

*Design Heuristics push you to think beyond your initial ideas*



# COMBINATORIAL OPTIMIZATION AND METAHEURISTICS

*Prof. Eduardo Pécora*

# CALENDAR

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Lecture	Date	Theme
1	13/07/2021	Introduction
2	20/07/2021	Single Solution Metaheuristic methods for combinatorial problems
3	27/07/2021	Local search heuristic methods and the local optimal trap (VNS, ILS, GRASP)
4	03/08/2021	Tabu Search
5	10/08/2021	Performance Analysis
6	17/08/2021	Population Based Metaheuristics: Genetic Algorithms
7	24/08/2021	Ants Colony, Particle Cloud, BRKGA
8	31/08/2021	Parameter Settings - Irace
	07/09/2021	Holliday
9	14/09/2021	Very Large Neighborhood Search, Granular Tabu Search, Other Metaheuristics
10	21/09/2021	Hybridization: Heuristic and Exact methods working together
<b>11 and 12</b>	28/09/2021	Presentations of the Final Works

## EVALUATION

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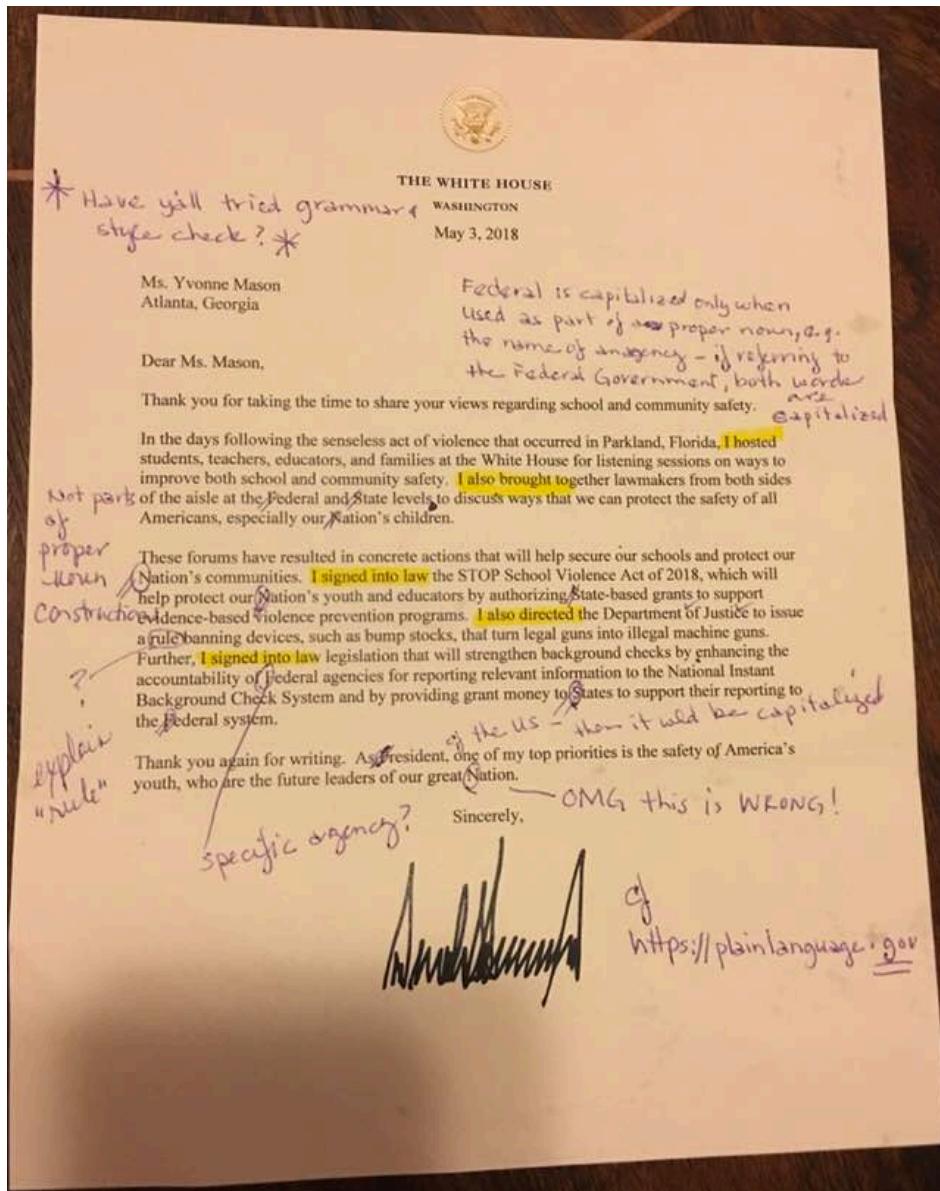
Evaluation	Percentage
LABs	40%
Final Project (article)	30%
Presentations	30%



# TEACHING CONTRACT

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*Prof. Eduardo Pécora*





## USEFUL LINKS

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- English Test: <https://www.efset.org/>
- skell
  - <https://skell.sketchengine.co.uk/run.cgi/skell>
- Dictionary -
  - <https://www.merriam-webster.com/>
- Thesaurus -
  - <http://www.thesaurus.com/>
- Google Translator
- DeepL



## GOOD HABITS

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- Keep an open mind! Interact with your classmates and professor!
- This class will help to improve your English! Let's learn together!
- Discuss how (and if) you want to be corrected!
- Keep a notepad with the vocabulary you do not know.
- At the end of the class, look for their meaning or ask a colleague or the professor.
- The primary focus of this class is to learn Metaheuristics.



## CONTRACT

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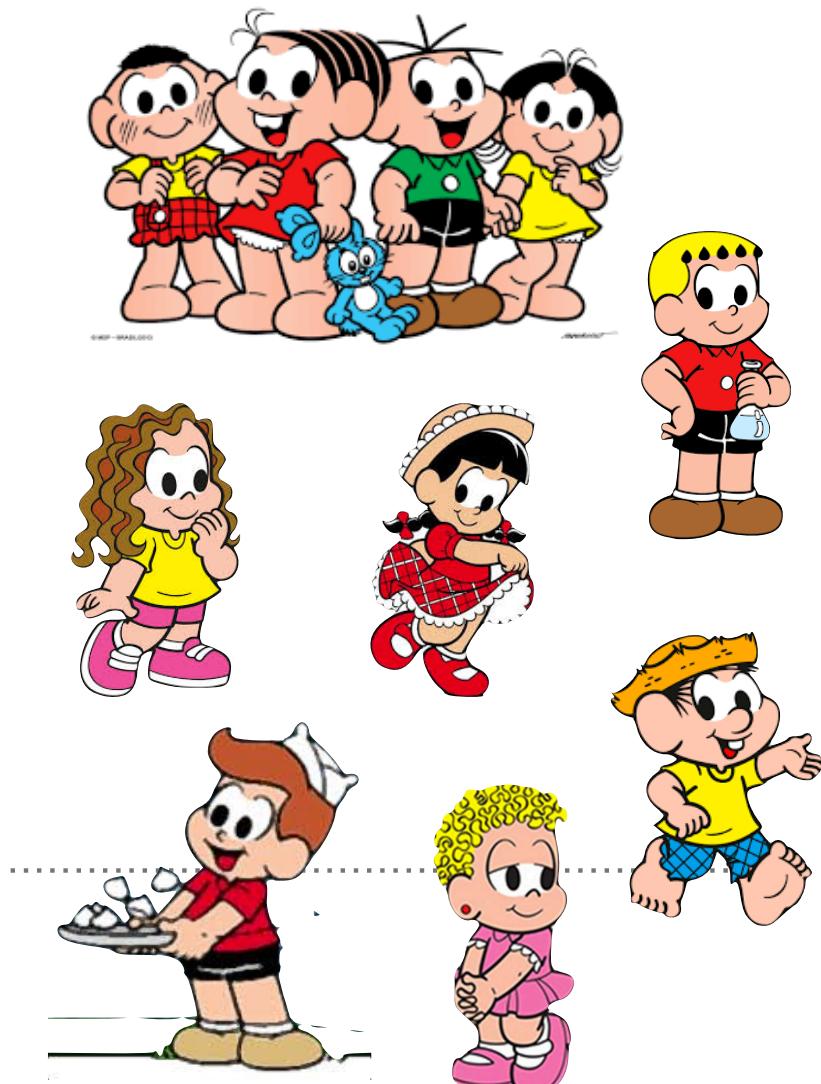
- Create a notepad for unknown words
- Be pro-active
- Teams



# COMBINATORIAL OPTIMIZATION

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*Prof. Eduardo Pécora*



	Chico Bento	Cascão	Cebolinha	Quinzinho	Franjinha
Mônica	3	7	1	2	3
Cascuda	9	8	8	3	2
Rosinha	8	5	6	1	8
Magali	6	9	4	3	5
Marina	8	5	5	7	3



	Chico Bento	Cascão	Cebolinha	Quinzinho	Franjinha
Mônica	3	7	1	2	3
Cascuda	9	8	8	3	2
Rosinha	8	5	6	1	8
Magali	6	9	4	3	5
Marina	8	5	5	7	3



## BIG NUMBERS

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- With 5 males and 5 females we may have 120 different combinations of couples.
- And if we had 70 males and 70 females. How many possible combinations will we have?

There are  $70!$  (seventy factorial) possible different combinations

How big is this number?

Just a hint!

$$70! > 10^{100}$$



## BIG NUMBERS

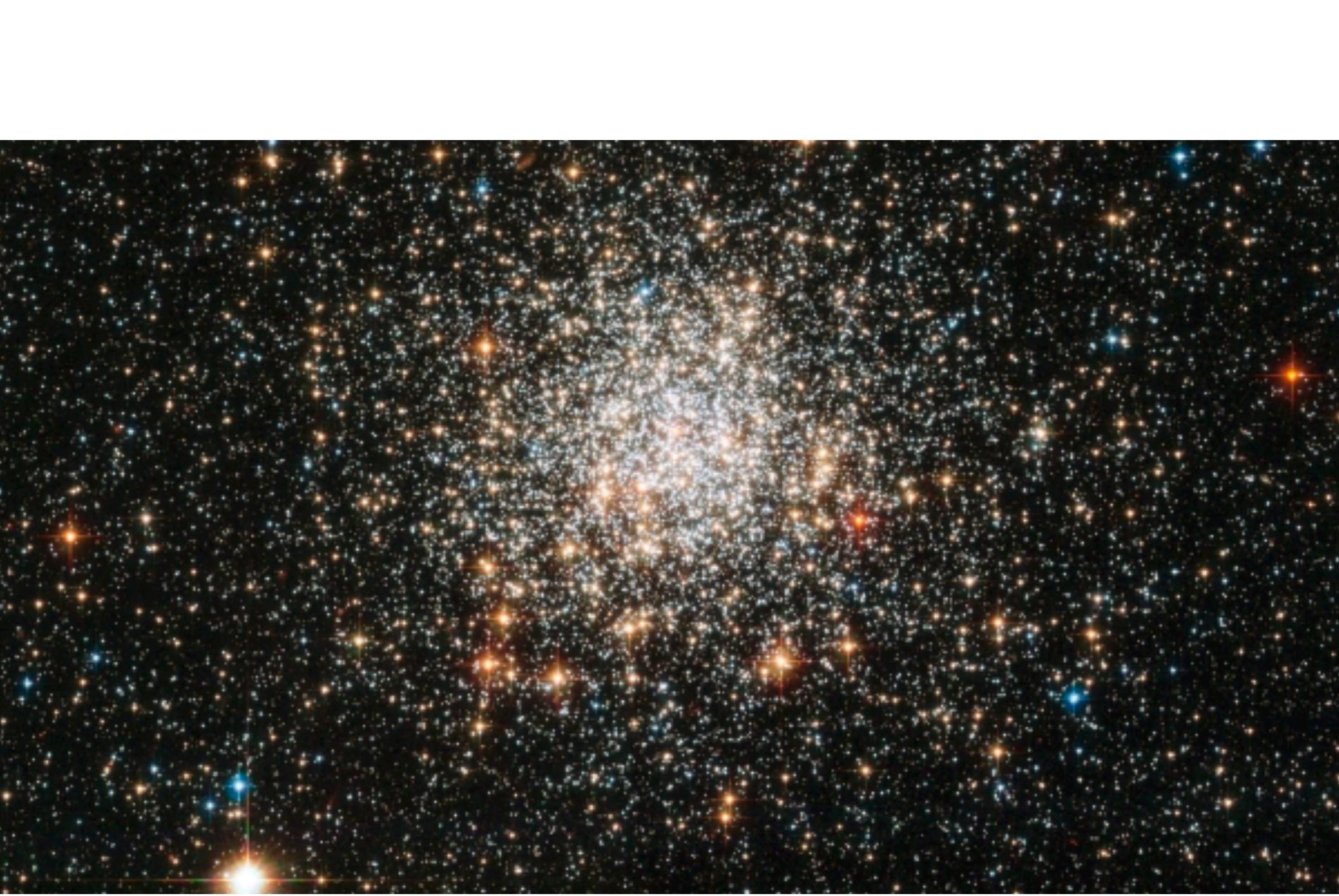
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Do you know this constant from physics?

$$7.1 \times 10^{79}$$

$$70! > 10^{100} > 7.1 \times 10^{79}$$







# BASICS

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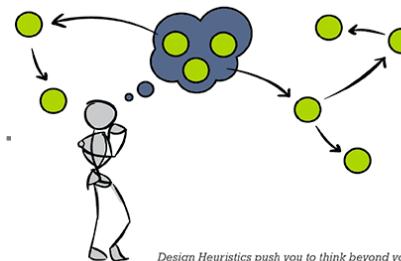
## WHAT IS A HEURISTIC?

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- Heuristic
- : involving or serving as an aid to learning, discovery, or problem-solving by experimental and especially trial-and-error methods <heuristic techniques> <a heuristic assumption>; also
- : of or relating to **exploratory problem-solving techniques** that utilize self-educating techniques (as the evaluation of feedback) to improve performance <a heuristic computer program>

Source: <http://www.merriam-webster.com/dictionary/heuristic>

# HEURISTIC METHODS



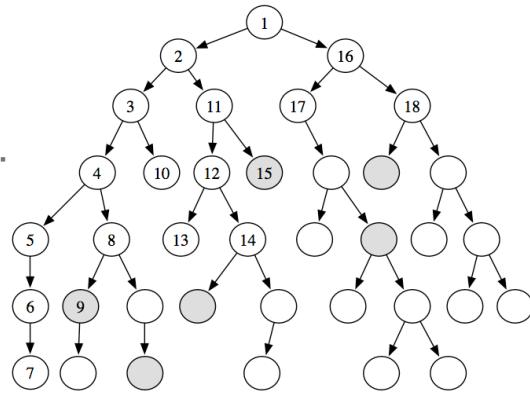
*Design Heuristics push you to think beyond your initial ideas*

- + empirically proven to find good solutions in a short time
- + exploit the problem characteristics for better performance
- do not guarantee the optimality
- may leave unexplored regions of the space

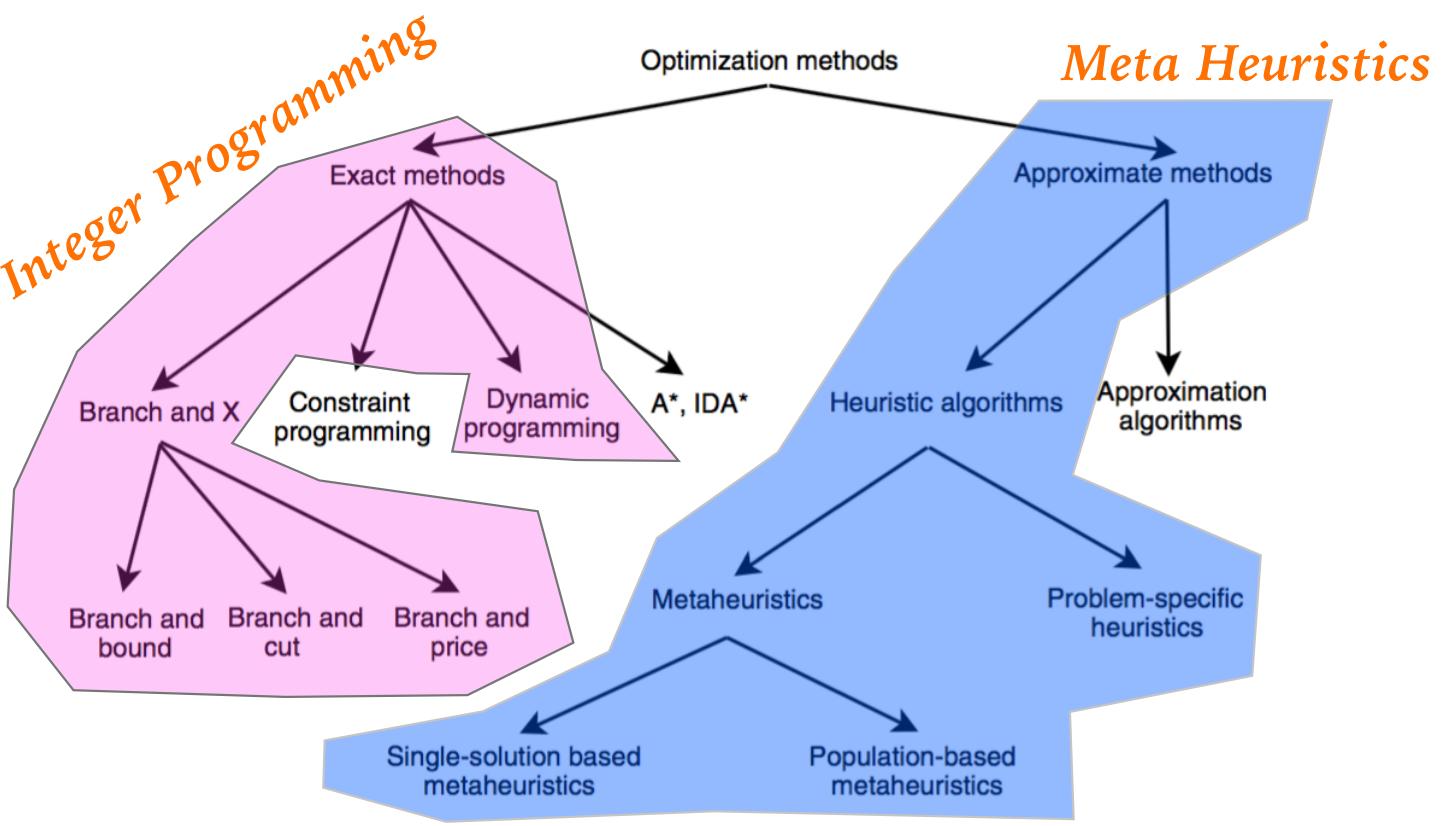


## EXACT METHODS

- + systematic exploration of the space
- + provides the optimal solution
- + very efficient for small sized instances
- very expensive computationally
- neither efficient nor fast enough for large scale problems



# SOLVING APPROACH TREE



**FIGURE 1.7** Classical optimization methods.



# DESIGN OF METAHEURISTICS

Conception

*Am I Exploring the problem's structure?  
Are there any constraints which may be relaxed?*

Programming

*Define Programming Language*

Small test

*Generate a small data instance  
Solve it*

Setting

*Are the parameters at their best values?  
May I prove it? Even empirically?*

Computational experiments

*Generate a large data instance  
Validate them  
Are my instances set large enough?  
How long takes to solve them?*



# DEFINITION

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## *Formal*

- Definition 1.1: Global optimum. A solution  $s^* \in S$  is a global optimum if it has a better objective function than all solutions of the search space, that is,  $\forall s \in S, f(s^*) \leq f(s)$ .

## *Casual*

- The best of all solutions ever!
- Nobody is better than me!
- I am so good!





# COMPLEXITY OF AN ALGORITHM

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# COMPLEXITY OF ALGORITHM

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- An algorithm needs two important resources to solve a problem: time and space.
- The time complexity of an algorithm is the number of steps required to solve a problem of size  $n$ . The complexity is generally defined in terms of the worst-case analysis.
- The goal in the determination of the computational complexity of an algorithm is not to obtain an exact step count but an asymptotic bound on the step count.
- The Big-O notation makes use of asymptotic analysis. It is one of the most popular notations in the analysis of algorithms.



**SS<->SS;**

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## SORT THIS LIST

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12

45

34

13

78

01

65

90

89

11

## ALGORITHM 01

12	OK	12	12	12
45		45	34	34
34		34	45	13
13		13	13	45
78		78	78	78
01		01	01	01
65		65	65	65
90		90	90	90
89		89	89	89
11		11	11	11

How many  
comparisons I  
will do in the  
worst case?

## ALGORITHM 02 – QUICK SORT

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12

45

34

13

78

01

65

90

89

11

How many  
comparisons I  
will do in the  
worst case?

# DEFINITION

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## *Formal*

- Definition 1.2: Big-O notation. An algorithm has a complexity  $f(n) = O(g(n))$  if there exist positive constants  $n_0$  and  $c$  such that  $\forall n > n_0, f(n) \leq c \cdot g(n)$ .

## *Casual*

- $f(n)$  is upper bounded by the function  $g(n)$
- From a certain point  $f(n)$  always loses



# DEFINITION

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## *Formal*

- **Definition 1.3 Polynomial-time algorithm.** An algorithm is a polynomial-time algorithm if its complexity is  $O(p(n))$ , where  $p(n)$  is a polynomial function of  $n$ .
- **Definition 1.4 Exponential-time algorithm.** An algorithm is an exponential-time algorithm if its complexity is  $O(c^n)$ , where  $c$  is a real constant strictly superior to 1.

## *Casual*

- Polynomial - piece of cake
- Exponential - OH My GOD! I have no memory, no time ...





## EXAMPLE EXPONENTIAL ALGORITHM

**TABLE 1.3 Search Time of an Algorithm as a Function of the Problem Size Using Different Complexities (from [299])**

Complexity	Size = 10	Size = 20	Size = 30	Size = 40	Size = 50
$O(x)$	0.00001 s	0.00002 s	0.00003 s	0.00004 s	0.00005 s
$O(x^2)$	0.0001 s	0.0004 s	0.0009 s	0.0016 s	0.0025 s
$O(x^5)$	0.1 s	0.32 s	24.3 s	1.7 mn	5.2 mn
$O(2^x)$	0.001 s	1.0 s	17.9 mn	12.7 days	35.7 years
$O(3^x)$	0.059 s	58.0 mn	6.5 years	3855 centuries	$2 \times 10^8$ centuries

M. Garey and D. Johnson. *Computers and Intractability: A Guide to the Theory on NP-Completeness*.  
W. H. Freeman and Co. Publishers, New York, 1979.



# COMPLEXITY OF A PROBLEM

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**SS<->SS;**

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## WORK IN PAIRS AND ANSWER THESE QUESTIONS!

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- What is a P class?
- What is a Non Deterministic Algorithm?
  - Can you give me an example?
- What is a NP class?
- What is a NP-HARD class?
- What is a NP-complete Class?





## COMPLEXITY OF A PROBLEM

- The complexity of a problem is equivalent to the complexity of the best algorithm TO SOLVE that problem.
- A problem is tractable (or easy) if there exists a polynomial-time algorithm to solve it.
- A problem is intractable (or difficult) if no polynomial-time algorithm exists to solve the problem.
- Attention!!! This is only a definition!!
- An algorithm that runs in time  $10^7 n$  is not efficient neither easy, although it is linear
- The same reasoning applies to  $O(n^{10})$  algorithms



## COMPLEXITY OF A PROBLEM

- P - Problems which may be solved by a deterministic polinomial algorithm
- NP - which may be solved by a non-deterministic polinomial algorithm
- NP-HARD: X is an NP-HARD problem if every problem in NP is polynomially deductible to X ("at least as hard as the hardest problems in NP")
- NP-COMPLETE: X is NP-COMPLETE if
  - (1) X belongs to NP and
  - (2) X is NP-HARD



# NON DETERMINISTIC ALGORITHM

Given a set of  $N$  objects. Each object  $O$  has a specified weight and a specified value. Given a capacity, which is the maximum total weight of the knapsack, and a quota, which is the minimum total value that one wants to get. The 0–1 knapsack decision problem consists in finding a subset of the objects whose total weight is at most equal to the capacity and whose total value is at least equal to the specified quota.

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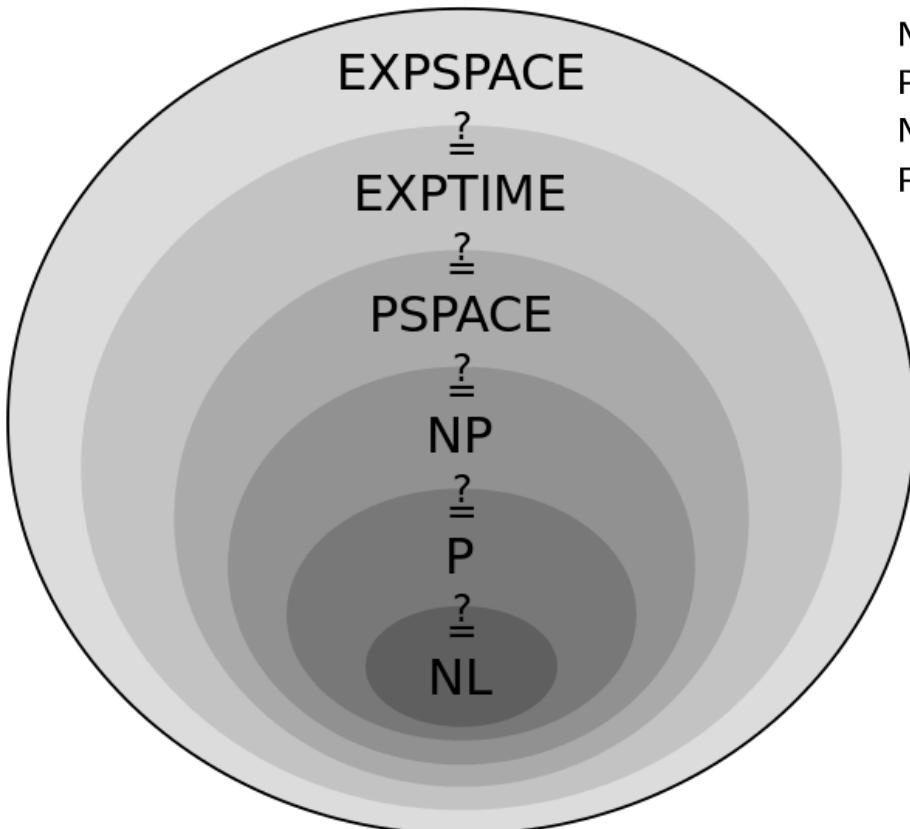
### Algorithm 1.1 Nondeterministic algorithm for the knapsack problem.

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```
Input OS : set of objects ; QUOTA : number ; CAPACITY : number.  
Output S : set of objects ; FOUND : boolean.  
S = empty ; total_value = 0 ; total_weight = 0 ; FOUND = false ;  
Pick an order L over the objects ;  
Loop  
    Choose an object O in L ; Add O to S ;  
    total_value = total_value + O.value ;  
    total_weight = total_weight + O.weight ;  
    If total_weight > CAPACITY Then fail  
    Else If total_value ≥ QUOTA  
        FOUND = true ;  
        succeed ;  
    Endif Endif  
    Delete all objects up to O from L ;  
Endloop
```

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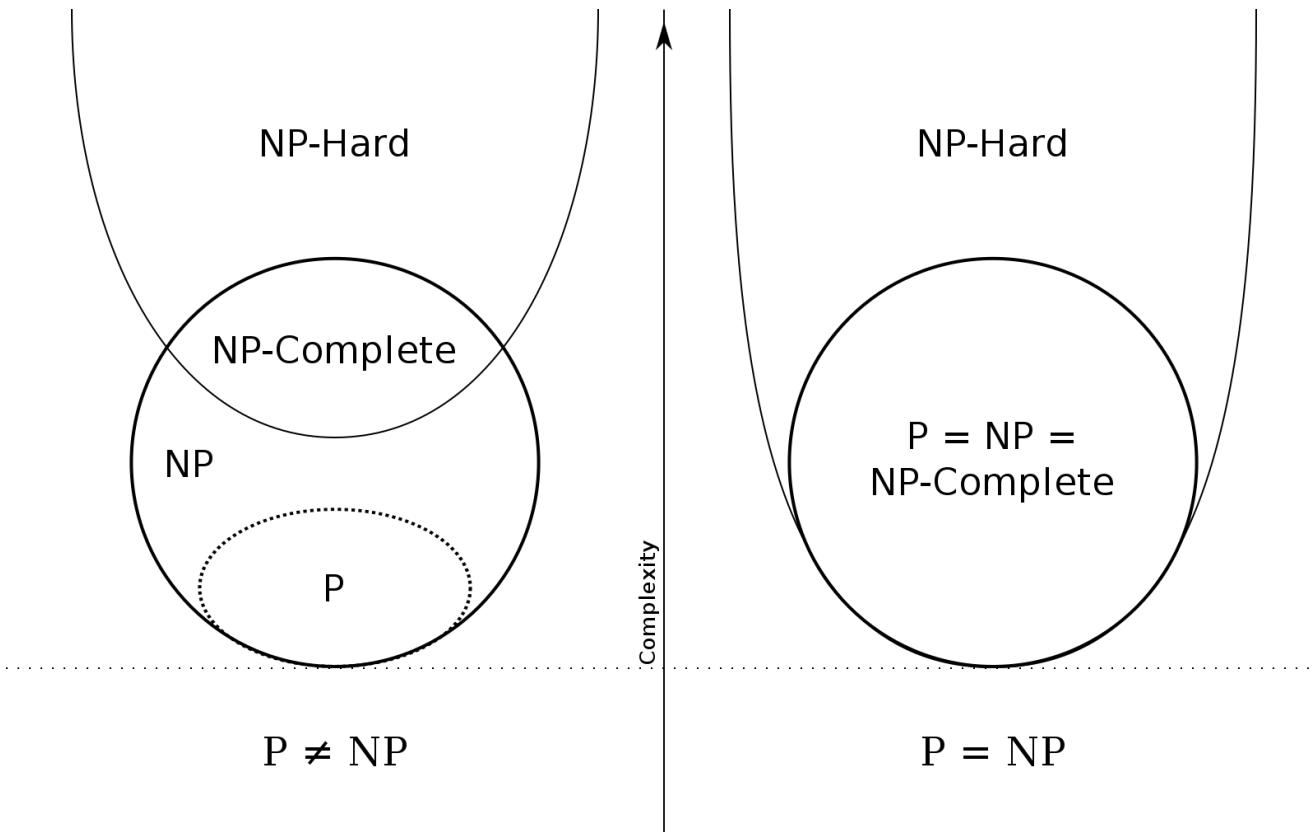
# COMPLEXITY OF A PROBLEM



$\text{NL} \subseteq \text{P} \subseteq \text{NP} \subseteq \text{PH} \subseteq \text{PSPACE}$   
 $\text{PSPACE} \subseteq \text{EXPTIME} \subseteq \text{EXPSPACE}$   
 $\text{NL} \subsetneq \text{PSPACE} \subsetneq \text{EXPSPACE}$   
 $\text{P} \subsetneq \text{EXPTIME}$



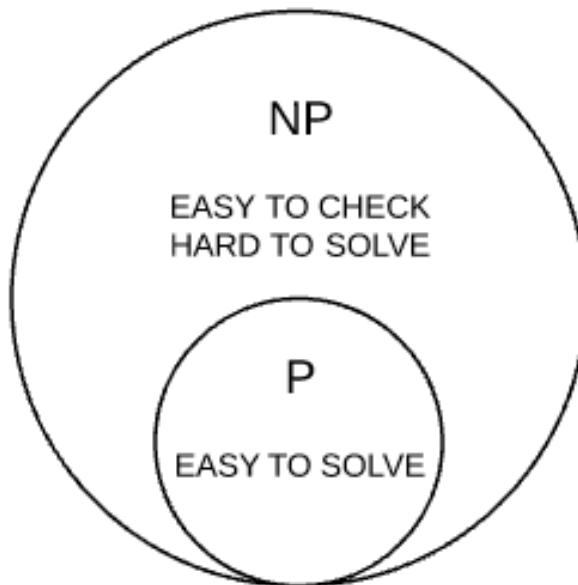
# COMPLEXITY OF A PROBLEM



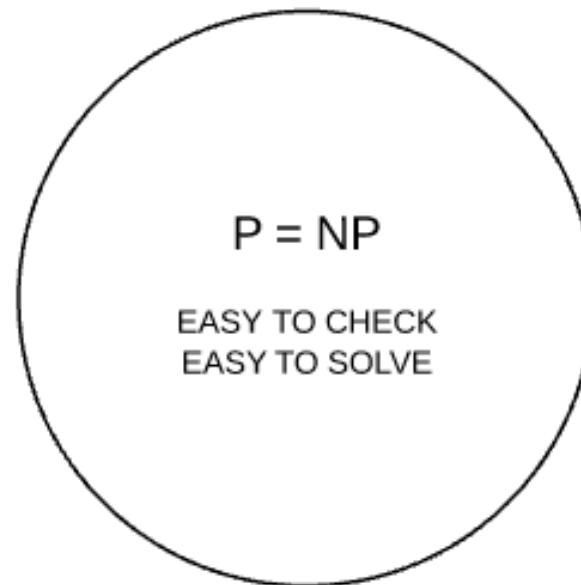
# COMPLEXITY OF A PROBLEM

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Right now



If  $P = NP$





## EXAMPLES OF PROBLEM'S COMPLEXITY

- Class P.
  - Some classical problems belonging to class P are minimum spanning tree, shortest path problems, maximum flow network, maximum bipartite matching, and linear programming continuous models.
- Class NP complete:
  - Sequencing and scheduling problems such as flow-shop scheduling, job-shop scheduling, or open-shop scheduling.
  - Assignment and location problems such quadratic assignment problem(QAP), generalized assignment problem (GAP), location facility, and the p-median problem.
  - Grouping problems such as data clustering, graph partitioning, and graph coloring.
  - Routing and covering problems such as vehicle routing problems (VRP), set covering problem (SCP), Steiner tree problem, and covering tour problem (CTP).
  - Knapsack and packing/cutting problems, and so on.

# P = NP ?



ABOUT PROGRAMS MILLENNIUM PROBLEMS PEOPLE PUBLICATIONS EVENTS EUCLID

## Millennium Problems

### Yang–Mills and Mass Gap

Experiment and computer simulations suggest the existence of a "mass gap" in the solution to the quantum versions of the Yang–Mills equations. But no proof of this property is known.

### Riemann Hypothesis

The prime number theorem determines the average distribution of the primes. The Riemann hypothesis tells us about the deviation from the average. Formulated in Riemann's 1859 paper, it asserts that all the 'non-obvious' zeros of the zeta function are complex numbers with real part 1/2.

### P vs NP Problem

If it is easy to check that a solution to a problem is correct, is it also easy to solve the problem? This is the essence of the P vs NP question. Typical of the NP problems is that of the Hamiltonian Path Problem: given N cities to visit, how can one do this without visiting a city twice? If you give me a solution, I can easily check that it is correct. But I cannot so easily find a solution.

### Navier–Stokes Equation

This is the equation which governs the flow of fluids such as water and air. However, there is no proof for the most basic questions one can ask: do

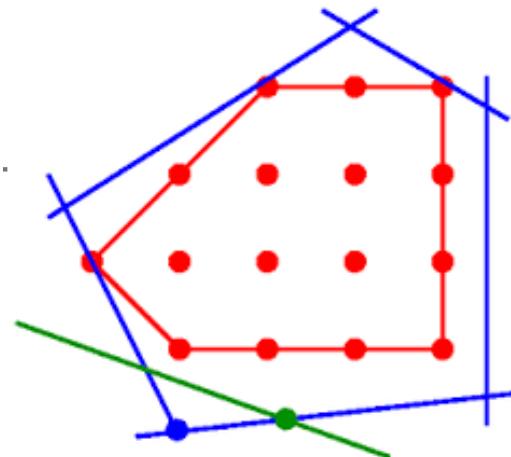
# INTEGER PROGRAMMING

- Integer programming?
- P or NP?

A matrix  $A$  is totally unimodular if the determinant of each square submatrix of  $A$  is 0, 1, or +1.

Theorem 1: If  $A$  is totally unimodular, then every vertex solution of  $Ax \geq b$  is integer.

- Conclusion ?
- !&#Y©ßð¬^Ø
- Search for theory of Matroids too ...





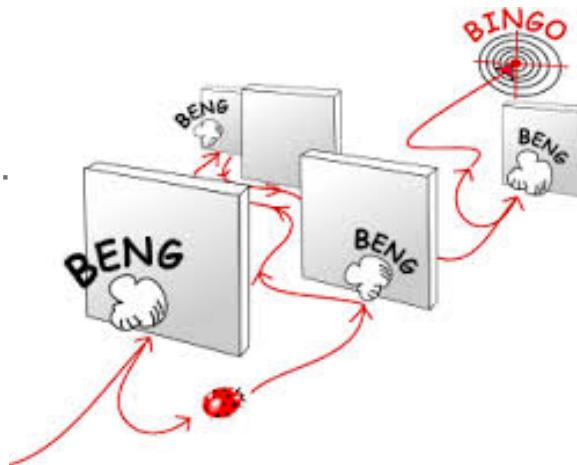
# HEURISTICS' CLASSIFICATION

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# BASIC HEURISTICS

BALL, M., and M. MAGAZINE (1981)

- CONSTRUCTION
- IMPROVEMENT
- MATHEMATICAL PROGRAMMING
- DECOMPOSITION
- PARTITIONING
- RESTRICTION OF FEASIBLE SOLUTION SPACE
- RELAXATION OF FEASIBLE SOLUTION SPACE



**SS<->T;  
YOU READ THE  
ARTICLE. CAN YOU  
EXPLAIN THEM TO  
ME?**

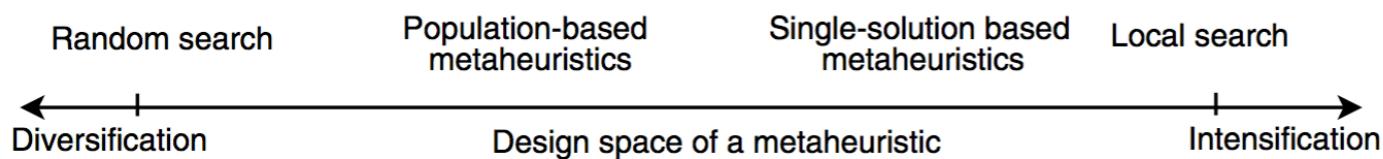
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# INTENSIFICATION – DIVERSIFICATION PARADIGM

- In designing a metaheuristic, two contradictory criteria must be taken into account: exploration of the search space (diversification) and exploitation of the best solutions found (intensification).
- Promising regions are determined by the obtained “good” solutions. In intensification, the promising regions are explored more thoroughly in the hope to find better solutions. In diversification, nonexplored regions must be visited to be sure that all regions of the search space are evenly explored and that the search is not confined to only a reduced number of regions.
- Random search Population-based Single-solution based Local search metaheuristics metaheuristics.





## CLASSIFICATION OF METAHEURISTICS

- **Nature inspired versus non nature inspired:** Many metaheuristics are inspired by natural processes: evolutionary algorithms and artificial immune systems from biology; ants, bees colonies, and particle swarm optimization from swarm intelligence into different species (social sciences); and simulated annealing from physics.
- **Memory usage versus memoryless methods:** Some metaheuristic algorithms are memoryless; that is, no information extracted dynamically is used during the search. Some representatives of this class are local search, GRASP, and simulated annealing. While other metaheuristics use a memory that contains some information extracted online during the search. For instance, short-term and long-term memories in tabu search.

# CLASSIFICATION OF METAHEURISTICS

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- **Deterministic versus stochastic:** A deterministic metaheuristic solves an optimization problem by making deterministic decisions (e.g., local search, tabu search). In stochastic metaheuristics, some random rules are applied during the search (e.g., simulated annealing, evolutionary algorithms). In deterministic algorithms, using the same initial solution will lead to the same final solution, whereas in stochastic metaheuristics, different final solutions may be obtained from the same initial solution.
- **Iterative versus greedy:** In iterative algorithms, we start with a complete solution (or population of solutions) and transform it at each iteration using some search operators. Greedy algorithms start from an empty solution, and at each step a decision variable of the problem is assigned until a complete solution is obtained.

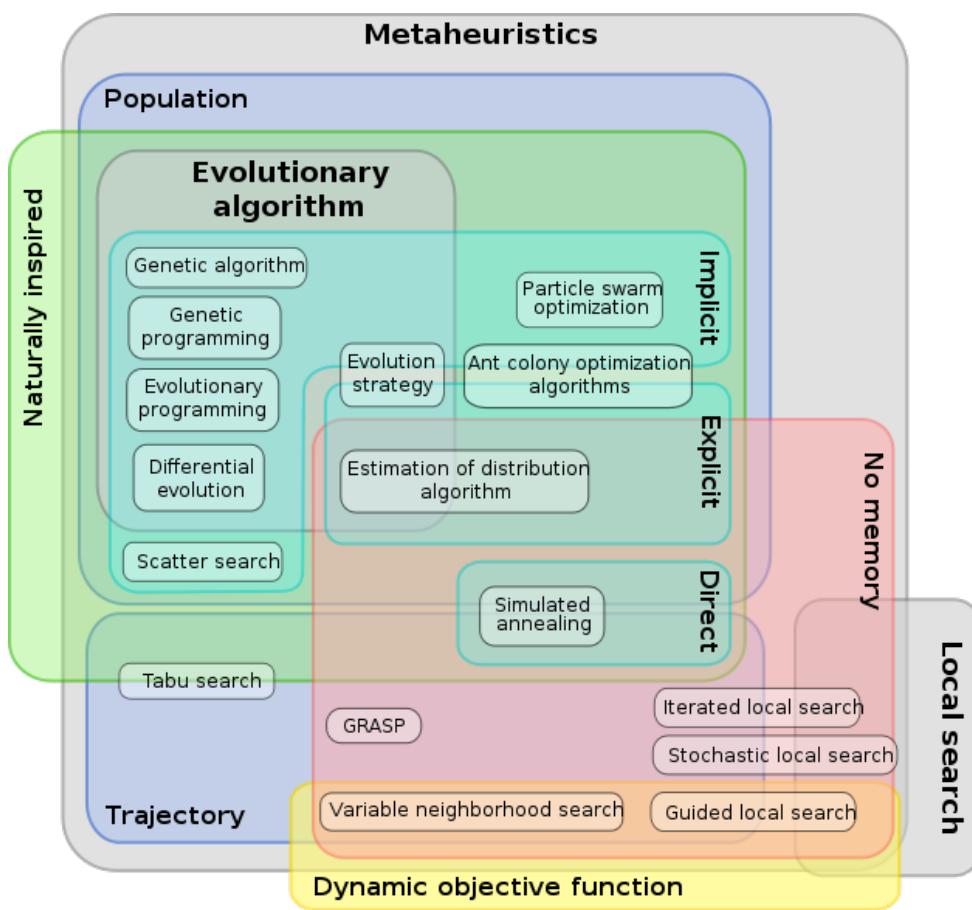


# CLASSIFICATION OF METAHEURISTICS

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- **Population-based search versus single-solution based search:** Single-solution based algorithms (e.g., local search, simulated annealing) manipulate and transform a single solution during the search while in population-based algorithms (e.g., particle swarm, evolutionary algorithms) a whole population of solutions is evolved.





*I picked this image  
from wikipedia!!  
At least I  
referenced it!*

(S)

# HOME WORK

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# LAB 1

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**Chose three of the following problems:**

- Knapsack Problem
  - Single Machine
  - Parallel Machines
  - Travelling Salesman Problem
  - Location and Allocation Problem
- 
- (1) Provide a Mathematical formulation;
  - (2) Identify the complexity of the problem;
  - (3) Propose a constructive heuristic;
  - (4) Classify your method into diversification and intensification;

**(Deliver before Class 3).**

