Optimization with Constraint Learning LAB

Part I

Speaker: Donato Maragno
University of Amsterdam

February 8, 2023

Before starting

https://github.com/ordavidov/ocl_lab

Agenda

- Introduction to mathematical optimization
- Introduction to Constraint Learning
- Chemotherapy case study
- Embedding Predictive Models
- Trust region constraints
- Hands-on tutorial

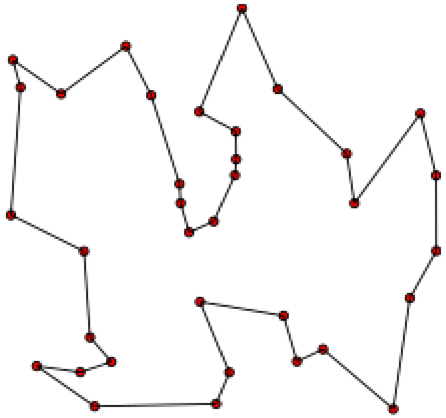
Mathematical Optimization

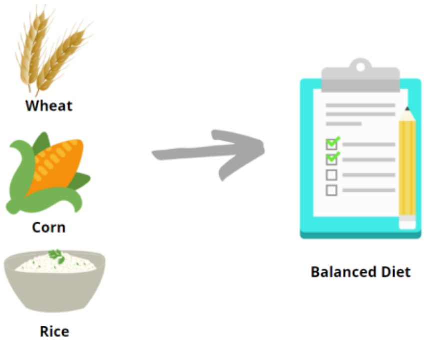
An optimization problem seeks to find the best (smallest or largest) value of a quantity given certain limits to the problem.

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





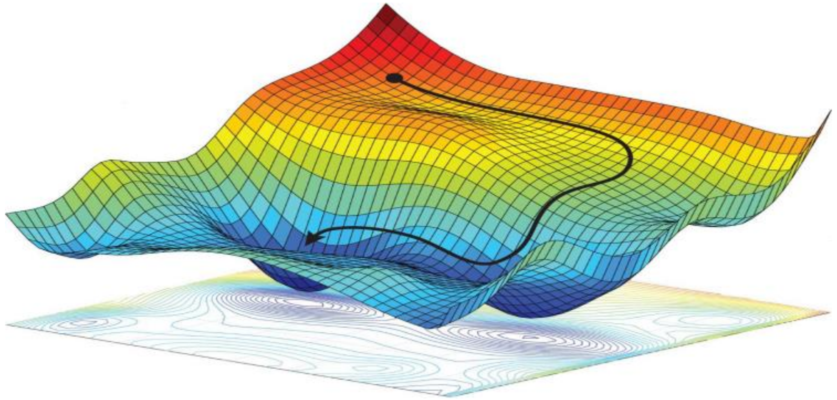
Mathematical Optimization

The general form of an optimization model is:

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

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

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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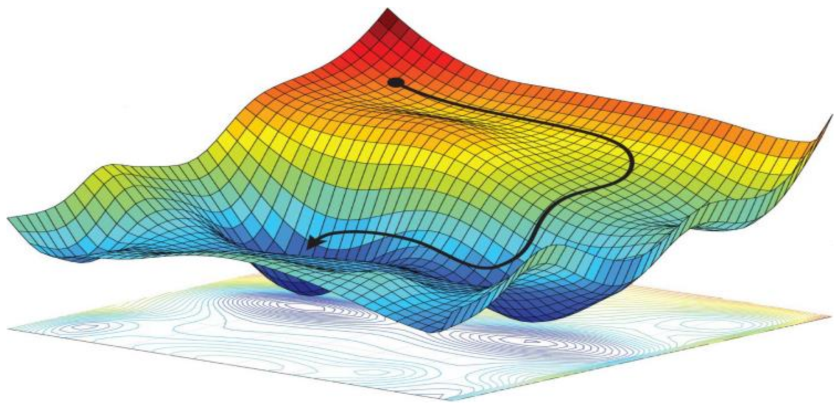

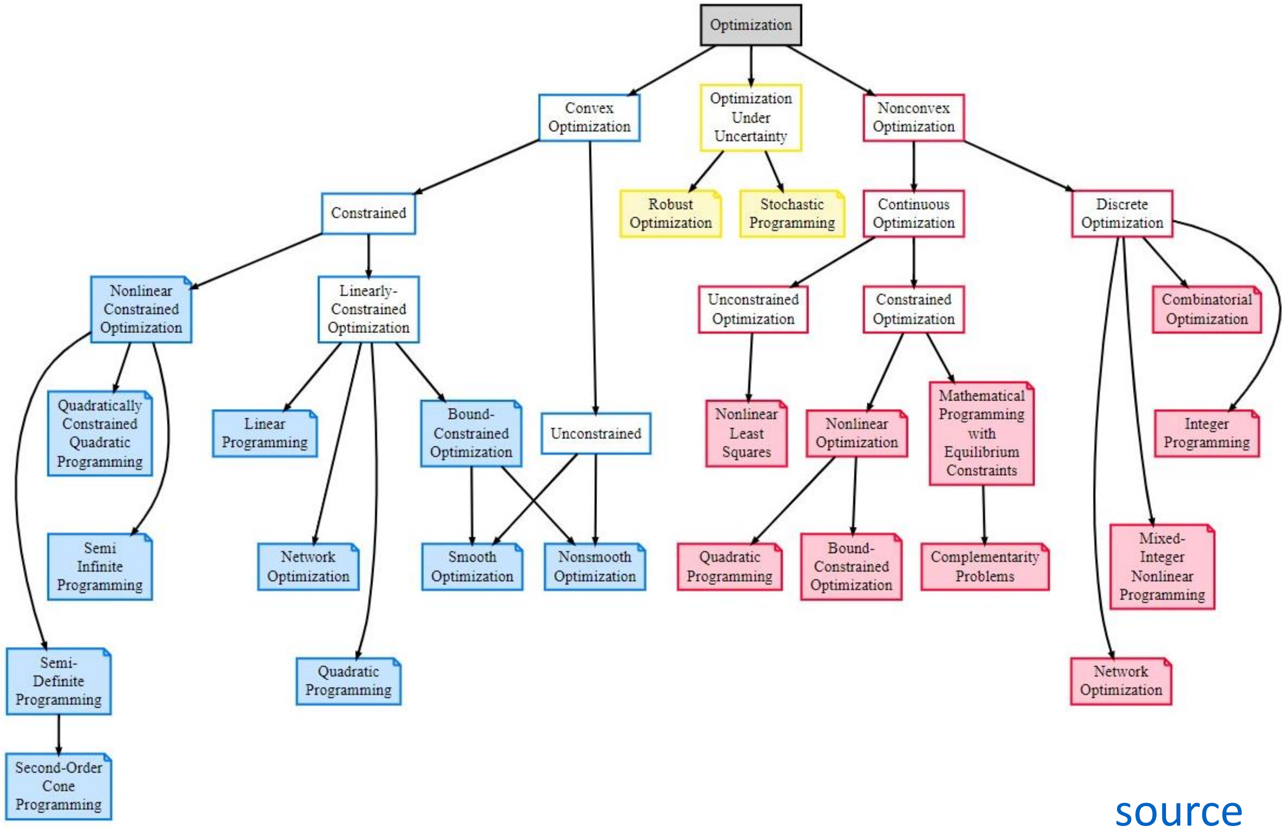

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Constraint Learning

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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.**

Case Study

Optimize the food baskets delivered by WFP to population groups in need.

- Minimize the procurement costs.
- Nutrient requirements constraints
- The food basket must be palatable

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$$\underset{x \in \mathbb{R}^n_{\geq 0}}{\text{minimize}} \quad f(\boldsymbol{x}) \longrightarrow \textit{Procurement costs}$$

Beans	Fish	...	Oil

Case Study

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Energy	Fat	...	Vitamin C

$$\underset{\boldsymbol{x}\in\mathbb{R}^n_{\geq 0}}{minimize} \quad f(\boldsymbol{x})$$ *Procurement costs*

$$subject\ to \quad \boldsymbol{NutVal}_i^T \boldsymbol{x} \geq NutReq_i \quad \forall\, i \in \mathcal{N}$$ *Nutrient requirements constraints*

Beans	Fish	...	Oil

Case Study

WFP

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IBM

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Procurement costs

Nutrient requirements constraints

No explicit formula but data is available

Beans	Fish	...	Oil

Applications of Constraint Learning

Table 1: Methods used for constraint learning

	Neural Networks	Decision Trees	Random Forest	Other Ensemble	Support Vector Machines	Clustering	(M)ILP	Other
Bergman et al. (2019)	x							x
Biggs et al. (2018)		x	x					
Chen et al. (2020)	x							
Chi et al. (2007)					x			
Cozad et al. (2014)							x	x
Cremer et al. (2018)		x		x				
De Angelis et al. (2003)	x							
Fahmi and Cremaschi (2012)	x							x
Garg et al. (2018)					x			
Grimstad and Andersson (2019)	x							
Gutierrez-Martinez et al. (2010)	x							
Halilbašić et al. (2018)		x						
Jalali et al. (2019)					x			
Kudła and Pawlak (2018)		x						
Lombardi et al. (2017)	x	x						
Maragno et al. (2022)	x	x	x	x	x	x		x
Mišić (2020)		x	x					
Paulus et al. (2021)	x							
Pawlak and Krawiec (2017a)							x	
Pawlak and Krawiec (2017b)								x
Pawlak and Krawiec (2018)								x
Pawlak (2019)								x
Pawlak and Litwiniuk (2021)						x		x
Pawlak and O'Neill (2021)							x	x
Prat and Chatzivasileiadis (2020)		x						
Say et al. (2017)	x							
Schede et al. (2019)		x					x	
Schweidtmann and Mitsos (2019)	x							
Spyros (2020)	x	x						
Sroka and Pawlak (2018)						x		x
Thams et al. (2017)		x						
Venzke et al. (2020b)	x							
Verwer et al. (2017)								
Xavier et al. (2021)								
Yang and Bequette (2021)	x							

Fajemisin A, Maragno D, den Hertog D (2021) Optimization with constraint learning: A framework and survey. URL https://arxiv.org/abs/2110.02121.

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Optimal planning using mixed integer linear optimization and a fitted deep network transition model

Global Optimization via Optimal Decision Trees

Dimitris Bertsimas

Sloan School of Management, Massachusetts Institute of Technology, Cambridge, MA, USA, dbertsim@mit.edu

Berk Öztürk

Department of Aeronautics and Astronautics, Massachusetts Institute of Technology, Cambridge, MA, USA, bozturk@mit.edu

Approximate non-convex function with Decision trees

Fajemisin A, Maragno D, den Hertog D (2021) Optimization with constraint learning: A framework and survey. URL https://arxiv.org/abs/2110.02121.

Constraint Learning

$\boldsymbol{x}$ Decision variables

$\boldsymbol{w}$ Contextual variables

$\boldsymbol{y}$ Predicted outcomes

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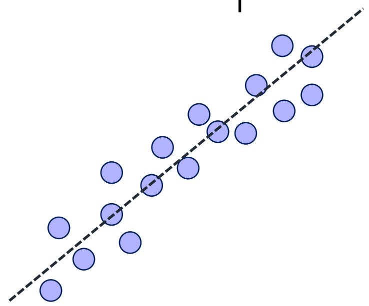
$$\boldsymbol{y} = \hat{\boldsymbol{h}}_{\mathcal{D}}(\boldsymbol{x}, \boldsymbol{w})$$

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



Constraint Learning

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

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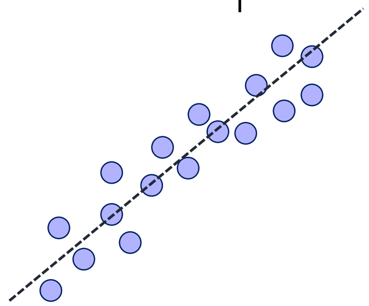

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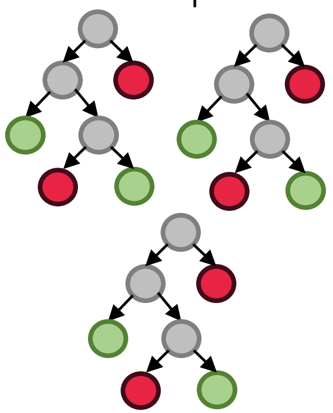

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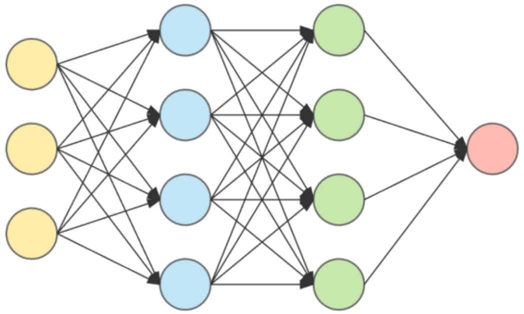

Chemotherapy Case Study

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**.

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

$$\boxed{\begin{aligned} \min_{\boldsymbol{x},\boldsymbol{y}} \quad & y_{OS} \\ \text{s.t.}\, & y_i \le \tau_i, && i \in \mathcal{Y}_C, \\ & y_i = \hat{h}_i(\boldsymbol{x}, \boldsymbol{w}), && i \in \mathcal{Y}_C, \\ & y_{OS} = \hat{h}_{OS}(\boldsymbol{x}, \boldsymbol{w}), \end{aligned}}$$

$$\begin{aligned} & \sum_d \boldsymbol{x}_b^d \le 3, \\ & \boldsymbol{x}_b \in \{0,1\}^d, \\ & \boldsymbol{x} \in \mathcal{X}(\boldsymbol{w}). \end{aligned}$$

(*) 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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Overall Survival

$$\begin{aligned}
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Toxicities

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

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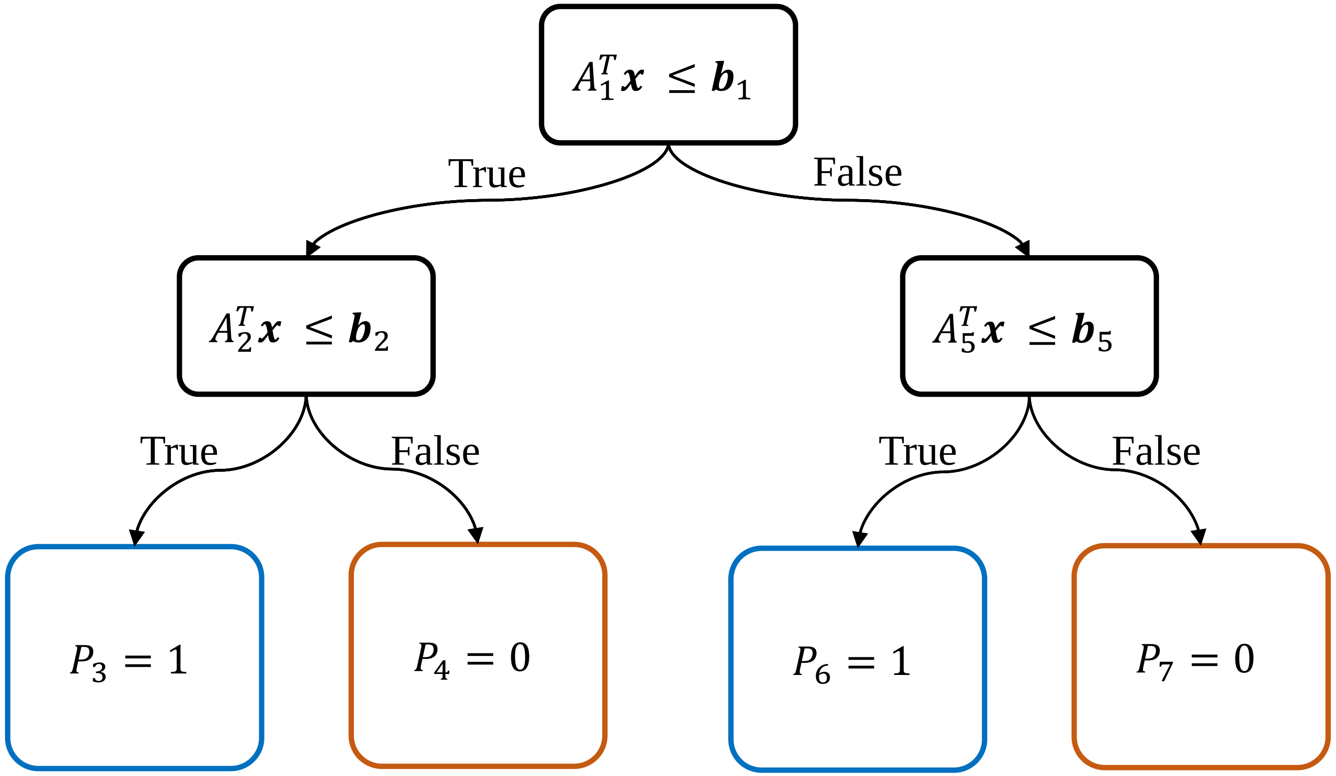
Embedding Decision Trees



Embedding Decision Trees

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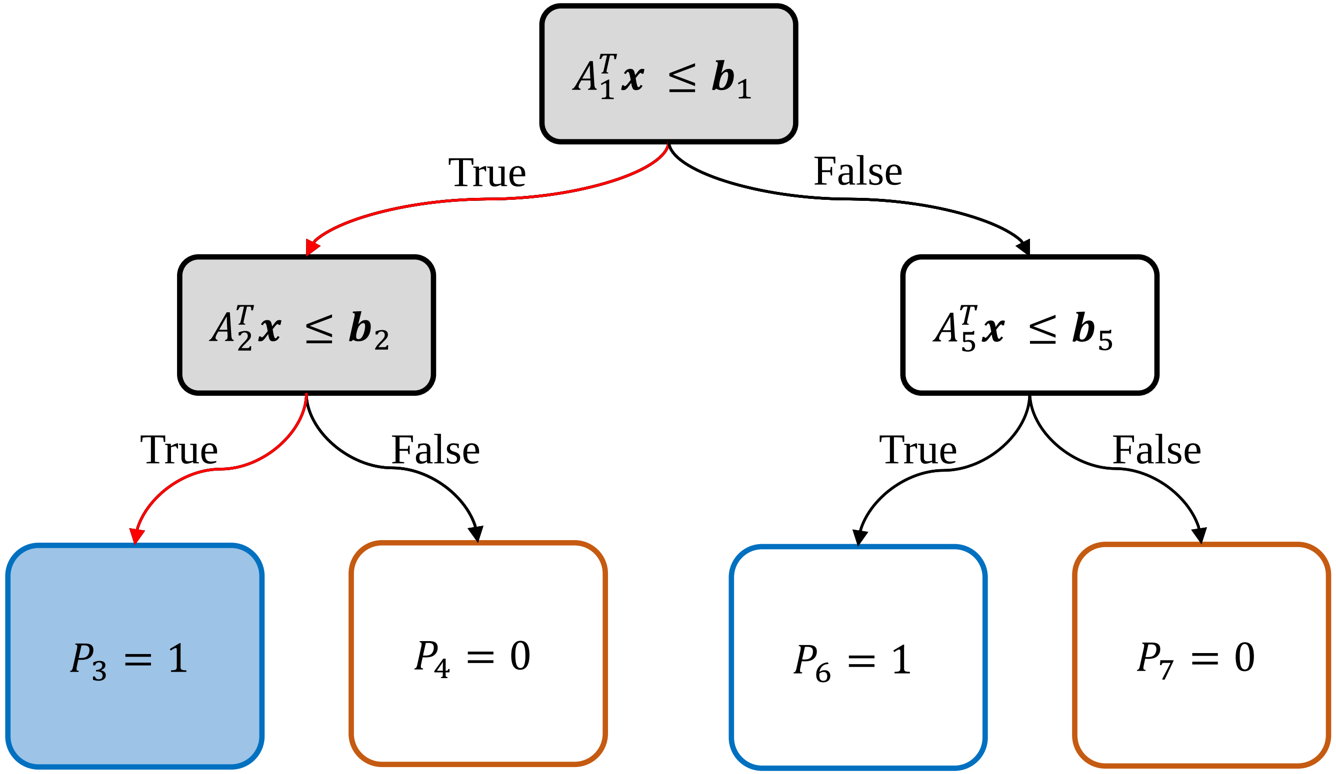


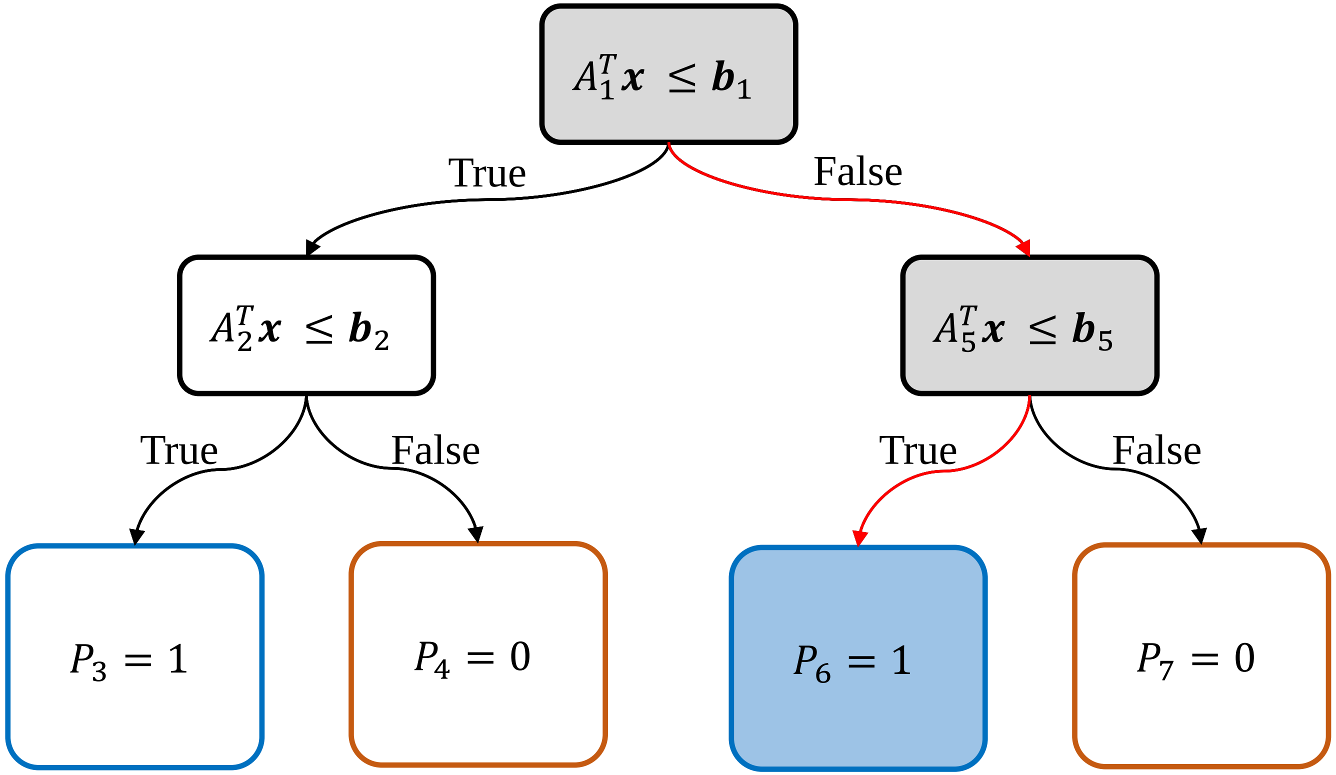
Conceptual model

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

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

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

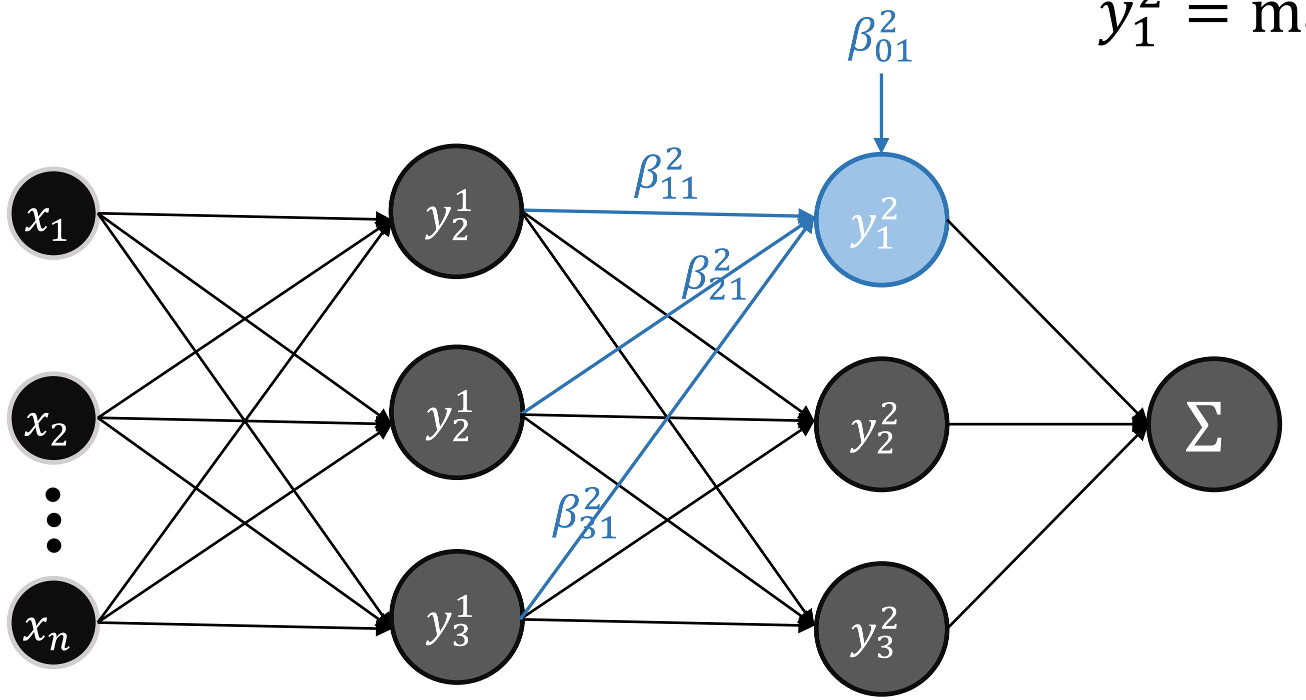
P_6

$$A_1^T\boldsymbol{x} \geq \boldsymbol{b}_1$$
$$A_5^T\boldsymbol{x} \leq \boldsymbol{b}_5$$

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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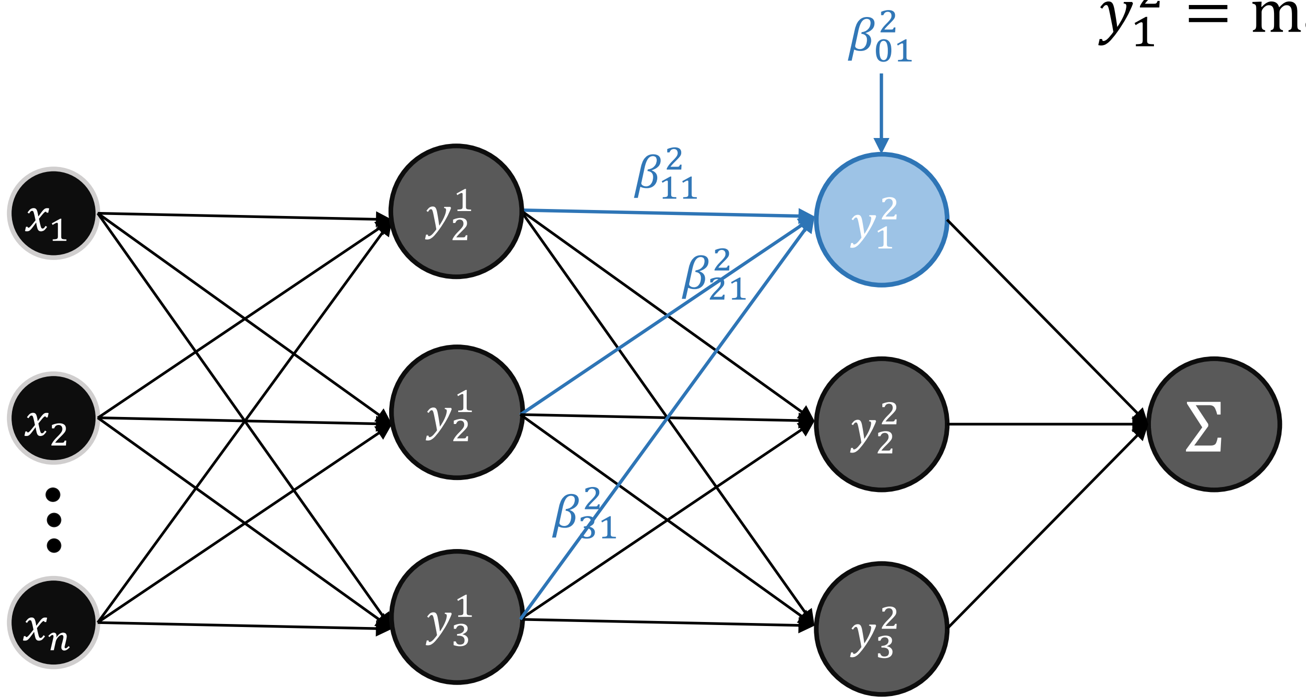
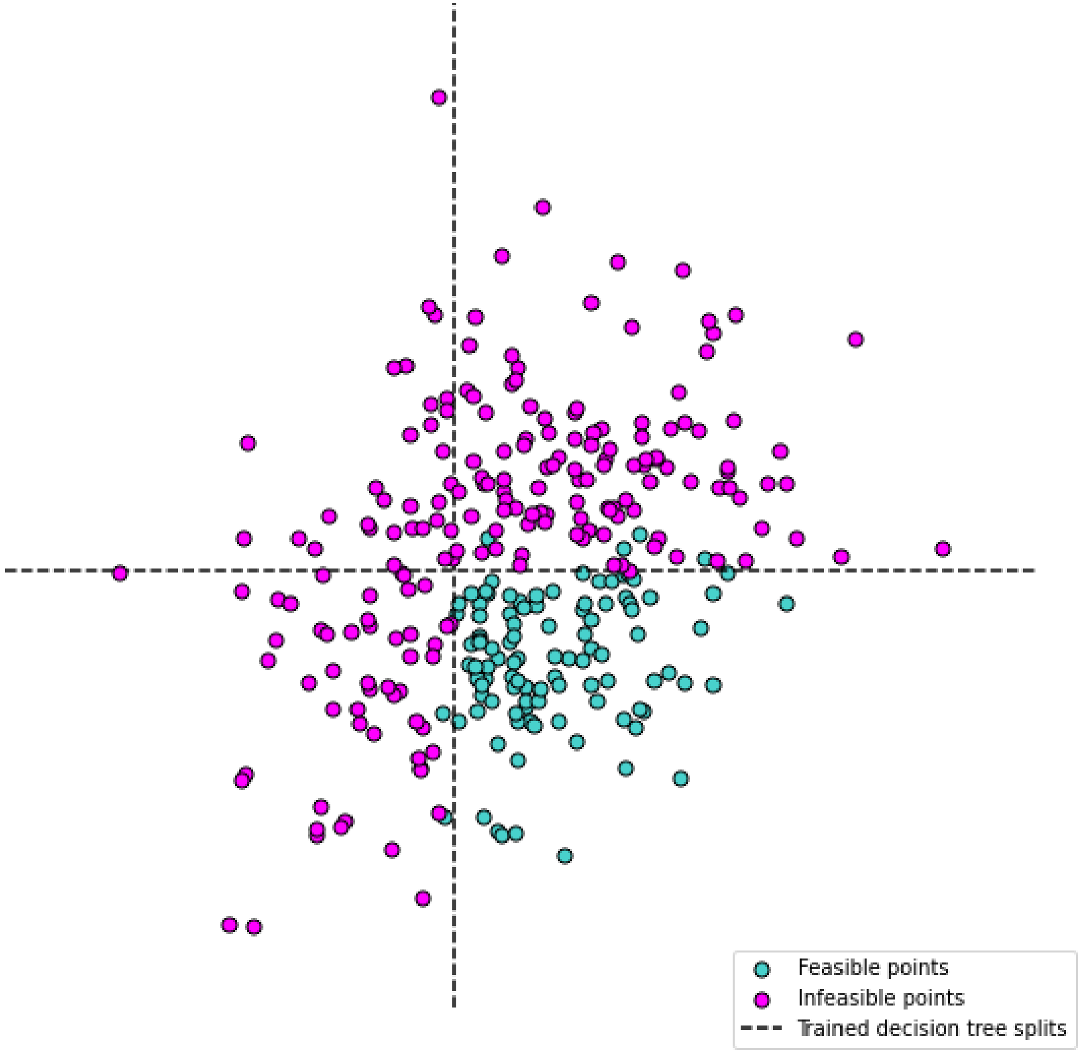


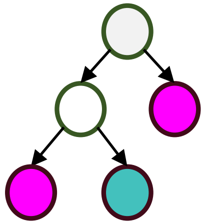
$y = \max\{0, x\}$ can also be written as:

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

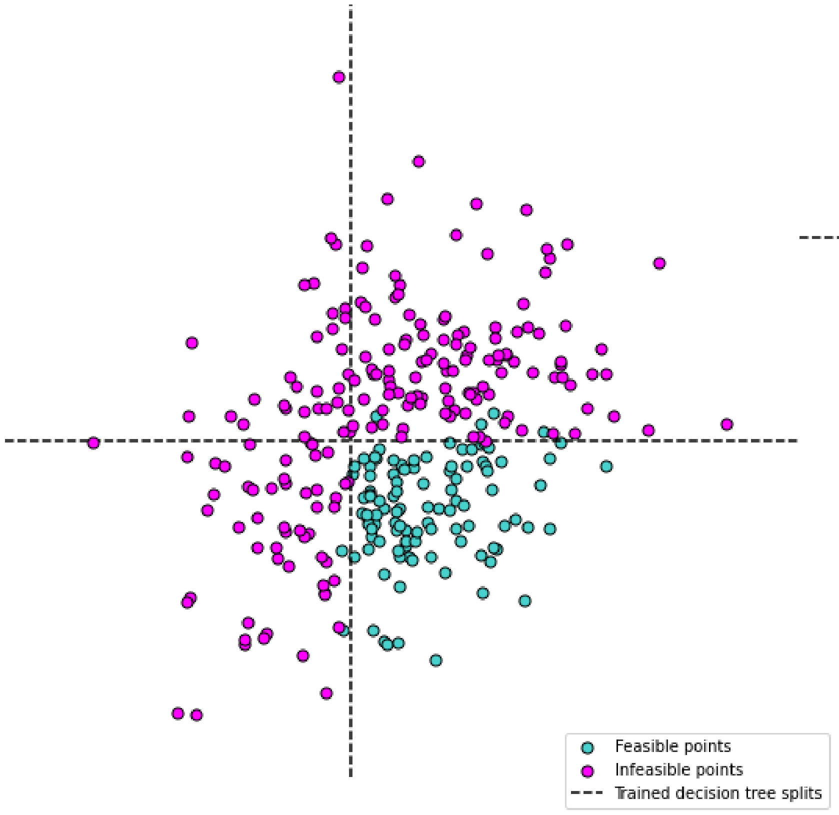
where $M_L < 0$ is a lower bound on all possible values of x, and $M_U > 0$ is an upper bound.

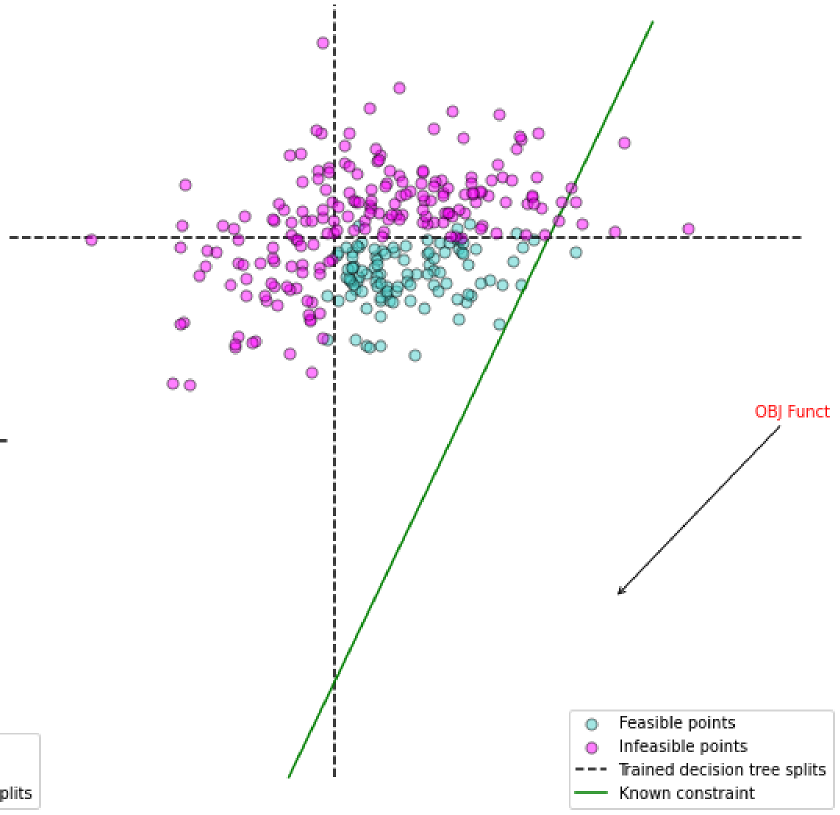
Trust region constraints

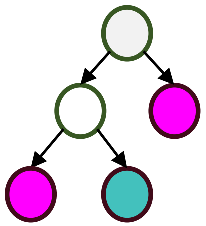




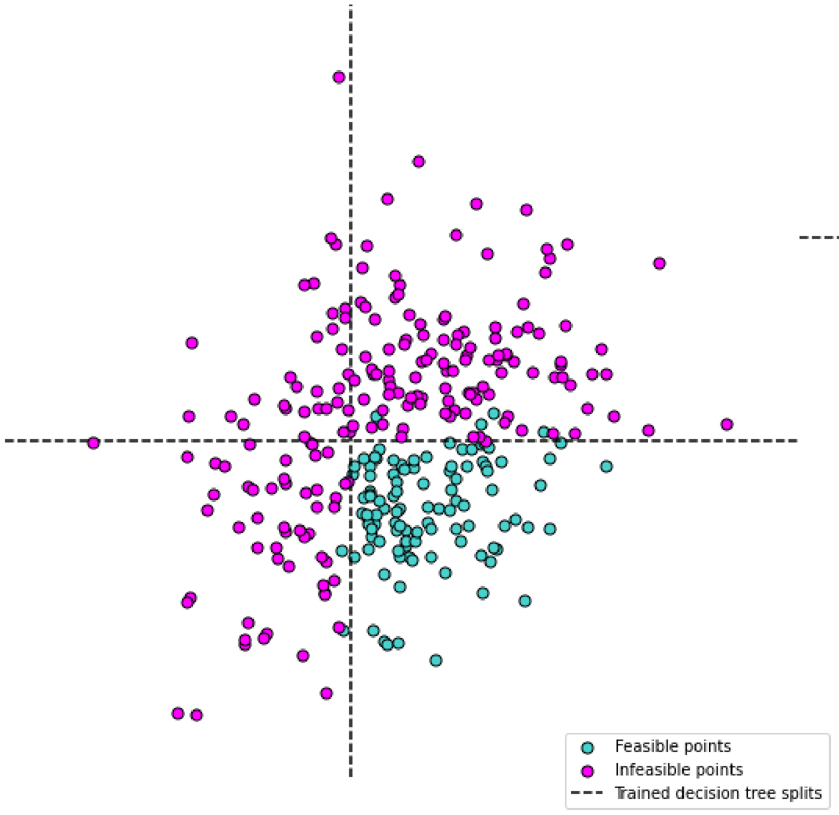
Trust region constraints

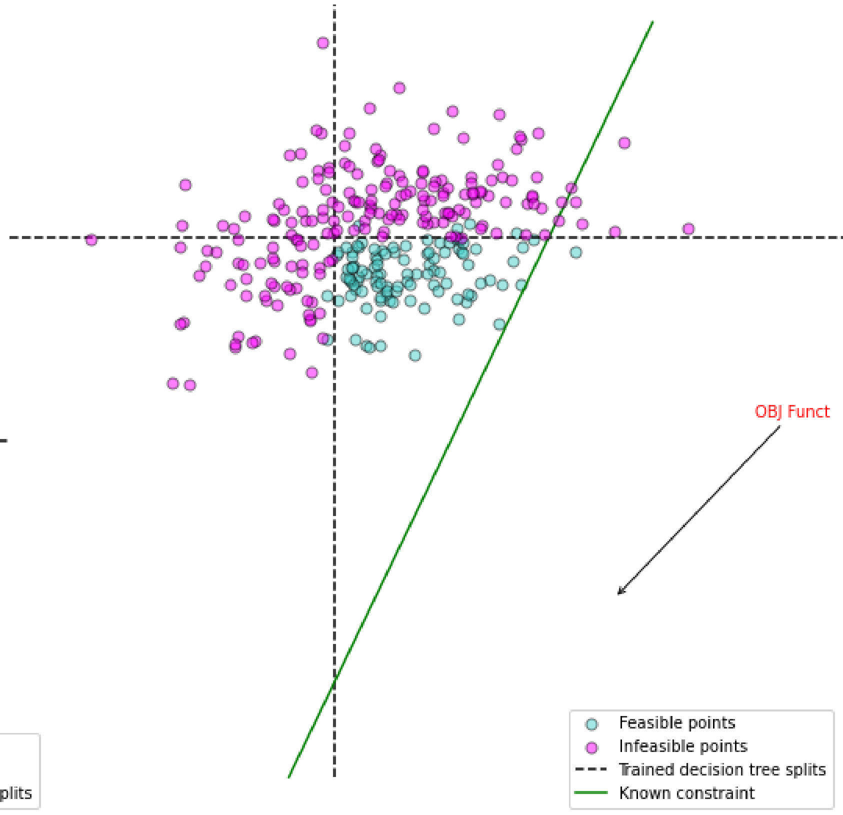


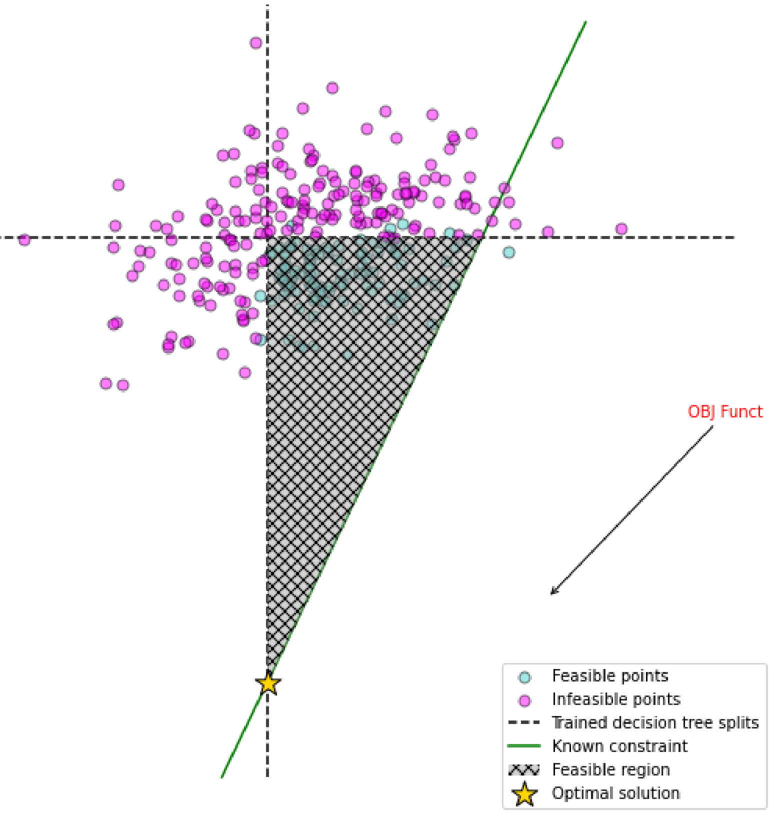


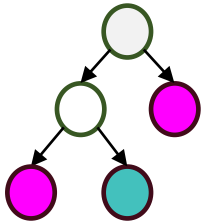


Trust region constraints

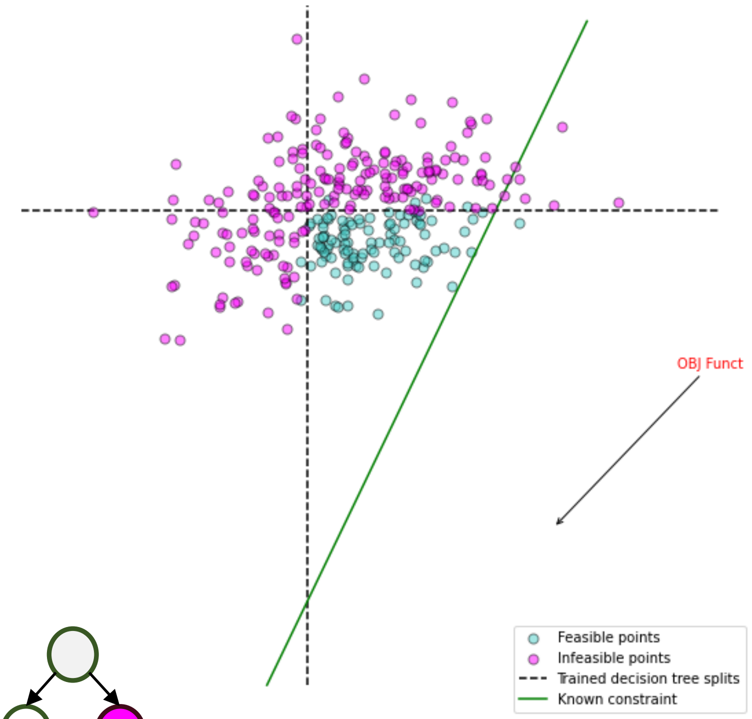


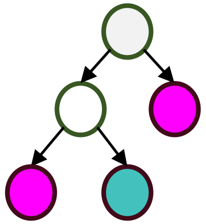






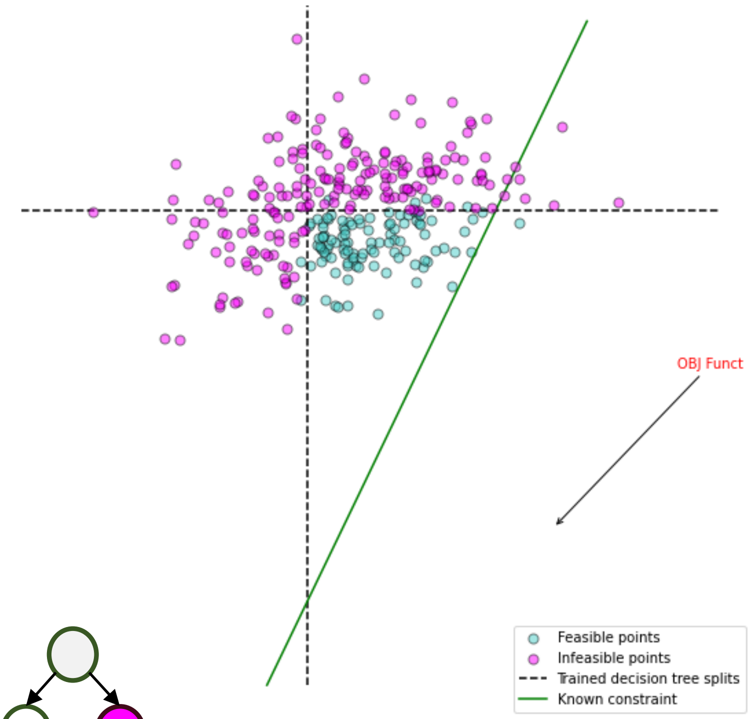
Trust region constraints

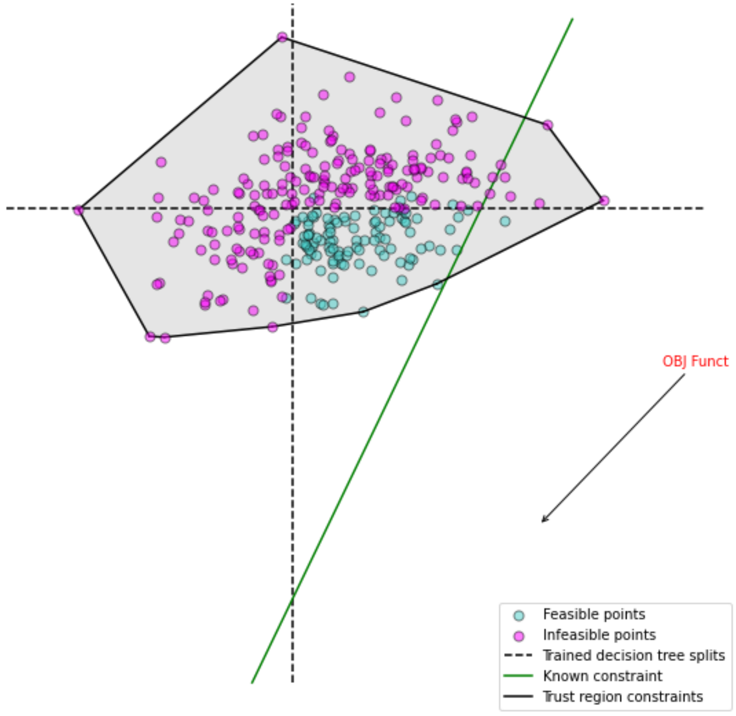


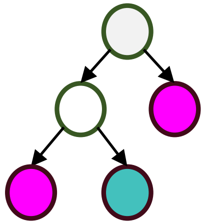


Trust region constraints

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







Trust region constraints

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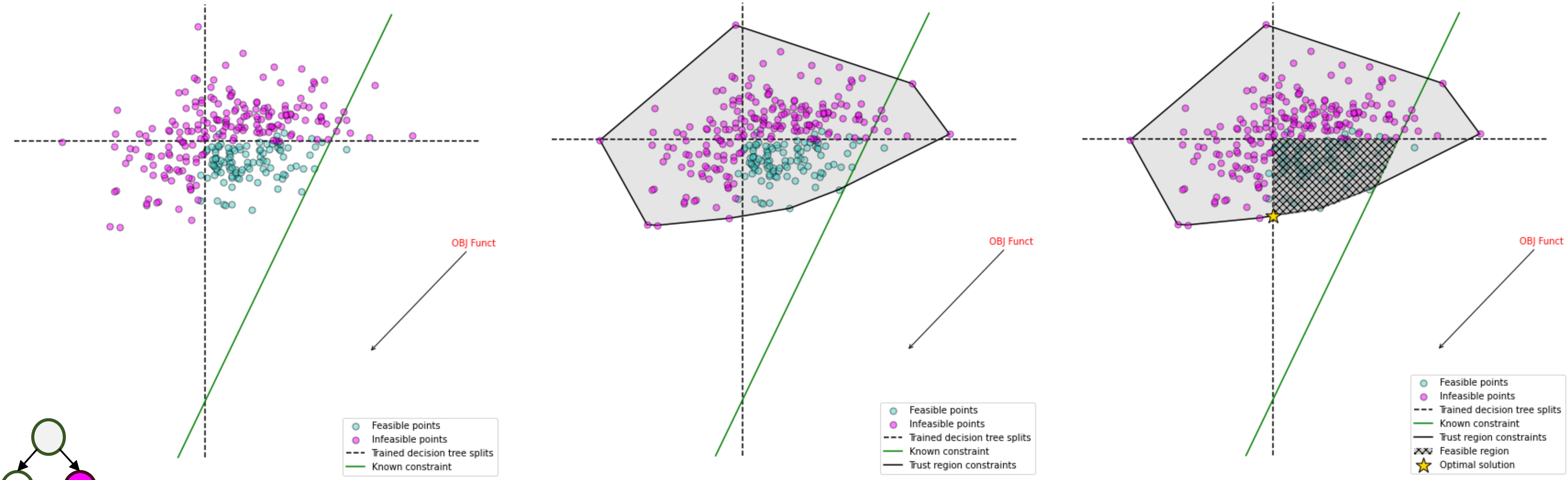

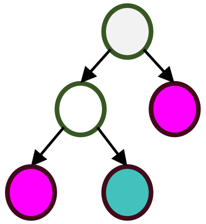

OptiCL

A Python Package for Optimization with Constraint Learning

https://github.com/hwiberg/OptiCL

OptiCL

A Python Package for

Optimization with **C**onstraint **L**earning

https://github.com/hwiberg/OptiCL

Hands-on tutorial on the

diet problem

Thank you!

Q&A

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