AI505

Optimization

Course Introduction

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University of Southern Denmark

Outline

1. Course Organization

2. Introduction

Who is here?

42 in total registered in ItsLearning

- **AI505 (7.5 ECTS)**
  34 from Bachelor in AI

- **AI505 (7.5 ECTS) + IAAI501 (2.5 ECTS)**
  9 from Master in Mathematics and Economics

Prerequisites

- Calculus
- Linear Algebra
- Programming

Outline

Aims of the course

Learn about **optimization**:

- continuous multivariate optimization
- discrrete optimization

Optimization is an important tool in machine learning, decision making and in analyzing physical systems.
In mathematical terms, an optimization problem is the problem of finding the best solution from the set of all feasible solutions.

The first step in the optimization process is constructing an appropriate mathematical formulation.
The second is devising an algorithm for solving the mathematical formulation.

Contents of the Course (Pensum)

Unit	Main topic
1	Introduction, Univariate Problems
2	Multivariate Problems, Gradient-Based Methods
3	Derivative-Free Methods
4	Optimization for Machine Learning
5	Constrained Optimization, Linear Programming
6	Sampling Methods
7	Discrete Optimization and Heuristics

Practical Information

Teacher: Marco Chiarandini (imada.sdu.dk/u/marco/)
Instructor: Bonnie Liefting (H21)

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Schedule, alternative views:

- mitsdu.sdu.dk, SDU Mobile
- Official course description (læserplanen)
- ItsLearning
- https://ai-505.github.io

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Schedule (16 weeks):

- Introductory classes: 40 hours (20 classes)
- Training classes: 30 hours (15 classes)
- Scheduled: $16 \times 4 = 64$ hours
- No classes in week 8

Communication Means

- ItsLearning $\Leftrightarrow$ External Web Page
  (link `https://ai-505.github.io`)
- Announcements in ItsLearning
- Write to Marco (`marco@imada.sdu.dk`) or to instructor
- Collaborate with peers

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$\rightsquigarrow$ It is good to ask questions!!

$\rightsquigarrow$ Let me know if you think we should do things differently!

Sources — Reading Material

Main reference:

[KW] Mykel J. Kochenderfer, Tim A. Wheeler. Algorithms for Optimization 2019. The MIT Press.

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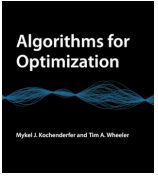
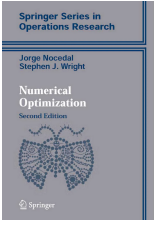


Others

[NW] J. Nocedal and S. J. Wright, Numerical Optimization, Second Edition. Springer Series in Operations Research, 2006



Course Material

External Web Page is the main reference for list of contents (ie[1], syllabus, pensum).

It will collect:

- slides
- list of topics and references
- exercises
- links
- tutorials for programming tasks

[1] ie = id est = that is, eg = exempli gratia = for example, wrt = with respect to, et al. = et alii = and others

Assessment

Portfolio consisting of:

- mandatory assignments in groups of 2:
  1. assignment
  2. assignment
  3. assignment
  4. assignment

  Time line to be announced.

- oral exam on June 11-13, 2025

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- oral exam on June 11-13, 2025

The oral examination consists of questions on the basis of the handed in assignments and can be extended to other parts of the course curriculum.

Final grade: starting from the grade of the assignments overall evaluation can move up or down by at most two levels.

(language: Danish and/or English)

Exercise Sessions (1/2)

For exercises in general:

- Both theoretical, modeling and programming tasks
- No mandatory hand-ins, voluntary participation, but all lectures and exercises are relevant for to exam
- Help each other! Teaching others is the best form of learning
- Bonnie will be there to help
- Exercises should help you to learn - don't hesitate to find a work setting or extend with other material that works better for you

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Exercises are group work

- Exercises best done in pairs of 2-3 people
- Try to gather in different groups every now and then

Exercise Sessions (1/2)

Notation: $^{+}$, *, ' '

- plus exercises are to be done before the class
- starred exercises are done in class
- unmarked exercises are for self study
- starred exercises are examples of asssignment questions

Coding

Set up your local Python programming environment and use the available tutorial to:

- Brush up some knowledge on Python-IDEs and Git
- Grasp some basics on jupyter notebooks
- Recap basics of data processing and visualisation

We will span several programming modes, functional, imperative, object oriented, small scripts large code bases, use pf modules and packages. We will use git.

Outline

Introduction

- Applications of Optimization
  - Physics
  - Business
  - Biology
  - Engineering
  - Machine Learning
  - Logistics and Scheduling
- Objectives to Optimize
  - Efficiency
  - Safety
  - Accuracy
- Constraints
  - Cost
  - Weight
  - Structural Integrity
- Challenges
  - High-Dimensional Search Spaces
  - Multiple Competing Objectives
  - Model Uncertainty

A Brief History

- Algebra, study of the rules for manipulating mathematical symbols

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- Artificial intelligence

Real World vs Model vs Representation vs Implementation

The Real World: That messy thing we are trying to study (with computers).

Model: Mathematical object in some class M.

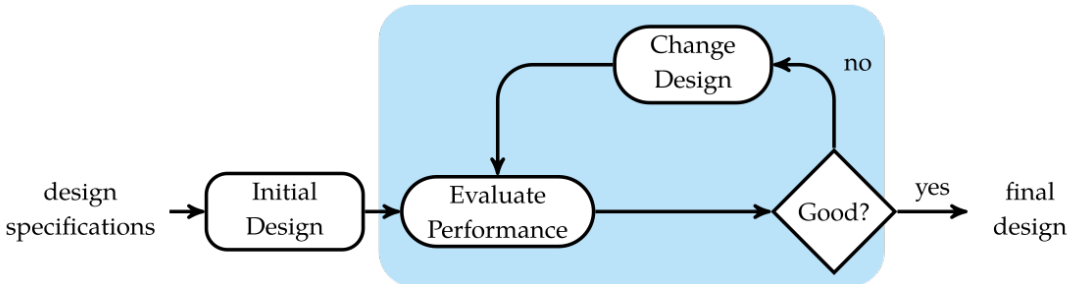
Representation: An object of an abstract data type R used to store the model.

Implementation: An object of a concrete type used to store the model.

Any object from the real world might have different models.
Any model might have several representations (exact).
And representation might have different implementations (exact).

We will focus on the algorithmic aspects of optimization that arise after the problem has been properly formulated

Optimization Process



An optimization algorithm is used to incrementally improve the design until it can no longer be improved or until the budgeted time or cost has been reached.

Search the space of possible designs with the aim of finding the best one.
Depending on the application, this search may involve:

- evaluating an analytical expression (white or glass box)
- running physical experiments, such as wind tunnel tests (black box)
- running computer simulations

Modern optimization techniques can be applied to problems with millions of variables and constraints.

Basic Optimization Problem

$$\begin{aligned} &\underset{\boldsymbol{x}}{\text{minimize}} && f(\boldsymbol{x}) \\ &\text{subject to} && \boldsymbol{x} \in \mathcal{X} \end{aligned}$$

- Design Point
- Design Variables
- Objective Function
- Feasible Set
- Minimizer

Any value of $\boldsymbol{x}$ from among all points in the feasible set $\mathcal{X}$ that minimizes the objective function is called a solution or minimizer. A particular solution is written $\boldsymbol{x}^*$.

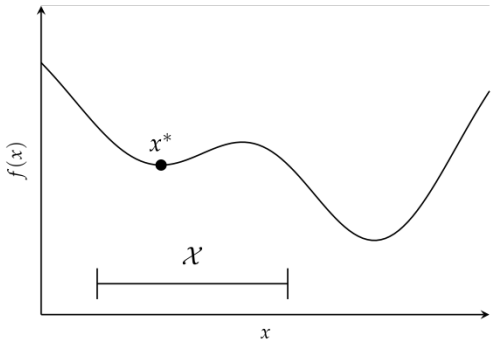
$$\boldsymbol{x}^* = \operatorname{argmin} f(\boldsymbol{x}) \text{ subject to } \boldsymbol{x} \in \mathcal{X}$$

There is only one minumum but there can be many minimizers

maximize $\boldsymbol{x}$ $f(\boldsymbol{x})$ subject to $\boldsymbol{x} \in \mathcal{X} \equiv$ minimize $\boldsymbol{x}$ $-f(\boldsymbol{x})$ subject to $\boldsymbol{x} \in \mathcal{X}$

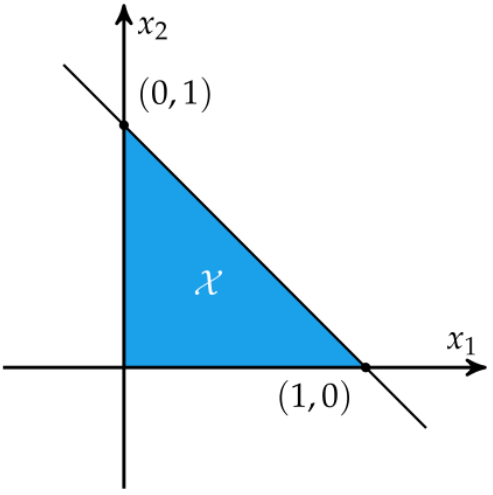
Basic Optimization Problem

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & f(x) \\ \text{subject to} \quad & x \in \mathcal{X} \end{aligned}$$



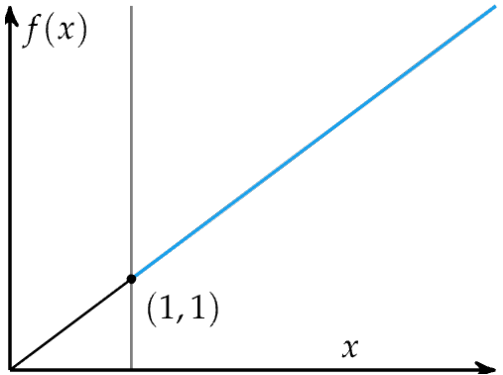
Constraints

$$\begin{aligned} \underset{x_1, x_2}{\text{minimize}} \quad & f(x_1, x_2) \\ \text{subject to} \quad & x_1 \geq 0 \\ & x_2 \geq 0 \\ & x1_+x_2 \leq 1 \end{aligned}$$



Constraints

$$\begin{aligned} &\underset{x}{\text{minimize}} && f(x) \\ &\text{subject to} && x > 1 \end{aligned}$$



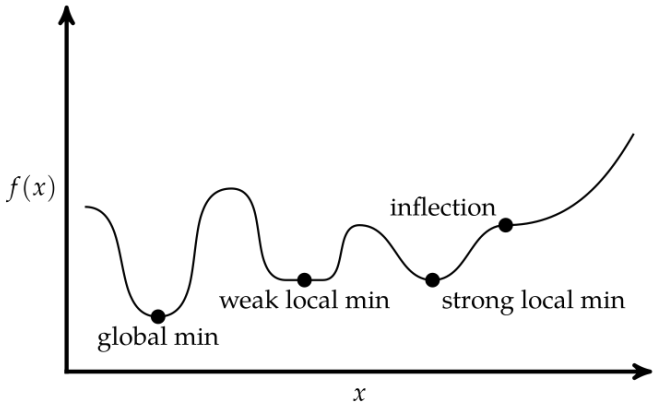
$x = 1$ would not be feasible.
$x = 1$ would be the solutions to

$$\underset{x}{\text{infimum}}\ f(x) \text{ subject to } x > 1$$

infimum of a subset $\mathcal{X}$ of a partially ordered set $\mathcal{P}$ is the greatest element in P that is less than or equal to each element of $\mathcal{X}$, if such an element exists. Aka, greatest lower bound.

Critical Points

Univariate function
global vs local minimum
Def. A point x^* is at a local minimum (or is a local minimizer) if there exists a $\delta > 0$ such that $f(x^*) \leq f(x)$ for all x with $\|x - x^*\| < \delta$.

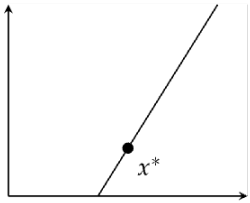


Conditions for Local Minima

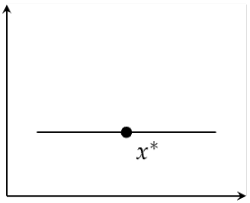
Univariate objective functions, assuming they are differentiable (Derivatives exist), without constraints

Local minimum: Necessary condition but not sufficient condition:

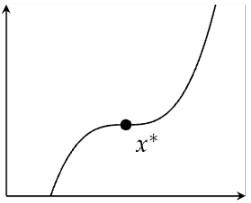
1. $f'(x^*) = 0$, the first-order necessary condition (FONC)
2. $f''(x^*) \geq 0$, the second-order necessary condition (SONC)



SONC but not FONC



FONC and SONC



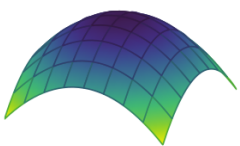
FONC and SONC

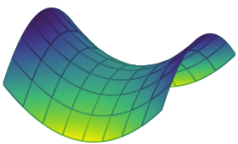
Conditions for Local Minima

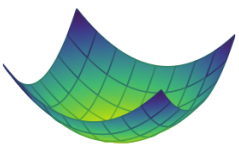
Multivariate objective functions, assuming they are differentiable (gradients and Hessians exist), without constraints

Local minimum: Necessary condition but not sufficient condition:

1. $\nabla f(x^*) = 0$, the first-order necessary condition (FONC)
2. $\nabla^2 f(x^*) \geq 0$, the second-order necessary condition (SONC)



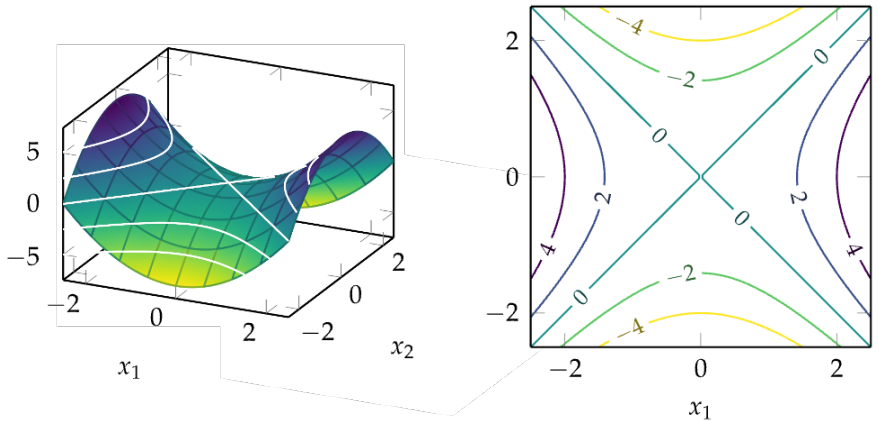




Contour Plots

$$f(x_1, x_2) = x_1^2 - x_2^2$$

can be rendered in a 3D space but convenient to represent it also in 2D showing the lines of constant output value



Taylor Expansion

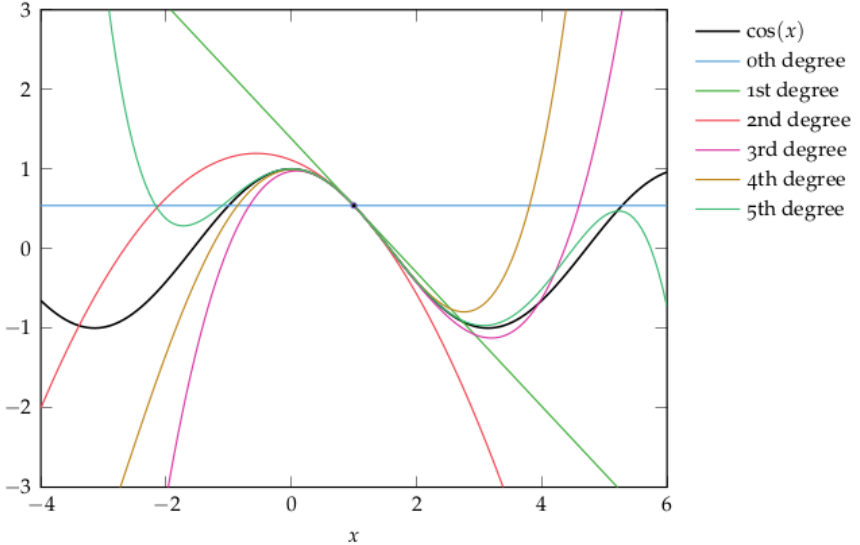
From the *first fundamental theorem of calculus*,[2] we know that

$$f(x+h) = f(x) + \int_0^h f'(x+a)\,da$$

Nesting this definition produces the Taylor expansion of f about x:

$$\begin{aligned}
f(x+h) &= f(x) + \int_0^h \left(f'(x) + \int_0^a f''(x+b)\,db \right) da \\
&= f(x) + f'(x)h + \int_0^h \int_0^a f''(x+b)\,db\,da \\
&= f(x) + f'(x)h + \int_0^h \int_0^a \left(f''(x) + \int_0^b f'''(x+c)\,dc \right) db\,da \\
&= f(x) + f'(x)h + \frac{f''(x)}{2!}h^2 + \int_0^h \int_0^a \int_0^b f'''(x+c)\,dc\,db\,da \\
&\;\;\vdots \\
&= f(x) + \frac{f'(x)}{1!}h + \frac{f''(x)}{2!}h^2 + \frac{f'''(x)}{3!}h^3 + \dots \\
&= \sum_{n=0}^{\infty} \frac{f^{(n)}(x)}{n!}h^n
\end{aligned}$$

Taylor Expansion



Example: Rosenbrock function

$$f(x, y) = (a - x)^2 + b(y - x^2)^2$$

It has a global minimum at $(x, y) = (a, a^2)$, where $f(x, y) = 0$. Usually, these parameters are set such that $a = 1$ and $b = 100$. Only in the trivial case where $a = 0$ the function is symmetric and the minimum is at the origin.

Multivariate generalization
sum of $N/2$ uncoupled 2D Rosenbrock problems, and defined only for even N:

$$f(\mathrm{x}) = f(x_1, x_2, \ldots, x_N) = \sum_{i=1}^{N/2} \left[100(x_{2i-1}^2 - x_{2i})^2 + (x_{2i-1} - 1)^2\right] .[3]$$

This variant has predictably simple solutions.

Example: Rosenbrock function

Consider the Rosenbrock banana function,

$$f(\mathbf{x}) = (1 - x_1)^2 + 5(x_2 - x_1^2)^2$$

Does the point $(1, 1)$ satisfy the FONC and SONC?

The gradient is:

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2\left(10x_1^3 - 10x_1x_2 + x_1 - 1\right) \\ 10(x_2 - x_1^2) \end{bmatrix}$$

and the Hessian is:

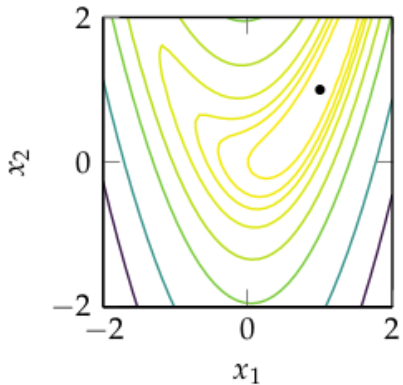
$$\nabla^2 f(\mathbf{x}) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2 \partial x_2} \end{bmatrix} = \begin{bmatrix} -20(x_2 - x_1^2) + 40x_1^2 + 2 & -20x_1 \\ -20x_1 & 10 \end{bmatrix}$$

We compute $\nabla(f)([1, 1]) = 0$, so the FONC is satisfied. The Hessian at $[1, 1]$ is:

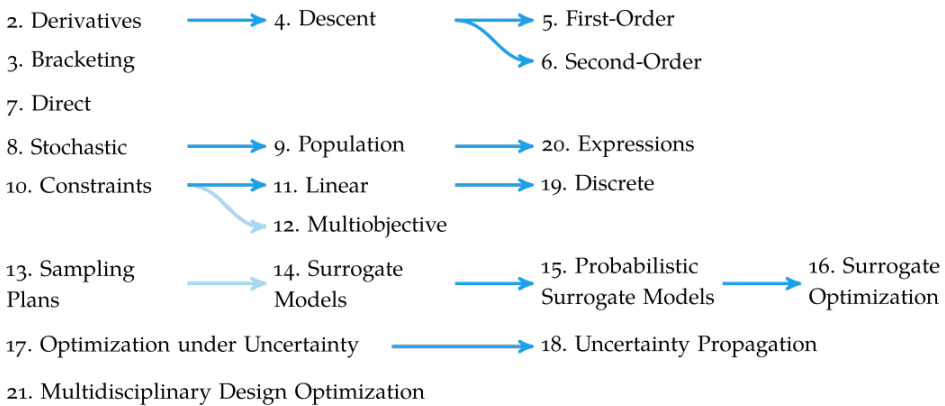
$$\begin{bmatrix} 42 & -20 \\ -20 & 10 \end{bmatrix}$$

which is positive definite, so the SONC is satisfied.

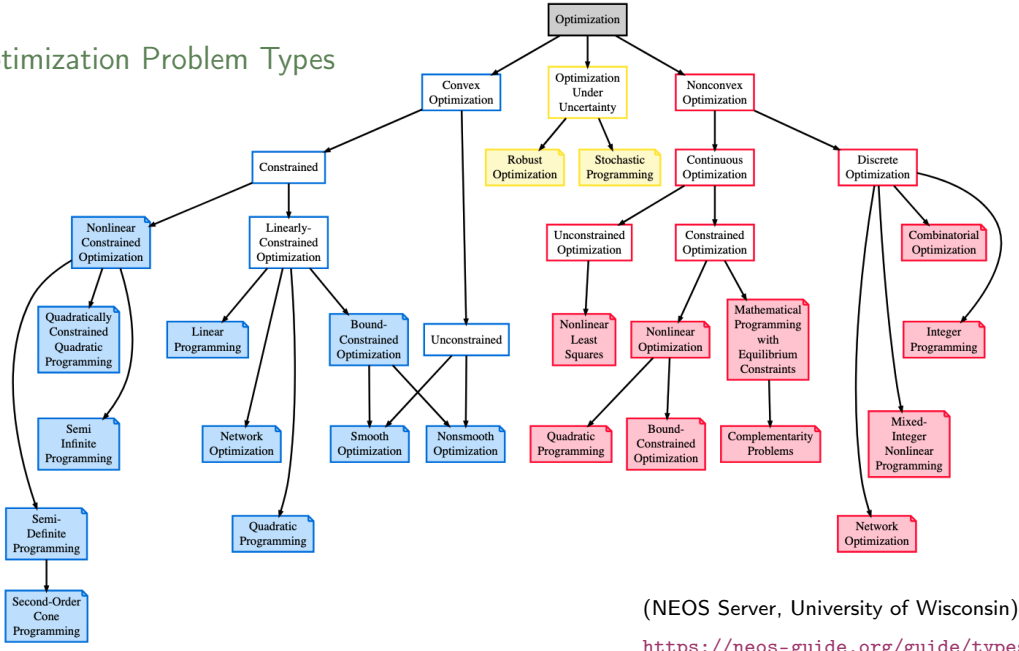
Example: Rosenbrock function



Overview


2. Derivatives
3. Bracketing
4. Descent
5. First-Order
6. Second-Order
7. Direct
8. Stochastic
9. Population
20. Expressions
10. Constraints
11. Linear
19. Discrete
12. Multiobjective
13. Sampling Plans
14. Surrogate Models
15. Probabilistic Surrogate Models
16. Surrogate Optimization
17. Optimization under Uncertainty
18. Uncertainty Propagation
21. Multidisciplinary Design Optimization

Optimization Problem Types



(NEOS Server, University of Wisconsin)

https://neos-guide.org/guide/types/

Application Example

In robotics, an autonomous agent (e.g., a drone, robotic arm, or self-driving car) needs to determine an optimal path from a starting position to a target while satisfying constraints such as avoiding obstacles, minimizing energy consumption, or optimizing smoothness.

Application Example

In robotics, an autonomous agent (e.g., a drone, robotic arm, or self-driving car) needs to determine an optimal path from a starting position to a target while satisfying constraints such as avoiding obstacles, minimizing energy consumption, or optimizing smoothness.
Formulating the Optimization Problem
The goal is to find a smooth trajectory $x(t)$ that minimizes a cost function:

$$J = \int_{t_0}^{t^f} C(x(t), u(t))dt$$

$x(t)$ is the state (e.g., position, velocity), $u(t)$ is the control input (e.g., force, acceleration), $C(x, u)$ is the cost function, which could represent energy usage, time, or distance.
Constraints:

- Dynamic Constraints: Governed by the system's physics (e.g., Newton's laws for a robot arm or quadcopter): x'=f(x,u)
- Obstacle Avoidance: Ensures that the trajectory does not collide with obstacles: $g(x(t)) \geq 0, \forall t$
- Boundary Conditions: The system must start and end at given positions with certain velocities.

Summary

- Optimization is the process of finding the best system design subject to a set of constraints
- Optimization is concerned with finding global minima of a function
- Minima can occur where the gradient is zero, but zero-gradient does not imply optimality