

# AGILE WORKFLOWS & GENERATIVE AI in A New Era of Autonomous Optimization

Seyedali Mirjalili

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Óbudai  
Egyetem  
OBUDA UNIVERSITY



TORRENS  
UNIVERSITY  
AUSTRALIA

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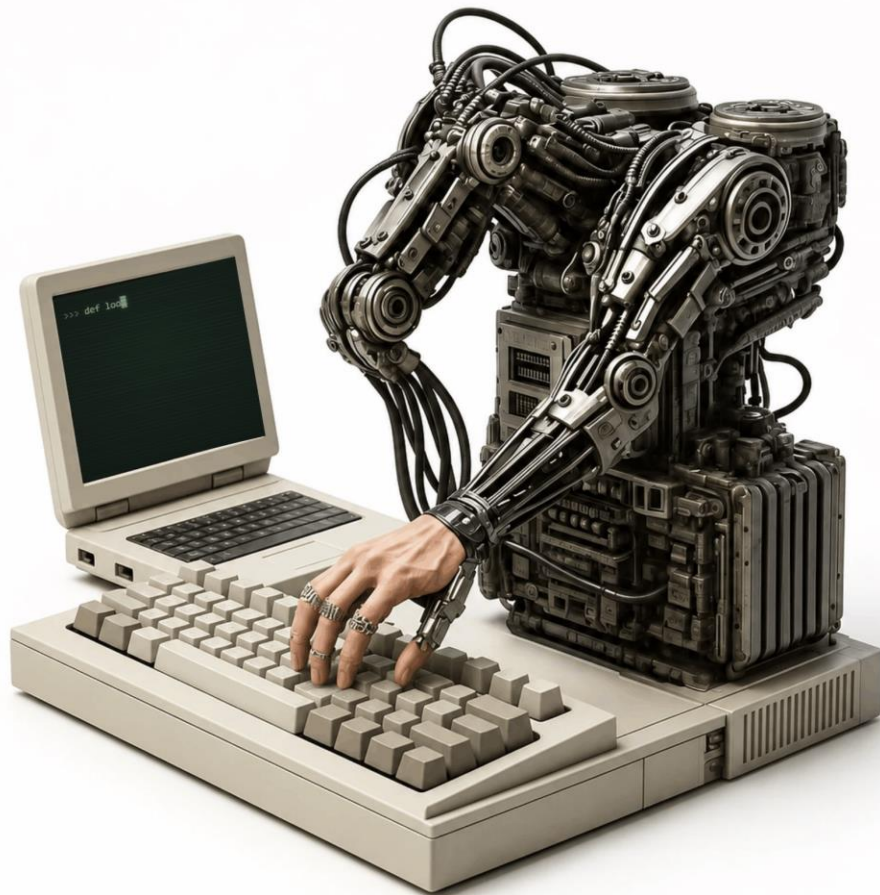
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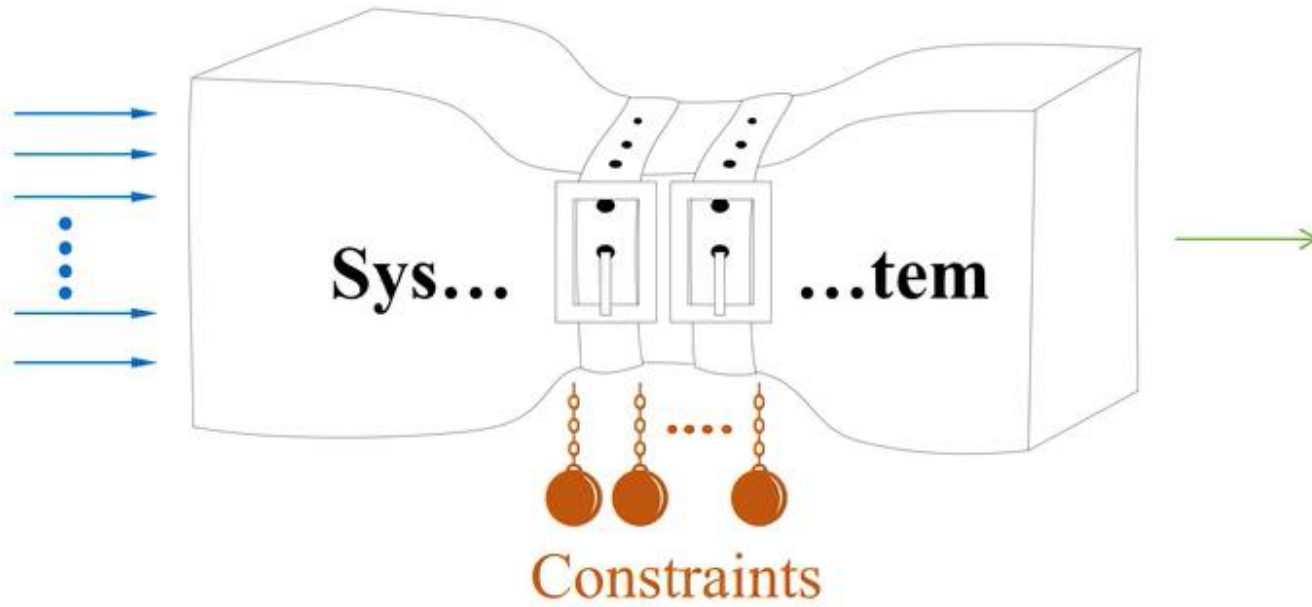
# OPTIMIZATION PROBLEMS

The background of the slide is composed of two large, overlapping, curved shapes. The top-left portion is a solid orange color, while the bottom-right portion is a solid blue color. The boundary between the two colors is a smooth, flowing curve that starts near the bottom center and extends towards the top right corner.

# MAIN COMPONENTS OF AN OPTIMIZATION PROBLEM

Inputs

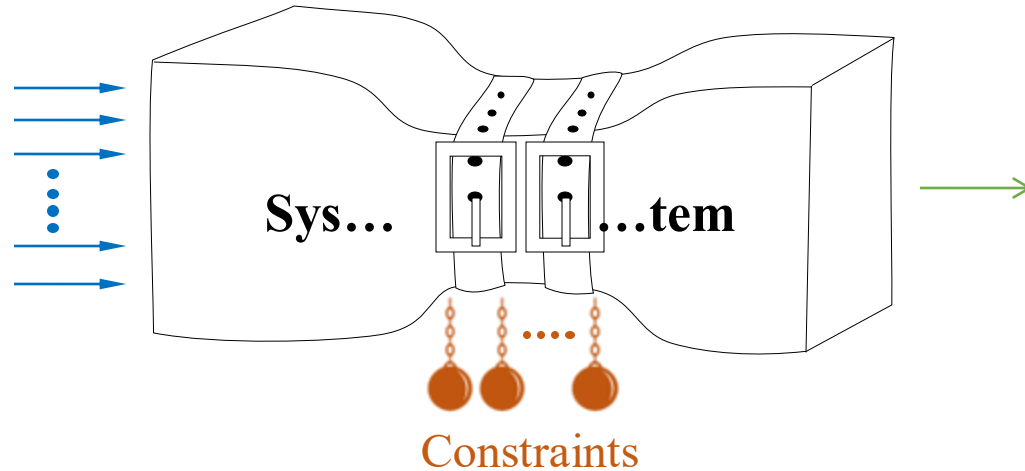
Output



# FORMULATION OF AN OPTIMIZATION PROBLEM

Inputs

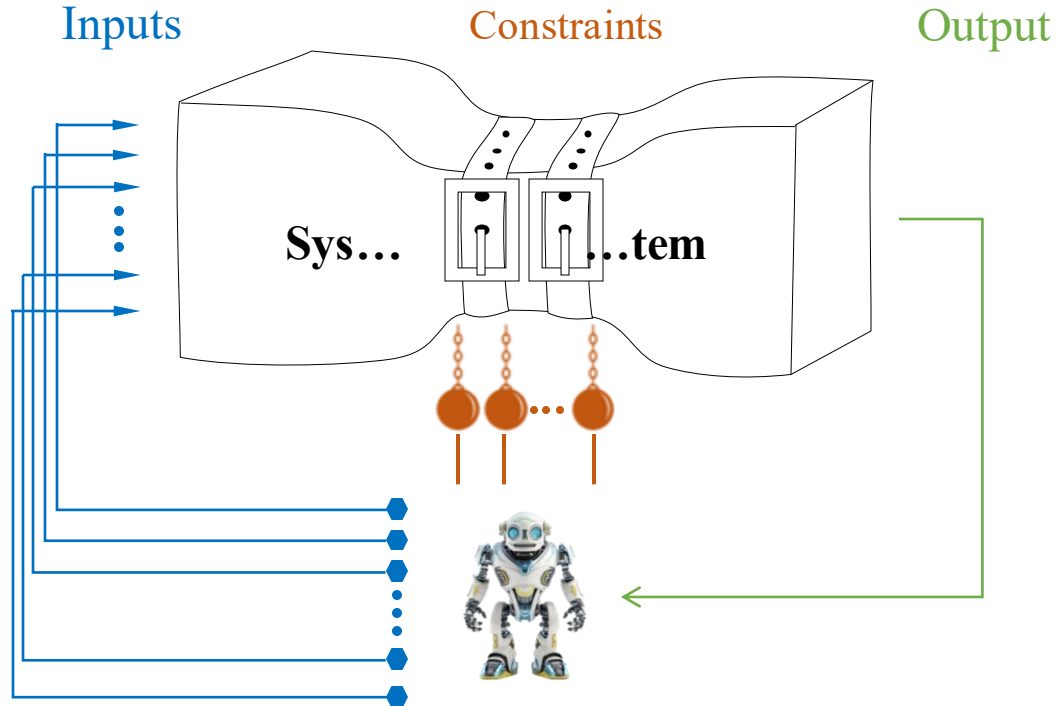
Output



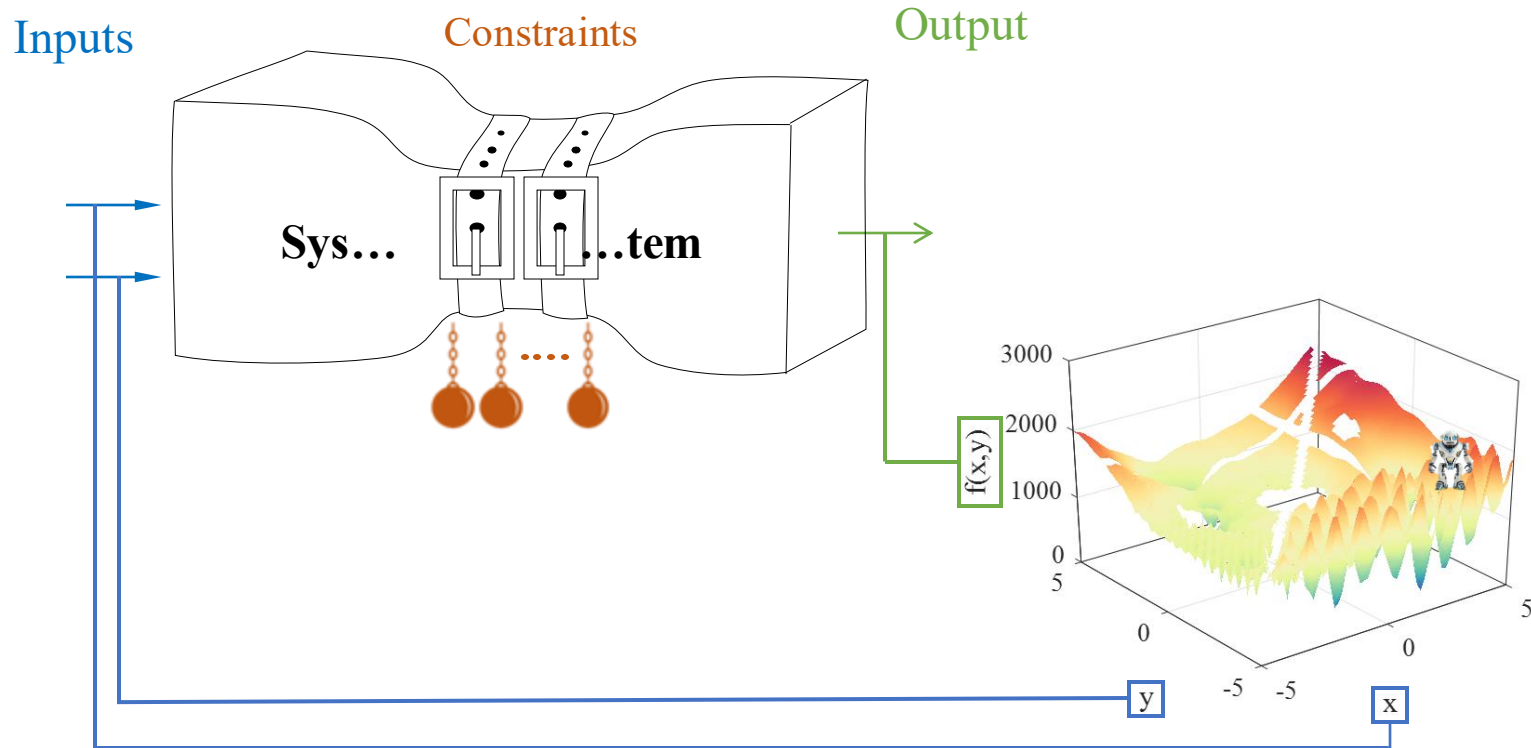
Minimise:  $f(x_1, x_2, \dots, x_n)$

Subject to: **Constraints**

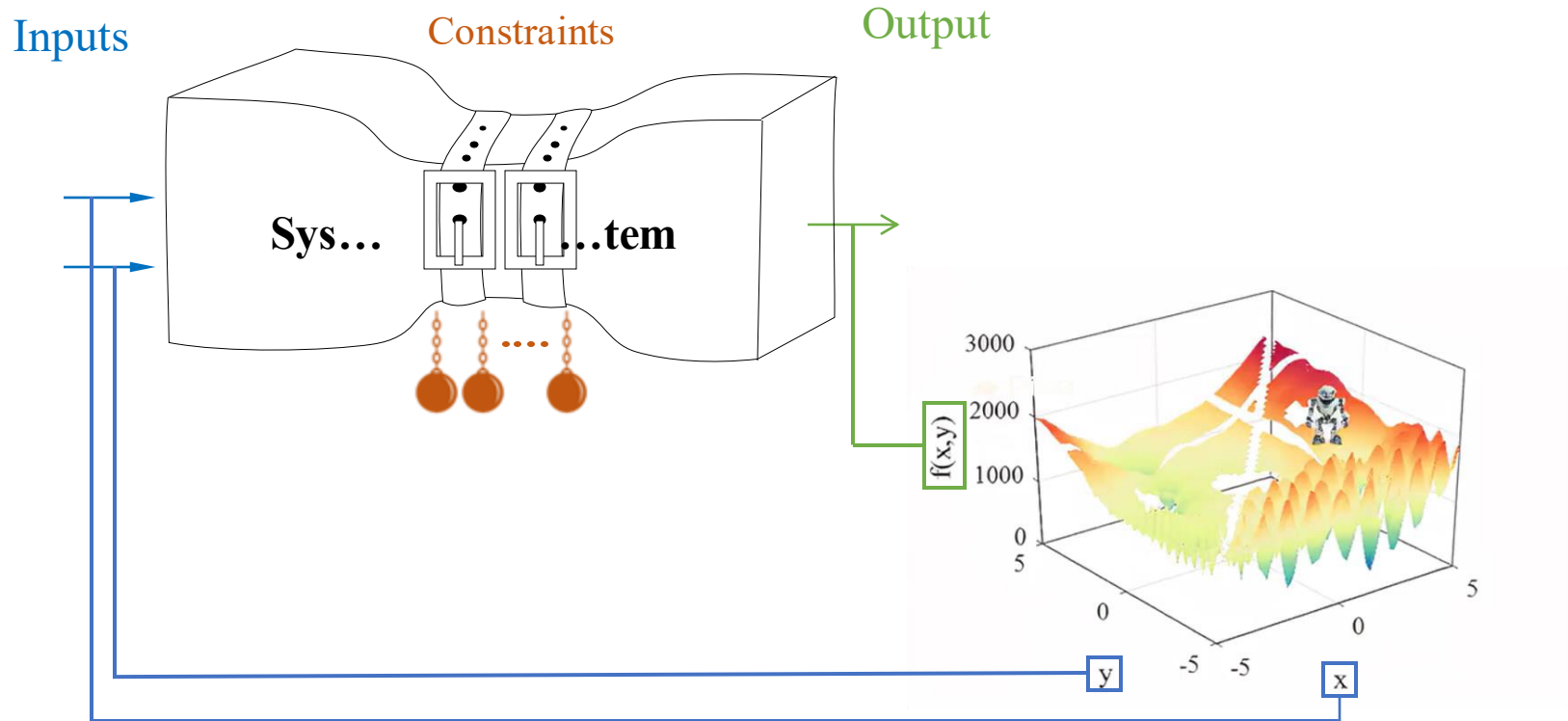
# THE ROLE OF AN OPTIMIZATION ALGORITHM



# WHAT ARE WE ACTUALLY TRYING TO DO?

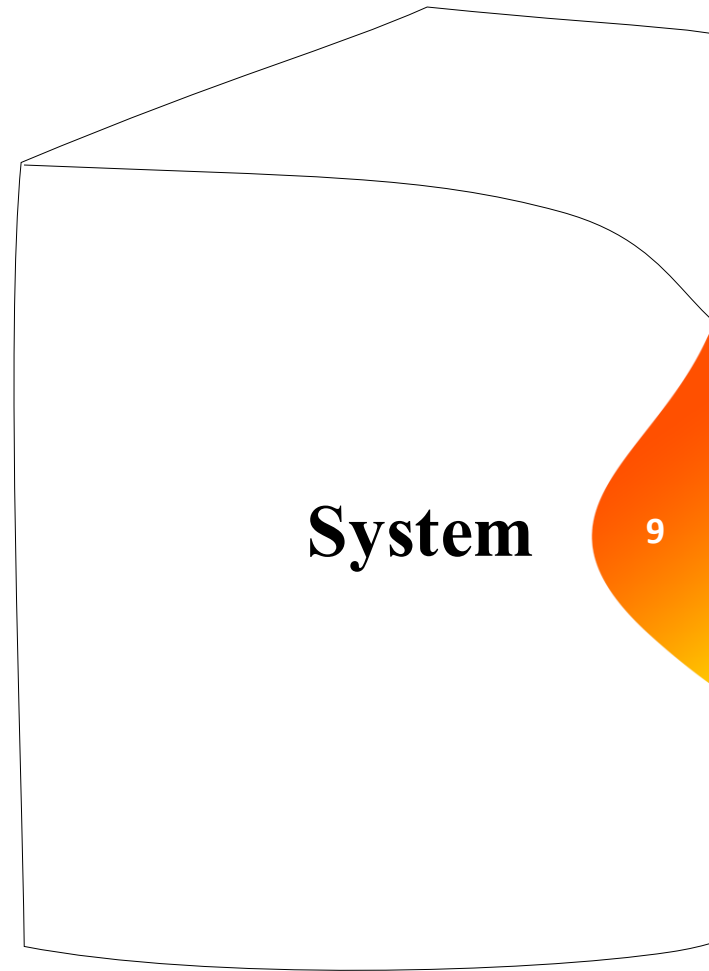
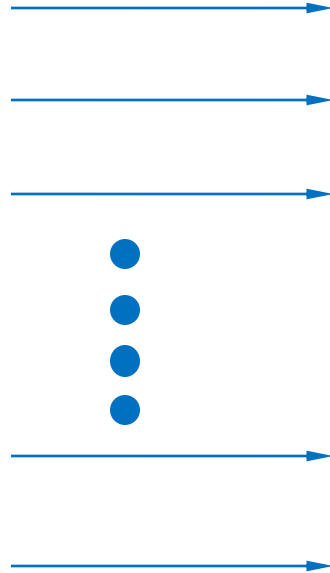


# WHAT ARE WE ACTUALLY TRYING TO DO?



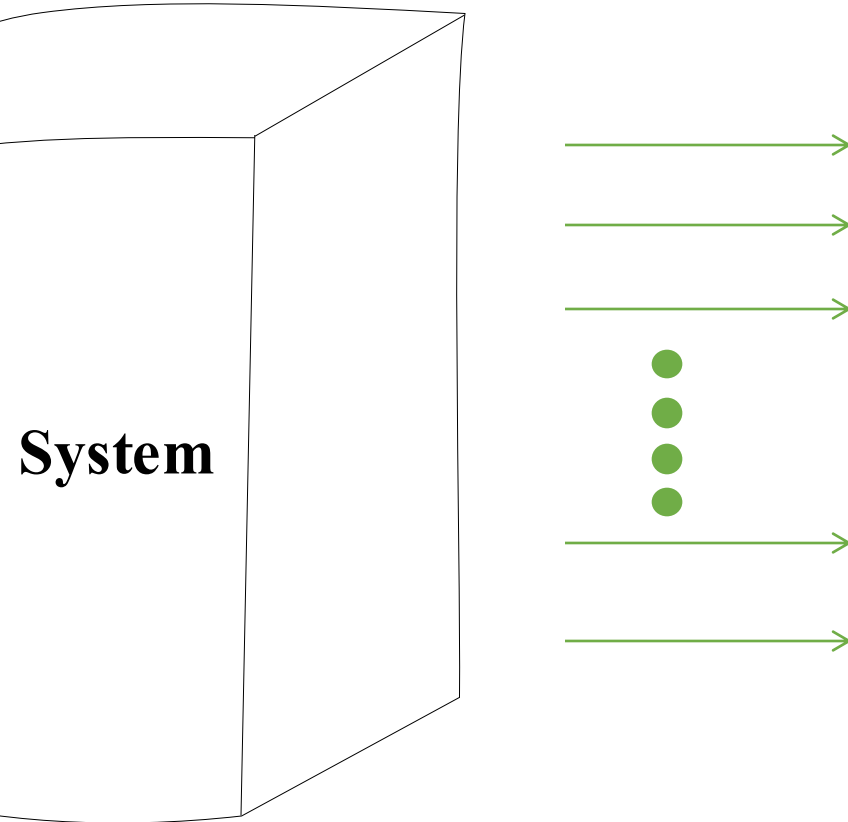
# DECISION SPACE COMPLEXITY

- Large number of inputs
- Variables with different ranges
- Dependency between the inputs
- Discrete variables
- Mix variables
- Noisy inputs
- ....



From small, homogeneous decision spaces → large-scale, mixed, interconnected and uncertain variables.

# OBJECTIVE SPACE COMPLEXITY

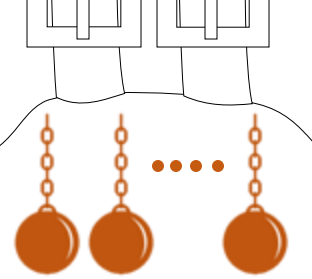


- Multiple/many objectives
- Conflicting objectives
- Dynamic objectives
- Difficult-to-Measure Objectives
- ...

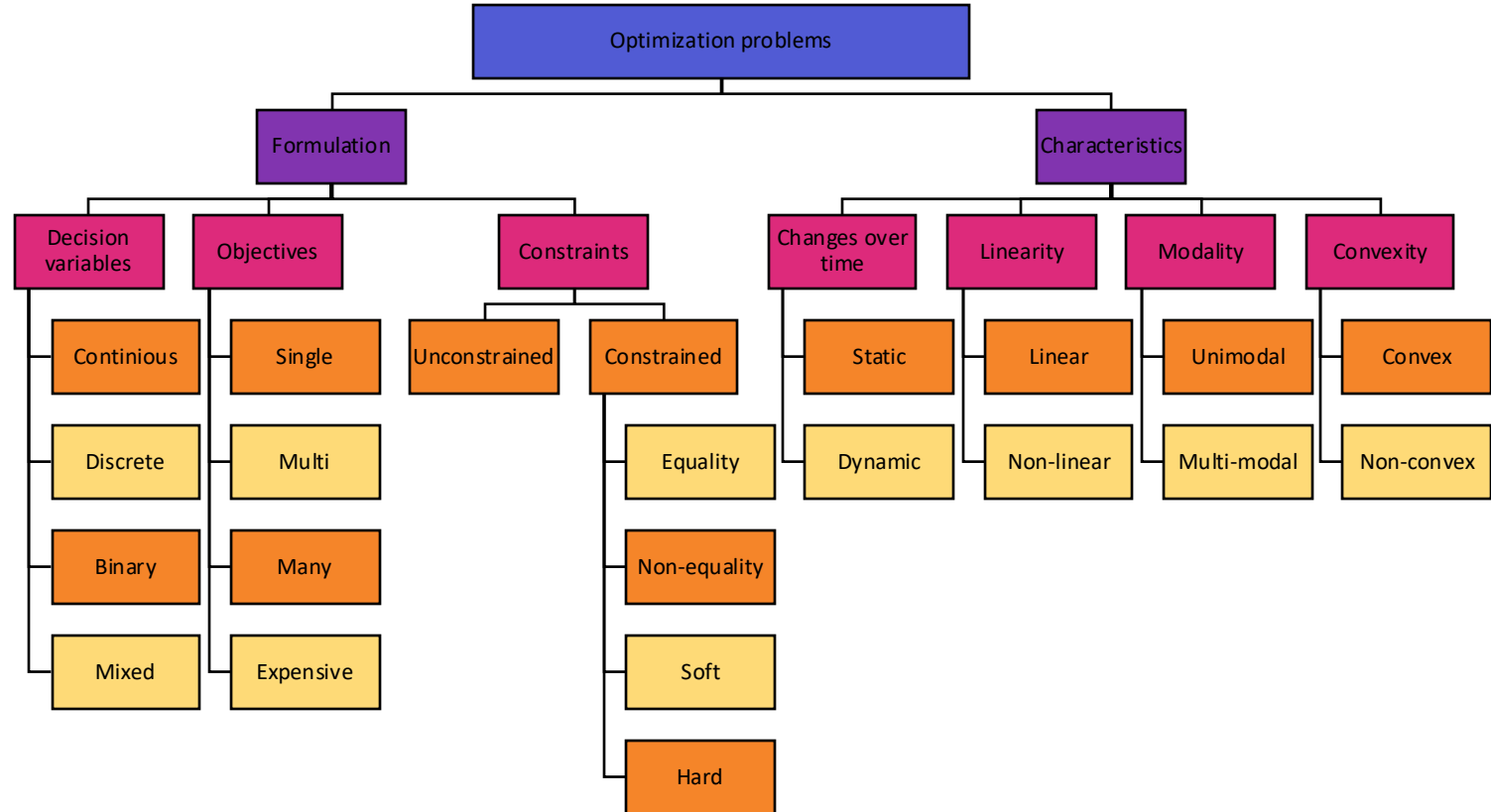
# CONSTRAINT SPACE COMPLEXITY

- Highly constrained landscape
- Equality constraint
- Inequality constraint
- Priority (soft vs. hard)
- Non-linear constraints
- Dynamic constraints
- ...

System

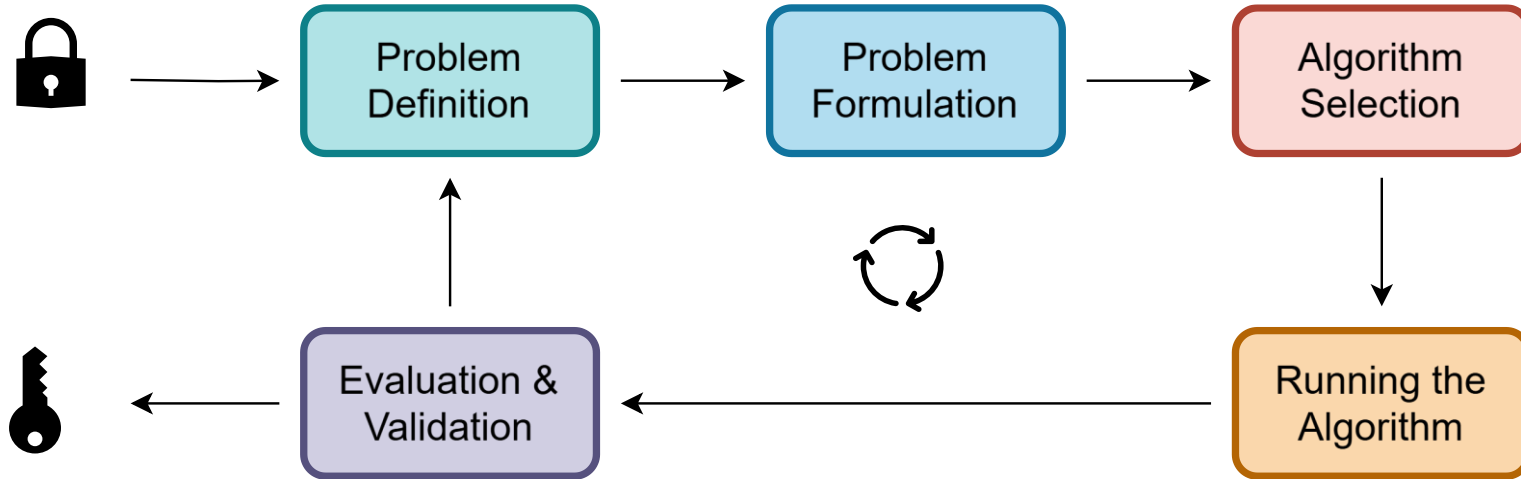


# A TAXONOMY

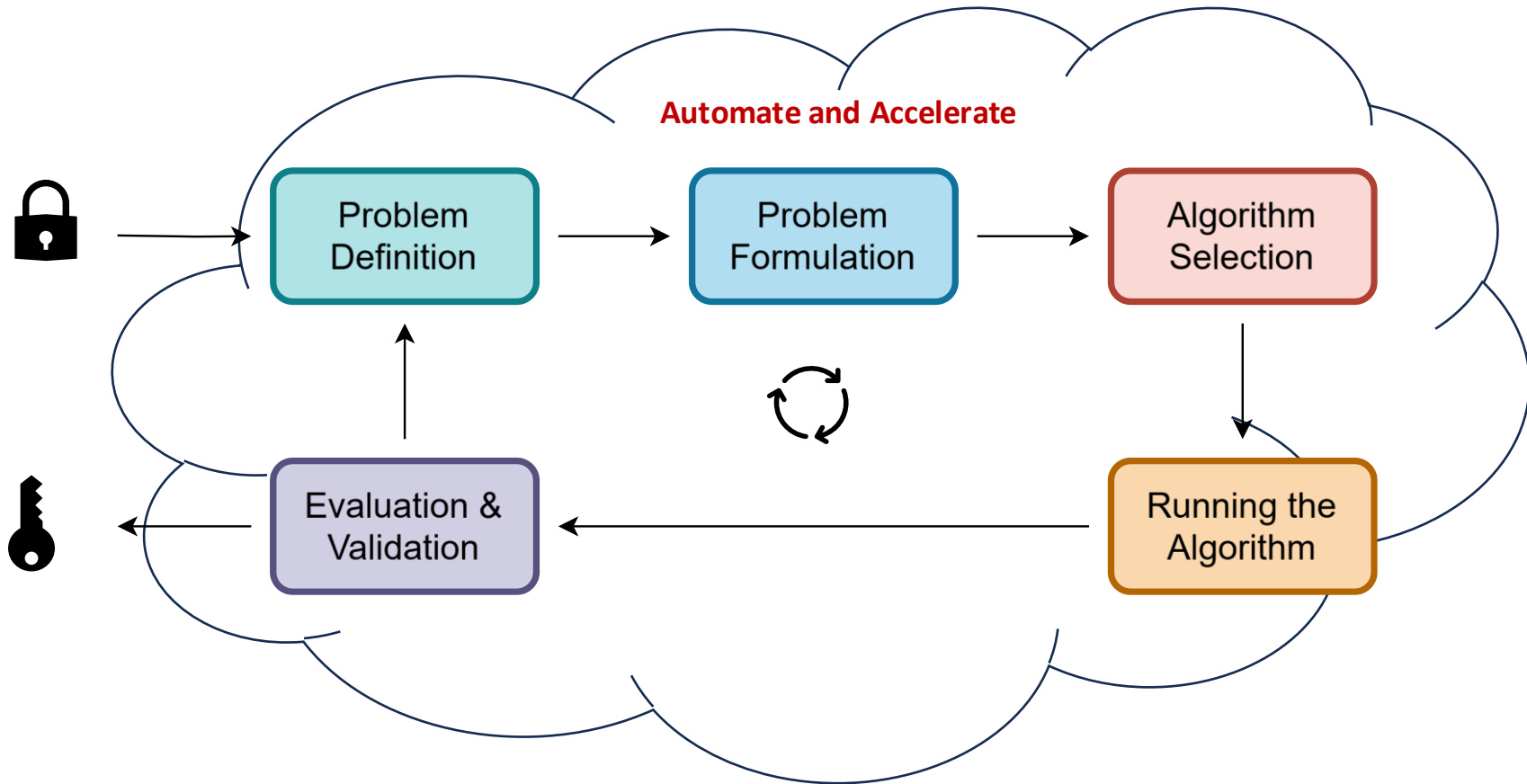




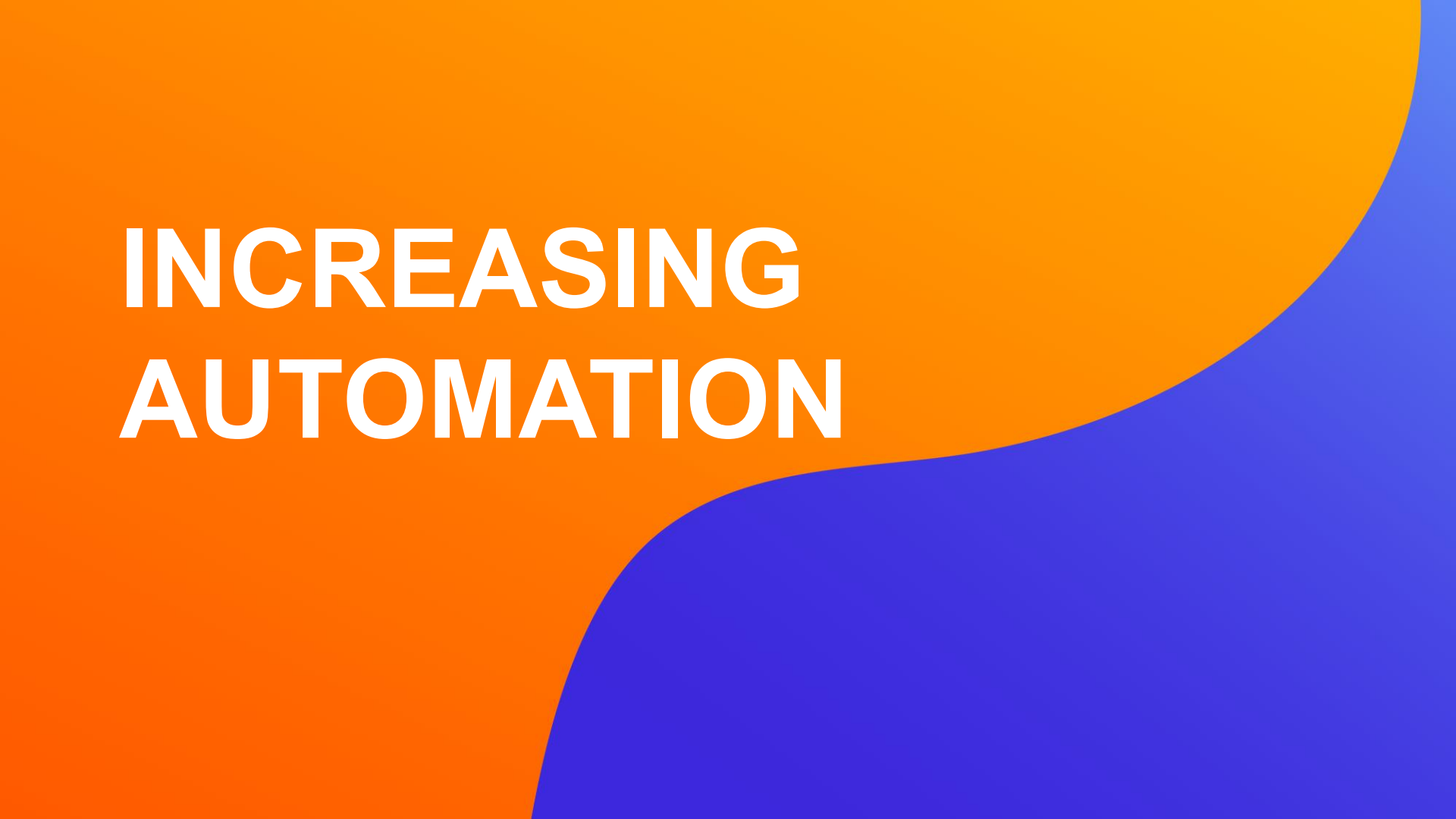
# OPTIMIZATION LIFECYCLE



# OPTIMIZATION LIFECYCLE



# INCREASING AUTOMATION

The background features a large, vibrant orange shape on the left and top, which transitions into a deep blue shape on the right and bottom. The boundary between the two colors is a smooth, flowing curve that starts near the bottom left and arcs towards the top right, creating a dynamic, modern aesthetic.

# CONVENTIONAL ALGORITHMS

## Gradient-based

$\nabla f(x)$  guides

Uses derivative information to move downhill in the objective landscape.

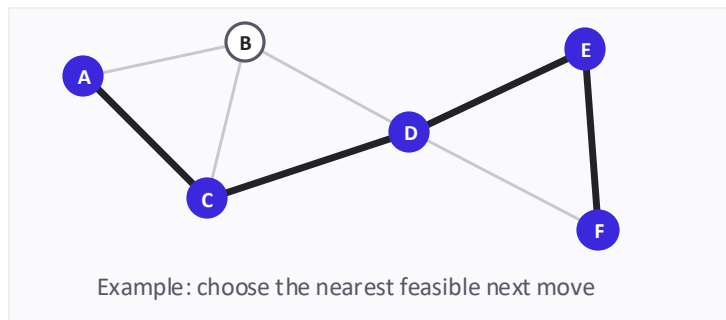


- Fast and precise when the problem is smooth and differentiable.
- Performance can depend on initialisation, scaling and step size.
- Can converge to a local stationary point in non-convex landscapes.

## Heuristics

domain knowledge

Uses a practical, problem-specific rule to construct or improve a solution.

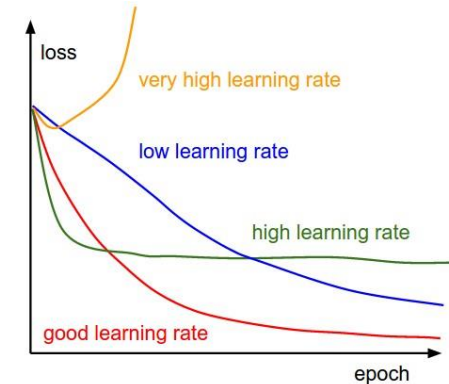
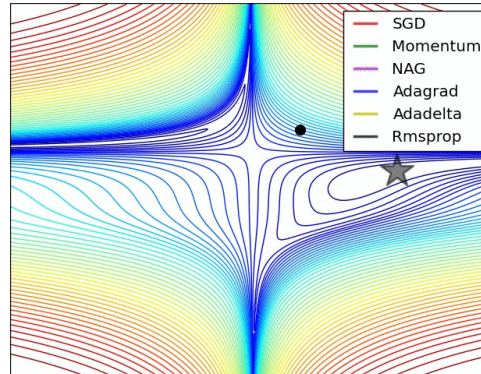
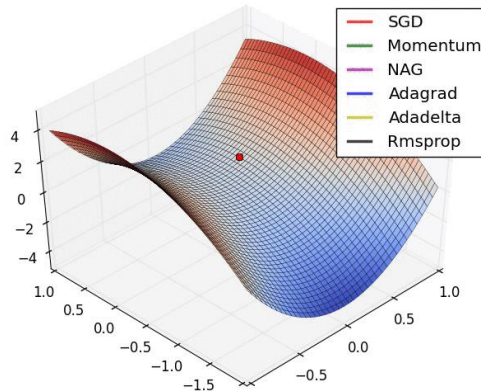
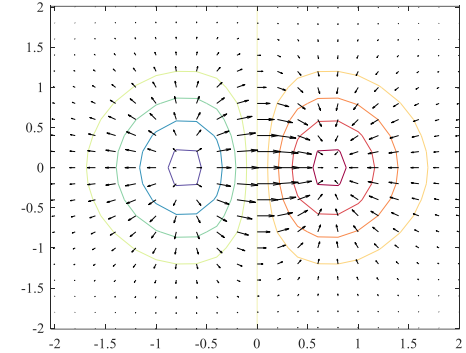
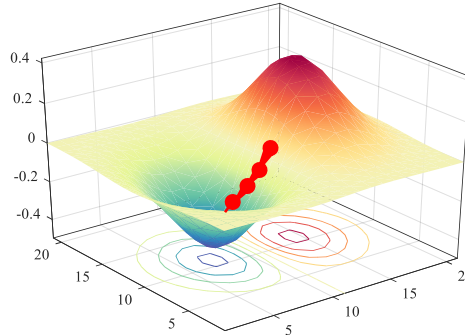


- Very fast and easy to apply when good domain knowledge exists.
- Usually designed for one problem or problem family.
- Solution quality depends strongly on the rule that was chosen.

Both search directly in the solution space

# CONVENTIONAL ALGORITHMS

1. Most Gradient-based
2. Sensitive to learning rate
3. Local optima
4. Saddle points
5. Not very practical in most problems



# META-HEURISTICS

A high-level, problem-independent strategy that guides search across complex solution spaces.

GA

DE

PSO

SA

GWO

WOA

SEARCH SPACE

EXPLORE



EXPLOIT

diversify search ← balance → intensify around promising regions

## Problem independent

The same framework can be adapted to many domains.

## Black-box friendly

Works without analytical gradients and tolerates non-smooth objectives.

## Approximate global search

Prioritises robust near-optimal solutions over guarantees of exact optimality.

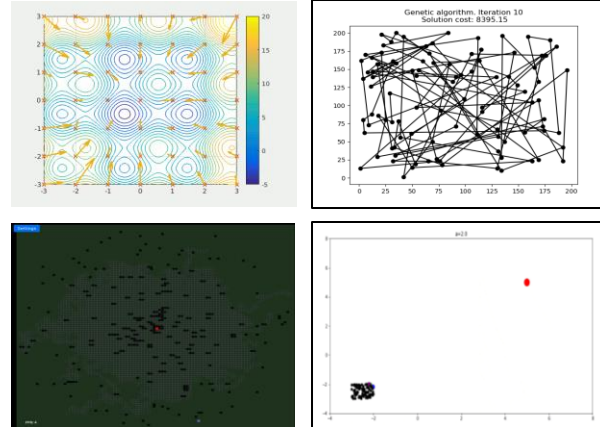
# META-HEURISTICS

## Advantages:

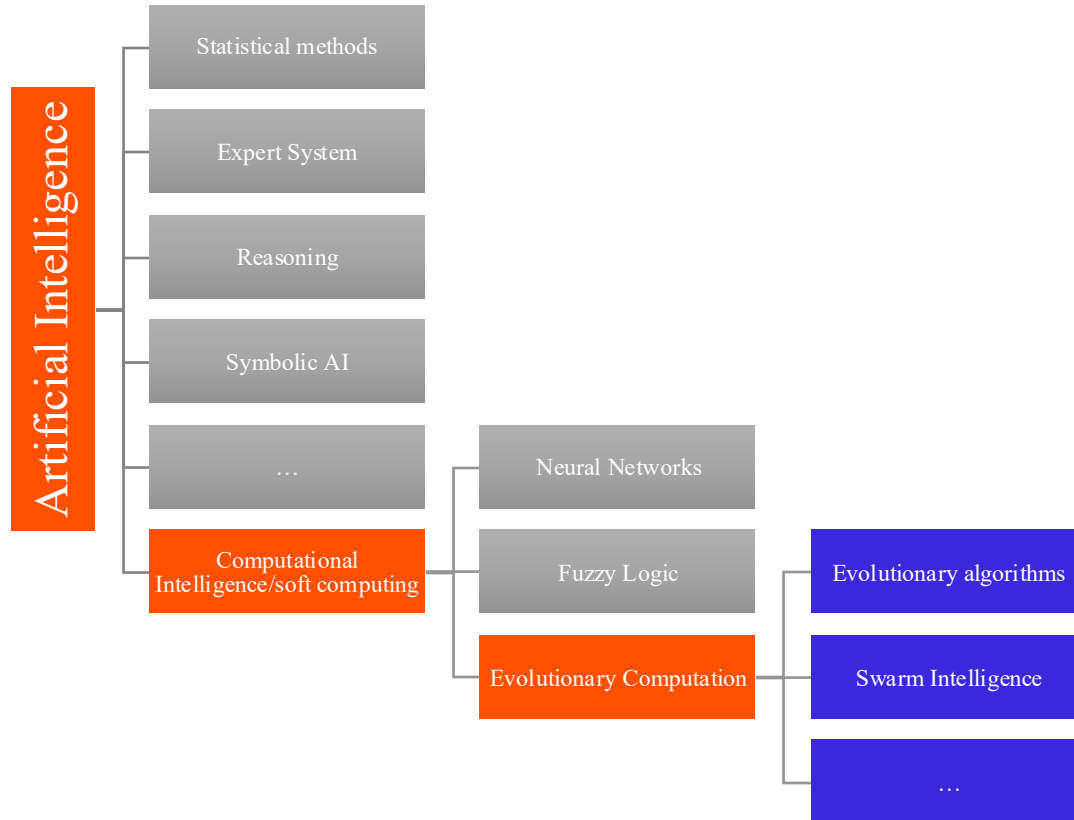
1. Avoid local solutions
2. Higher chance of finding the global optimum
3. Low dependency on the initial solution
4. Mostly do not need gradient

## Drawbacks:

1. Slow convergence speed
2. Finding different answers in each run

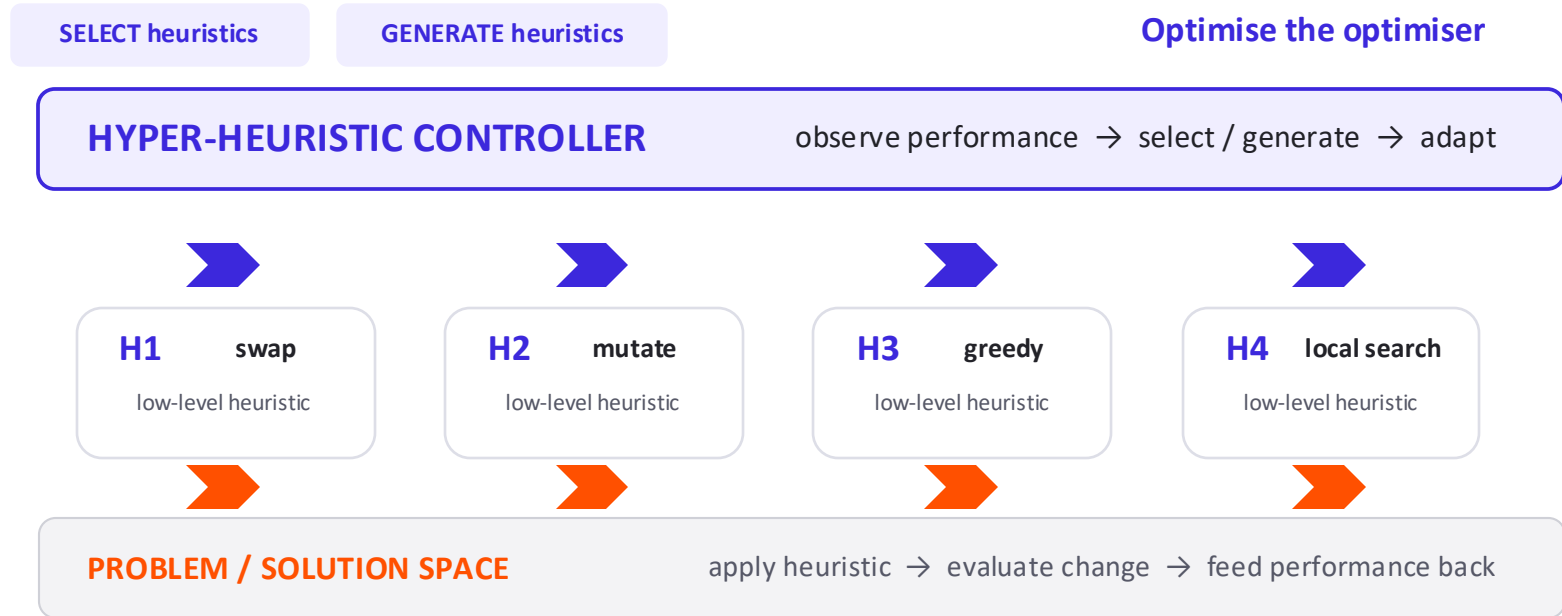


# EVOLUTIONARY COMPUTATION & SOFT COMPUTING



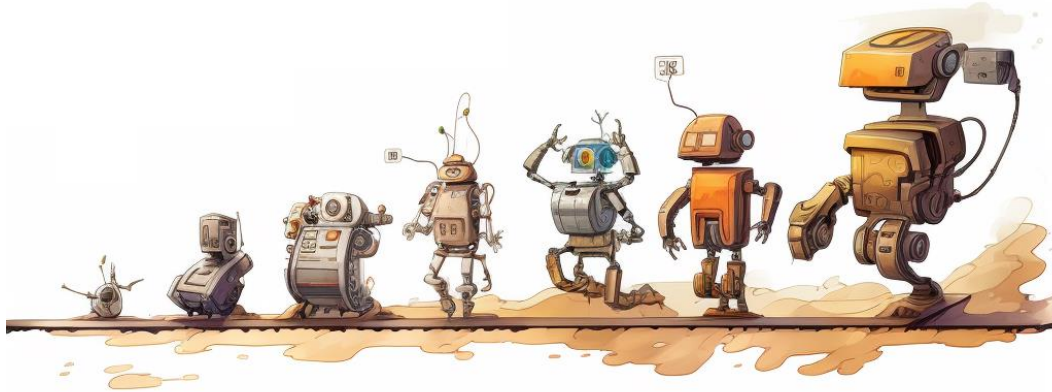
# HYPER-HEURISTICS

Search the space of heuristics rather than searching the solution space directly.



# WHERE WER ARE HEADING?

Gradient-based → Heuristic → Meta-heuristic → Hyper-heuristic → ?????

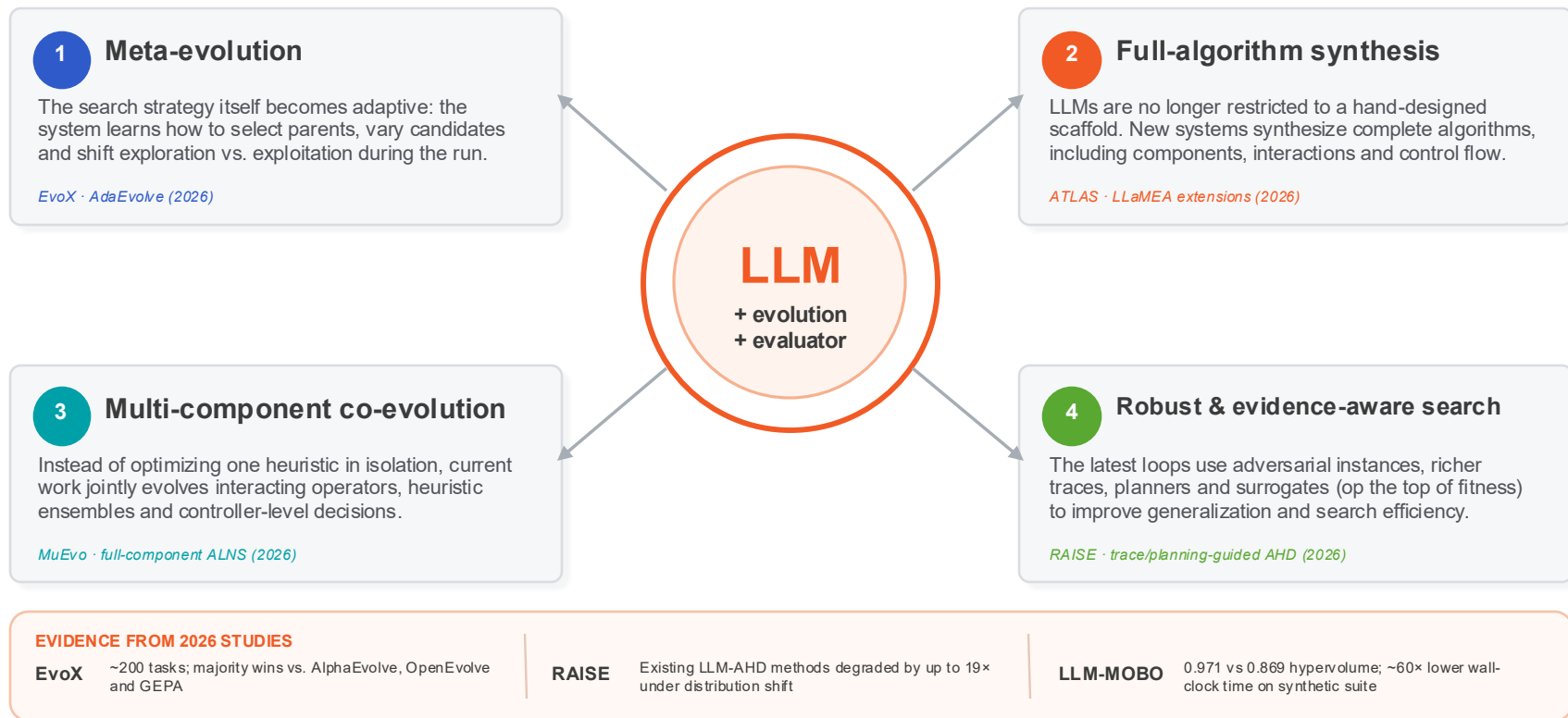


Increased Automation

Less Human Involvement

# LATEST DEVELOPMENTS IN LLM-DRIVEN META-HEURISTICS

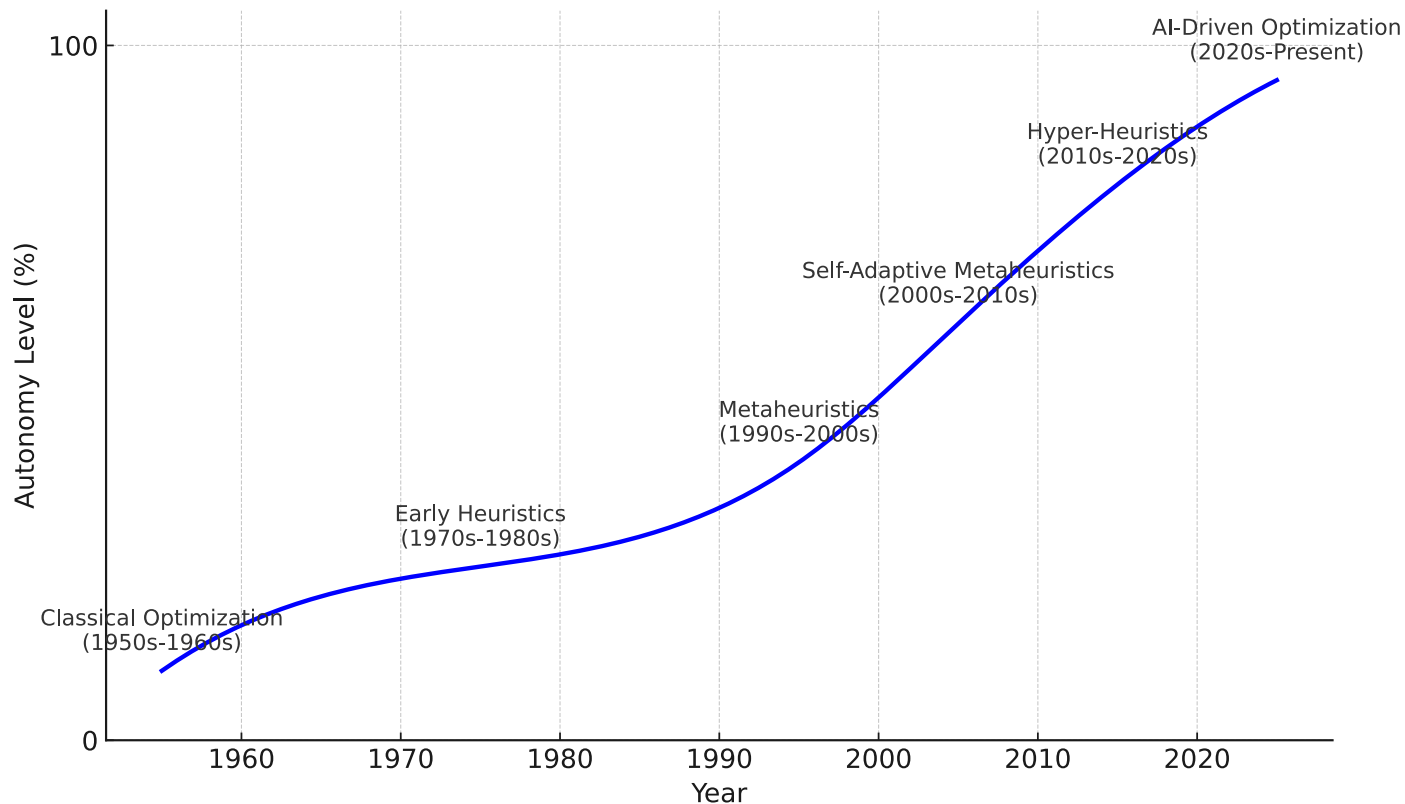
The frontier is moving from LLM-generated code to adaptive, multi-component and full-algorithm discovery.



**KEY SHIFT** LLM as code generator → LLM as strategic meta-optimizer and autonomous algorithm designer

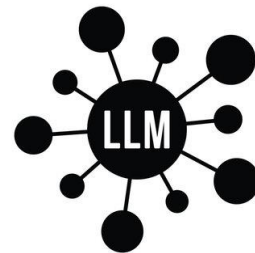
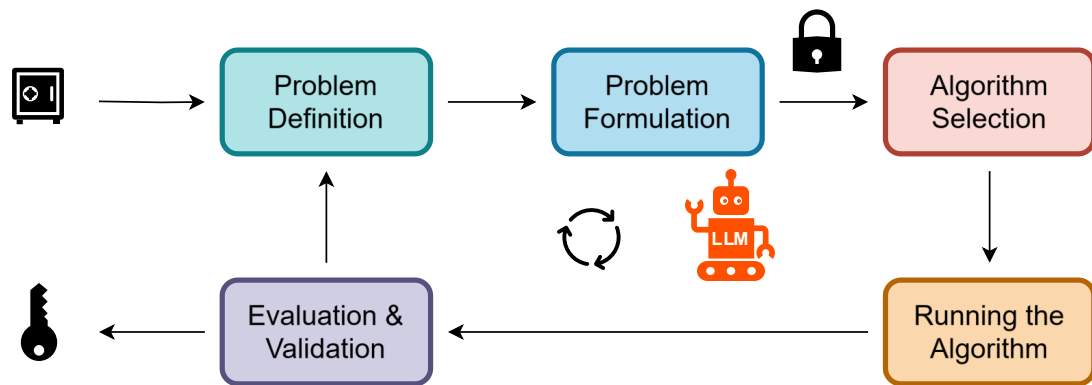
Recent primary studies: ATLAS (arXiv:2608.15546); MuEvo (2608.03636); EvoX (2602.23413); RAISE (2606.31801); Laskaris et al. MOBO (2607.08791).

# WHERE WER ARE HEADING?



## OPEN RESEARCH QUESTIONS

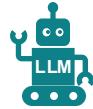
1. How to automate algorithm development and improvement?
2. How to automate problem formulation?
3. How to reduce human involvement in both?



# HOW GENAI CAN BE USED?

1. **GenAI-powered problem definition:**
  - Gathers and structures qualitative data for precise requirement modeling.
  - Maximizes stakeholder input and validates requirements for optimization.
2. **GenAI-powered problem formulation:**
  - Creates accurate mathematical models from detailed requirements.
  - Refines models iteratively to match real-world conditions effectively.
3. **GenAI-powered algorithm design and development:**
  - Generates, analyzes, and refines code for algorithm development.
  - Enables rapid exploration of innovative meta-heuristic solutions.
4. **GenAI-powered algorithm executor:**
  - Optimizes hardware and algorithm settings for efficient execution.
  - Monitors and improves execution by addressing inefficiencies.
5. **GenAI-powered solution evaluator:**
  - Evaluates results, identifies patterns, and suggests improvements.
  - Accelerates iterative optimization with expert-level insights.

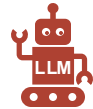
Problem  
Definition



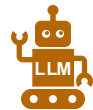
Problem  
Formulation



Algorithm  
Selection



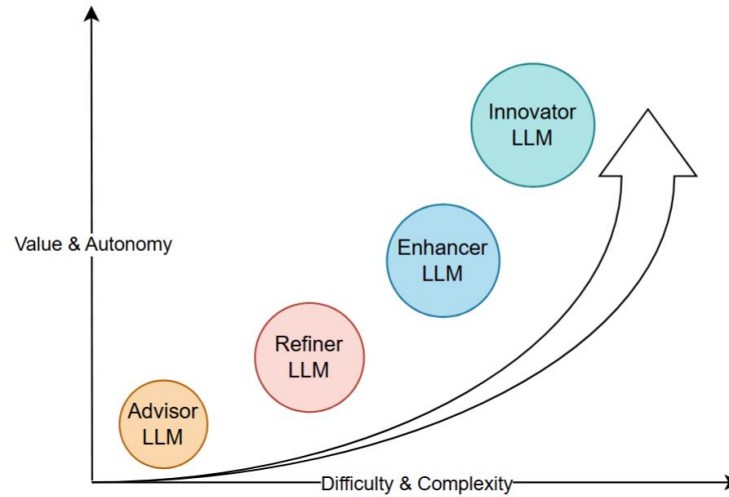
Running the  
Algorithm



Evaluation &  
Validation



# HOW **GENAI** CAN BE IN ALGORITHM DESIGN AND DEVELOPMENT?

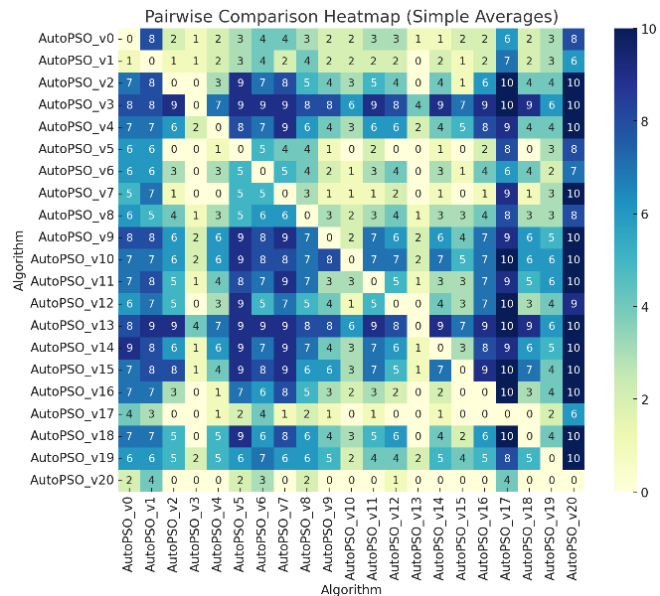
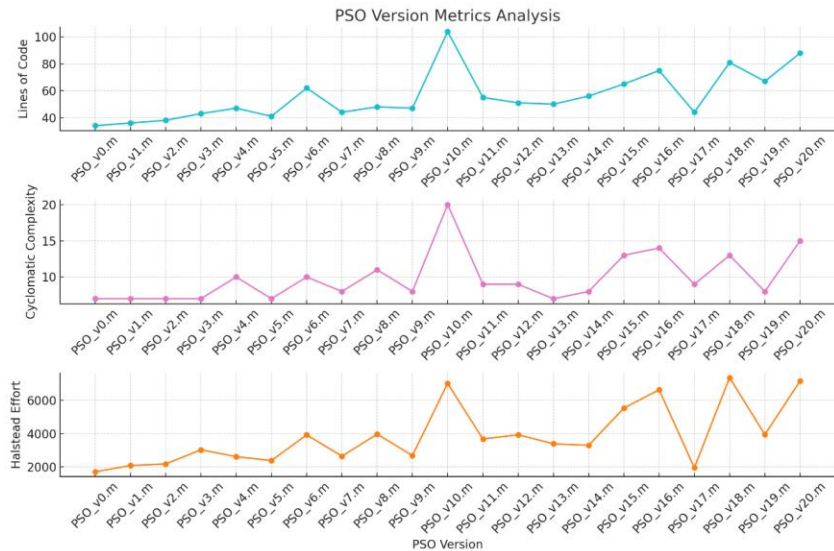


**Figure 14:** Visualisation of LLM Roles in metaheuristic optimisation where Advisor, Refiner, Enhancer, and Innovator roles each contribute uniquely to improving algorithm performance and adaptability.

# EXAMPLE I



Improving PSO 20 times without human intervention using GPT 4o (temperature 0.7)



# EXAMPLE II

## Sustainable Facility Site Location Selection

Problem  
Formulation

Algorithm  
Development

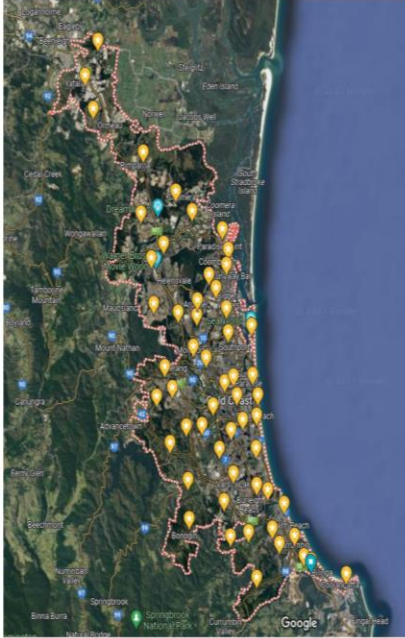


Figure 6. All DCs available for Gold Coast City (source Google Maps)[32]

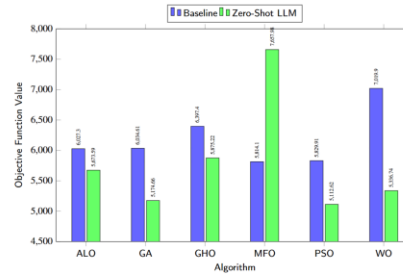
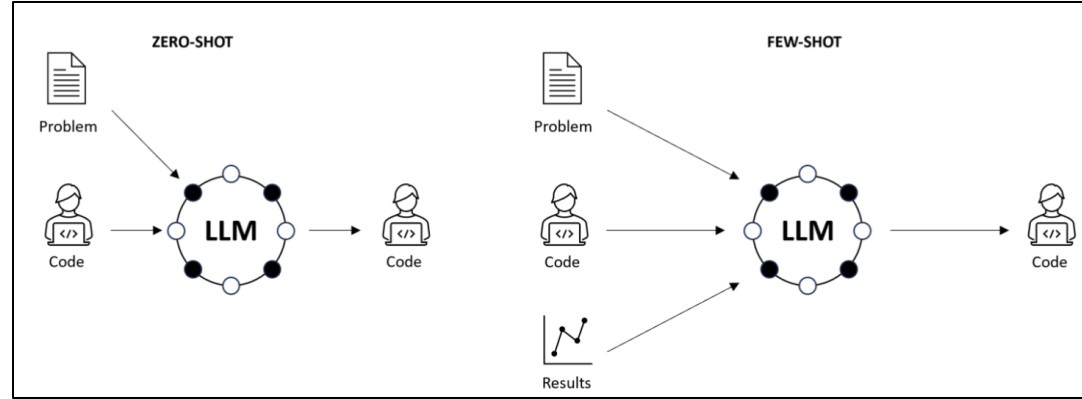


Figure 17: Performance comparison of baseline and zero-shot LLM-enhanced algorithms under Configuration B

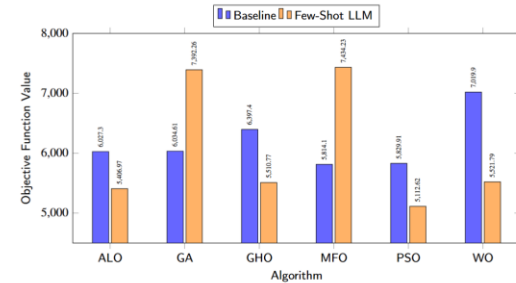


Figure 25: Performance comparison of baseline and few-shot LLM-enhanced algorithms under Configuration B

# EXAMPLE III: A NEW PROMPTING FRAMEWORK

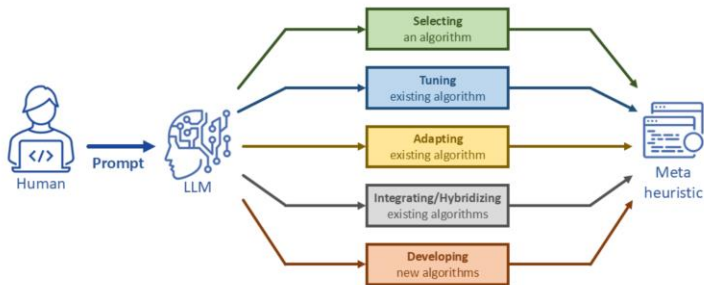


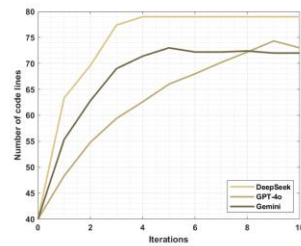
Figure 2: Human and LLM Collaboration in Meta-Heuristic Optimization Across Five Levels: Selection Level, Tuning Level, Adapting Level, Integration Level, and Developing Level

## RESOLUTION Prompt (Adapting Existing Algorithms for Solving Traveling Salesman Problem)

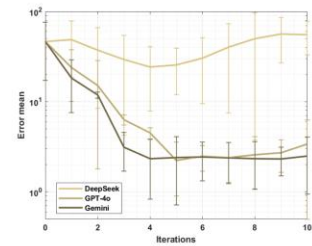
Consider the following as an input prompt and do so carefully to the end. **Roles** phase (You act as a code developer. You act as an optimization expert.) **Explanation** phase (I am looking for an optimized binary GA code based on the provided code to use in my project.) **InStances** phase (To solve a TSP problem instance with the given distance matrix.) **Algorithms** phase (I would like you to precisely adjust the parameters of the code and the operators used in the code.) **Variables** phase (Consider tuning all parameters and variables.) **Modules** phase (Consider all possible operators could be found in MH literature.) **DeTails** phase (I require a detailed Python code, with extensive comments to explain each part.) **Architecture** phase (Revising the structure of the code is also allowed.) **Score** phase (Revise the original code to enhance it based on a metric defined as the product of the answer error and the number of lines of the code) **Return** phase (1- Provide the revised code. 2- Highlight any tuning made. 3- Run both the original and the revised codes for 10 times to solve the instance with the given distance matrix. 4- Which algorithm do you suggest based on the mentioned score average? 5- Provide a table of the number of lines and the tour distance mean and standard deviation for both codes confirming your answer.)

Table 2  
RESOLUTION Hyper-Framework Aspects Across Levels

| RESOLUTION      | Aspects                                                                                                          | Selection Level | Tuning Level | Adapting Level | Integration Level | Developing Level |
|-----------------|------------------------------------------------------------------------------------------------------------------|-----------------|--------------|----------------|-------------------|------------------|
| R: Role         | Explaining roles                                                                                                 | *               | *            | *              | *                 | *                |
| E: Explanation  | Explaining what we require                                                                                       | *               | *            | *              | *                 | *                |
| S: inStances    | Defining the optimization problem instance                                                                       | *               | *            | *              | *                 | *                |
| O: algOrithms   | Introducing the algorithm(s)                                                                                     | *               | *            | *              | *                 | *                |
| L: variables    | Determining variables to be tuned                                                                                | -               | *            | *              | *                 | *                |
| U: modUles      | Introducing the pool of modules                                                                                  | -               | -            | *              | *                 | *                |
| T: deTails      | Determining details of the desired output code                                                                   | *               | *            | *              | *                 | *                |
| I: architecture | Determining structure or architecture of the output code                                                         | *               | *            | *              | *                 | *                |
| O: scOre        | Defining the scoring criteria                                                                                    | *               | *            | *              | *                 | *                |
| N: returN       | Explaining what we require as the output, including algorithm(s), experimental confirmation, final code(s), etc. | *               | *            | *              | *                 | *                |

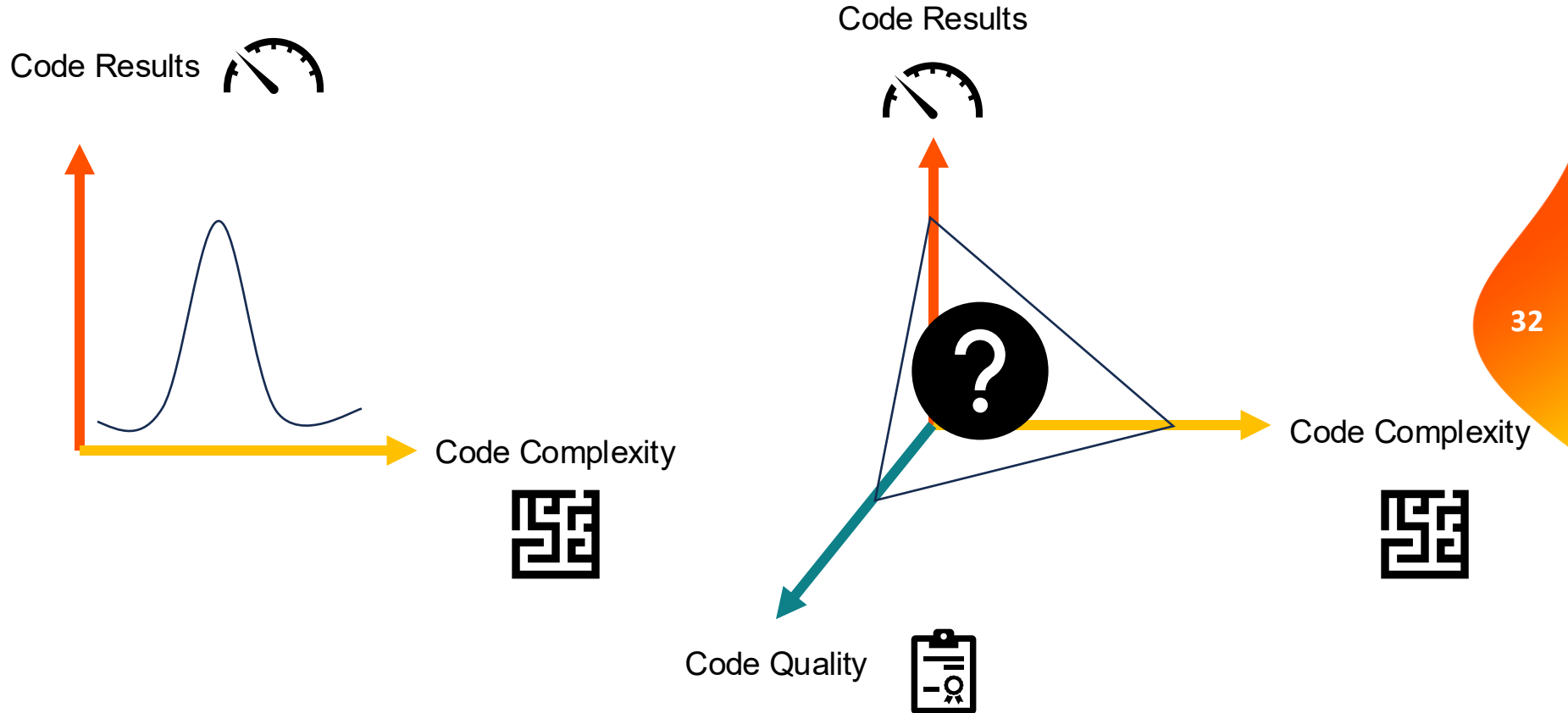


(a) Number of code lines.



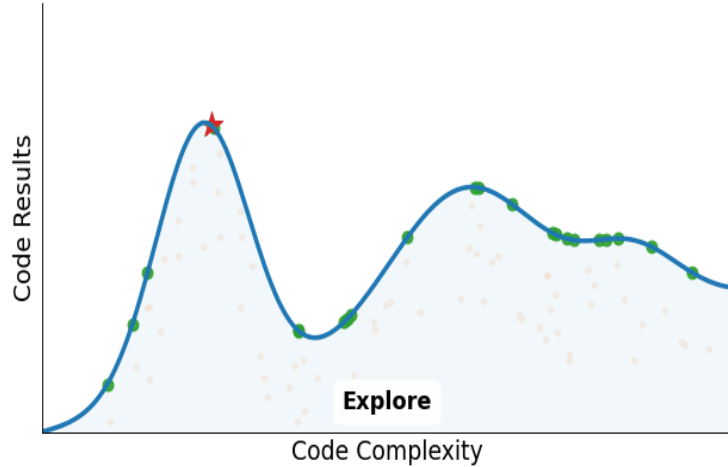
(b) Error mean.

# EXAMPLE IV: A NEW SET OF PERFORMANCE METRICS

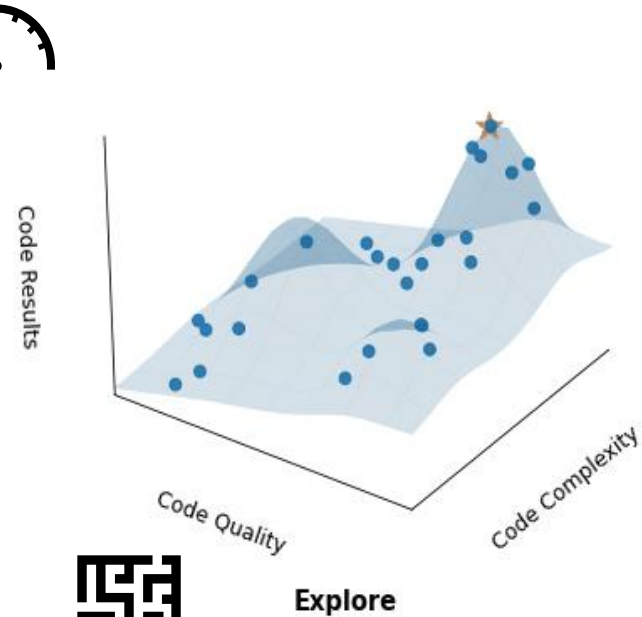


# EXAMPLE IV: A NEW SET OF PERFORMANCE METRICS

## Discovering Better Algorithms



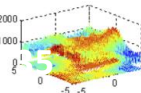
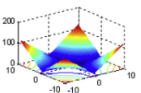
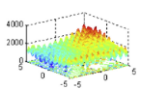
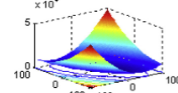
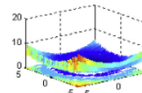
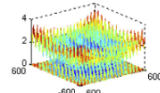
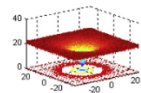
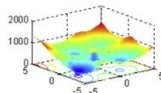
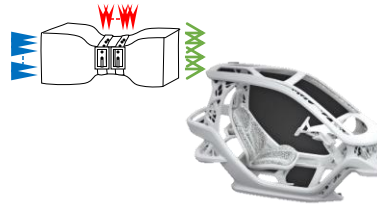
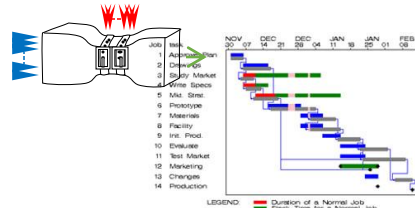
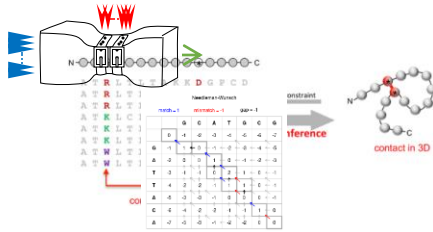
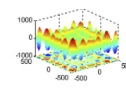
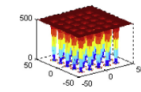
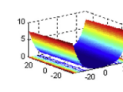
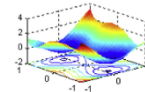
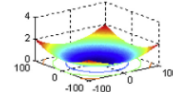
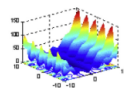
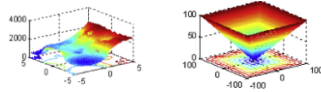
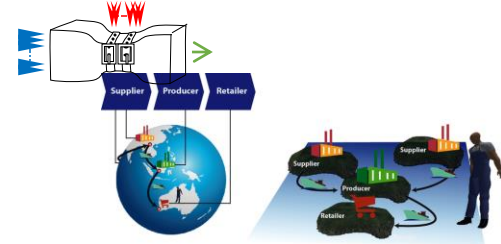
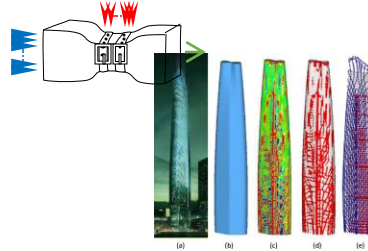
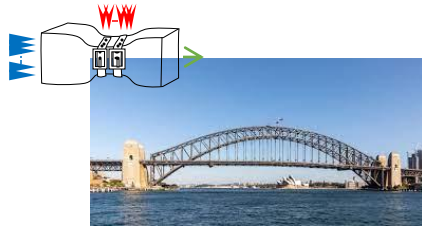
## Evolution Through Algorithm Space



# THE RISK OF OVER OPTIMIZATION?

The background of the slide features two large, overlapping, wavy shapes. The top-left portion is a solid orange color, while the bottom-right portion is a solid blue color. The boundary between the two colors is a smooth, flowing curve that starts near the bottom left and extends towards the top right.

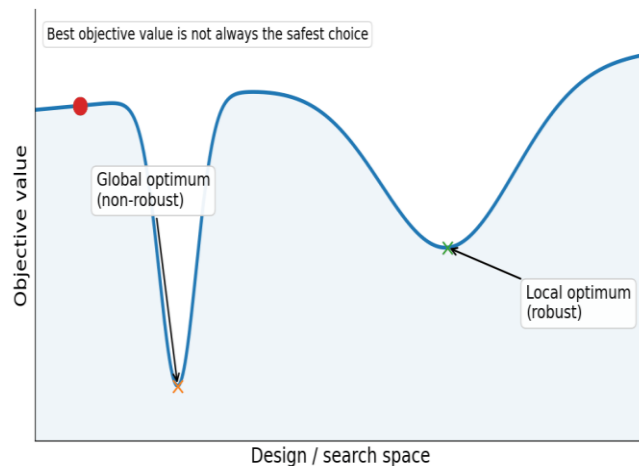
# EVERYTHING CAN BE OPTIMIZED, BUT SHOULD WE?



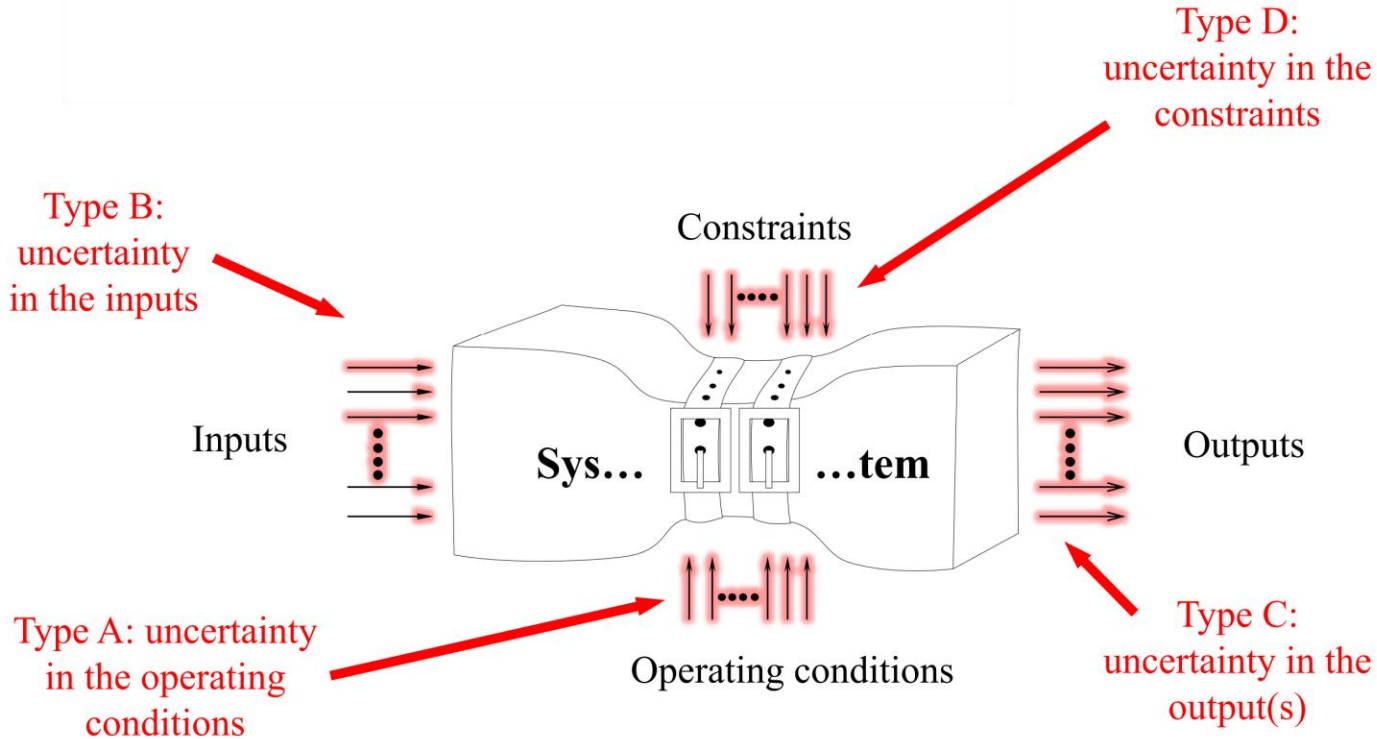
# WHAT IF WE OVER OPTIMIZE?

- **Small errors can lead to big failures:** Tiny mistakes in how we set up the problem or prompt the model can grow into serious issues later, like wrong or unsafe solutions.
- **Chain reaction of errors:** If we use LLMs in several steps of optimization, a small error early on can spread and affect the final outcome without being noticed.
- **Too tuned to the simulator:** If we train or test the optimiser only using a simulator, it might learn tricks that work there but fail in the real world, because it's just fitting to the simulator's rounding errors or unrealistic assumptions.

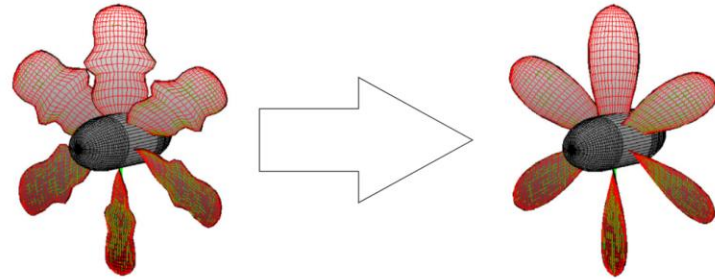
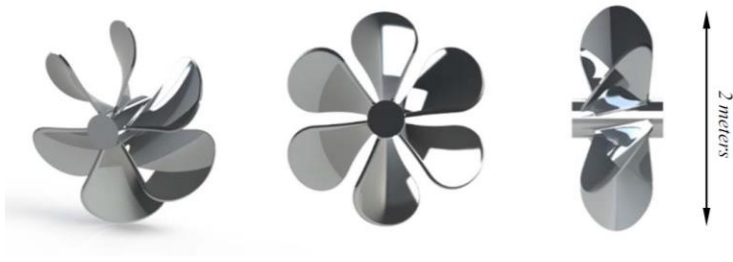
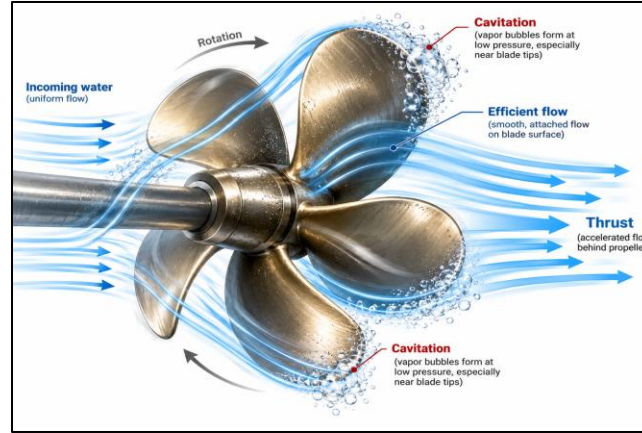
## Global Non-Robust vs Local Robust Solution



# DIFFERENT TYPES OF UNCERTAINTIES

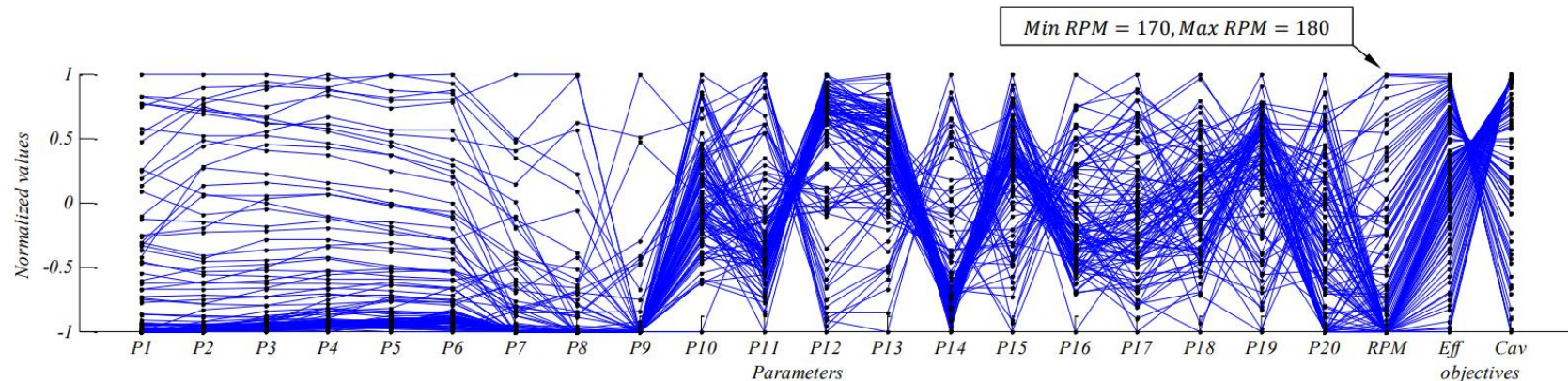
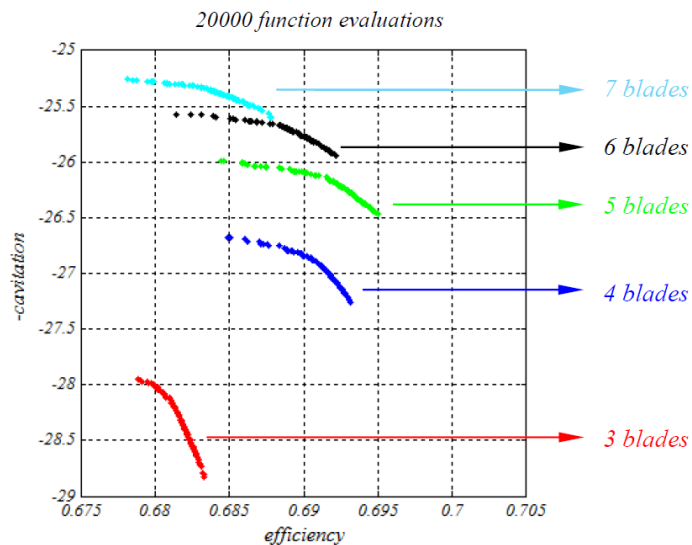
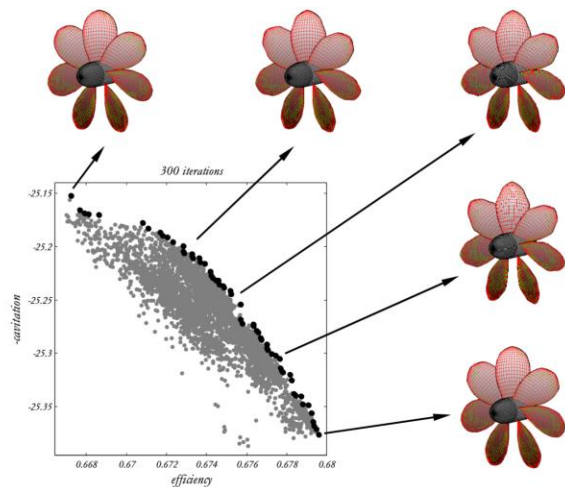


# AN EXAMPLE



Propeller efficiency is the ratio of thrust power to shaft power; every extra percentage point is real fuel money unless it comes with cavitation).

# AN EXAMPLE



# Effects of uncertainties in variables on the objectives

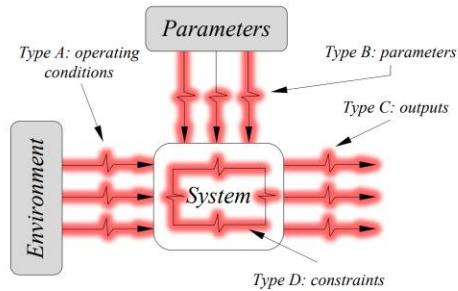


Figure 2.8: Different categories of uncertainties and their effects on a system: Type A, Type B, and Type C

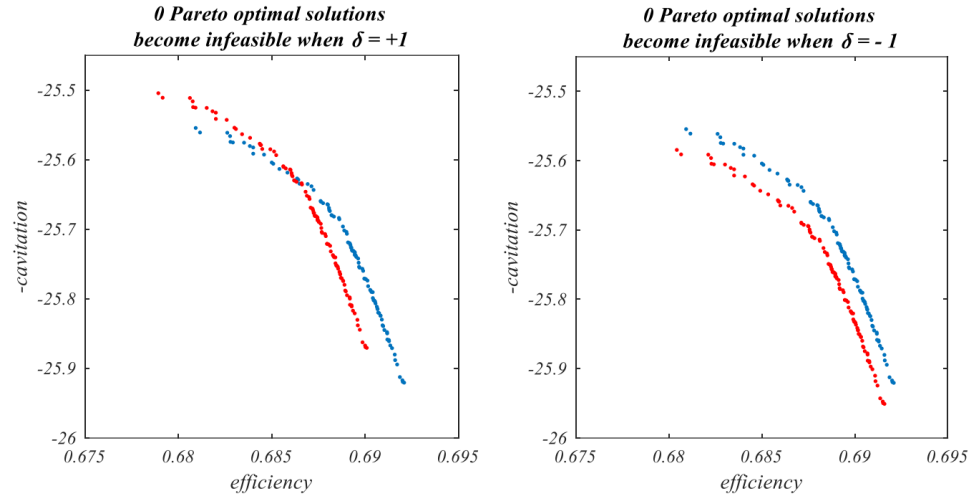
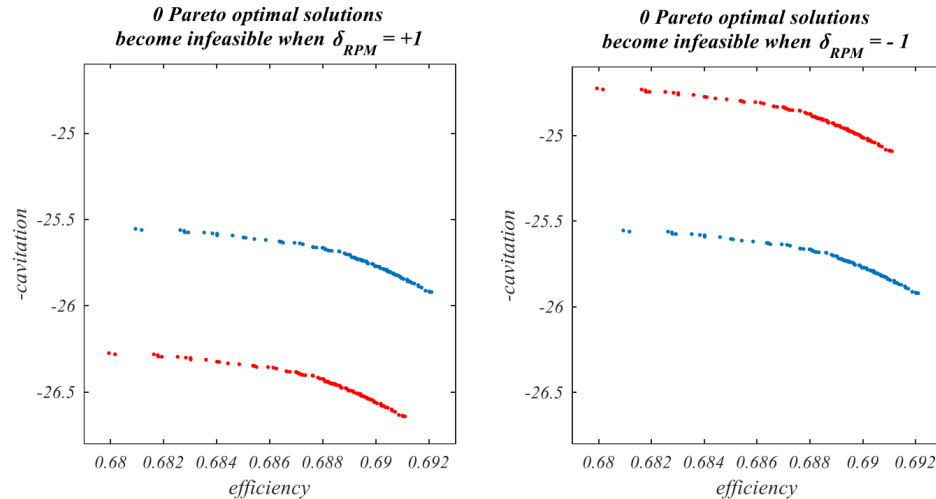


Figure 9.8: Pareto optimal solutions in case of (left)  $\delta = +1.5\%$  (right)  $\delta = -1.5\%$  perturbations in parameters. Original values are shown in blue, perturbed results in red.

# Effects of uncertainties in operating conditions on the objectives



**Perturbation may cause  
extra 40 liter of fuel  
consumption per day!!!**

Figure 9.7: Pareto optimal solutions in case of (left)  $\delta_{RPM} = +1$ , (right)  $\delta_{RPM} = -1$  fluctuations in RPM (right). Original values are shown in blue, perturbed results in red.

# Considering 1.5% noise according to ISO 484/2-1981

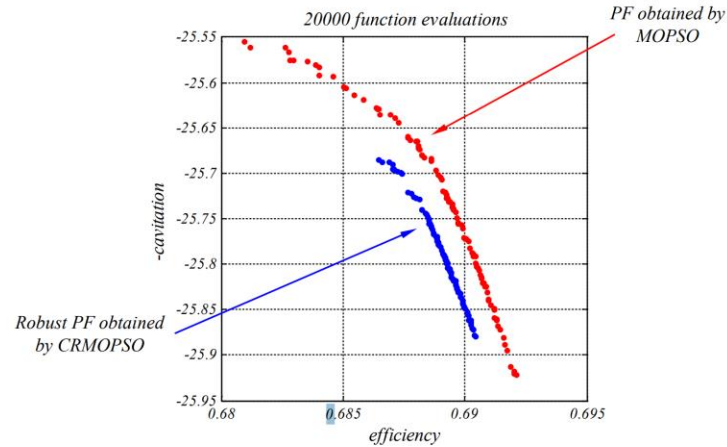


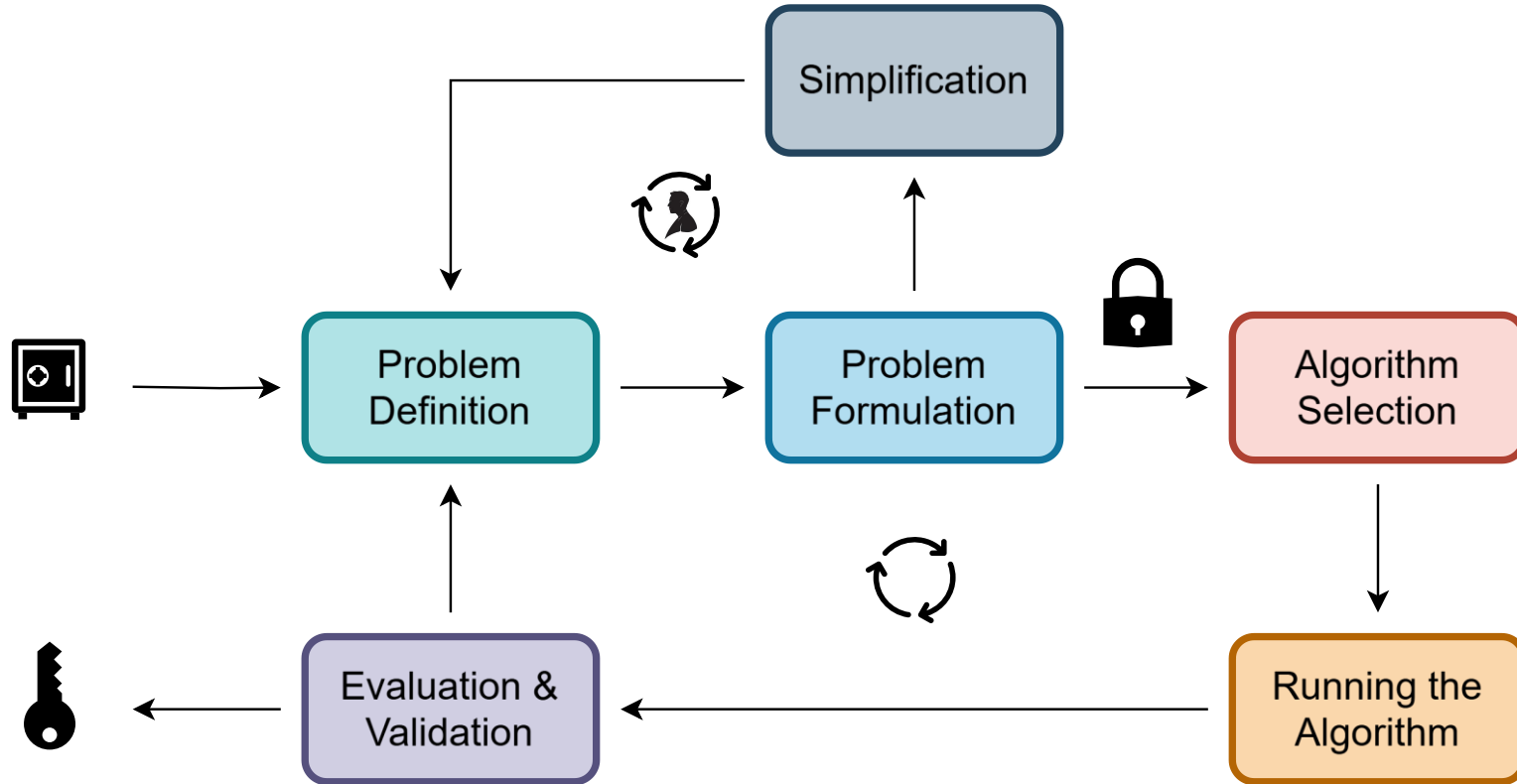
Figure 9.9: Robust front obtained by CRMOPSO versus global front obtained by MOPSO

Table 9.1: Fuel consumption discrepancy in case of perturbation in all of the structural parameters for both PS obtained by MOPSO and RPS obtained by CRMOPSO

| Algorithm | average | min    | max    |
|-----------|---------|--------|--------|
| MOPSO     | 0.1735  | 0.1676 | 0.1851 |
| CRMOPSO   | 0.0825  | 0.0805 | 0.0863 |

**WHAT TO DO TO  
MINIMIZE THE  
RISK?**

# A **REVISED** OPTIMIZATION LIFECYCLE/WORKFLOW

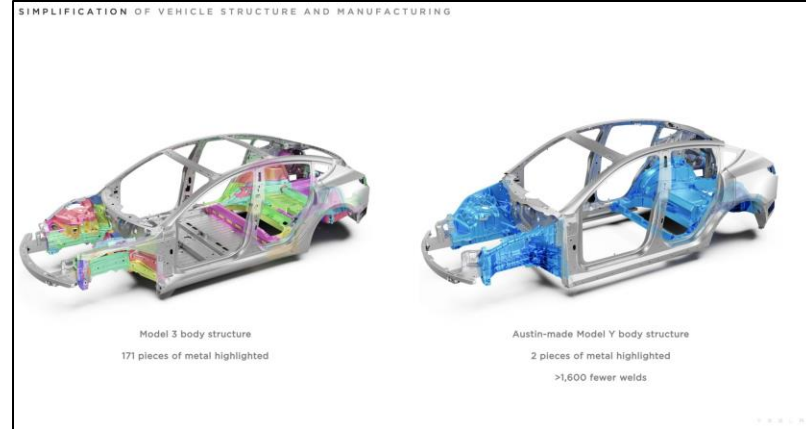
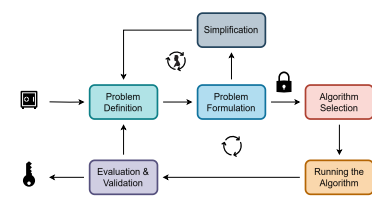


# AGILE WORKFLOW

1. **Make the requirements less dumb:** *“your requirements are definitely dumb, it does not matter who gave them to you”, so question the question.*
2. **Delete the part or process:** *“If you’re not adding things back in at least 10% of the time, you’re clearly not deleting enough”, so regularly review and remove parts or processes that don’t add significant value.*
3. **Simplify or optimize the design:** *“Possibly the most common error of a smart engineer is to optimize a thing that should not exist”, so focus on essential elements*
4. **Accelerate cycle time:** *“Every process can be speeded up. But only do this after you have followed the first three steps. In the Tesla factory, I mistakenly spent a lot of time accelerating processes that I later realized should have been deleted.”, so focus on valuable progress instead of mere speed.*
5. **Automate:** *“That comes last. The big mistake in Nevada and at Fremont was that I began by trying to automate every step. We should have waited until all the requirements had been questioned, parts and processes deleted, and the bugs were shaken out.”, so only automate after the first four steps.*



# EXAMPLES



**TAKE AWAYS?**

# KEY TAKE AWAYS

1. AI can automate the whole optimization lifecycle
2. Early evidences are convincing
3. Open challenges remain: fully automating algorithm improvement and problem formulation while keeping humans only where their insight truly matters.
4. Question requirements, delete what doesn't add value, simplify first, speed up second, automate last.



**Bottom line:** anything can be optimized, but not everything should be. Beware the “too-perfect” solution. Over-optimization can make systems fragile and expensive when real-world noise or constraints shift.

Love what  
you do



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