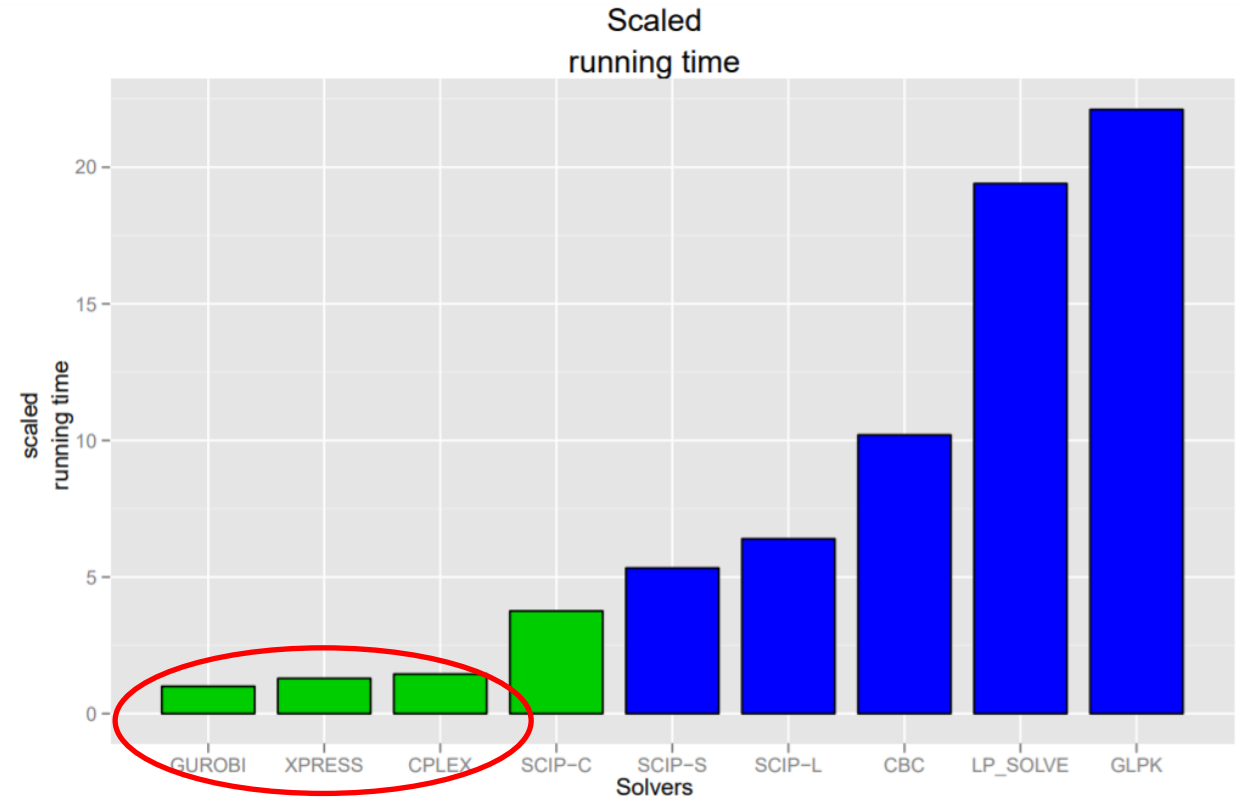
Assistant Professor



# Optimization Software

## Optimization Solver

- Gurobi
- Cplex **Paid Software**
- Xpress **Free Academic License**
- GLPK
- LP\_SOLVE
- CLP **Free Software**
- SCIP
- SoPlex



Running times of several solvers applied to benchmark test data

**Source: Analysis of commercial and free and open source solvers for linear optimization problems B. Meindl and M. Tempel**

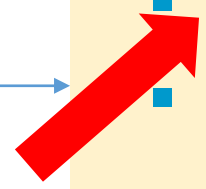
# Optimization Software

## Optimization Solver

- Gurobi
- Cplex
- Xpress
- GLPK
- LP\_SOLVE
- CLP
- SCIP
- SoPlex

## Programming Language

- Gurobi **Paid Software**
- IBM CPLEX **Free Academic License**
- Mosel
- GAMS
- AMPL **Paid Software**
- AIMSS
- **Pyomo - Python** **Free Software**
- Google OR Tools – Python, C++, Java
- NEOS\* **Online Server**  
[\\*https://neos-server.org/neos/](https://neos-server.org/neos/)



# Pyomo Overview

- Pythonic framework for formulating optimization models
  - Provide a natural syntax to describe mathematical models
  - Formulate large models with a concise syntax
  - Separate modeling and data declarations
  - Enable data import and export in commonly used formats
- Pyomo Documentation:
  - [Pyomo Documentation 6.1.2](#)



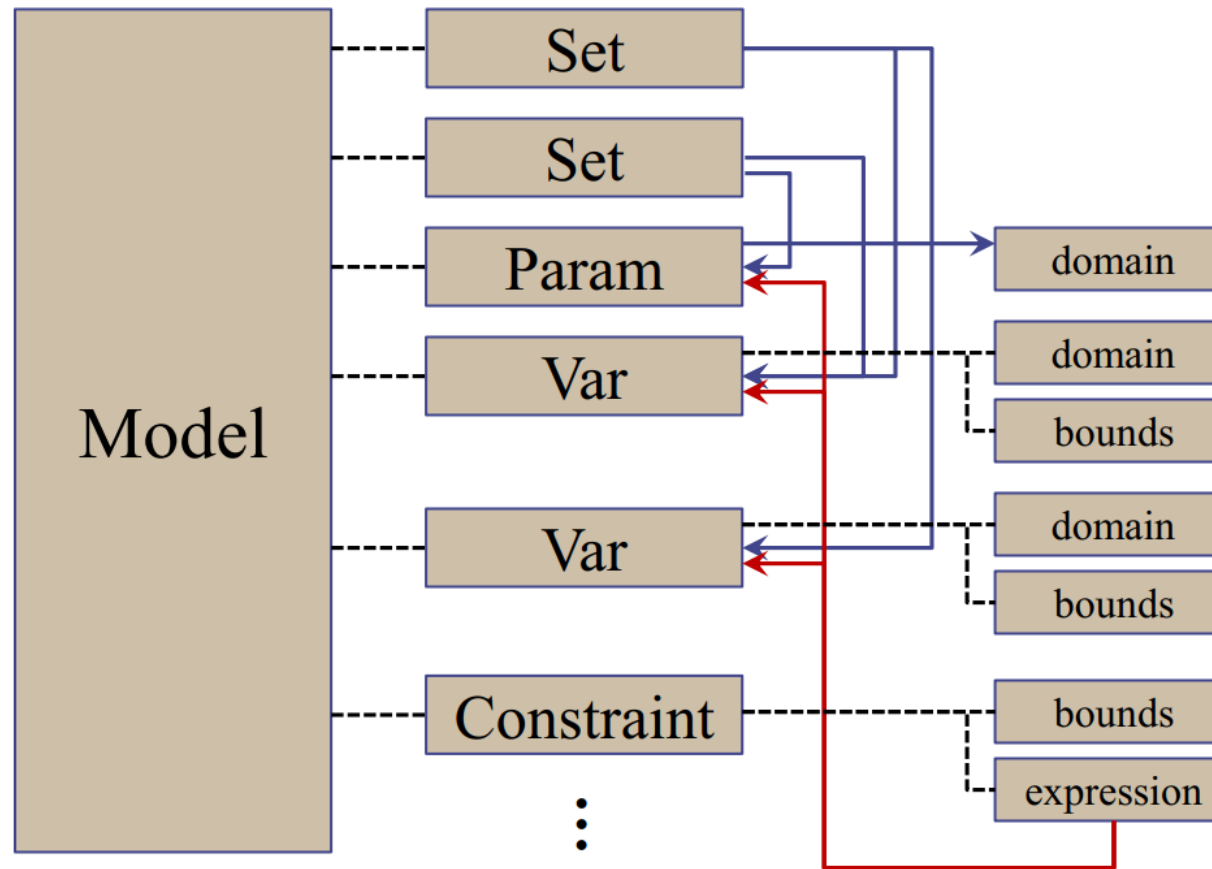
```
# simple.py
from pyomo.environ import *

M = ConcreteModel()
M.x1 = Var()
M.x2 = Var(bounds=(-1,1))
M.x3 = Var(bounds=(1,2))
M.o = Objective(
    expr=M.x1**2 + (M.x2*M.x3)**4 + \
        M.x1*M.x3 + \
        M.x2*sin(M.x1+M.x3) + M.x2)

model = M
```

# Fundamental Pyomo Components

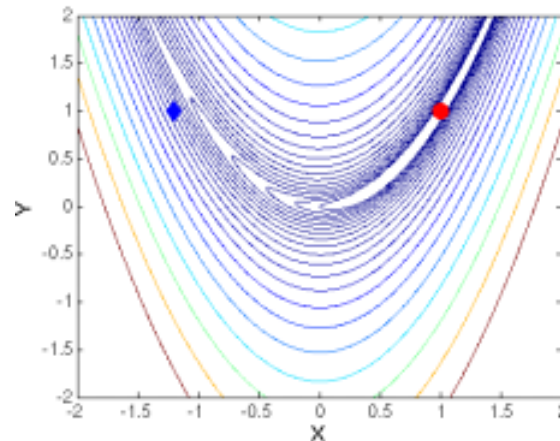
- Pyomo is an object model for describing optimization problems



# A simple Pyomo Model

- Rosenbrock.py

```
from pyomo.environ import *  
  
model = ConcreteModel()  
  
model.x = Var( initialize=-1.2, bounds=(-2, 2) )  
model.y = Var( initialize= 1.0, bounds=(-2, 2) )  
  
model.obj = Objective(  
    expr= (1-model.x)**2 + 100*(model.y-model.x**2)**2,  
    sense= minimize )
```



# Getting Started: the Model

- Import pyomo environ and create model instance

```
from pyomo.environ import *
```

← Every Pyomo model starts with this; it tells Python to load the Pyomo Modeling Environment

```
model = ConcreteModel()
```

↑ Create an instance of a *Concrete* model

- Concrete models are immediately constructed
- Data must be present *at the time* components are defined

↑ Local variable to hold the model we are about to construct

- While not required, by convention we use “model”
- If you choose to name your model something else, you will need to tell the Pyomo script the object name through the command line

# Modeling the Decision Variables

- Declare the decision variables

```
model.a_variable = Var(within = NonNegativeReals)
```

↑  
The name you assign the object to becomes the object's name, and must be unique in any given model.

↑  
"within" is optional and sets the variable domain ("domain" is an alias for "within")

↑  
Several pre-defined domains, e.g., "Binary"

```
model.a_variable = Var(bounds = (0, None))
```

↑  
Same as above: "domain" is assumed to be Reals if missing

# Modeling the Objective Function

- Formulate the objective function

```
model.x = Var( initialize=-1.2, bounds=(-2, 2) )  
model.y = Var( initialize= 1.0, bounds=(-2, 2) )
```

```
model.obj = Objective(  
    expr= (1-model.x)**2 + 100*(model.y-model.x**2)**2,  
    sense= minimize )
```

If “sense” is omitted, Pyomo assumes minimization

“expr” can be an expression, or any function-like object that returns an expression

Note that the Objective expression is not a *relational expression*



# Modeling the Constraints

- Formulate the model constraints

```
model.a = Var()  
model.b = Var()  
model.c = Var()  
model.c1 = Constraint(  
    expr = model.b + 5 * model.c <= model.a )
```

↑  
“expr” can be an expression,  
or any function-like object  
that returns an expression

# Modeling the Sets (Indices)

- Declare the sets of the decision variables and parameters

```
model.IDX = range(10)
model.a = Var()
model.b = Var(model.IDX)
model.c1 = Constraint(
    expr = sum(model.b[i] for i in model.IDX) <= model.a )
```

Python *list comprehensions* are very common for working over indexed variables and nicely parallel mathematical notation:

$$\sum_{i \in IDX} b_i \leq a$$



# Solving Optimization Problems using Pyomo

Nuno Antunes Ribeiro

Assistant Professor

# Facility Location Optimization Problem

- Location planning involves specifying the physical position of facilities that provide demanded services.
  - Urban and Regional Planning - location of schools, hospitals, bus stops, electric charging stations, solid waste landfills, etc.
  - Business Logistics and Supply Chains – location of industrial facilities, warehouses, distribution centres, hubs, offices, etc.
  - Defence and National Security – location of military bases, anti-missile systems, fire watchtowers, etc.
  - Electronics Industry- placement of interconnected electronic components onto a printed circuit board or on a microchip
  - Clustering techniques - cluster analysis problems can be viewed as facility location problems. The objective is to partition data points into equivalence classes such that points assigned of the same class are close to one another
- There are a variety of different models to solve this problem (**p-median problem**, quadratic assignment problem, capacitated location problem, etc.)

# P-Median Formulation

## □ Sets

*Set of candidate locations:  $i = 1, 2, \dots, i$*

*Set of costumers:  $j = 1, 2, \dots, j$*

## □ Parameters

*$d_j$  = demand of costumer  $j$*

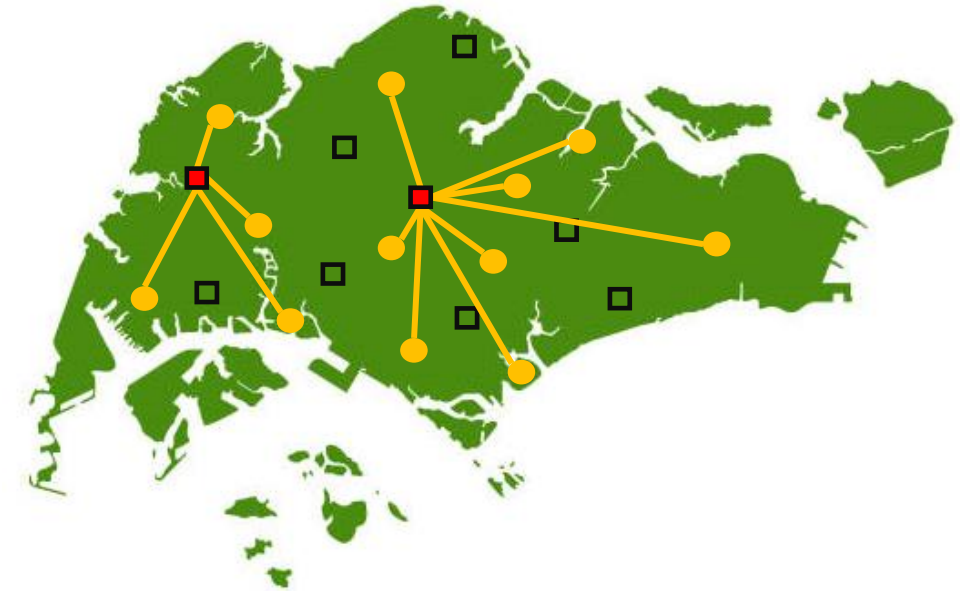
*$c_{ij}$  = unit cost of satisfying customer  $j$  from facility  $i$*

*$p$  = number of locations to open*

## □ Decision Variables

*$x_{ij} = 1$  if customer  $j$  is supplied by location  $i$ , 0 otherwise*

*$y_i = 1$  if a facility is located at location  $i$ , 0 otherwise*



# P-Median Formulation

$$\min z = \sum_{i \in I} \sum_{j \in J} d_j c_{ij} x_{ij}$$

**Minimize the demand-weighted total cost**

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

**All of the demand for customer j must be satisfied**

$$\sum_{i \in I} y_i = p$$

**Exactly p facilities are located**

$$x_{ij} \leq y_i, \quad \forall i \in I, j \in J$$

**Demand nodes can only be assigned to open facilities**

*$x_{ij}, y_i$  is binary*

**All variables are binary**

# Pyomo P-Median Formulation

## Inputs

```
#Generate Data Inputs

# Select random seed
random.seed(1)

# Number of candidate Locations
#n=100
n=1000

#Number of Locations to open
openfac=30

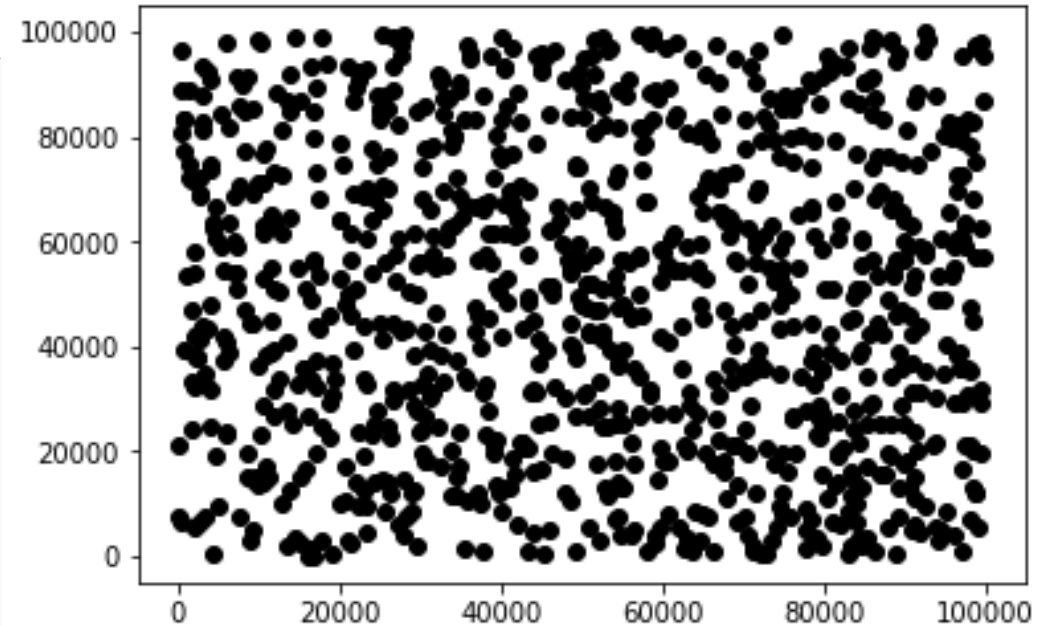
#Coordinate Range
rangelct=100000

#Generate random Locations
coordlct_x = random.choices(range(0, rangelct), k=n)
coordlct_y = random.choices(range(0, rangelct), k=n)

#Compute distance between Locations
distancelct=np.empty([n, n])
for i_index in range(n):
    for j_index in range(n):
        distancelct[i_index,j_index]=(math.sqrt(((coordlct_x[i_index]-coordlct_x[j_index])**2) +((coordlct_y[i_index]-coordlct_y

df = pd.DataFrame(distancelct)
df.index += 1
df.columns += 1
cij_model=df.stack().to_dict()

#Generate demand between locations
demandlct = random.choices(range(1, 50), k=n)
demanddf = pd.DataFrame(demandlct)
demanddf.index += 1
dj_model=demanddf.to_dict()
dj_model=dj_model[0]
```



# Pyomo P-Median Formulation

## Sets

```
# Create Model  
model = AbstractModel()
```

*Set of candidate locations:  $i = 1, 2, \dots, i$*

```
# Set of candidate locations
```

```
model.M = RangeSet(n)
```

```
# Set of customer nodes
```

```
model.N = RangeSet(n)
```

*Set of costumers:  $j = 1, 2, \dots, j$*

## Parameters

```
# Number of facilities
```

```
model.p = openfac
```

```
#  $d[j]$  - demand of customer  $j$ 
```

```
model.d = Param(model.N, initialize=dj_model)
```

```
#  $c[i,j]$  - unit cost of satisfying customer  $j$  from facility  $i$ 
```

```
model.c = Param(model.M, model.N, initialize=cij_model)
```

*$p$  = number of locations to open*

*$d_j$  = demand of customer  $j$*

*$c_{ij}$  = unit cost of satisfying customer  $j$   
from facility  $i$*

## Decision Variables

```
#  $x[i,j]$  - 1 if customer  $j$  is supplied by location  $i$ 
```

```
model.x = Var(model.M, model.N, within=Binary)
```

*$x_{ij} = 1$  if customer  $j$  is supplied by  
location  $i$ , 0 otherwise*

```
#  $y[i]$  - a binary value that is 1 if a facility is located at location  $i$ 
```

```
model.y = Var(model.M, within=Binary)
```

*$y_i = 1$  if a facility is located at  
location  $i$ , 0 otherwise*



# Pyomo P-Median Formulation

## Objective Function

```
# Minimize the demand-weighted total cost
def cost_(model):
    return sum(model.d[j]*model.c[i,j]*model.x[i,j] for i in model.M for j in model.N)
model.cost = Objective(rule=cost_)
```

$$\min z = \sum_{i \in I} \sum_{j \in J} d_j c_{ij} x_{ij}$$

## Constraints

```
# All of the demand for customer j must be satisfied
def demand_(model, j):
    return sum(model.x[i,j] for i in model.M) == 1.0
model.demand = Constraint(model.N, rule=demand_)
```

$$\sum_{i \in I} x_{ij} = 1, \quad \forall j \in J$$

```
# Exactly p facilities are located
def facilities_(model):
    return sum(model.y[i] for i in model.M) == model.p
model.facilities = Constraint(rule=facilities_)
```

$$\sum_{i \in I} y_i = p$$

```
# Demand nodes can only be assigned to open facilities
def openfac_(model, i, j):
    return model.x[i,j] <= model.y[i]
model.openfac = Constraint(model.M, model.N, rule=openfac_)
```

$$x_{ij} \leq y_i, \quad \forall i \in I, j \in J$$

# Pyomo P-Median Solve Model

## Solve Model

```
instance = model.create_instance()
opt = pyo.SolverFactory('gurobi')
opt.solve(instance, options={'TimeLimit': 10000}, tee=True)
```

Solved with barrier

Root relaxation: objective 1.613801e+08, 30112 iterations, 157.47 seconds

Nodes		Current Node			Objective Bounds			Work	
Expl	Unexpl	Obj	Depth	IntInf	Incumbent	BestBd	Gap	It/Node	Time
	0	0	1.6138e+08	0	538	2.3800e+08	1.6138e+08	32.2%	- 180s
H	0	0			1.615296e+08	1.6138e+08	0.09%	-	182s
H	0	0			1.613936e+08	1.6138e+08	0.01%	-	188s

Explored 1 nodes (30112 simplex iterations) in 188.72 seconds  
Thread count was 4 (of 4 available processors)

Solution count 3: 1.61394e+08 1.6153e+08 2.37999e+08

Optimal solution found (tolerance 1.00e-04)

Best objective 1.613935998492e+08, best bound 1.613800660278e+08, gap 0.0084%

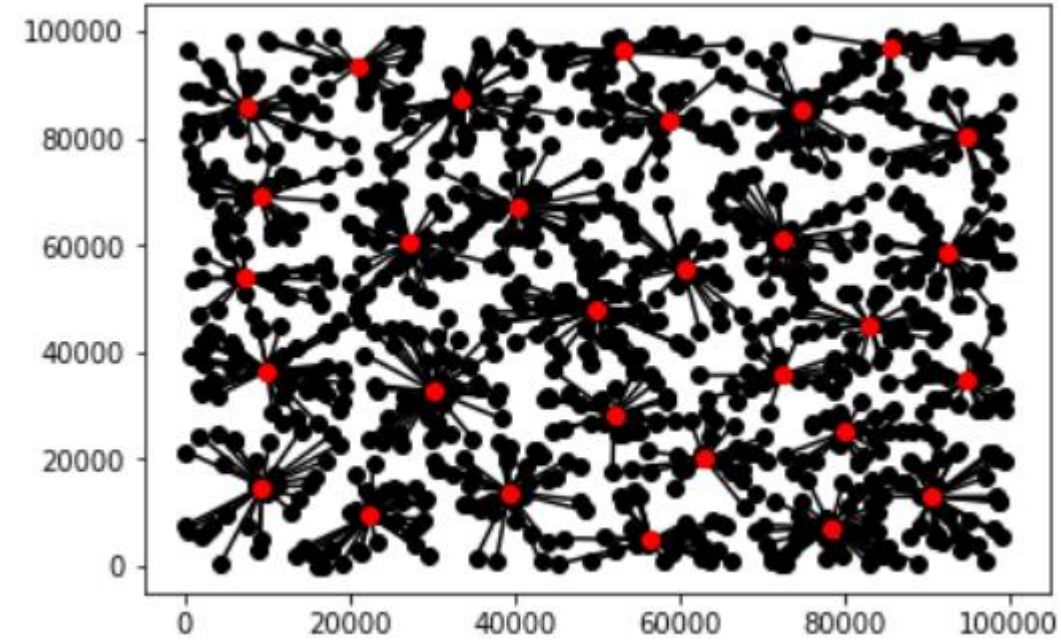
# Pyomo P-Median Outputs

## Read output variables

```
xij_dic = {i:int(value(j)) for (i,j) in instance.x.items()}  
xij = pd.DataFrame(xij_dic.values(), index = xij_dic.keys()).unstack()  
linkindex = np.where(xij == 1)
```

## Plot results

```
def connectpoints(x,y,p1,p2):  
    x1, x2 = x[p1], x[p2]  
    y1, y2 = y[p1], y[p2]  
    plt.plot([x1,x2],[y1,y2], 'k-')  
  
for i_index in range(len(linkindex[0])):  
    connectpoints(coordlct_x,coordlct_y,linkindex[0][i_index],linkindex[1][i_index])  
  
plt.plot(coordlct_x, coordlct_y, 'o', color='black');  
  
yi_dic = {i:int(value(j)) for (i,j) in instance.y.items()}  
yi = pd.DataFrame(yi_dic.values(), index = yi_dic.keys()).unstack()  
facilityindex = np.where(yi == 1)  
  
for i_index in range(len(facilityindex[0])):  
    plt.plot(coordlct_x[facilityindex[0][i_index]], coordlct_y[facilityindex[0][i_index]], 'o', color='red');
```





# Travelling Salesman Problem

- Much of the work on the TSP is motivated by its use as a platform for the study of general methods that can be applied to a wide range of discrete optimization problems. This is not to say, however, that the TSP does not find applications in many fields.
- The TSP naturally arises as a **subproblem in many transportation and logistics applications**, for example the problem of arranging school bus routes to pick up the children in a school district.
- Other applications: scheduling of service calls at cable firms, the delivery of meals to homebound persons, the scheduling of stacker cranes in warehouses, the routing of trucks for parcel post pickup
- Also: genome sequencing, NASA Starlight space interferometer program, semi-conductor manufacturing, compute DNA sequences, fiber optical networks, deliver power to electronic devices
- <https://www.math.uwaterloo.ca/tsp/apps/index.html>

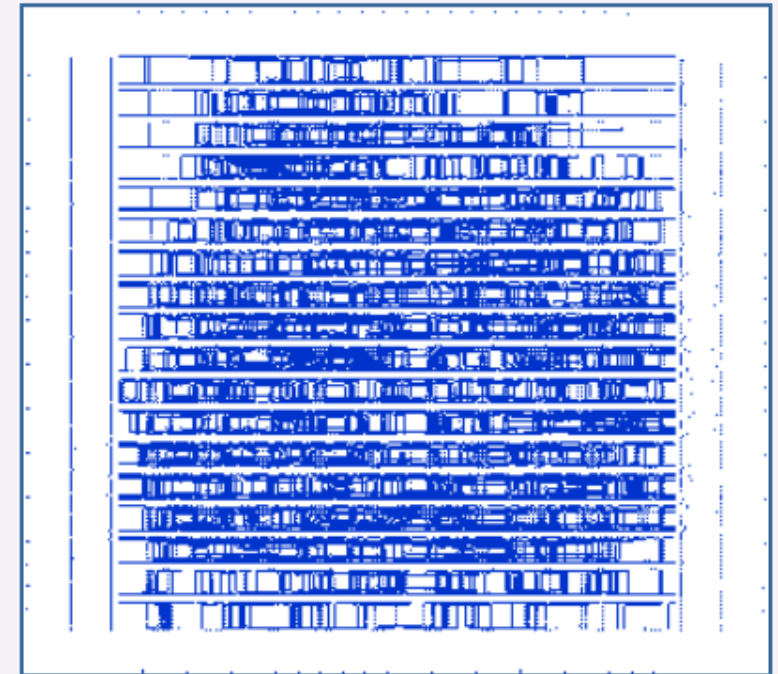
# Solving the Travelling Salesman Problem



24,978 Cities in Sweden  
Solved in 2004



15,112 Cities in Germany  
Solved in 2001

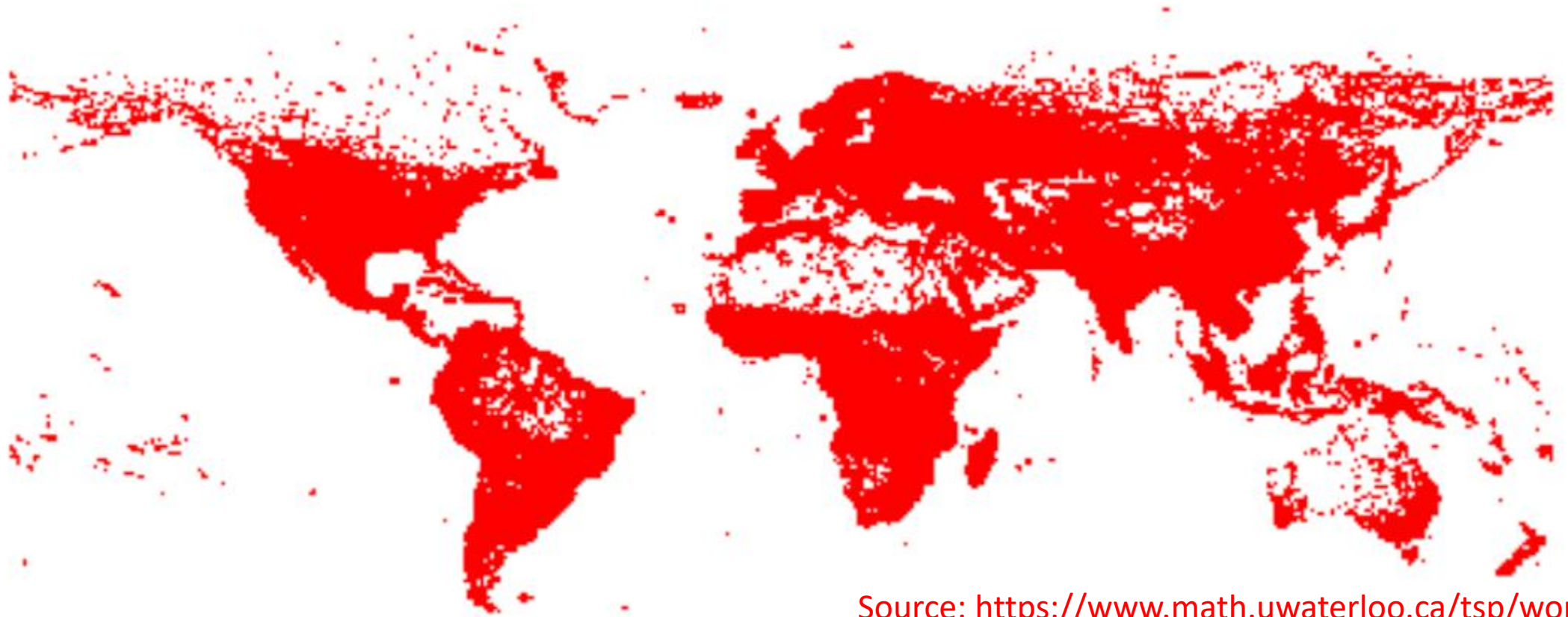


85,900 Locations in a VLSI Application  
Solved in 2006

1954	1962	1977	1987	1987	1987	1994	1998	2001	2004
n=49	n=33	n=120	n=532	n=666	n=2392	n=7397	n=13509	n=15112	n=24978

<https://www.math.uwaterloo.ca/tsp/apps/index.html>

# Solving the Travelling Salesman Problem



Source: <https://www.math.uwaterloo.ca/tsp/world/>

- Size: 1,904,711-cities
- Best lower bound: 7,512,218,268 (June, 2007)
- Best solution: 7,515,755,956 (February, 2021) --- Gap 0.0471%

# TSP Formulation

## □ Sets

*Set of cities to visit:  $i = 1, 2, \dots, i$*

## □ Parameters

*$c_{ij}$  = distance from  $i$  and  $j$*

## □ Decision Variables

*$x_{ij} = 1$  if city  $j$  is visited right after city  $i$ , 0 otherwise*

*$u_i$  = Auxiliary variable indicating tour ordering*





# TSP Formulation

$$\min z = \sum_{i,j \in I} c_{ij} x_{ij}$$

Minimize the total distance

$$s.t. \quad \sum_{j \in I} x_{ij} = 1, \quad \forall i \in I$$

There is only one departure  
from each city

$$\sum_{i \in I} x_{ij} = 1, \quad \forall j \in I$$

There is only one arrival to  
each city

$$u_i - u_j + nx_{ij} \leq (n - 1), \quad \forall i, j \in I \mid 2 \leq i \neq j \leq n$$

There is only a  
single tour covering  
all cities, and not  
two or more  
disjointed tours

$$n = \text{card}(J)$$

$x_{ij}$ , is binary

$$0 \leq u_i \leq n, \quad \forall i \in I$$

# Pyomo TSP Formulation

## Inputs

```
#Generate Data Inputs

# Select random seed
random.seed(1)

# Number of cities
n=100

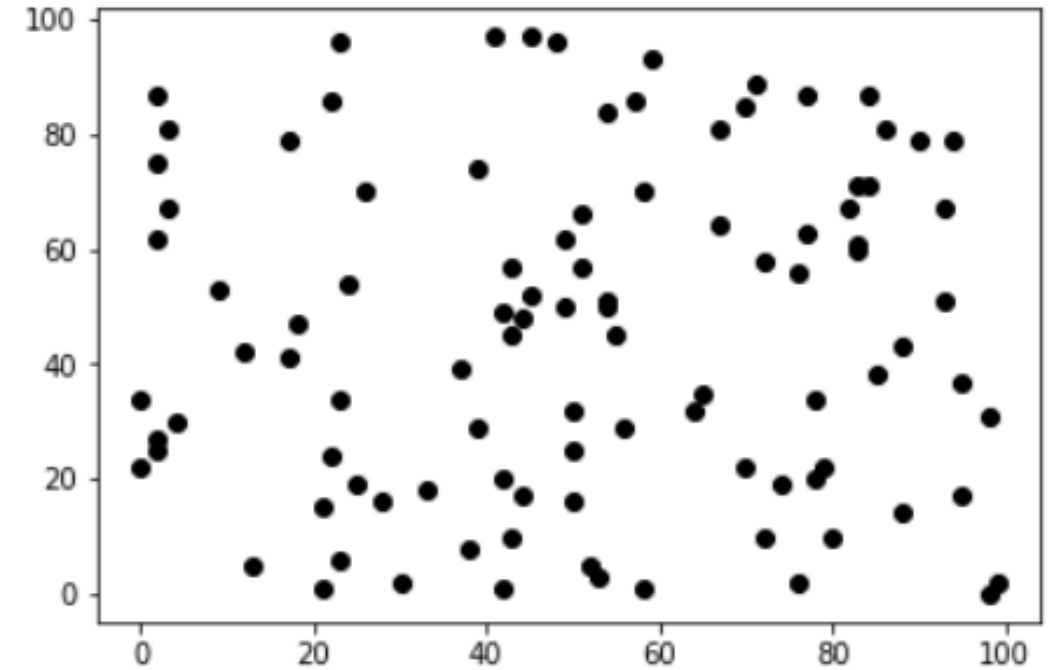
#Coordinate Range
rangelct=100

#Generate random locations
coordlct_x = random.choices(range(0, rangelct), k=n)
coordlct_y = random.choices(range(0, rangelct), k=n)

#Compute distance between locations
distancelct=np.empty([n, n])
for i_index in range(n):
    for j_index in range(n):
        distancelct[i_index,j_index]=(math.sqrt(((coordlct_x[i_index]-coordlct_x[j_index])**2) +((coordlct_y[i_index]-coordlct_y[j_index])**2)))

distancelct[np.diag_indices_from(distancelct)] = 99999

df = pd.DataFrame(distancelct)
df.index += 1
df.columns += 1
cij_model=df.stack().to_dict()
```



# Pyomo TSP Formulation

## Sets

```
# Create Model
model = AbstractModel()

# Set of cities to visit
model.N = RangeSet(n)
model.U = RangeSet(2,n)
```

*Set of cities to visit:  $i = 1, 2, \dots, i$*   
*Set of cities to visit w/o considering origin:  $i = 2, 3, \dots, i$*

## Parameters

```
# c[i,j] - distance from i and j
model.c = Param(model.N, model.N, initialize=cij_model)
```

*$c_{ij} = \text{distance from } i \text{ and } j$*

## Decision Variables

```
# x[i,j] - 1 if city j is visited right after city i, 0 otherwise
model.x = Var(model.N, model.N, within=Binary)

# u[i] - auxiliary variable indicating tour ordering
model.u = Var(model.N, within=Integers, bounds=(0,n))
```

*$x_{ij} = 1$  if city  $j$  is visited right after city  $i$ , 0 otherwise*  
 *$u_i = \text{Auxiliary variable indicating tour ordering}$*

# Pyomo TSP Formulation

## Objective Function

```
# Minimize total distance
def cost_(model):
    return sum(model.c[i,j]*model.x[i,j] for i in model.N for j in model.N)
model.cost = Objective(rule=cost_)
```

$$\min z = \sum_{i,j \in I} c_{ij} x_{ij}$$

## Constraints

```
# There is only one departure from each city
def arrive_(model, j):
    return sum(model.x[i,j] for i in model.N if i!=j) == 1
model.arrive = Constraint(model.N, rule=arrive_)
```

$$\sum_{i \in I} x_{ij} = 1, \quad \forall j \in I$$

```
# There is only one arrival to each city
def depart_(model, i):
    return sum(model.x[i,j] for j in model.N if j!=i) == 1
model.depart = Constraint(model.N, rule=depart_)
```

$$\sum_{j \in I} x_{ij} = 1, \quad \forall i \in I$$

```
# There is only a single tour covering all cities, and not two or more disjointed tours
def singletour_(model,i,j):
    if i!=j:
        return model.u[i] - model.u[j] + model.x[i,j] * n <= n-1
    else:
        return model.u[i] - model.u[j] == 0
model.singletour = Constraint(model.U,model.N,rule=singletour_)
```

$$u_i - u_j + nx_{ij} \leq (n - 1)$$

$$, \forall i, j \in I \mid 2 \leq i \neq j \leq n$$

# Pyomo TSP Formulation

```
instance = model.create_instance()
opt = pyo.SolverFactory('gurobi')
opt.solve(instance, options={'TimeLimit': 3600*500}, tee=True)
```

Root relaxation: objective 6.532166e+02, 355 iterations, 0.02 seconds

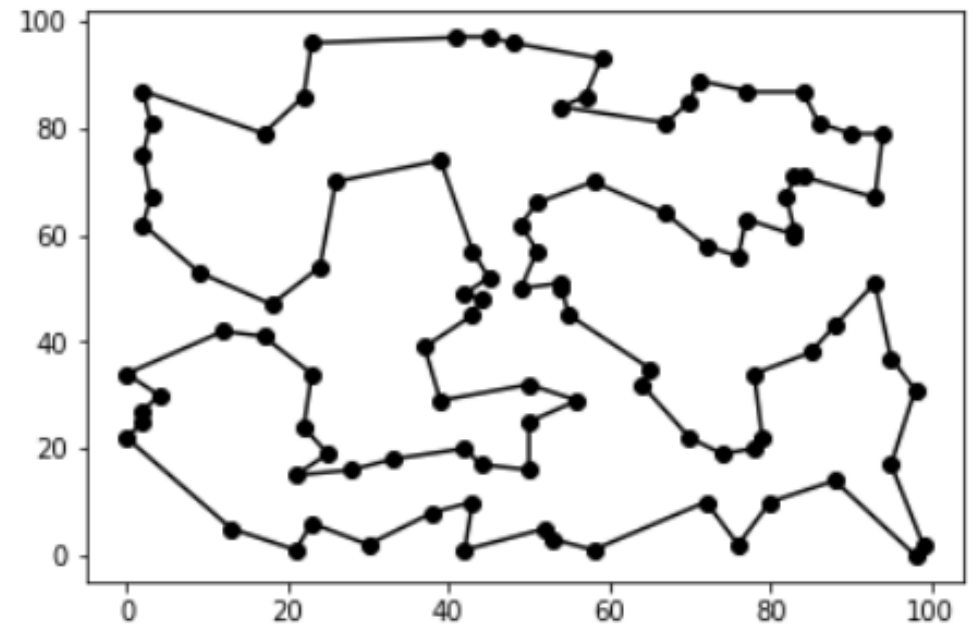
Nodes		Current Node			Objective Bounds			Work	
Expl	Unexpl	Obj	Depth	IntInf	Incumbent	BestBd	Gap	It/Node	Time
0	0	653.21664	0	195	4921.99004	653.21664	86.7%	-	0s
0	0	743.92129	0	254	4921.99004	743.92129	84.9%	-	1s
0	0	743.95035	0	271	4921.99004	743.95035	84.9%	-	1s
0	0	743.95035	0	273	4921.99004	743.95035	84.9%	-	1s
0	0	751.90069	0	243	4921.99004	751.90069	84.7%	-	2s
0	0	752.86330	0	233	4921.99004	752.86330	84.7%	-	2s
0	0	752.89659	0	240	4921.99004	752.89659	84.7%	-	2s
0	0	752.89659	0	240	4921.99004	752.89659	84.7%	-	2s
969	603	809.00378	200	244	809.00378	775.49354	4.14%	31.4	110s
H 975	576				794.3991143	775.77367	2.34%	31.3	112s
998	592	794.39911	248	118	794.39911	775.86216	2.33%	39.9	115s
H 1077	604				792.4346674	776.39951	2.02%	44.2	119s
1280	648	789.86207	74	187	792.43467	776.59202	2.00%	42.8	120s
2661	443	cutoff	80		792.43467	779.77907	1.60%	48.2	125s
* 4316	300		76		786.7827327	784.41635	0.30%	47.4	129s
4611	272	786.45151	88	62	786.78273	784.70306	0.26%	46.0	130s
* 4716	230		72		785.9523981	784.75775	0.15%	45.6	130s
* 4849	86		81		785.5122306	785.15006	0.05%	45.1	130s

# Pyomo TSP Outputs

## Read output variables

```
xij_dic = {i:int(np.round(value(j))) for (i,j) in instance.x.items()}  
xij = pd.DataFrame(xij_dic.values(), index = xij_dic.keys()).unstack()  
linkindex = np.where(xij == 1)
```

```
ui_dic = {i:int(value(j)) for (i,j) in instance.u.items()}  
ui = pd.DataFrame(ui_dic.values(), index = ui_dic.keys()).unstack()  
sequence = np.where(ui == 1)  
uidf=pd.DataFrame(ui)  
uidf=uidf.sort_values(by=[0])  
  
pd.set_option('display.max_rows', uidf.shape[0]+1)
```



# Vehicle Routing Problem

- In the Vehicle Routing Problem (VRP), the goal is to find optimal routes for multiple vehicles visiting a set of locations. (When there's only one vehicle, it reduces to the Travelling Salesman Problem)



# TSP Formulation

## □ Sets

*Set of cities to visit:  $i = 1, 2, \dots, i$*

## □ Parameters

*$c_{ij}$  = distance from  $i$  and  $j$*

*$d_i$  = demand of customer in city  $i$*

*$nvhc$  = number of vehicles*

*$cvhc$  = vehicle capacity*

## □ Decision Variables

*$x_{ij} = 1$  if city  $j$  is visited right after city  $i$ , 0 otherwise*

*$u_i$  = Auxiliary variable indicating tour ordering*





# VRP Formulation

$$\min z = \sum_{i,j \in I} c_{ij} x_{ij}$$

Minimize the total distance

$$s.t. \quad \sum_{j \in I} c_{ij} x_{ij} = 1, \quad \forall i \in I$$

Each city there is a departure to exactly one other city

$$\sum_{i \in I} c_{ij} x_{ij} = 1, \quad \forall j \in I$$

Each city is arrived at from exactly one other city

$$\sum_{j \in I} x_{nj} = nvhc$$

Only nvhc vehicles leave the depot (last city)

$$\sum_{i \in I} x_{in} = nvhc$$

Only nvhc vehicles return to the depot (last city)

$$u_i - u_j + nx_{ij} \leq (n - 1) y_i, \quad \forall i, j \in I \mid 1 \leq i \neq j \leq n - 1$$

All tours start and end in the depot (i.e. no subtours)

$$n = \text{card}(J) \quad x_{ij}, \text{ is binary} \quad 0 \leq u_i \leq n, \quad \forall, ji \in I$$

# Pyomo VRP Formulation

```
#Generate Data Inputs

# Number of cities
n=20

# Number of Vehicles
nvhc=3

# Vehicle capacity
cvhc=230

#Coordinate Range
rangelct=10000

coordlct_x = random.sample(range(0, rangelct), n)
coordlct_y = random.sample(range(0, rangelct), n)

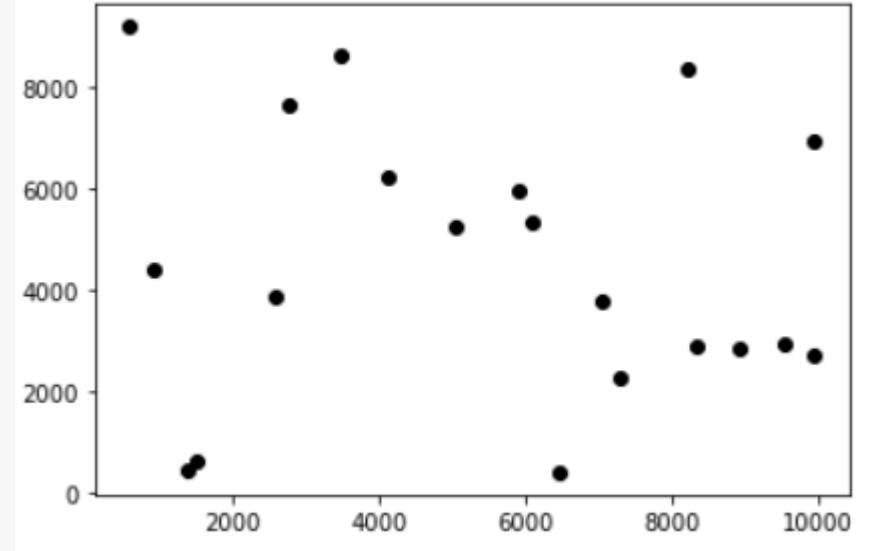
distancelct=np.empty([n, n])
for i_index in range(n):
    for j_index in range(n):
        distancelct[i_index,j_index]=(math.sqrt(((coordlct_x[i_index]-coordlct_x[j_index])**2) +((coordlct_y[i_index]-coordlct_y

distancelct[np.diag_indices_from(distancelct)] = 99999

distancelctdf = pd.DataFrame(distancelct)
distancelctdf.index += 1
distancelctdf.columns += 1
cij_model=distancelctdf.stack().to_dict()

cij_model

#Generate Demand
demandlct = random.sample(range(1, 50), n)
demanddf = pd.DataFrame(demandlct)
demanddf.index += 1
dj_model=demanddf.to_dict()
dj_model=dj_model[0]
```



# Pyomo VRP Formulation

## Sets

```
model = AbstractModel()

# Set of candidate cities
model.N = RangeSet(n)
model.M = RangeSet(n-1)
```

## Parameters

```
#  $c[i,j]$  - distance from  $i$  and  $j$ 
model.c = Param(model.N, model.N, initialize=cij_model)

#  $d[j]$  - demand of customer  $j$ 
model.d = Param(model.N, initialize=dj_model)
```

## Decision Variables

```
#  $x[i,j]$  - 1 if city  $j$  is visited right after city  $i$ , 0 otherwise
model.x = Var(model.N, model.N, within=Binary)

#  $u[i]$  - auxiliary variable indicating tour ordering
model.u = Var(model.N, within=NonNegativeReals)
```

# Pyomo VRP Formulation

## Objective Function

```
# Minimize the demand-weighted total cost
def cost_(model):
    return sum(model.c[i,j]*model.x[i,j] for i in model.N for j in model.N)
model.cost = Objective(rule=cost_)
```

## Constraints

```
# Only 1 departs from each city
def departs_(model, j):
    return sum(model.x[i,j] for i in model.N if i!=j) == 1
model.departs = Constraint(model.M, rule=departs_)
```

```
# Only 1 arrives from each city
def arrives_(model, i):
    return sum(model.x[i,j] for j in model.N if j!=i) == 1
model.arrives = Constraint(model.M, rule=arrives_)
```

```
# Only nvhc vehicles arrive to the depot (city with index n)
def arrivesdepot_(model):
    return sum(model.x[i,n] for i in model.N) == nvhc
model.departsdepot = Constraint(rule=arrivesdepot_)
```

```
# Only nvhc vehicles depart to the depot (city with index n)
def departdepot_(model):
    return sum(model.x[n,j] for j in model.N) == nvhc
model.arrivesdepot = Constraint(rule=departdepot_)
```

```
def singletour_(model,i,j):
    if i!=j:
        return model.u[i] - model.u[j] +cvhc*model.x[i,j] <= cvhc-model.d[i]
    else:
        return model.u[n]== 0

model.singletour = Constraint(model.M,model.M,rule=singletour_)
```

# Pyomo VRP Formulation

## Solve Model

```
instance = model.create_instance()
opt = pyo.SolverFactory('gurobi')
opt.solve(instance, options={'TimeLimit': 10000}, tee=True)
```

1898020	119535	cutoff	48		58996.2502	57755.5710	2.10%	10.2	550s
1918105	114070	58376.2388	53	24	58996.2502	57796.2967	2.03%	10.2	555s
1936846	108570	cutoff	60		58996.2502	57835.7144	1.97%	10.2	560s
1955533	102850	58968.5048	52	22	58996.2502	57877.0488	1.90%	10.1	565s
1976102	96126	cutoff	50		58996.2502	57926.6680	1.81%	10.1	570s
1993836	89929	58775.7200	57	23	58996.2502	57970.7462	1.74%	10.1	575s
2009394	84243	cutoff	87		58996.2502	58011.0204	1.67%	10.1	580s
2023335	78812	infeasible	60		58996.2502	58051.1434	1.60%	10.1	585s
2036836	73501	58926.5236	49	15	58996.2502	58090.8971	1.53%	10.1	590s
2049888	67946	58912.9060	61	12	58996.2502	58135.4420	1.46%	10.1	595s
2063176	61976	infeasible	50		58996.2502	58181.1793	1.38%	10.1	600s
2077785	55086	cutoff	48		58996.2502	58237.1841	1.29%	10.1	605s
2090984	48282	infeasible	69		58996.2502	58295.4634	1.19%	10.0	610s
2107780	38888	cutoff	51		58996.2502	58381.3247	1.04%	10.0	615s
2123286	29412	58612.6235	58	18	58996.2502	58481.8104	0.87%	10.0	620s
2136164	20201	cutoff	62		58996.2502	58594.4752	0.68%	10.0	625s
2151717	7282	cutoff	67		58996.2502	58804.9760	0.32%	10.0	630s

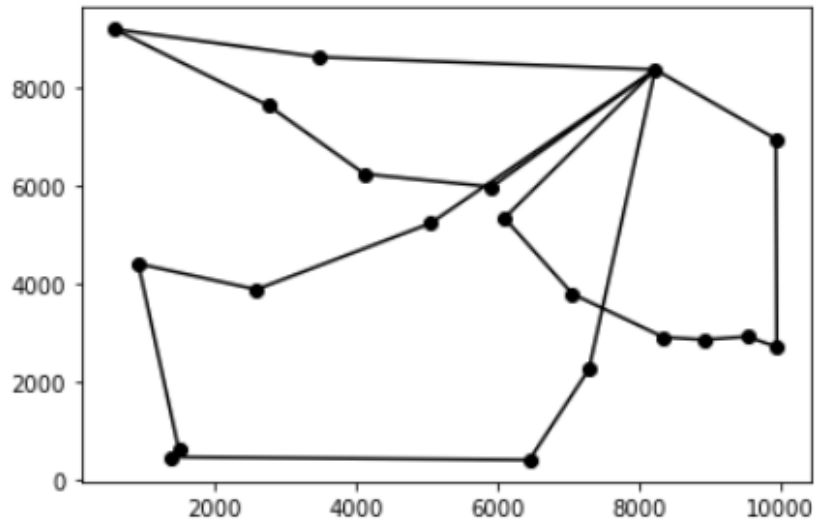
Cutting planes:

Loaded: 45

# Pyomo VRP Formulation

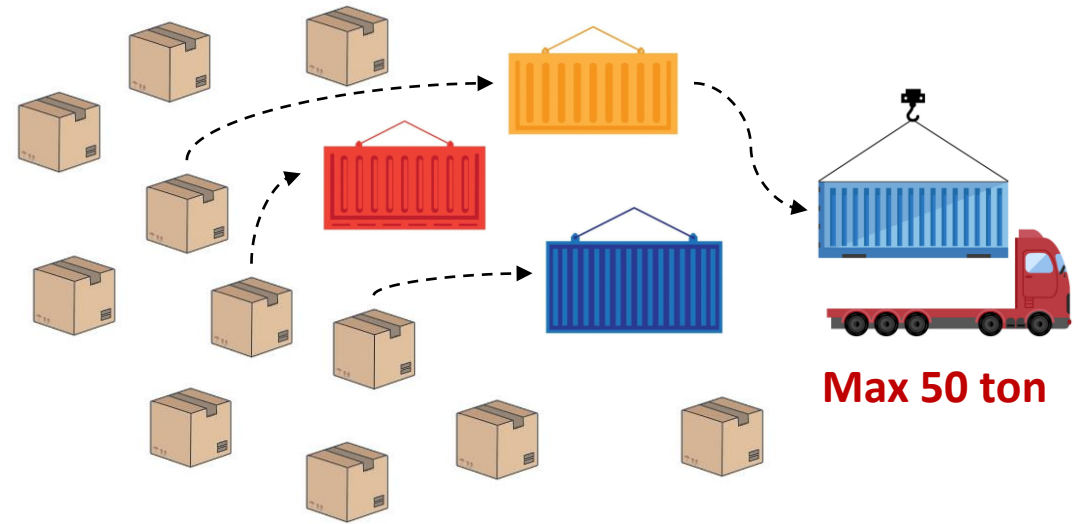
## Plot results

```
def connectpoints(x,y,p1,p2):  
    x1, x2 = x[p1], x[p2]  
    y1, y2 = y[p1], y[p2]  
    plt.plot([x1,x2],[y1,y2], 'k-')  
  
for i_index in range(len(linkindex[0])):  
    connectpoints(coordlct_x,coordlct_y,linkindex[0][i_index],linkindex[1][i_index])  
  
plt.plot(coordlct_x, coordlct_y, 'o', color='black');
```



# Activity 1

- Consider the following problem: Given a set of  $n$  packages with profit  $p_j$  and weight  $w_j$ , and a set of  $m$  containers with weight capacity  $c_i$ , select  $m$  disjoint subsets of packages so that the total profit of the selected packages is maximum, while ensuring the containers' capacity is never exceeded
- Exercise 1: Formulate the problem mathematically
- Exercise 2: Solve the problem using pyomo (instances in the next slide)



# Activity 1 - Instances

- Instance 1

```
random.seed(1)
```

```
n = 100 #number of objects
```

```
b= 5 #number of bins
```

```
cap=50
```

```
#Generate random locations
```

```
value = random.choices(range(10, 100), k=n)
```

```
weights = random.choices(range(5, 20), k=n)
```

- Instance 2

```
random.seed(1)
```

```
n = 10000 #number of packages
```

```
m= 200 #number of containers
```

```
cap=50
```

```
#Generate random locations
```

```
profit = random.choices(range(10, 100), k=n)
```

```
weights = random.choices(range(5, 20), k=n)
```



# Happy Chinese New Year!

