Optimization with Constraint Learning LAB

Part I

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University of Amsterdam

February 8, 2023

Agenda

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- Introduction to mathematical optimization
- Introduction to Constraint Learning
- Chemotherapy case study
- Embedding Decision trees
- Embedding Neural networks
- Trust region constraints
- Hands-on tutorial

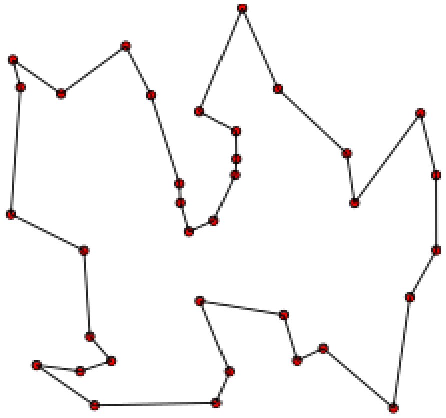
Mathematical Optimization

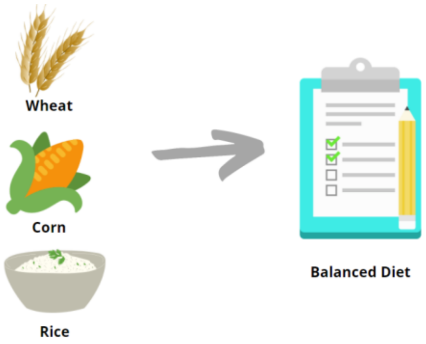
An optimization problem seeks to find the best (smallest or largest) value of a quantity given certain limits to the problem.

It can be expressed as a **minimization** (or maximization) of a quantity subject to a set of **constraints**.

Some examples:

- Travelling salesperson problem: minimize distance s.t. each city visited exactly once
- Diet problem: minimize cost s.t. nutrient requirements
- knapsack problem: maximize the value of objects in the knapsack s.t. capacity constraints





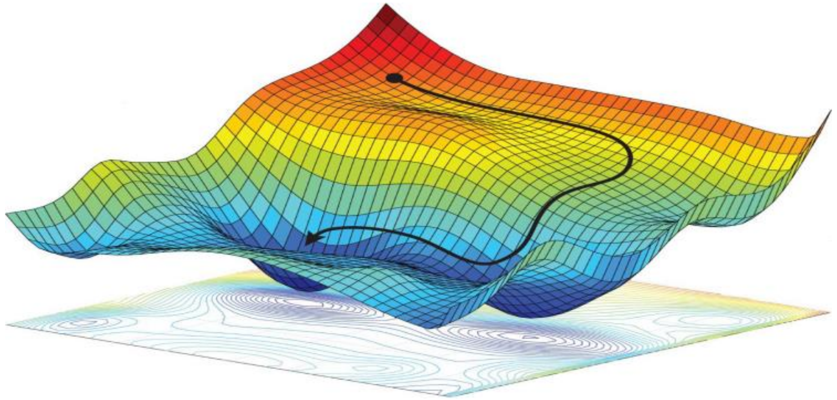
Mathematical Optimization

The general form of an optimization model is:

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} \; f(x_1,\dots,x_n) \rightarrow \textit{Objective function}$$

$$subject\ to \;\; g_i(x_1,\dots,x_n) \le 0,\; i=1,\dots,m \rightarrow \textit{Constraints}$$

where $x_1,\dots,x_n$ are the decision variables and the goal is to find a value for each of them such that the constraints are satisfied and the objective value is minimized.



Mathematical Optimization

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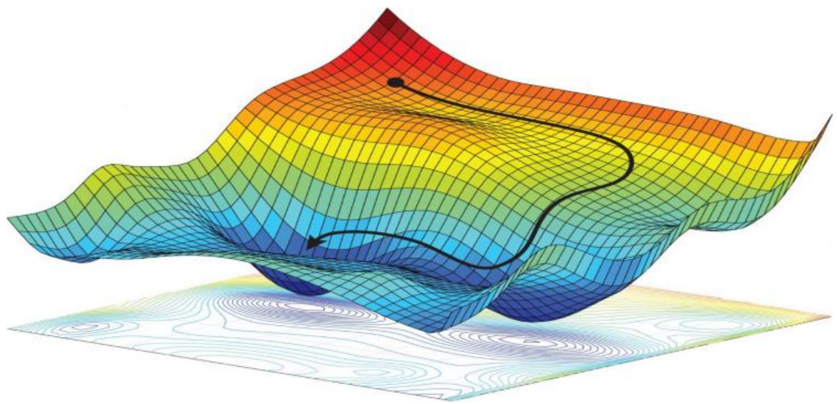

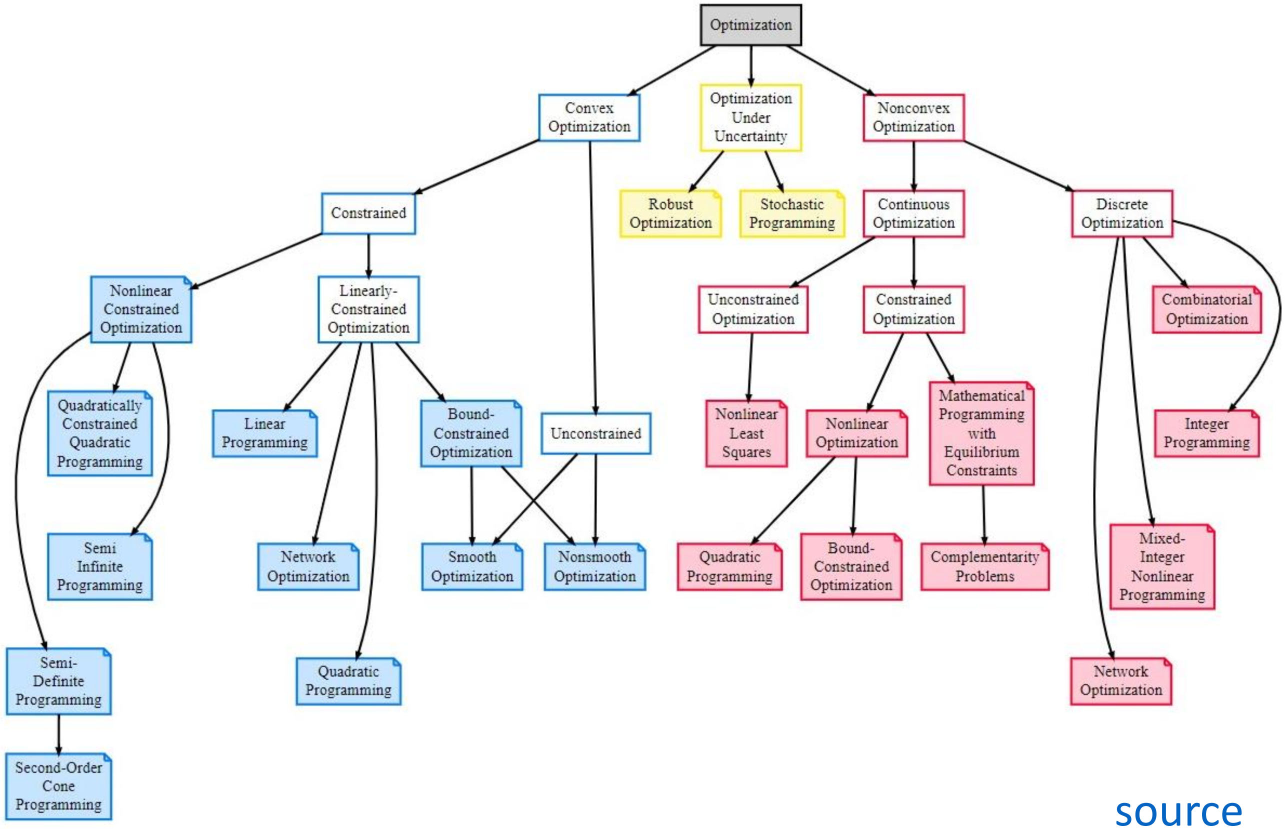

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Constraint Learning

Mixed-Integer Optimization (MIO)

Powerful tool that allows us to optimize a given objective subject to various constraints.

Many real-life optimization problems contain one or more constraints or objectives for which **there are no explicit formulae.**

Constraint Learning

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Machine Learning (ML)

Data is available and machine learning models can be used to **learn the constraints.**

Constraint Learning

$\boldsymbol{x}$ Decision variables

$\boldsymbol{w}$ Contextual variables

$\boldsymbol{y}$ Predicted outcomes

Constraint Learning

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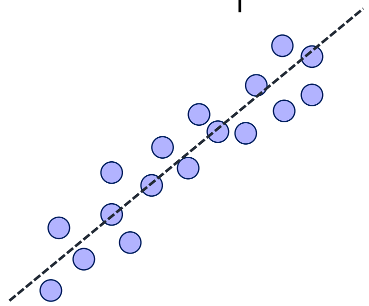
$$\boldsymbol{y} = \hat{\boldsymbol{h}}_{\mathcal{D}}(\boldsymbol{x}, \boldsymbol{w})$$

$$D = \{(\overline{\boldsymbol{x}}_i, \overline{\boldsymbol{w}}_i, \overline{\boldsymbol{y}}_{\boldsymbol{i}})\}_{i=1}^{N} \longrightarrow$$



Constraint Learning

$$\min_{\boldsymbol{x}\in\mathbb{R}^n,\boldsymbol{y}\in\mathbb{R}^k} \quad f(\boldsymbol{x},\boldsymbol{w},\boldsymbol{y})$$

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$$\text{s.t.} \quad \boldsymbol{g}(\boldsymbol{x},\boldsymbol{w},\boldsymbol{y}) \leq \boldsymbol{0}$$

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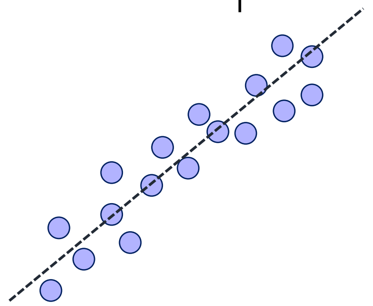

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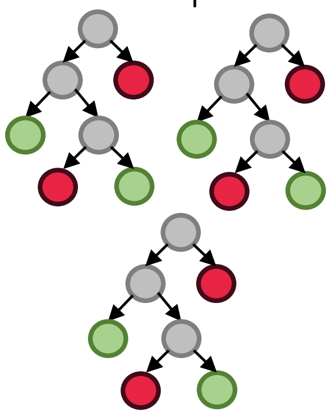

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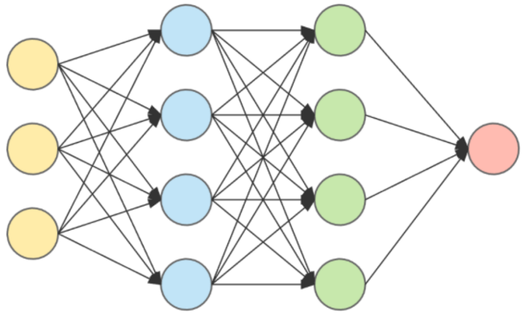

Chemotherapy Case Study

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In this case study, we extend the work of [Bertsimas et al. (2016)]* in the design of chemotherapy regimens for advanced gastric cancer. Given a new study cohort and study characteristics, we would like to optimize a chemotherapy regimen to **maximize the cohort's survival subject to constraint on different types of toxicity**.

$$\boldsymbol{x}_b^d = \mathbb{I}(\text{drug } d \text{ is administered}),$$
$$\boldsymbol{x}_a^d = \text{average daily dose of drug } d,$$
$$\boldsymbol{x}_i^d = \text{maximum instantaneous dose of drug } d.$$

$$\begin{aligned}
\min_{\boldsymbol{x},\boldsymbol{y}} \quad & y_{OS} \\
\text{s.t.}\; & y_i \le \tau_i, && i \in \mathcal{Y}_C, \\
& y_i = \hat{h}_i(\boldsymbol{x}, \boldsymbol{w}), && i \in \mathcal{Y}_C, \\
& y_{OS} = \hat{h}_{OS}(\boldsymbol{x}, \boldsymbol{w}), \\
& \sum_d \boldsymbol{x}_b^d \le 3, \\
& \boldsymbol{x}_b \in \{0,1\}^d, \\
& \boldsymbol{x} \in \mathcal{X}(\boldsymbol{w}).
\end{aligned}$$

(*) Bertsimas D, O'Hair A, Relyea S, Silberholz J (2016) An analytics approach to designing combination chemotherapy regimens for cancer. Management Science 62(5):1511–1531, ISSN 15265501

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Cohort contextual variables

- Gender
- Age
- primary site breakdown
- ecog score
- …

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Toxicities

- Grade 3/4 constitutional
- Infection
- Neurological
- Grade 4 blood
- …

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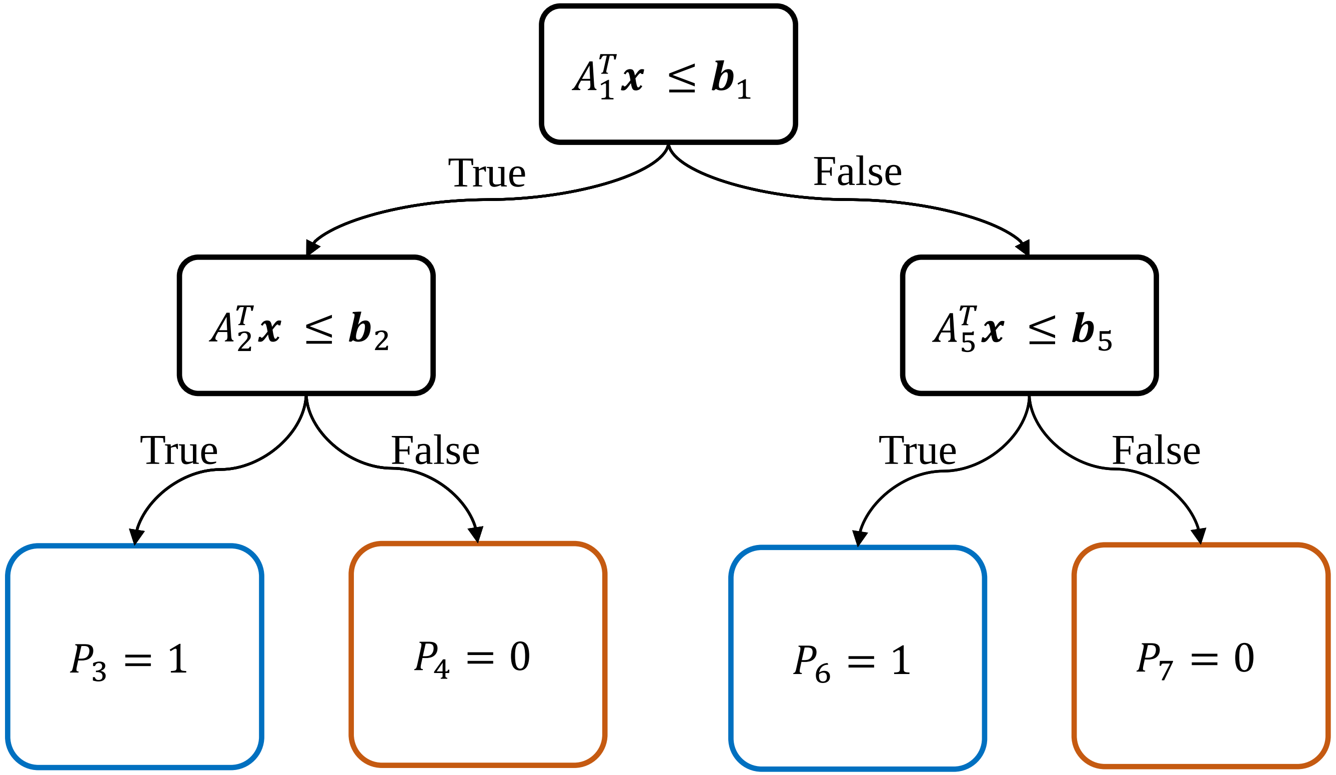
Embedding Decision Trees



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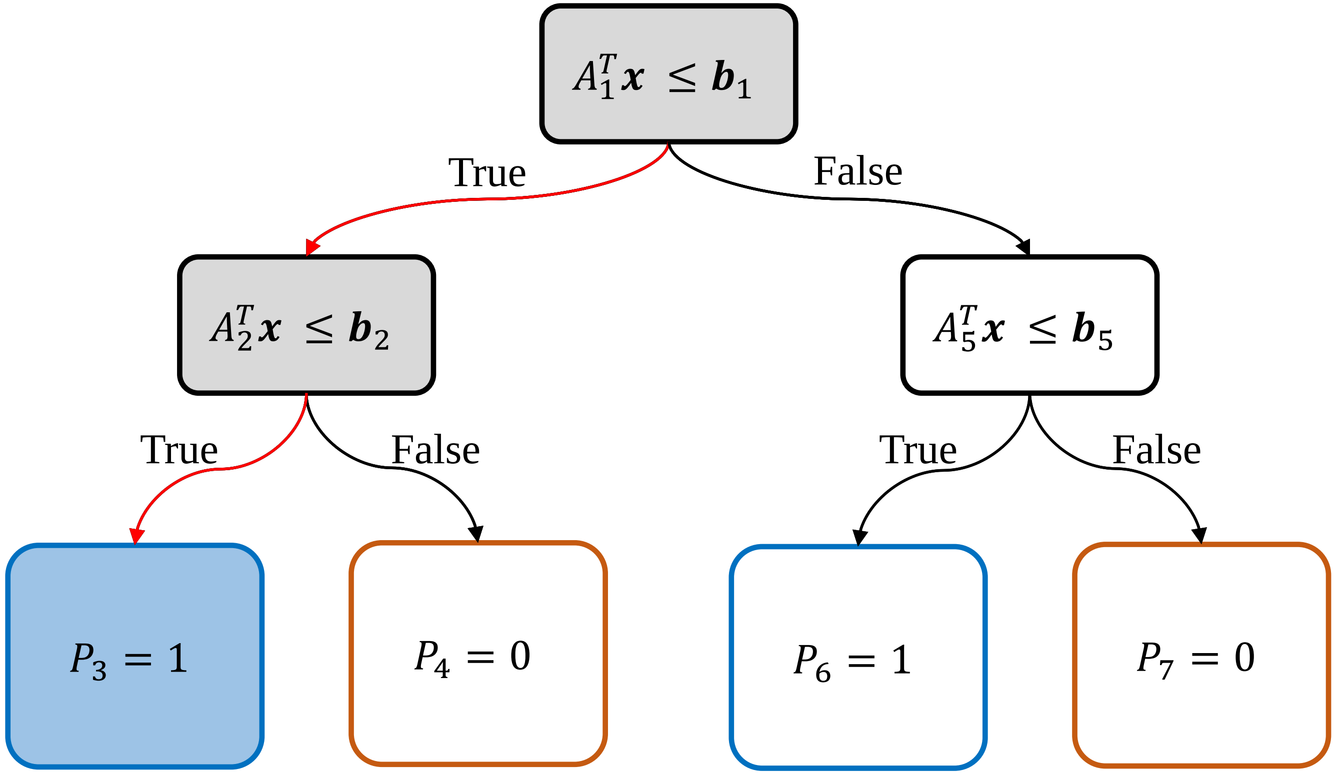


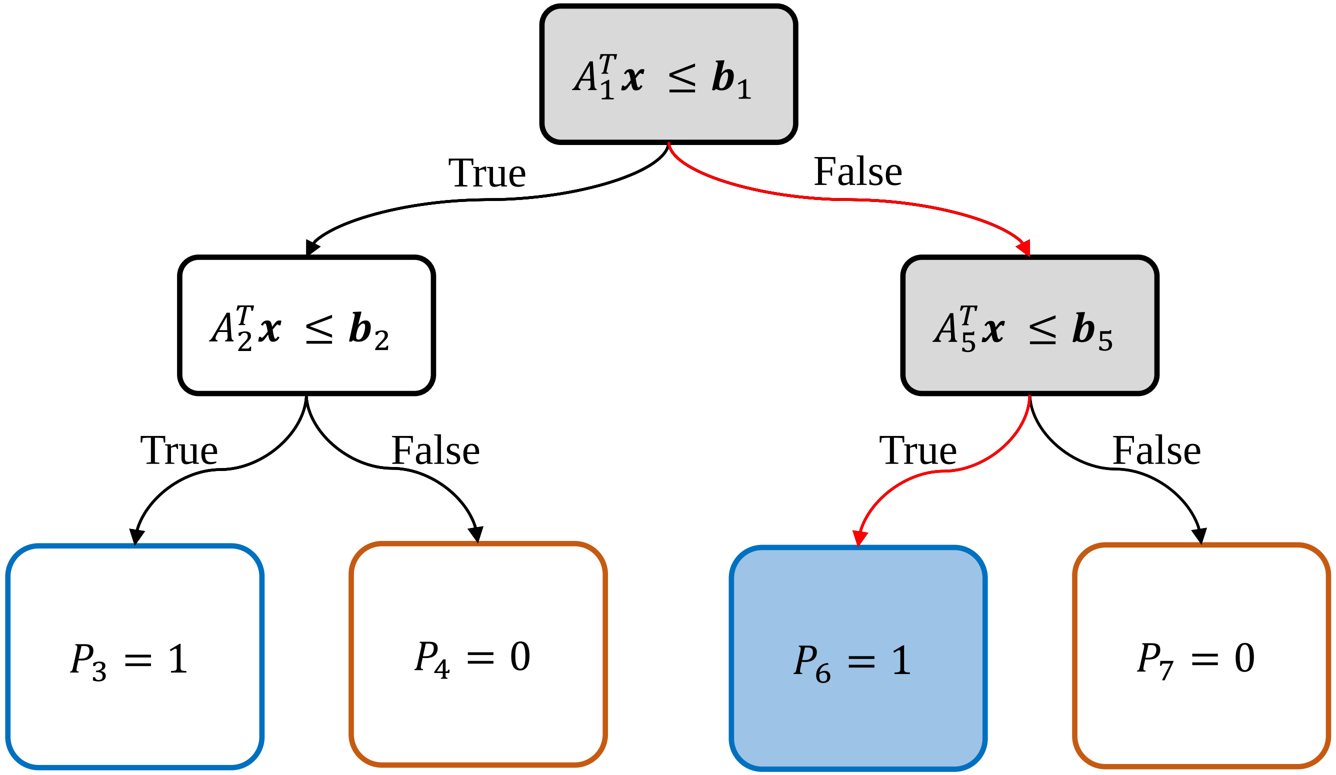
Conceptual model

$$\begin{aligned} \min_{\boldsymbol{x}} \quad & f(\boldsymbol{x}) \\ s.t. \quad & \boldsymbol{g}(\boldsymbol{x}) \le \boldsymbol{0} \end{aligned}$$

P_3

$$A_1^T \boldsymbol{x} \le \boldsymbol{b}_1$$
$$A_2^T \boldsymbol{x} \le \boldsymbol{b}_2$$

Embedding Decision Trees



Conceptual model

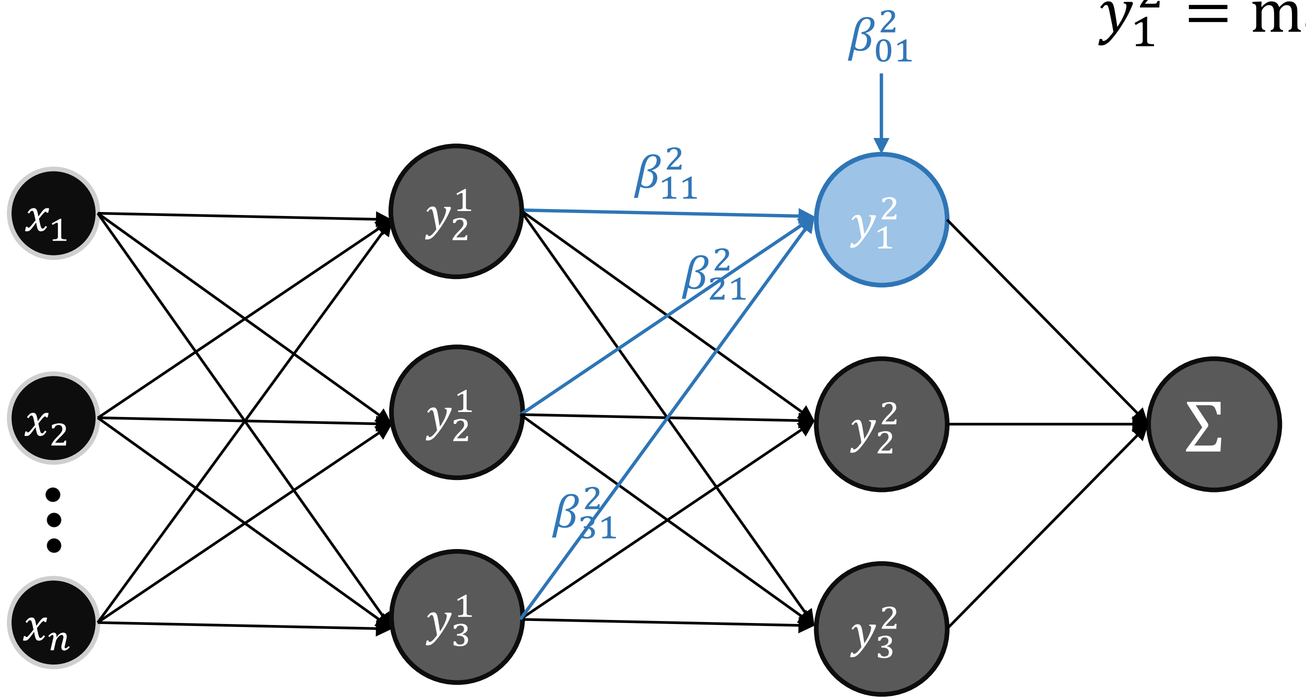
$$\left\{\begin{array}{ll} \min\limits_{\boldsymbol{x}} & f(\boldsymbol{x}) \\ s.t. & \boldsymbol{g}(\boldsymbol{x}) \le \boldsymbol{0} \end{array}\right.$$

P_6
$$A_1^T\boldsymbol{x} \ge \boldsymbol{b}_1$$
$$A_5^T\boldsymbol{x} \le \boldsymbol{b}_5$$

Embedding Neural Networks

ReLU activation function

$$y_1^2 = \max\left\{0, \beta_{01}^2 + \boldsymbol{\beta}_1^{2^T} \boldsymbol{y}^1\right\}$$



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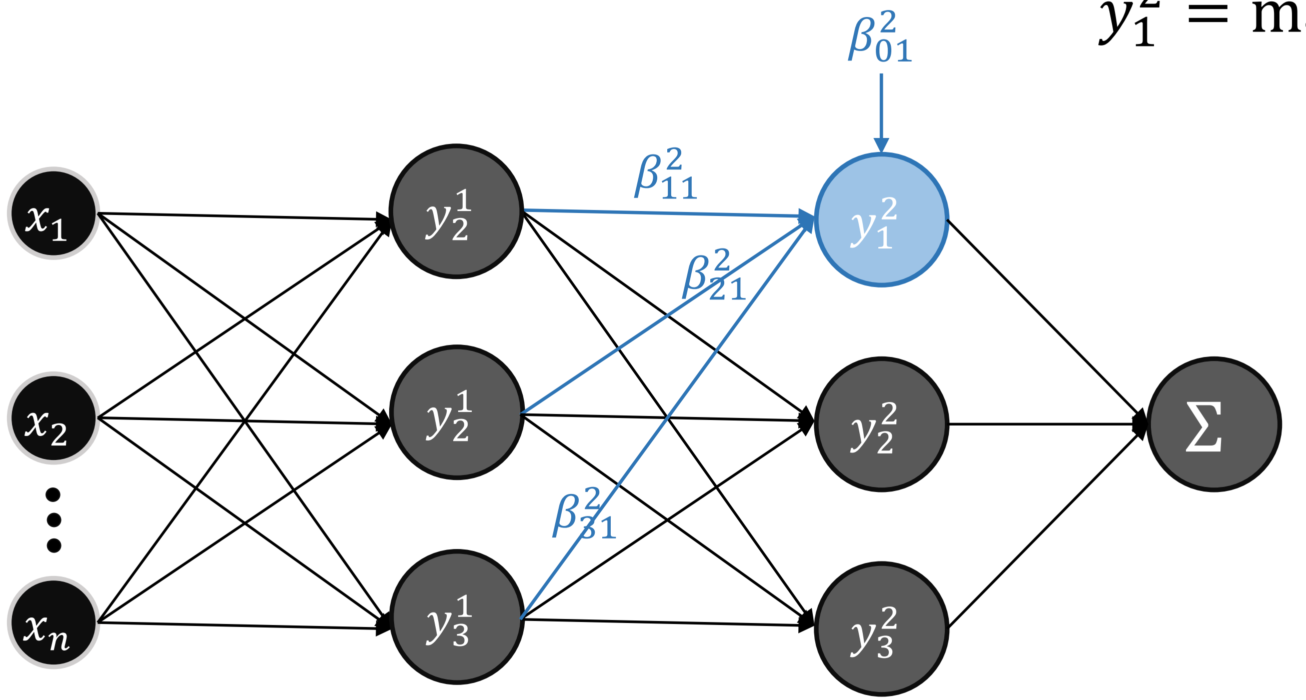

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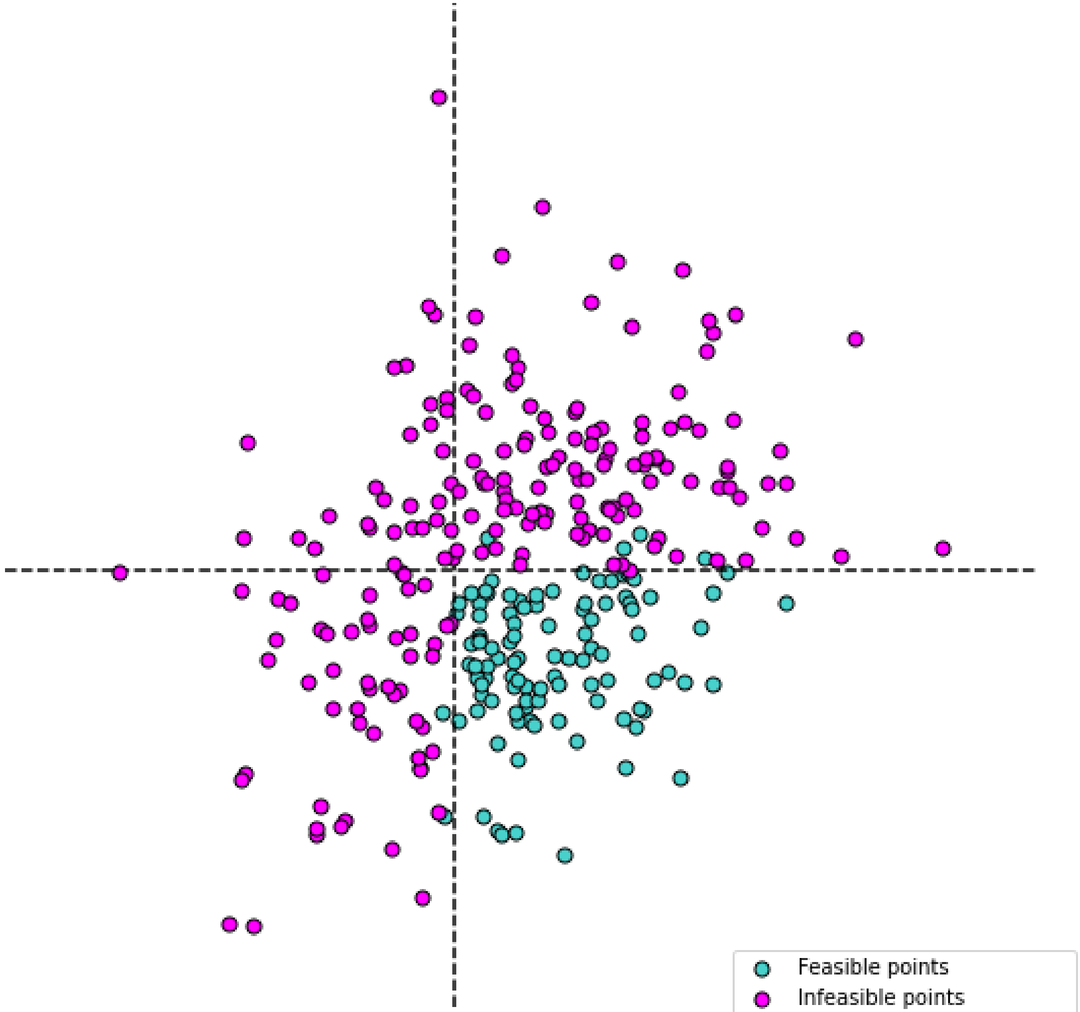
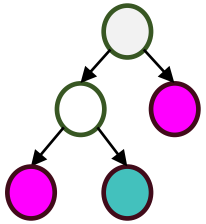
$y = \max\{0, x\}$ can also be written as:

$$\begin{cases} y \geq x, \\ y \leq x - M_L(1 - z), \\ y \leq M_U z, \\ y \geq 0, \\ z \in \{0, 1\}, \end{cases}$$

where $M_L < 0$ is a lower bound on all possible values of x, and $M_U > 0$ is an upper bound.

Trust region constraints





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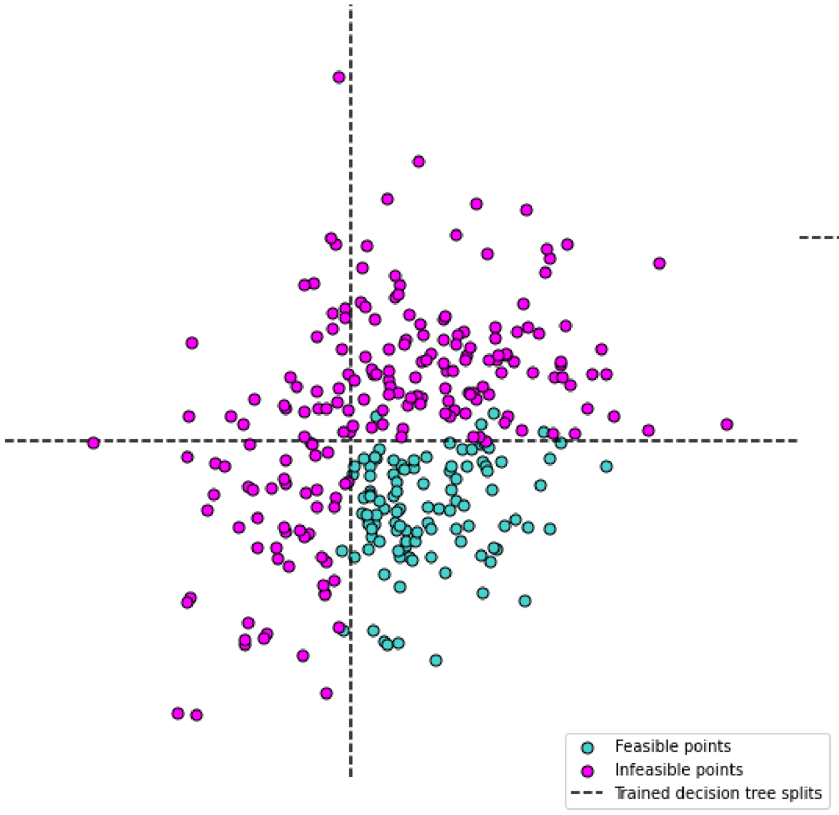

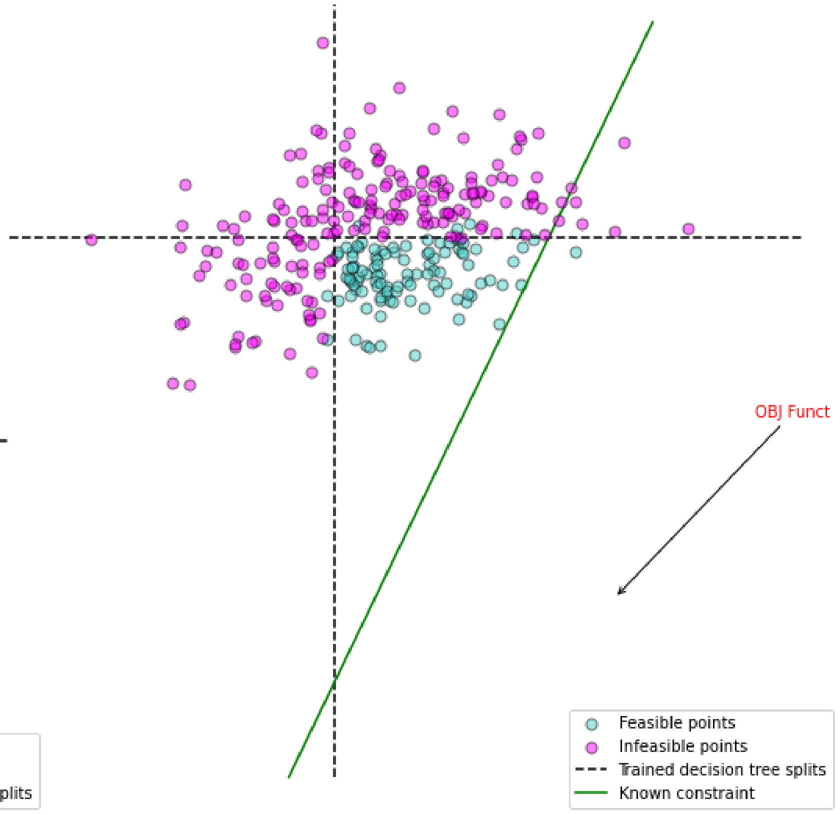

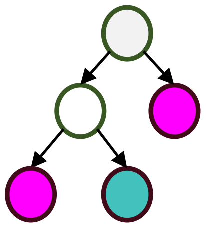

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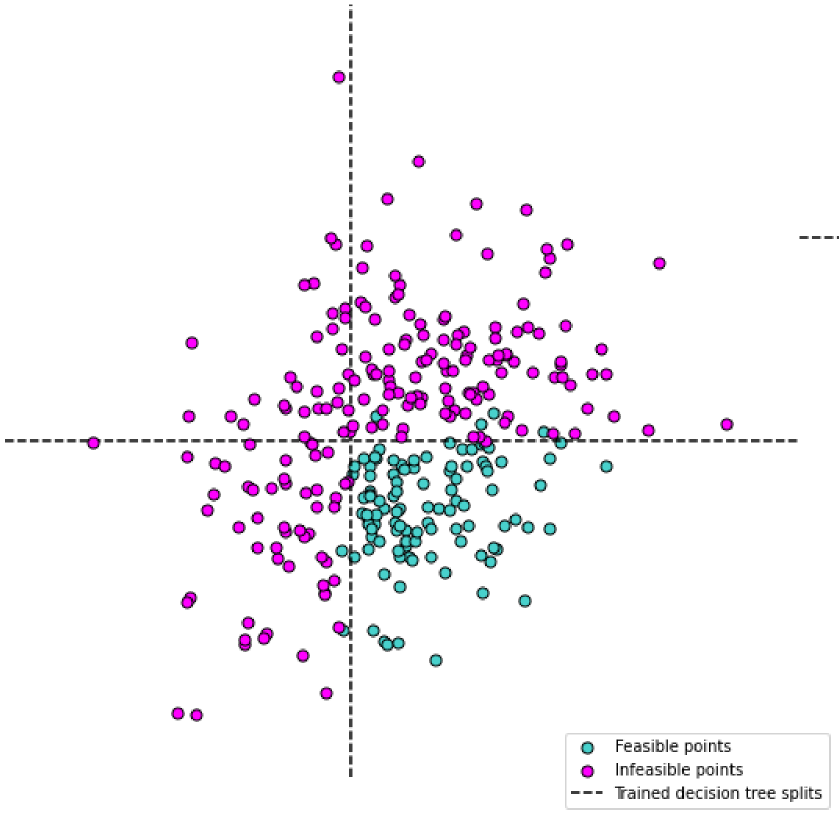

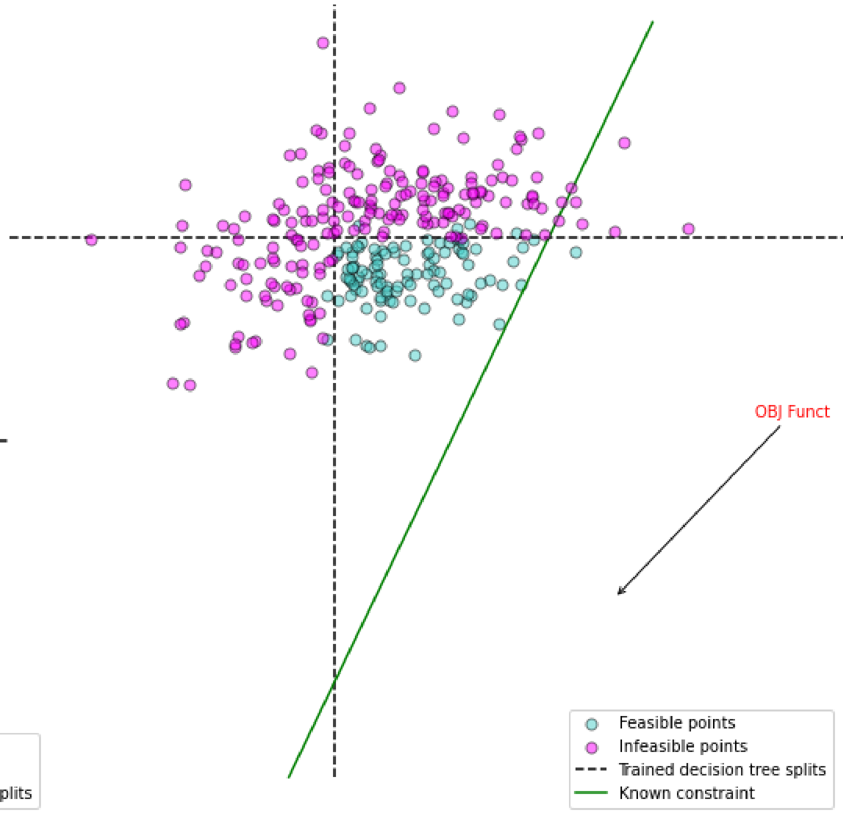

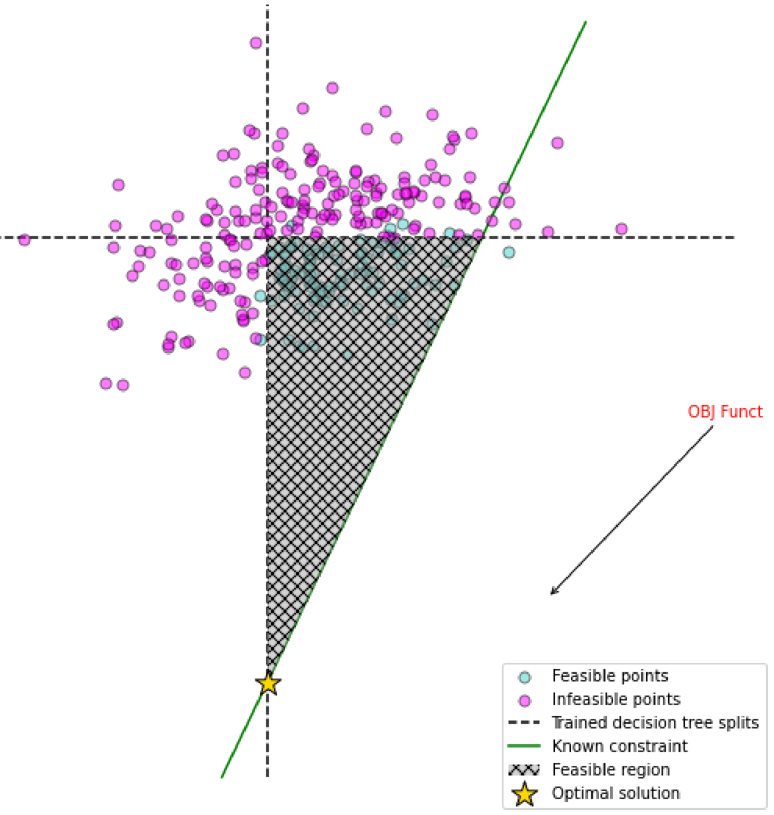

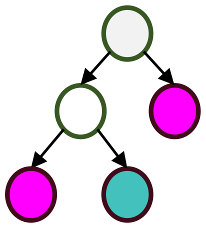

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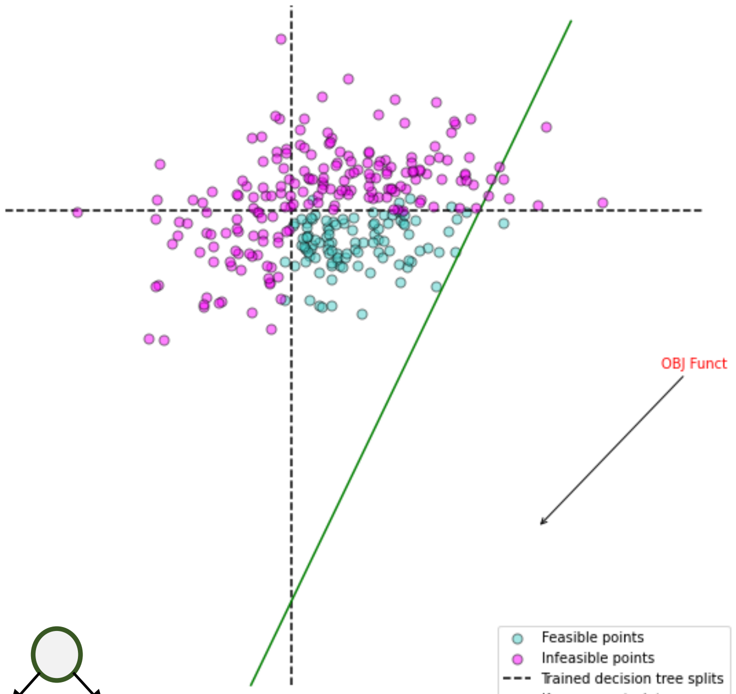

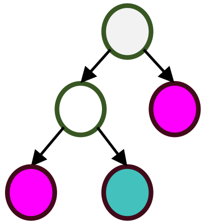

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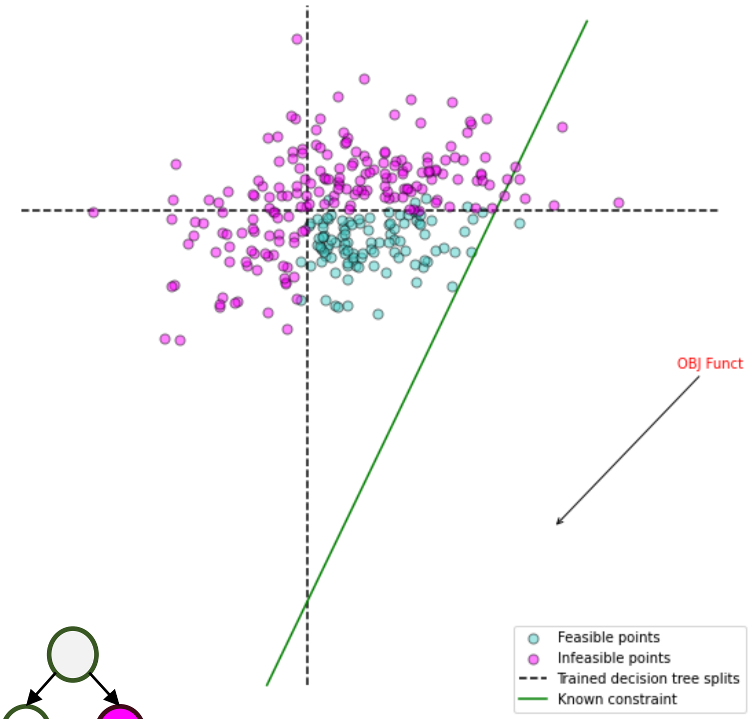
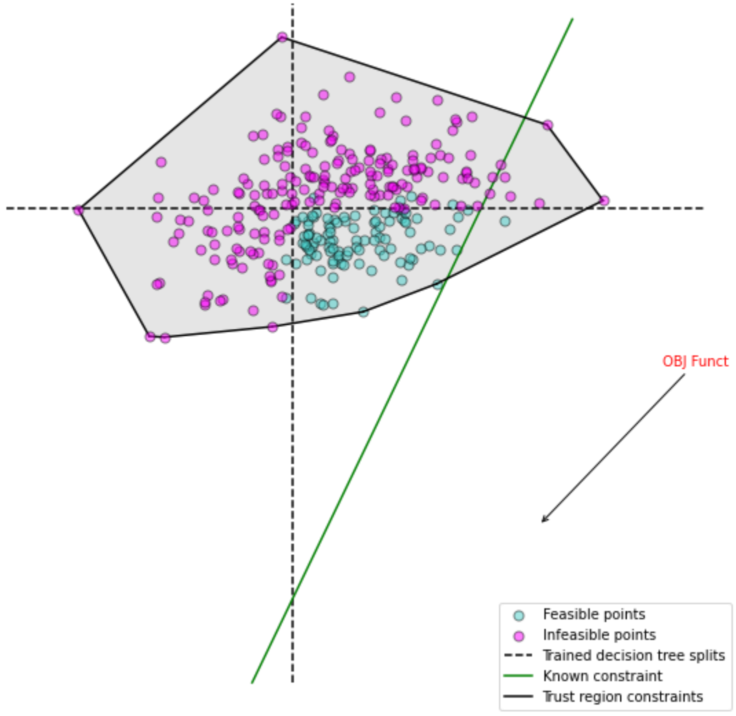
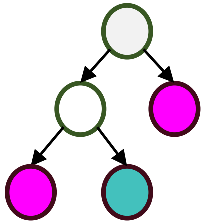
$$CH(\boldsymbol{x}) = \left\{ \boldsymbol{x} | \boldsymbol{x} = \sum_{i}^{N} \lambda_i \bar{\boldsymbol{x}}_i \,, \sum_{i}^{N} \lambda_i = 1 \,, \lambda_i \geq 0, i = 1, \dots, N \right\}$$







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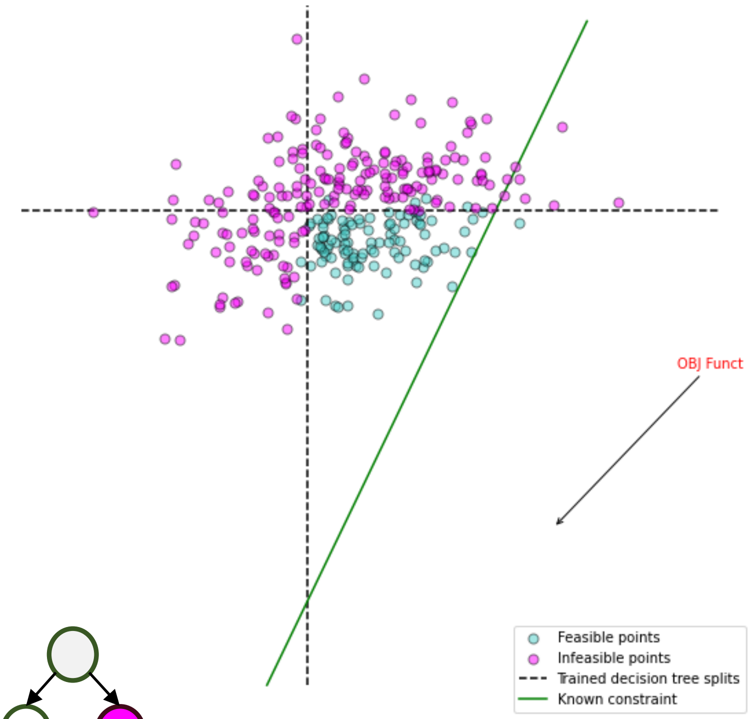

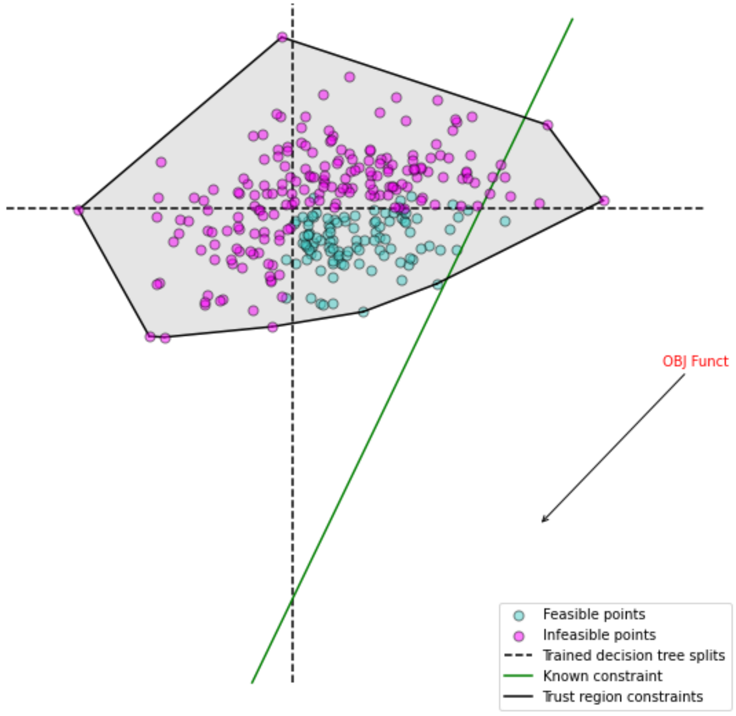

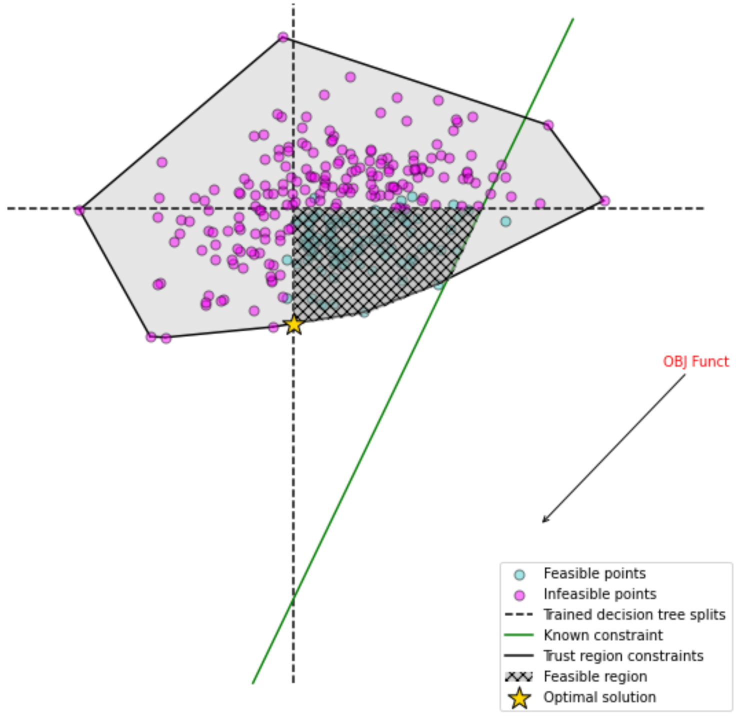

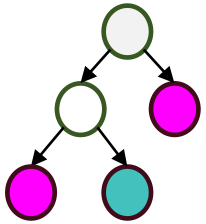

OptiCL

A Python Package for

Optimization with Constraint Learning

https://github.com/hwiberg/OptiCL

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Hands-on tutorial on the diet problem

Thank you!

Q&A

CONTACT ME

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