Pacific Northwest
NATIONAL LABORATORY

Mathematical Optimization in Python

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Agenda

- Introduction
- Optimization Problem
- Types of Optimization Problems
  - Linear Programming
  - Nonlinear Programming
  - Evolutionary Computing
- Conclusion

Introduction

- **Mathematical optimization** or **mathematical programming** is the selection of the best element, with regard to some criterion, from some set of available alternatives.
- Optimization problems arise in many quantitative disciplines including:
  - Computer science
  - Engineering
  - Operations research
  - Economics

Optimization Problem

- Mathematically speaking, an **optimization problem can be defined** as:
  - Given a function ***f*** from a set ***A***, look for an element $\boldsymbol{x_0}$ in ***A*** such that $f(\boldsymbol{x_0}) \leq f(\mathbf{x})$ or such that $f(\boldsymbol{x_0}) \geq f(\mathbf{x})$, for all **x** in *A*.
    - The first case is called **minimization** and the second **maximization**.
    - Note: $f(\boldsymbol{x_0}) \geq f(\mathbf{x}) \Leftrightarrow -f(\boldsymbol{x_0}) \leq -f(\mathbf{x})$
- Optimization problems can have many objective functions and many constraints.

$arg\ min\ x^2 + 1$	Objective function ***f***
$subject\ to{:}\ x > 1$	Constraint on ***x***

Optimization Problem (Cont.)

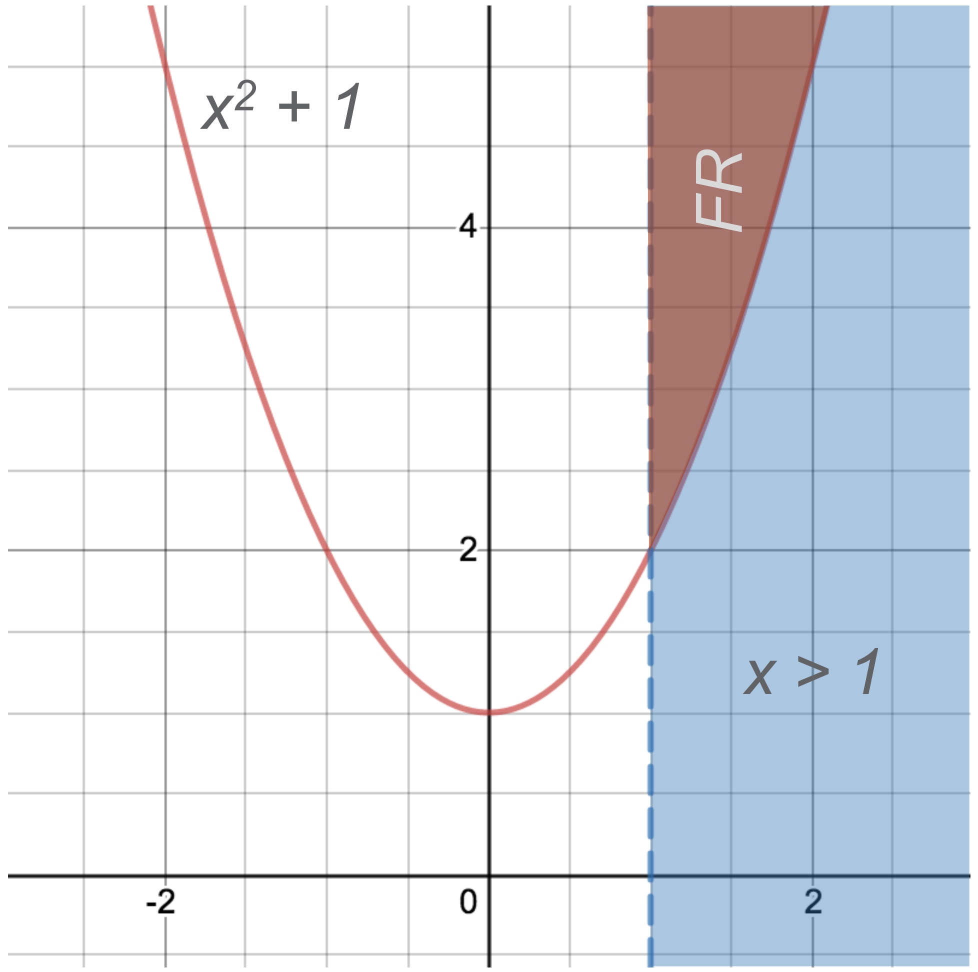
$$\underbrace{\begin{array}{l} \arg\min x^2 + 1 \\ \text{subject to: } x > 1 \end{array}}$$

Objective function ***f***

Constraint on ***x***

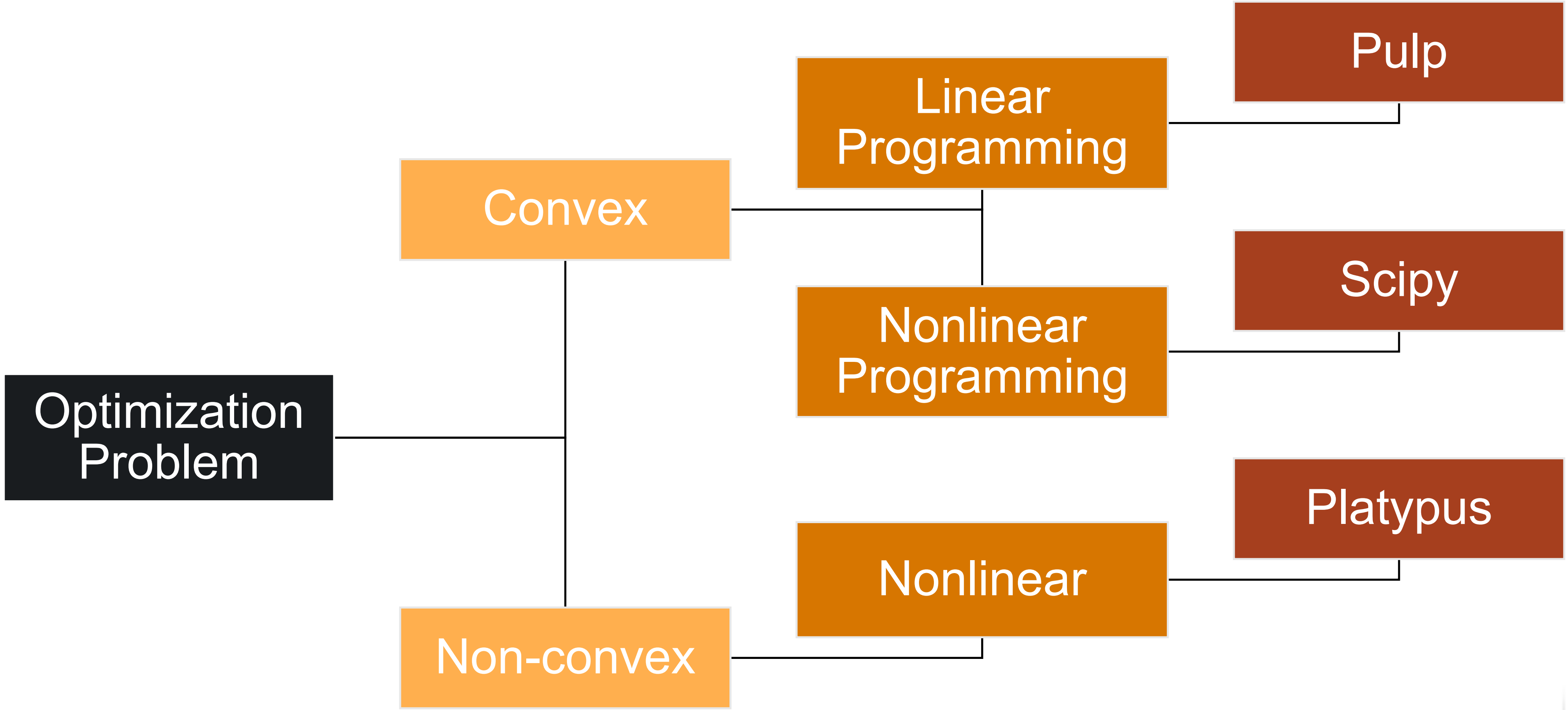
Mathematically

These define the **feasible region**.

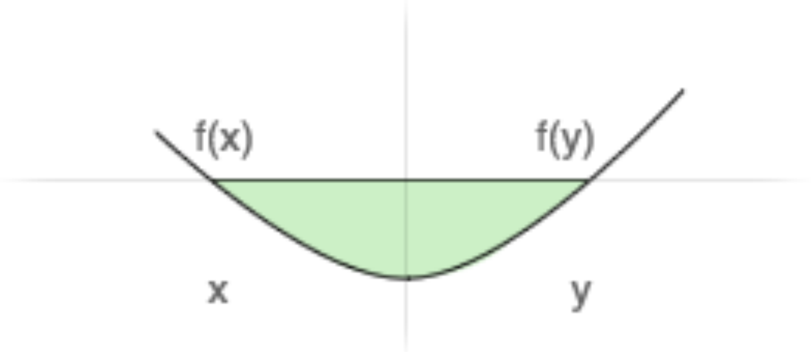


It is easy to verify that the solution to this "trivial" optimization problem is $x = 1^+$.

Some Types of Optimization Problems



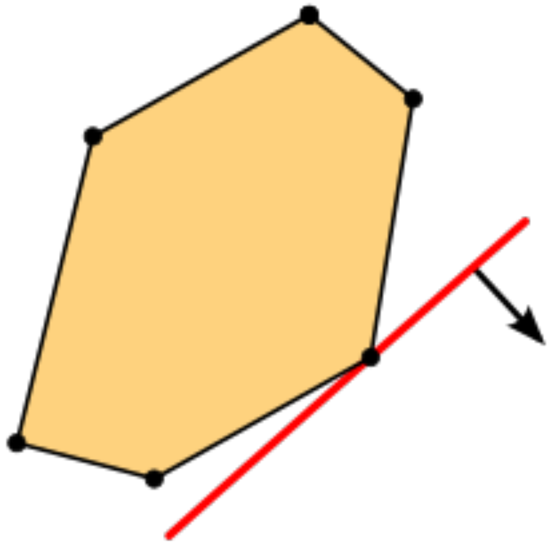
A **function is convex** if a line segment drawn from any point *(x, f(x))* to another point *(y, f(y))* lies on or above the graph of *f*.

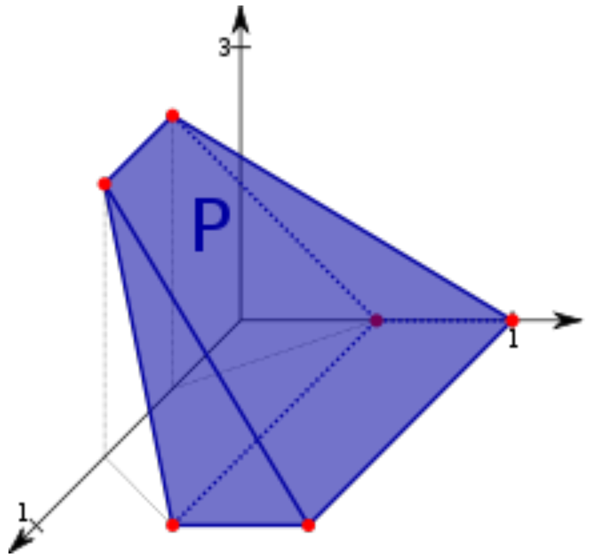


Lineal Programming

- Linear programming is a method to achieve the best outcome in a mathematical model **with objectives and constraints represented by linear relationships**.

$$\begin{aligned} &\arg\max\ \mathbf{c}^T\mathbf{x} \\ &\text{subject to: } A\mathbf{x} \le \mathbf{b} \\ &\qquad\qquad\quad \mathbf{x} \ge 0 \end{aligned}$$





Use case 1: LP Optimization Problem

Suppose you are a mechanic and your goal is to make cars run faster. The more cars you are able make faster, the better. Your secret behind making cars fasters is 2 gas additives, each of which uses special compounds. To create one unit of additive 1, you need 3.1 units of compound A and 2.4 units of compound B. Similarly, to create one unit of additive 2, you need 4.8 and 1 units of compound A and B, respectively. Now additive 1 can make a car faster by 7.5 speed units and additive 2 by 5.2. Furthermore, you only have 15 and 5 units of compound A and B at your disposal.

The question is, how much of each additive will you create to maximize the speed of the next car?

Use case 1: LP Optimization Problem (Cont.)

arg max $7.5\,a_1 + 5.2\,a_2$

subject to: $3.1\,a_1 + 4.8\,a_2 \leq 15$

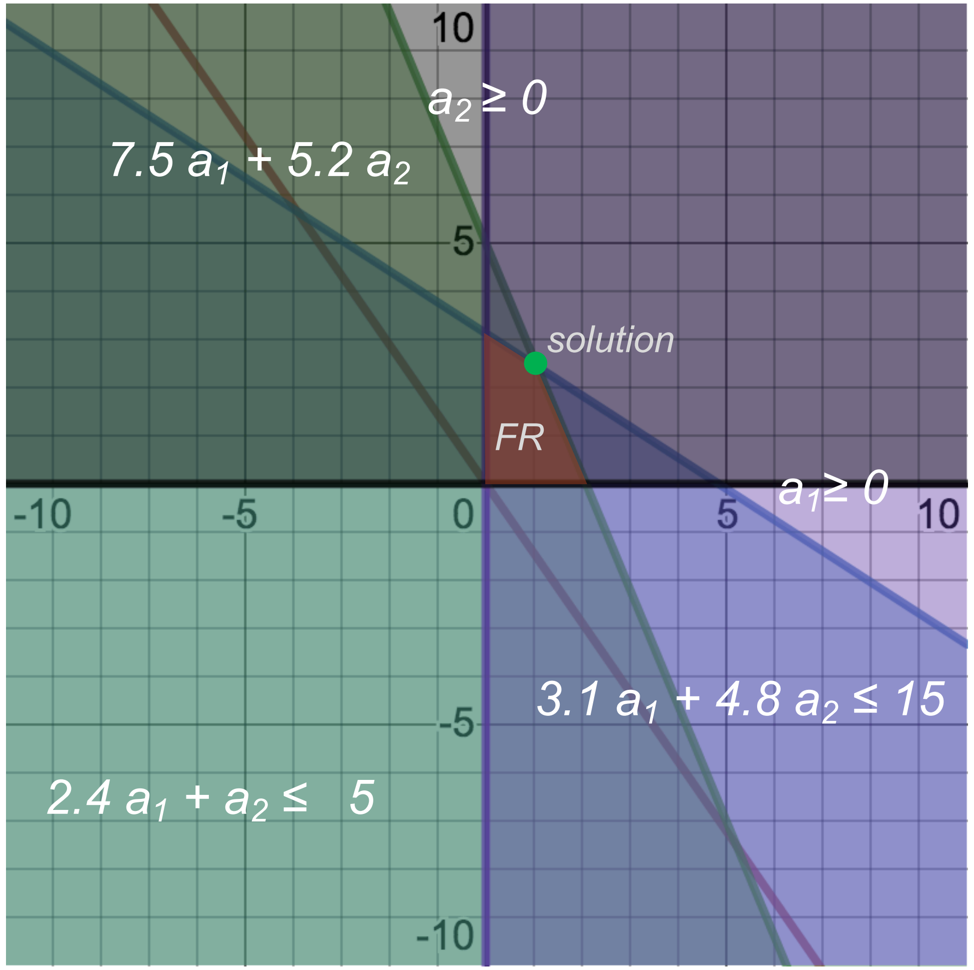
$2.4\,a_1 + a_2 \leq 5$

$a_1 \geq 0$

$a_2 \geq 0$

Solution: $a_1 = 1.07,\ a_2 = 2.43$

Speed can be maximized by 20.68 units!



Use case 1: LP Optimization Problem (Cont.)

What would happen if we change the speed coefficients of the objective?

arg max $1.2\,a_1 + 2.1\,a_2$

subject to: $3.1\,a_1 + 4.8\,a_2 \leq 15$

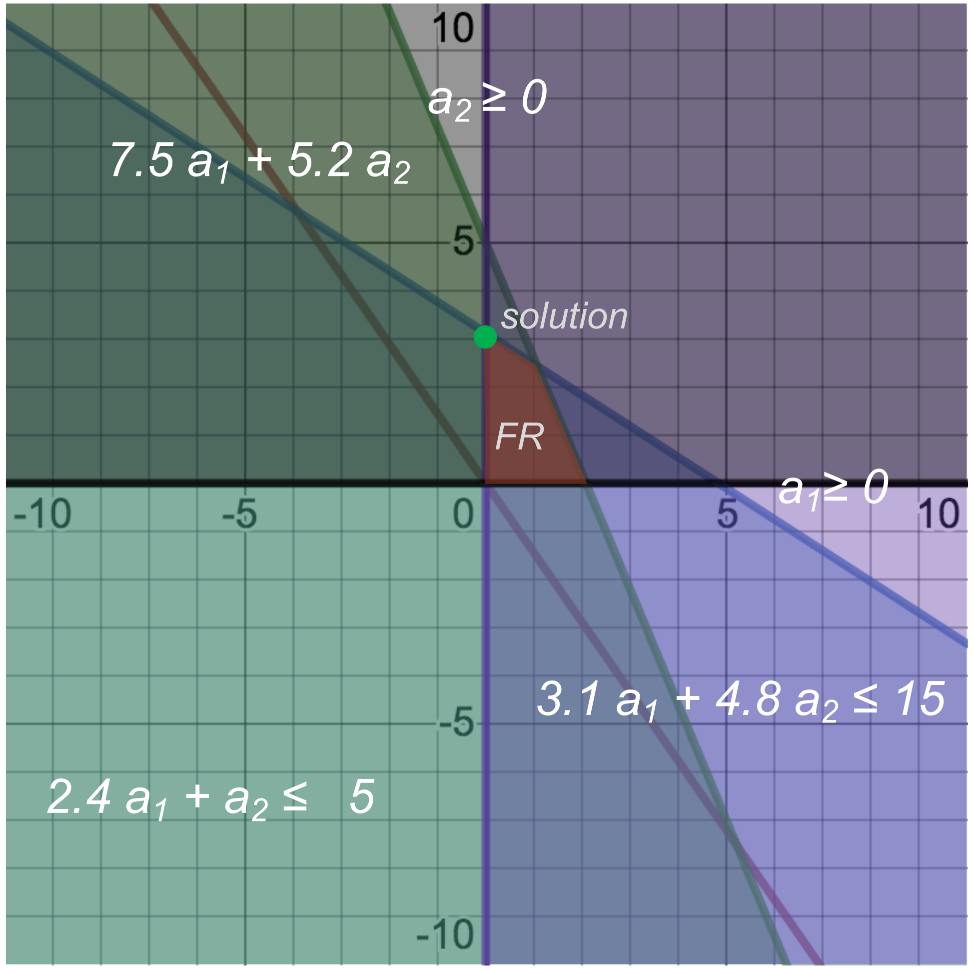
$2.4\,a_1 + a_2 \leq 5$

$a_1 \geq 0$

$a_2 \geq 0$

Solution: $a_1 = 0.00$, $a_2 = 3.12$

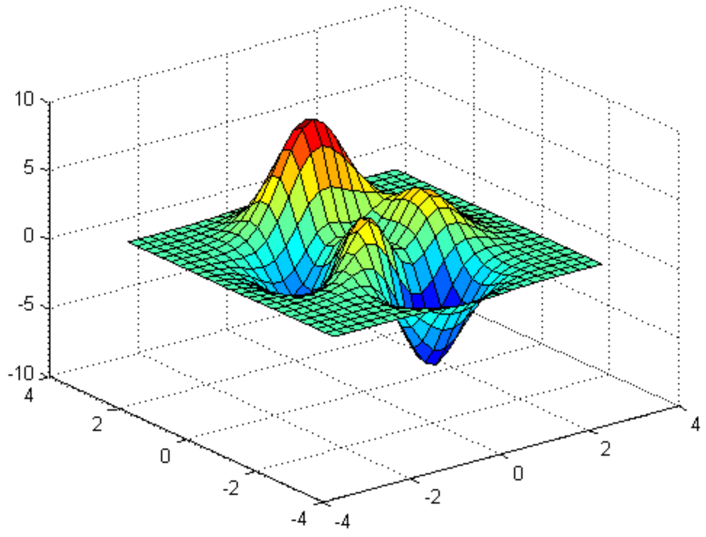
Speed can be maximized by 6.56 units!



Nonlinear Programming

- Nonlinear programming is the process of solving an optimization problem **where some of the constraints or the objective function are nonlinear**.

$$\begin{aligned} &\arg\min f(\mathbf{x}) \\ &\text{subject to: } g(\mathbf{x}) \leq 0 \\ &\qquad\qquad\quad h(\mathbf{x}) = 0 \end{aligned}$$



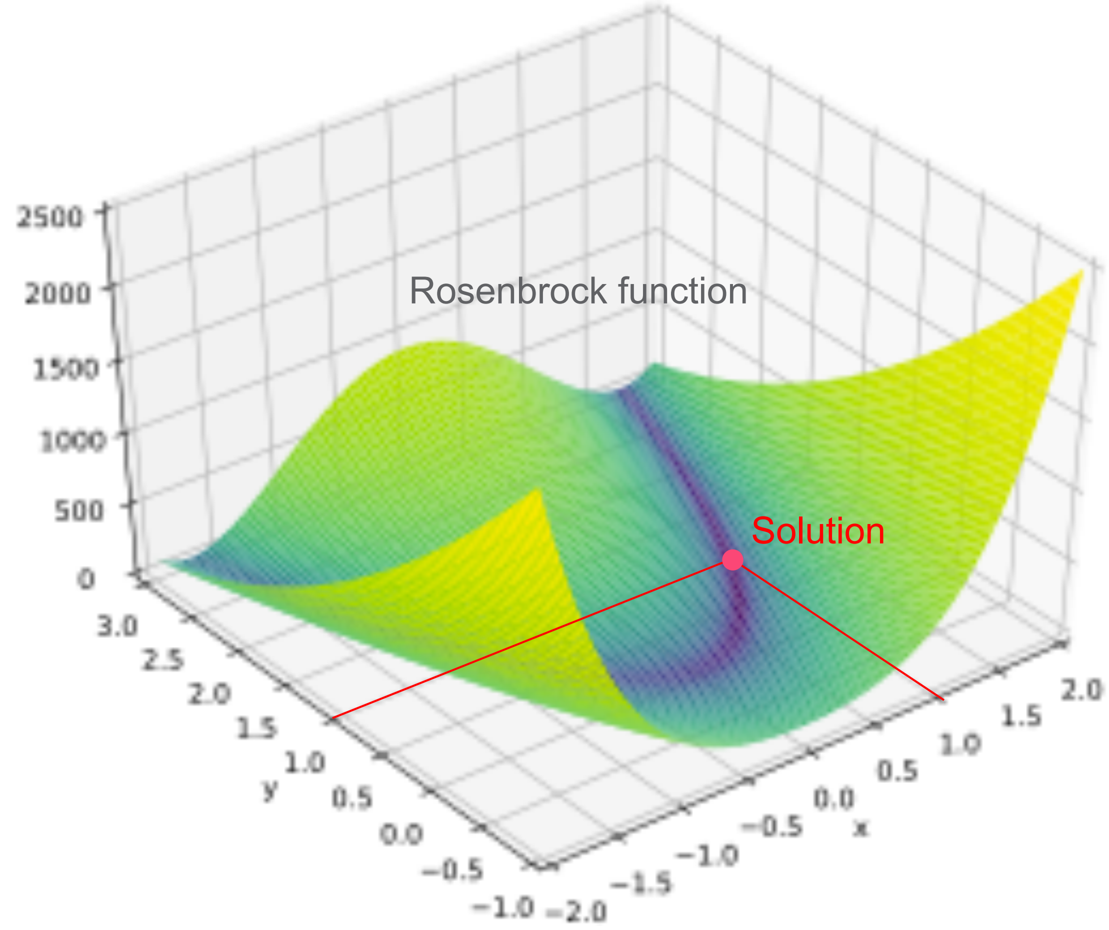
Use case 2: NLP Optimization Problem

- Let us consider the problem of minimizing the Rosenbrock function of variables:

$$\text{arg min} \sum_{i=2}^{N} 100\,(x_{i+1} - x_i^2)^2 + (1 - x_i)^2$$

- The Rosenbrock function is used as a **performance test problem for optimization algorithms**.

- The minimum value of this function is 0 which is achieved when $x_i = 1$.



Evolutionary Computing

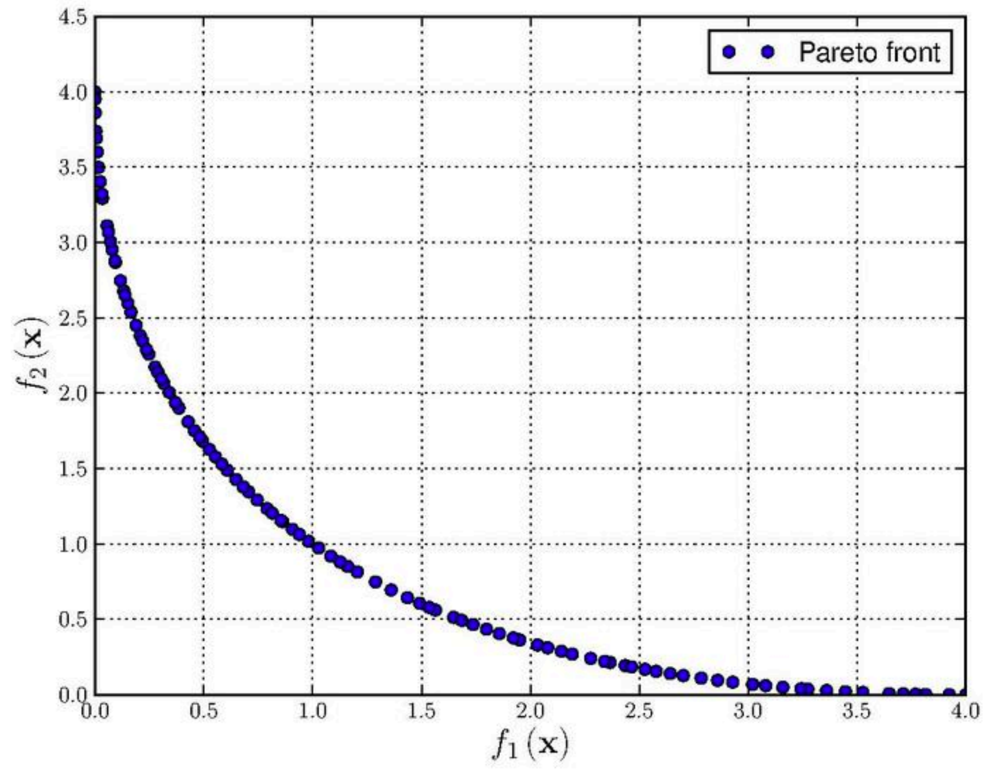
- Evolutionary computation is a family of algorithms for global optimization **inspired by biological evolution.**
  - Genetic Algorithms
    - Initialization: the population size and position is set within the FR.
    - Selection: a portion of the existing population is selected to breed a new generation
    - Genetic operators: i.e. crossover and mutation
    - Termination: if a solution satisfies a minimum criteria, the number of generations is reached, or the combinations of these two.

Use case 3: Evolutionary Computing

- Let us consider the problem of minimizing the Schaffer function:

$$\arg\min \begin{cases} f_1(x) = x^2 \\ f_2(x) = (x-2)^2 \end{cases}$$

- The Schaffer function is also used as a **performance test problem for optimization algorithms**.



Conclusion

- We discussed how to formulate and model optimization problems:
    - Convex and nonconvex
        - Linear
            - Single objective constrained
            - Multi-objective unconstrained
        - Nonlinear
            - Single objective unconstrained
- There are several Python optimization packages:
    - PuLP: A linear programming Python API
    - Scipy: A Python open-source software for mathematics
    - Platypus: A framework for evolutionary computing in Python
- The use of these packages depends on the nature of the problem at hand.

Links

- https://www.coin-or.org/PuLP
- https://docs.scipy.org/doc/scipy/reference/optimize.html
- https://platypus.readthedocs.io/en/latest/