TACTICAL TRANSPORT PLANNING UNDER IMPERFECT INFORMATION BY COMBINING MACHINE LEARNING AND DISCRETE OPTIMIZATION

EMMA FREJINGER

Associate Professor, Department of Computer Science and Operations Research, Université de Montréal

CN Chair in Optimization of Railway Operations

Large-scale real-world decision-making problems…

…are hard to solve, in fact, too hard to process or too time-consuming to solve for humans…

Operations Research

Machine Learning

… and they occur in an environment that changes over time and whose evolution is uncertain.

This talk is about combining machine learning and operations research to solve large-scale decision-making problems.

Second part: novel methodology in the context of a railway application

MACHINE LEARNING (ML)

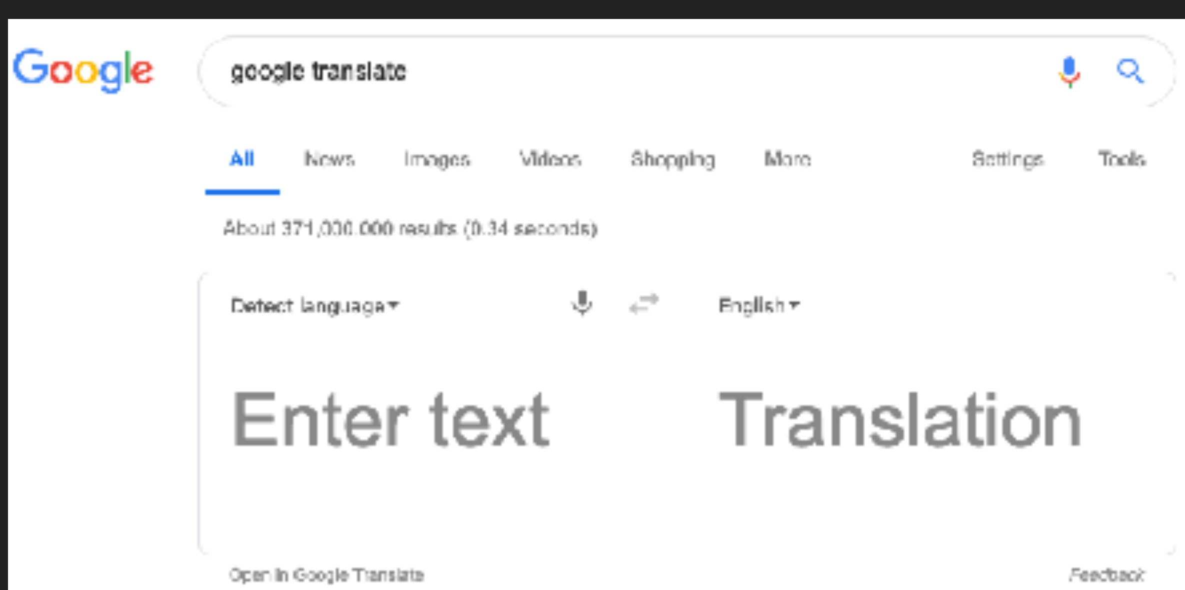
- Acquisition of knowledge by extracting patterns from data
- Ingredients of most machine/statistical learning algorithms: data, a model, means to link the two - infer values of parameters (cost function and optimization procedure)
- Supervised learning: data consists of examples that are described by certain features and a corresponding label

$$\mathbf{y} = f(\mathbf{x}; \boldsymbol{\theta})$$

$$(\mathbf{x}^{(i)}, \mathbf{y}^{(i)}) \quad i = 1, \ldots, m$$

MACHINE LEARNING – EXAMPLES OF EXTENSIVELY STUDIED PROBLEMS

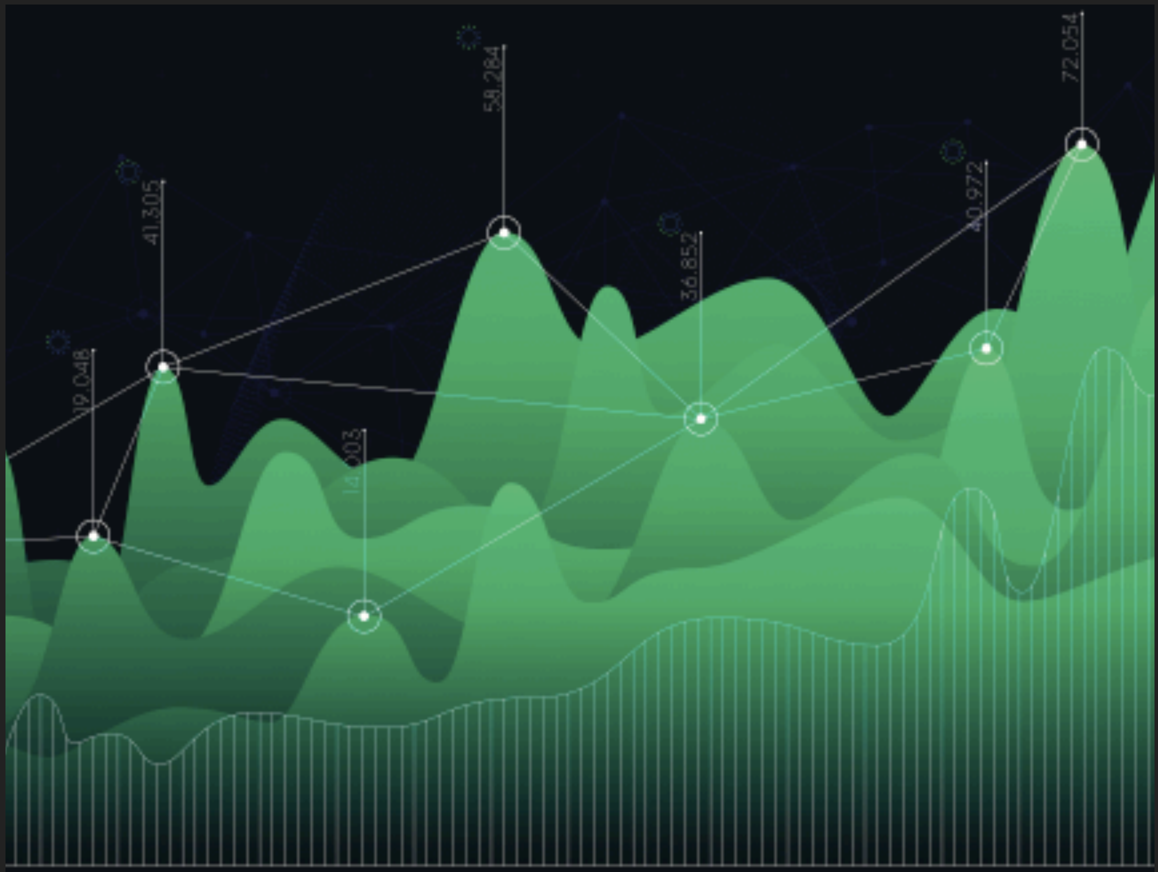
- Analyzing and describing visual content
- Machine Translation
- Important tasks in many applications

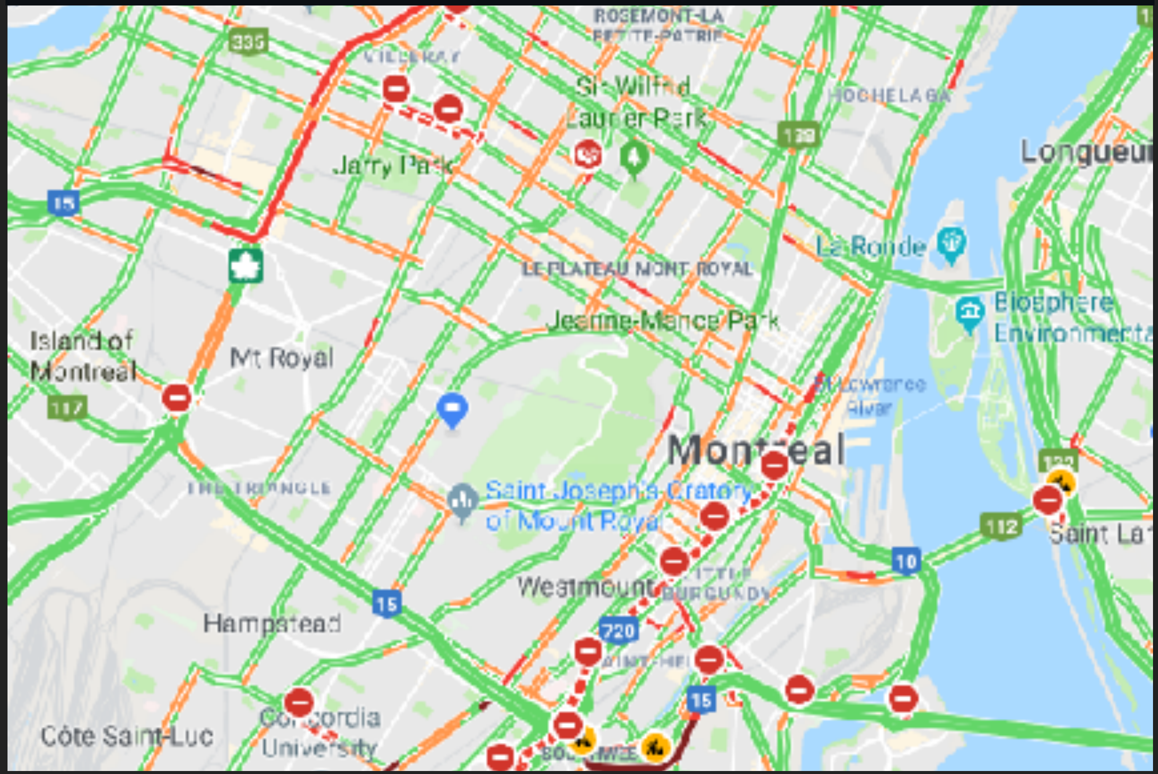


Xu et al., Show, attend and tell: Neural image caption generation with visual attention, 2016. ArXiv: 1502.03044v3

STATISTICAL LEARNING – DEMAND FORECASTING EXAMPLE

- Predict how demand varies over time, alternatives to statistical time series models
- Predict user behavior, e.g., choice of path and choice of transport service in a network
    - Route choice in transportation
    - Inverse reinforcement learning or imitation learning in ML

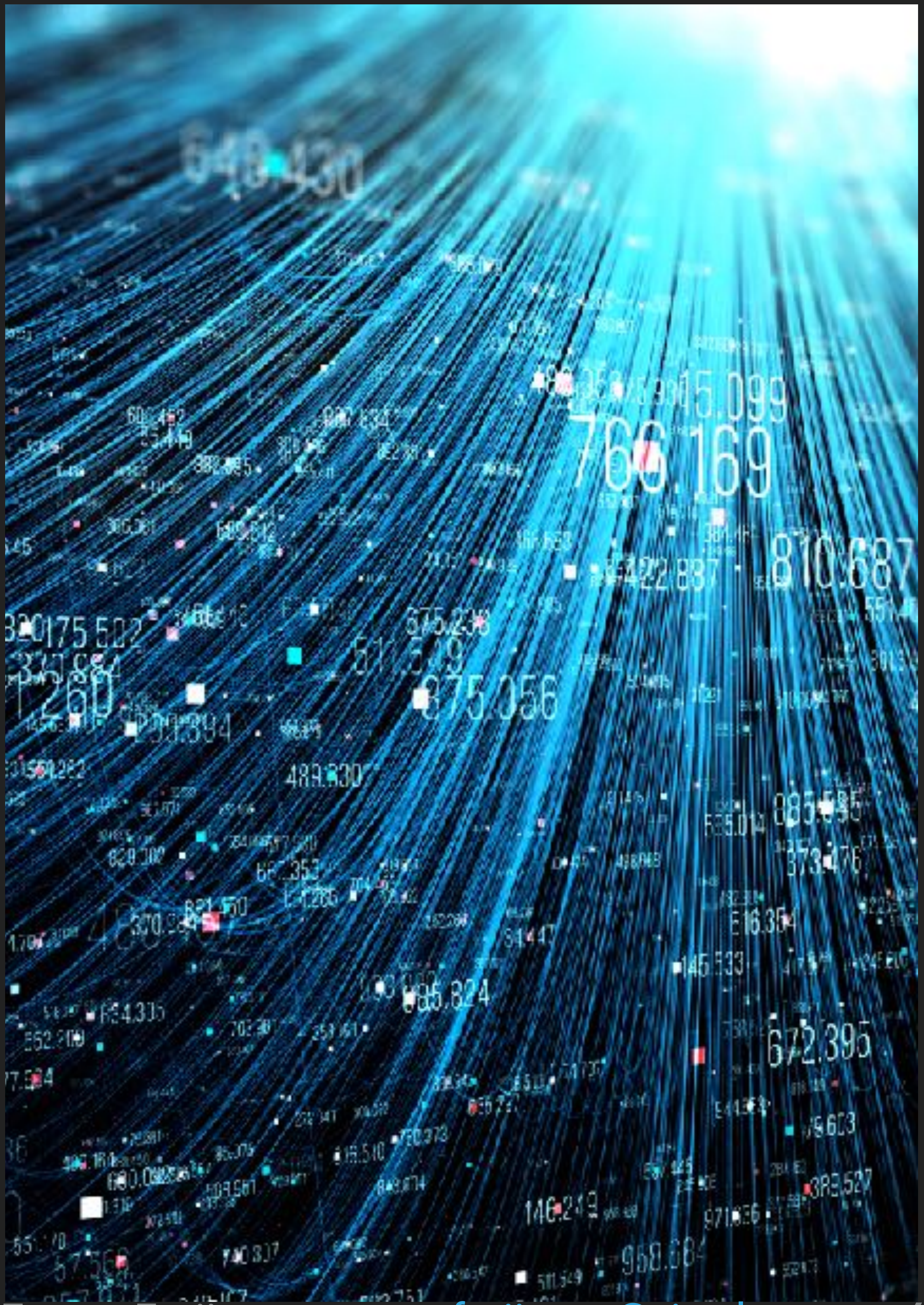




Huge success in automating tasks that are rather easy for humans but hard to formalize.

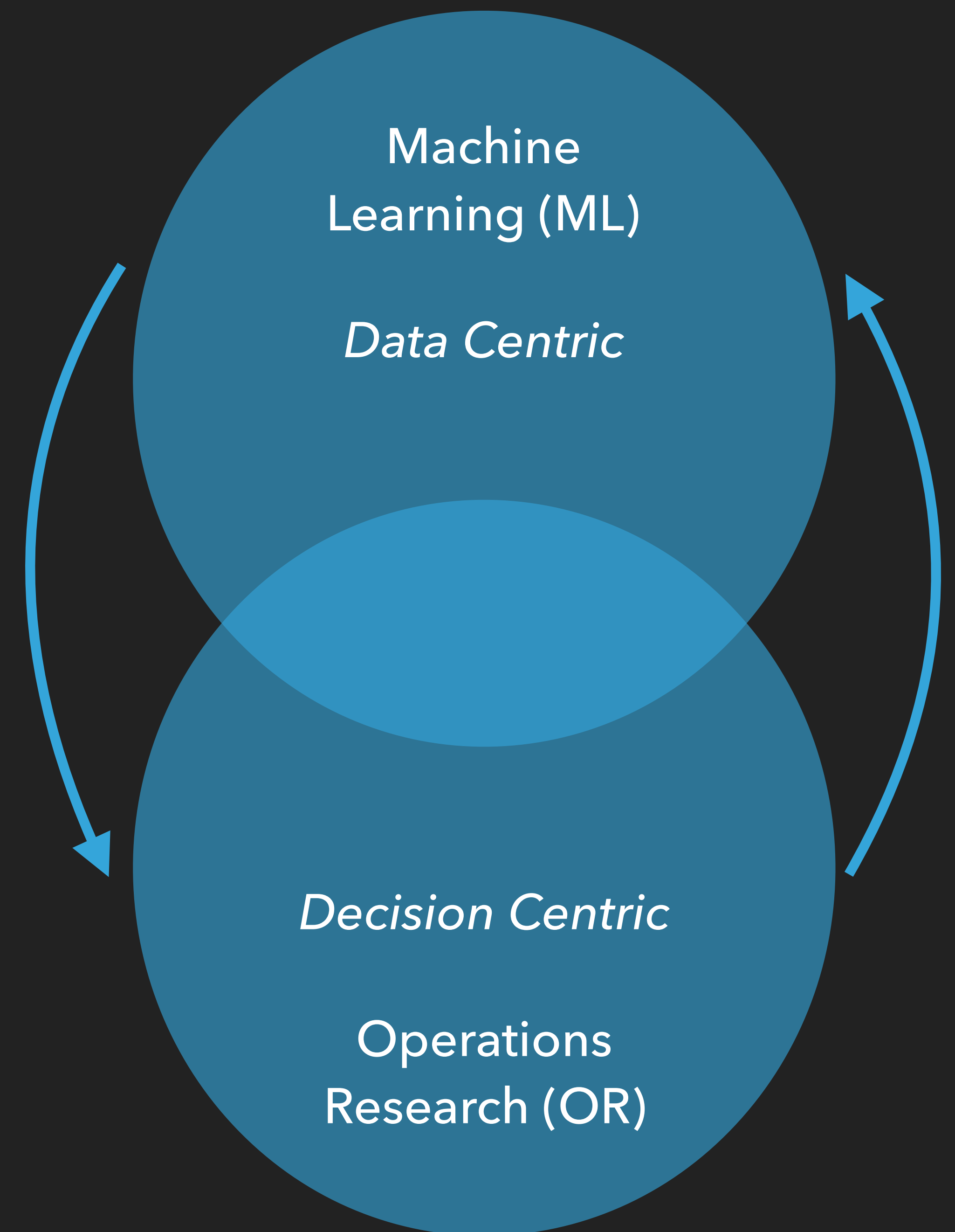
WHY ALL THE SUCCESS NOW?

- Massive amount of high quality data
- Flexible models
- Computing power
- Algorithms



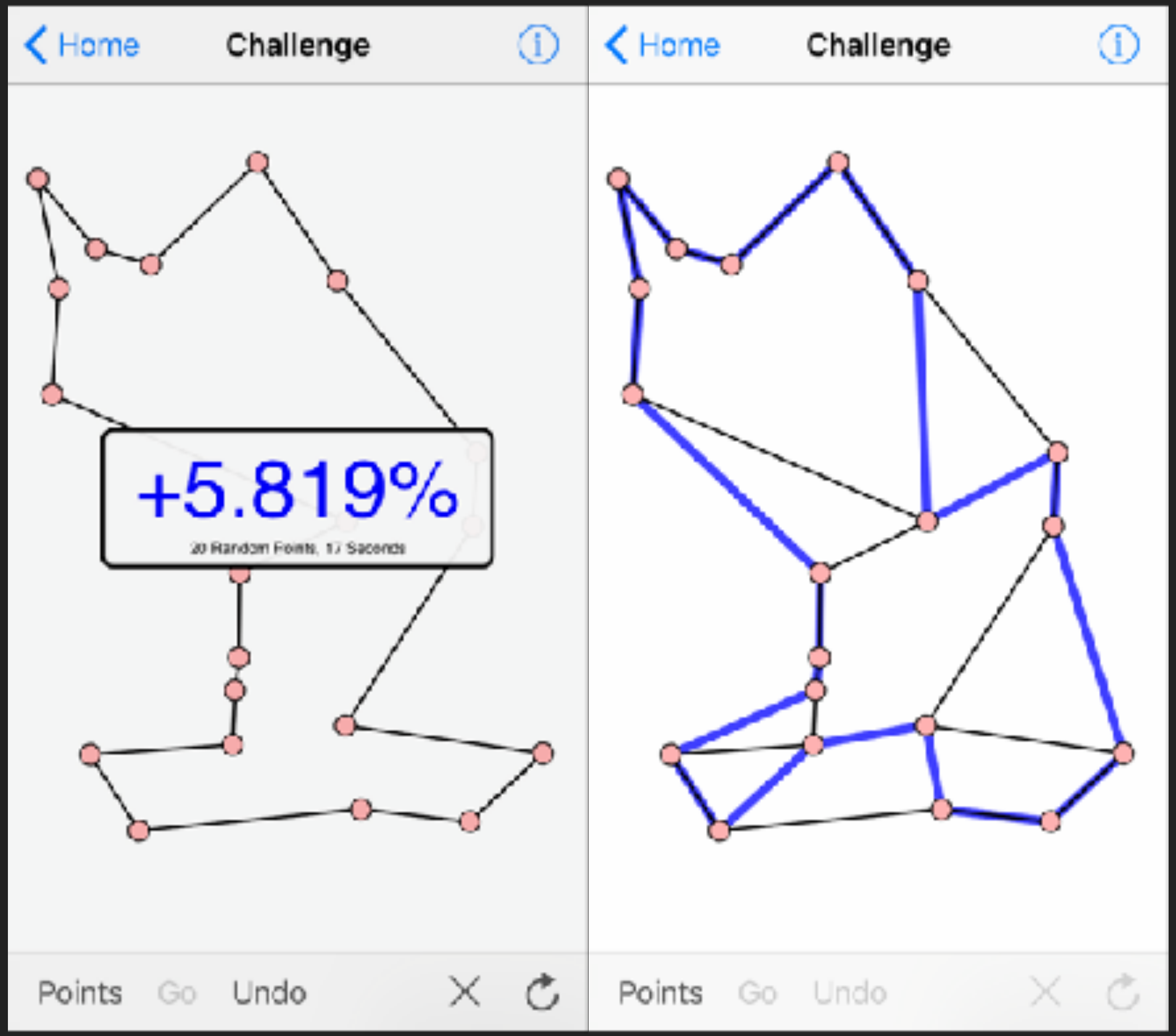
OPERATIONS RESEARCH

- Broad field focused on solving complex decision-making problems that are too hard or too time-consuming for humans to solve
- Non-linear continuous optimization algorithms are an essential ingredient of machine learning, here we focus on discrete optimization



A FAMOUS PROBLEM

- The traveling salesman problem: Given a list of cities and distances between each pair, find the shortest route that visits each city and returns to the original city.
- Easy to understand but hard to solve
- TSP with 20 cities has 19!/2 solutions = **60,822,550,000,000,000**
- Effective algorithms exist to solve large instances (one of the largest has 85,900 cities!)

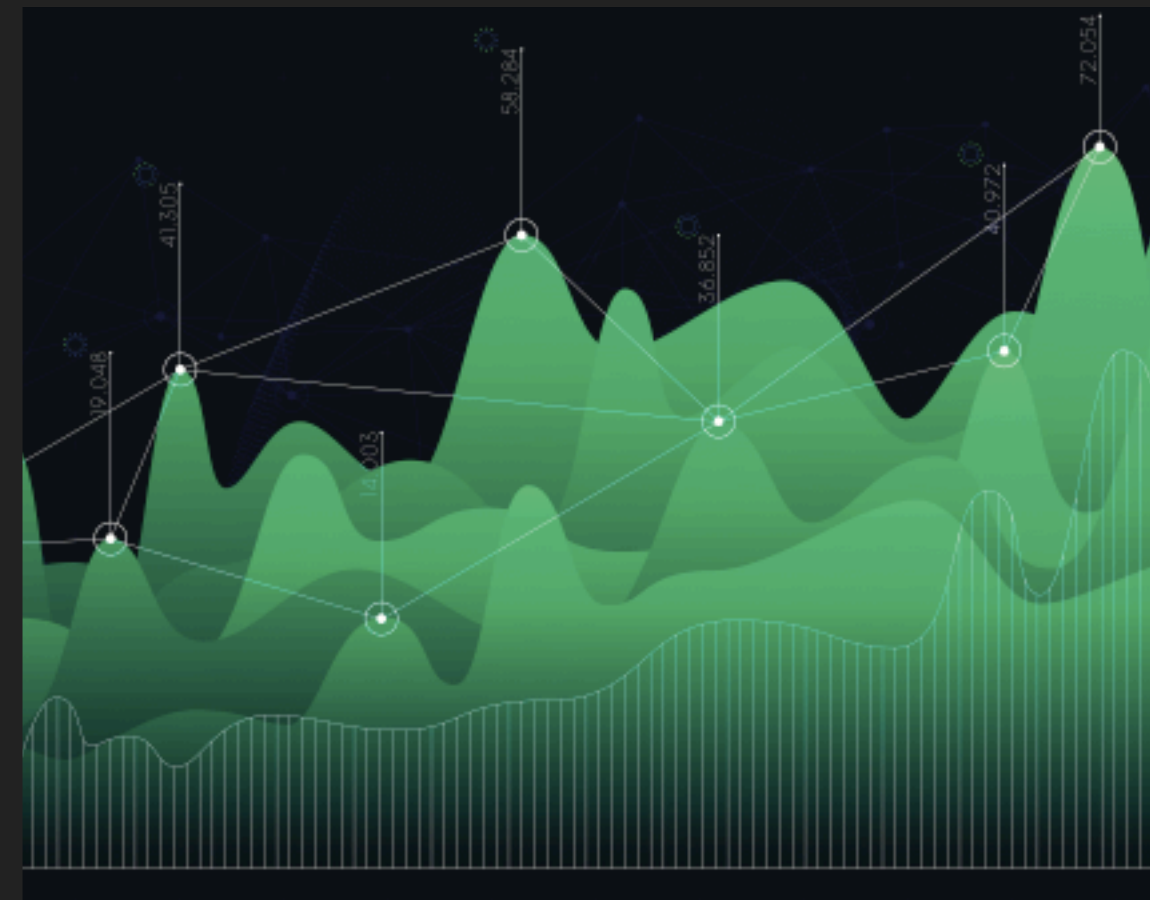


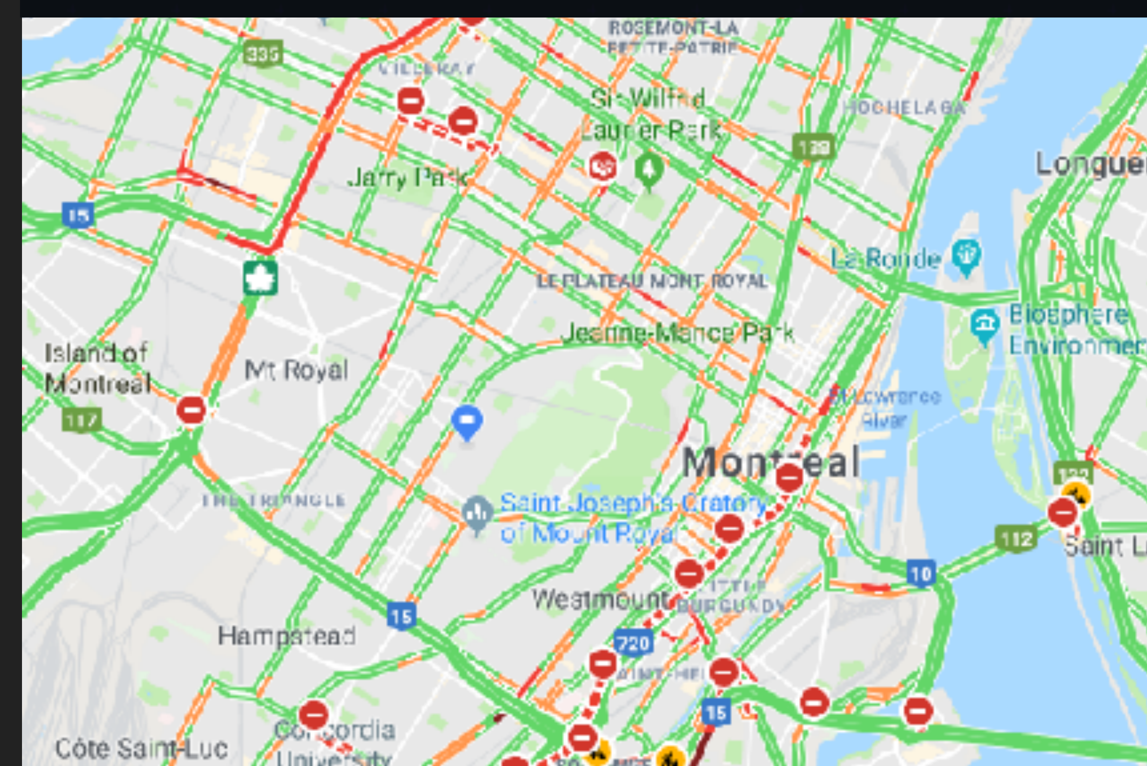
Don't get addicted!
Concorde TSP solver app

Book: In the pursuit of the traveling salesman: Mathematics at the limits of computation, William Cook, Princeton University Press, 2012.

EXAMPLE: DISCRETE OPTIMIZATION AND ML COMBINED

- ML algorithm predicts users' behavior in a transport network
- OR methodology solves a decision-making problem taking users' reactions into account
  - Pricing at certain arcs (network pricing)
  - Planning of new infrastructure (network design / facility location)
  - Control traffic flow (flow capture)





THE SUCCESS OF OR

- A wide range of real-word applications rely on operations research methodologies: scheduling, energy grid management, vehicle routing, service network design, fleet management, …
- Impressive results over the past two decades: more than 265,000x algorithmic speedup!
- The environment is assumed to be known perfectly in a majority of the applications.

Problems that would have taken 7 years to solve in 1991, take one second now [2003].

George Nemhauser
Georgia Institute of Technology

CPLEX and Gurobi solvers, assuming conservative 1000x machine speedup, 1991-2003.

MACHINE LEARNING + DISCRETE OPTIMIZATION

Interact

ML and optimization are integrated, interplay and conduct learning through interaction with the environment.
Example: integrated model adapts to a changing environment, e.g., user behavior is changing over time

Interplay

ML and optimization are integrated and interplay.
Examples: bilevel optimization, « hybrid » algorithms

Understand

ML is used to characterize uncertainty in the environment.
ML predictions and optimization are used in sequence.
Majority of models used in practice.

MACHINE LEARNING + DISCRETE OPTIMIZATION

Interplay ◯ Example

An example of bilevel optimization problem important to transport planning

Lower level is modelled with a probabilistic choice model: non-linear optimization problem with strong combinatorial features

Dan & Marcotte (2019) on competitive facility location

Gilbert, Marcotte, Savard (2014) on logit network pricing

Morin, Frejinger, Gendron (2019) on flow capture

LEADER first selects *y*, anticipating the follower's reaction *x*

$$\max_{x,y} f(x, y)$$

Subject to: $(x, y) \in Y$

$$x \in \arg \max_{x' \in X(y)} E_{\varepsilon}[U(x', y, \varepsilon)]$$

FOLLOWER selects x from lower level feasible set *X(y)* that maximizes expected utility

MACHINE LEARNING + DISCRETE OPTIMIZATION

Interplay ◯ A view - by no means exhaustive

- ML used as a tool for approximating complex and time-consuming tasks in OR algorithms, e.g, branching for enumerative approaches (survey by Lodi and Zarpellon, 2017)
- ML used to (heuristically) solve discrete optimization problems (survey by Bengio et al., 2018)
- Discrete optimization for ML algorithms (e.g., Bertsimas and Shioda, 2017; Grünlück et al., 2017)
- Learning optimization models from data
  - Constrained models (Lombardi et al., 2017; Hewitt and Frejinger, 2019)
  - Objective function: data-driven inverse optimization (e.g., Esfahani et al., 2017) inverse reinforcement learning (Ng and Russell, 2000), dynamic discrete choice models (Rust, 1986)

Predicting tactical solutions to operational planning problems under imperfect information

E. Larsen, S. Lachapelle, Y. Bengio,
E. Frejinger, S. Lacoste-Julien & A. Lodi
ArXiv:1807.11876v3

E. Larsen & E. Frejinger

In brief:

Combine machine learning and discrete optimization to solve a problem that we could not solve with any existing methodology.

Challenges:

Very restricted computing time budget.
Imperfect information.

CONTEXT

Planning horizon and increasing level of information

Long term
« strategic »

Medium term
« tactical »

Short term
« operational »

LEVEL OF DETAIL OF SOLUTION

Fully detailed solution - implementable

Description of solution - level of detail that is relevant to the tactical decision problem

Value of the solution

(c) Emma Frejinger emma.frejinger@cirrelt.ca

CONTEXT

Planning horizon and increasing level of information

Medium term
« tactical »

Compute description of solution to operational problem under imperfect information

Short term
« operational »

Operational problem of interest: Compute solution under perfect information

COMPUTING TIME BUDGET

seconds to minutes

milli-seconds

	Medium term « tactical »	Short term « operational »
seconds to minutes		*Reasonable computing time - within the time budget for the operational problem*
milli-seconds	*Much shorter than the time it takes to solve the full problem under perfect information*	

CONTEXT

Planning horizon and increasing level of information

Medium term « tactical »	**Short term « operational »**
Compute description of solution to operational problem under imperfect information	Operational problem of interest: Compute solution under perfect information
	High-precision solution Reasonable computing time *Solve deterministic optimization problem* ***mathematical programming***
High-level solution Very short computing time ***Stochastic programming*** ***Machine learning*** *predict the tactical solution descriptions*	

SOME NOTATION

Planning horizon and increasing level of information

	Medium term « tactical »		Short term « operational »	
Problem instance	Imperfect information	$\mathbf{x}_a$	Perfect information	$\mathbf{x} = [\mathbf{x}_a, \mathbf{x}_u]$
Solution		$\widehat{\mathbf{y}}^*(\mathbf{x}_\mathrm{a})$	Deterministic problem	$\mathbf{y}^*(\mathbf{x}) = \arg\min_{\mathbf{y}\in Y(\mathbf{x})} C(\mathbf{x}, \mathbf{y})$
	Tactical solution description	$\bar{\mathbf{y}}^* = g(\mathbf{y}^*(\mathbf{x}))$		

APPLICATION - LOAD PLANNING

Planning horizon and increasing level of information

Medium term
« tactical »

Capacity management, e.g., bookings

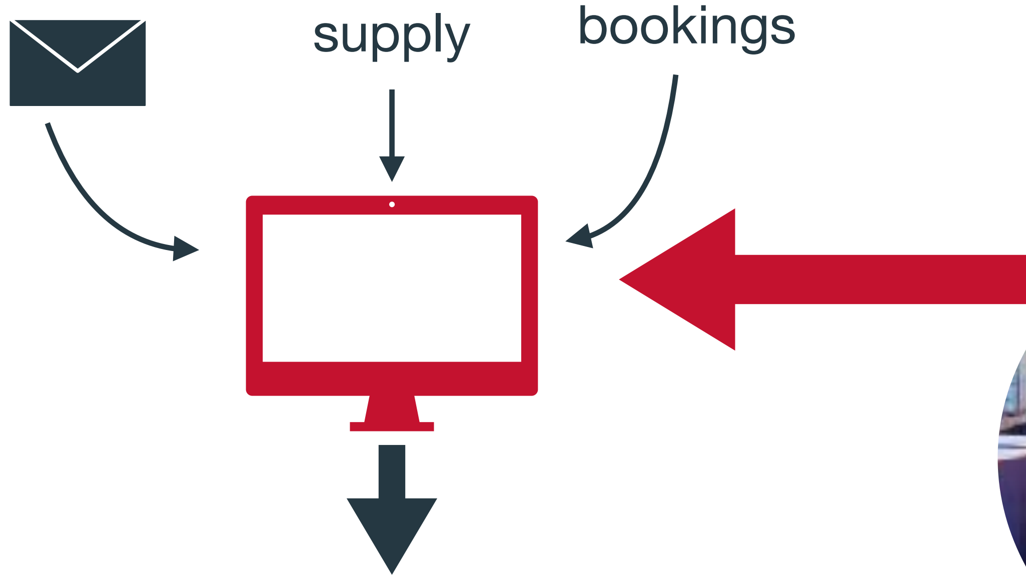
Short term
« operational »

Load planning for double-stack trains

Request

Railcar supply

Accepted bookings



Accept / reject

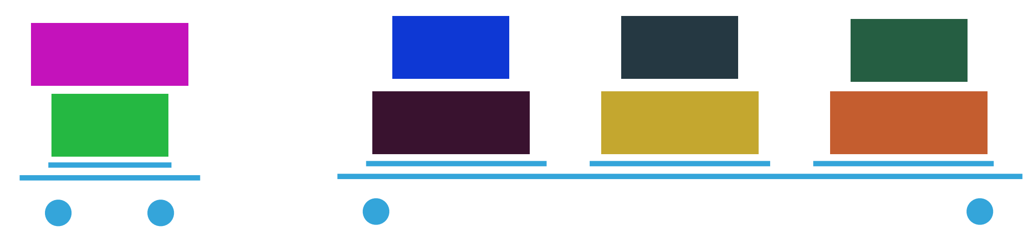
APPLICATION - LOAD PLANNING

Problem instance

$$\mathbf{x} = [\mathbf{x}_a, \mathbf{x}_u]$$

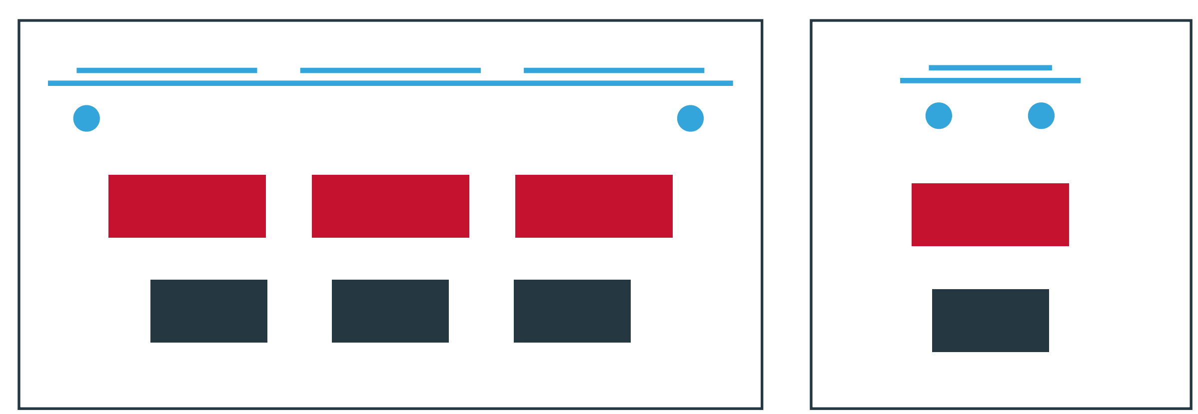
Operational solution

$$\mathbf{y}^*(\mathbf{x}) = \arg\min_{\mathbf{y} \in Y(\mathbf{x})} C(\mathbf{x}, \mathbf{y})$$



Tactical solution

$$\bar{\mathbf{y}}^* = g(\mathbf{y}^*(\mathbf{x}))$$



CN CHAIR IN OPTIMIZATION OF RAILWAY OPERATIONS

APPLICATION - LOAD PLANNING

- Containers have different characteristics, for example:
  - Size
  - Weight
- The loading (operational problem) of the containers onto railcars crucially depends on weight
- Weight is unknown at the tactical level

(c) Emma Frejinger emma.frejinger@cirrelt.ca

IDEA IN BRIEF

- We know how to solve the deterministic problem - let's use that!
  - Generate a lot of data and pretend that we have perfect information - solve the discrete optimization problem with an existing solver
- Let machine learning take care of the uncertain part: hide the information that is not available at prediction time - find best possible prediction of $\bar{\mathbf{y}}^*$

$$\widehat{\mathbf{y}}^*(\mathbf{x}_\mathrm{a}) \equiv f(\mathbf{x}_\mathrm{a};\boldsymbol{\theta})$$

State-of-the-art ML model　　Parameters

METHODOLOGY

Problem

Two-stage stochastic programming formulation

Optimal prediction conditional on $\mathbf{x}_a$, expectation over distribution of $\mathbf{x}_u$

Optimal solution to deterministic problem for given $\mathbf{x} = [\mathbf{x}_a, \mathbf{x}_u]$

Data

Problem instances and solutions (perfect information)

Machine learning training, validation, test data

Training & performance

Train and validate model

Assess predictive performance, e.g.

METHODOLOGY

Problem

$$\bar{\mathbf{y}}^*(\mathbf{x}_\mathrm{a}) :\equiv \arg \inf_{\bar{\mathbf{y}}(\mathbf{x}_\mathrm{a}) \in \bar{\mathcal{Y}}(\mathbf{x}_\mathrm{a})} \Phi_{\mathbf{x}_\mathrm{u}} \{ \|\bar{\mathbf{y}}(\mathbf{x}_\mathrm{a}) - g(\mathbf{y}^*(\mathbf{x}_\mathrm{a}, \mathbf{x}_\mathrm{u}))\| \mid \mathbf{x}_\mathrm{a} \}$$

$$\mathbf{y}^*(\mathbf{x}_\mathrm{a}, \mathbf{x}_\mathrm{u}) :\equiv \arg \inf_{\mathbf{y} \in \mathcal{Y}(\mathbf{x}_\mathrm{a}, \mathbf{x}_\mathrm{u})} C(\mathbf{x}_\mathrm{a}, \mathbf{x}_\mathrm{u}, \mathbf{y})$$

Data

Problem instances and solutions (perfect information)

Machine learning training, validation, test data

Training & performance

Train and validate model

Assess predictive performance, e.g.

METHODOLOGY

Problem

$$\bar{\mathbf{y}}^*(\mathbf{x}_\mathrm{a}) :\equiv \arg \inf_{\bar{\mathbf{y}}(\mathbf{x}_\mathrm{a}) \in \bar{\mathcal{Y}}(\mathbf{x}_\mathrm{a})} \Phi_{\mathbf{x}_\mathrm{u}} \{ \boxed{\|\bar{\mathbf{y}}(\mathbf{x}_\mathrm{a}) - g(\mathbf{y}^*(\mathbf{x}_\mathrm{a}, \mathbf{x}_\mathrm{u}))\|} \mid \mathbf{x}_\mathrm{a} \}$$

$$\boxed{\mathbf{y}^*(\mathbf{x}_\mathrm{a}, \mathbf{x}_\mathrm{u})} :\equiv \arg \inf_{\mathbf{y} \in \mathcal{Y}(\mathbf{x}_\mathrm{a}, \mathbf{x}_\mathrm{u})} C(\mathbf{x}_\mathrm{a}, \mathbf{x}_\mathrm{u}, \mathbf{y})$$

Data

Problem instances and solutions (perfect information)

$(\mathbf{x}^{(i)} , \mathbf{y}^{*(i)}) \quad i = 1,\ldots, m$

Machine learning training, validation, test data

$(\mathbf{x}_a^{(i)} , \bar{\mathbf{y}}^{*(i)}) \quad i = 1,\ldots, m$

Training & performance

Train and validate model

Assess predictive performance, e.g.

METHODOLOGY

Problem

$$\bar{\mathbf{y}}^*(\mathbf{x}_\mathrm{a}) :\equiv \arg \inf_{\bar{\mathbf{y}}(\mathbf{x}_\mathrm{a}) \in \bar{\mathcal{Y}}(\mathbf{x}_\mathrm{a})} \Phi_{\mathbf{x}_\mathrm{u}} \{ \boxed{\| \bar{\mathbf{y}}(\mathbf{x}_\mathrm{a}) - g(\mathbf{y}^*(\mathbf{x}_\mathrm{a}, \mathbf{x}_\mathrm{u})) \|} \mid \mathbf{x}_\mathrm{a} \}$$

$$\boxed{\mathbf{y}^*(\mathbf{x}_\mathrm{a}, \mathbf{x}_\mathrm{u})} :\equiv \arg \inf_{\mathbf{y} \in \mathcal{Y}(\mathbf{x}_\mathrm{a}, \mathbf{x}_\mathrm{u})} C(\mathbf{x}_\mathrm{a}, \mathbf{x}_\mathrm{u}, \mathbf{y})$$

Data

Problem instances and solutions (perfect information)

$$(\ \mathbf{x}^{(i)}\ ,\ \mathbf{y}^{*(i)}\ )\quad i = 1, \ldots, m$$

Machine learning training, validation, test data

$$(\ \widetilde{\mathbf{x}}_a^{(i)}\ ,\ \bar{\mathbf{y}}^{*(i)}\ )\quad i = 1, \ldots, m$$

Training & performance

Train and validate model

$$\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \frac{1}{m'} \sum_{i=1}^{m'} L\left(f(\mathbf{x}_a; \boldsymbol{\theta}), \bar{\mathbf{y}}^{*(i)}\right)$$

Assess predictive performance, e.g.

$$\mathbf{MAE}_{\mathbf{test}} = \frac{1}{n} \sum_{i=1}^{n} \left| f(\mathbf{x}_a^{(i)}; \hat{\boldsymbol{\theta}}) - \bar{\mathbf{y}}^{*(i)} \right|$$

(c) Emma Frejinger emma.frejinger@cirrelt.ca

METHODOLOGY

- **Data**
  - Historically observed instances and their solutions
    - Purpose: « mimic » behaviour in such data
  - Our approach: generate data by sampling problem instances and computing the corresponding solutions using existing optimization model and solver
    - Purpose: generalization over the domain of $\mathbf{x}$
- The **input structure** is governed by the information available at prediction time
- The **output structure** is governed by the choice of solution description and can be of fixed or variable size
- **Model architecture** depends on input and output structures and on constraints linking the two

RELATED LITERATURE

- Closest to our work are those based on supervised learning but they focus on deterministic problems
  - Fischetti and Fraccaro (2017) predict optimal objective function value
  - Vinyals et al. (2015) define pointer networks to solve a class of discrete optimization problems, constraints are imposed by changing the NMT model architecture
- Nair et al. (2017) propose a reinforcement learning algorithm combined with ILP solver for a two-stage binary stochastic program (unconstrained binary decisions)

DATA GENERATION

- Random sampling of container/railcar types and container weights

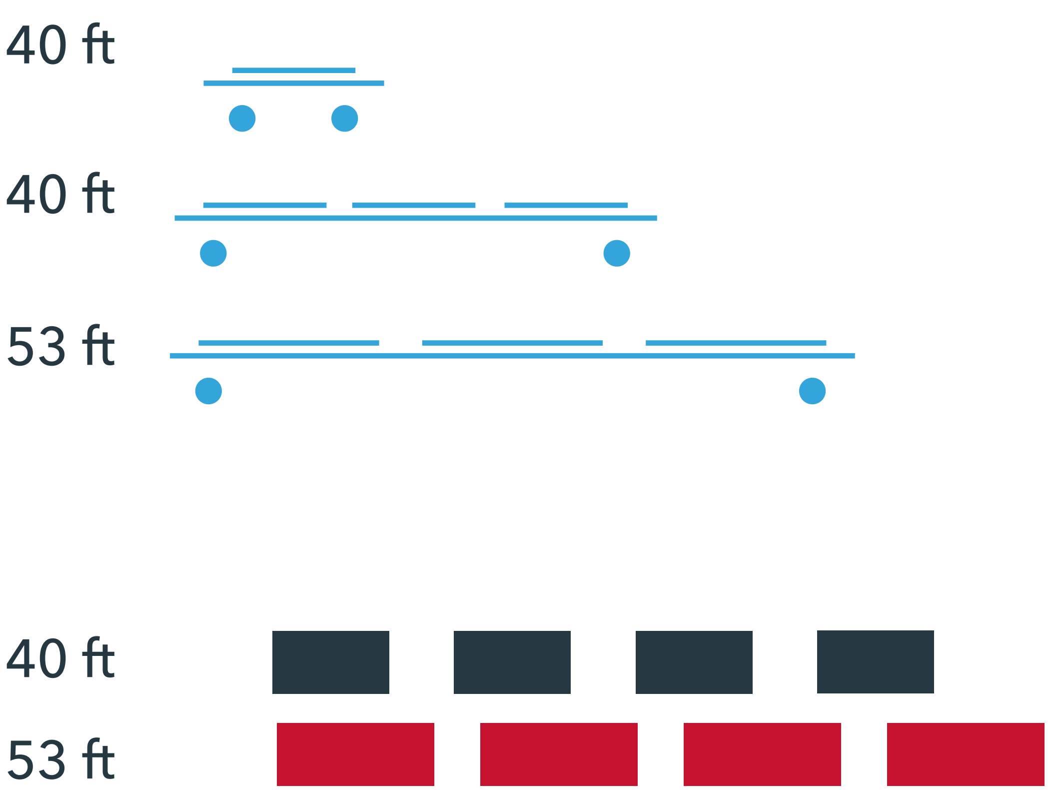
Class	Description	# of containers	# of platforms
A	Simple ILP	[1,150]	[1,50]
B	More containers than A (excess demand)	[151,300]	[1,50]
C	More platforms than A (excess supply)	[1,150]	[51,100]
D	Larger and harder	[151,300]	[51,100]

INPUT-OUTPUT

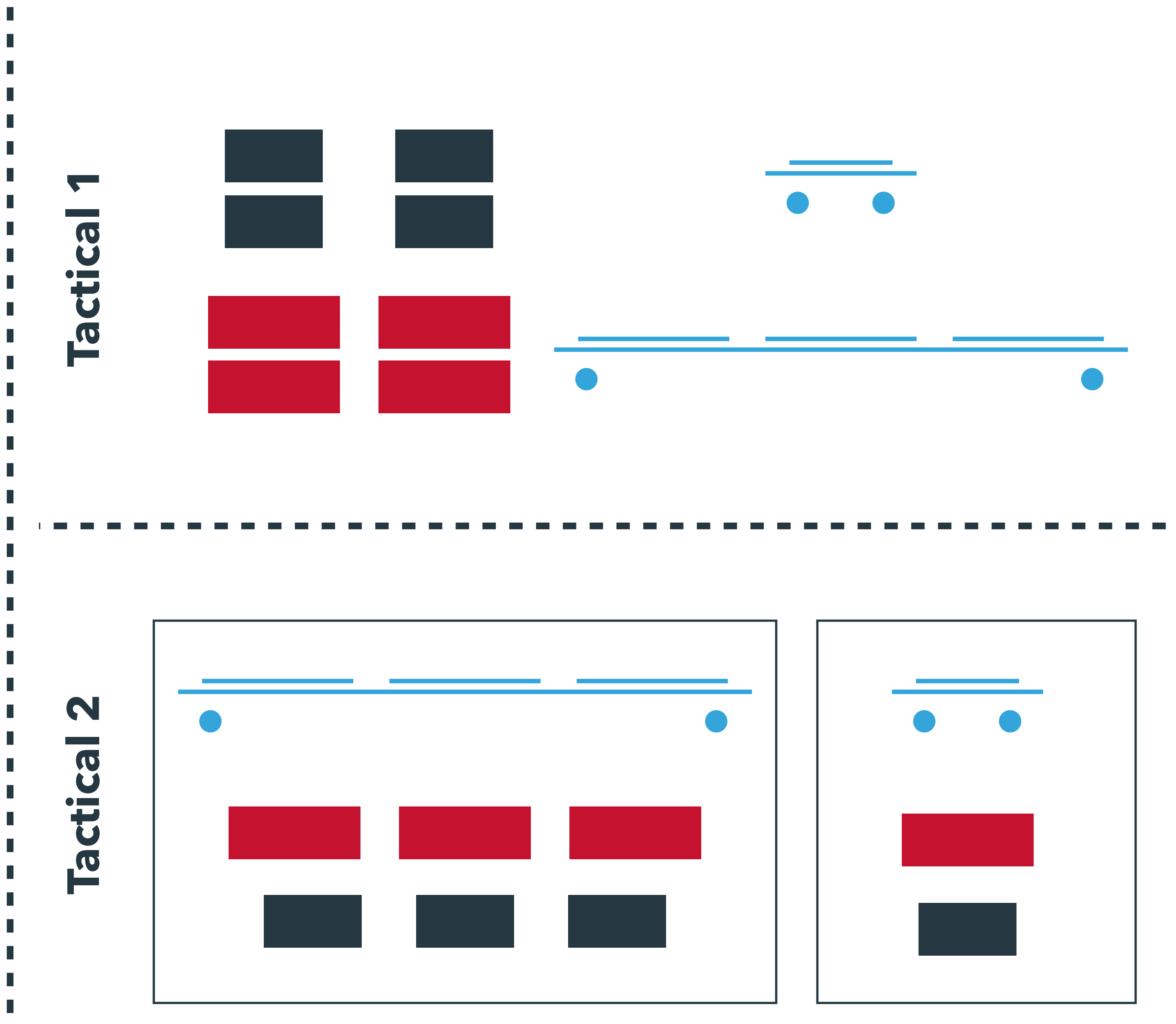
Input: problem instance

2 container types: 40 and 53 ft

10 railcar types: 10 most numerous in the North American fleet



Output: tactical solution



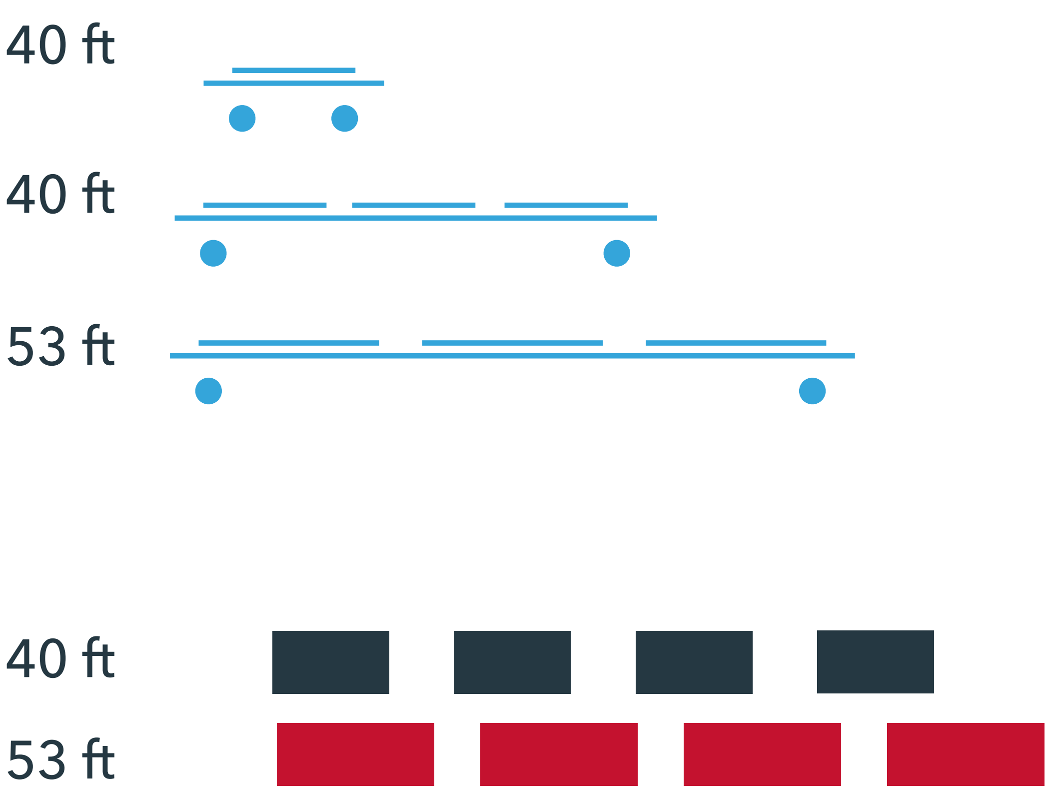
(c) Emma Frejinger emma.frejinger@cirrelt.ca

INPUT-OUTPUT

Input: problem instance

2 container types: 40 and 53 ft

10 railcar types: 10 most numerous in the North American fleet



Output: tactical solution

TACTICAL 1:
MULTILAYER PERCEPTRON /
FEED-FORWARD NETWORK

TACTICAL 2:
NEURAL MACHINE TRANSLATION (NMT) MODEL

(c) Emma Frejinger emma.frejinger@cirrelt.ca

TACTICAL 1: MULTILAYER PERCEPTRON

Input

Fixed-size vector

$\mathbf{x}_a$

Output

Fixed-size vector

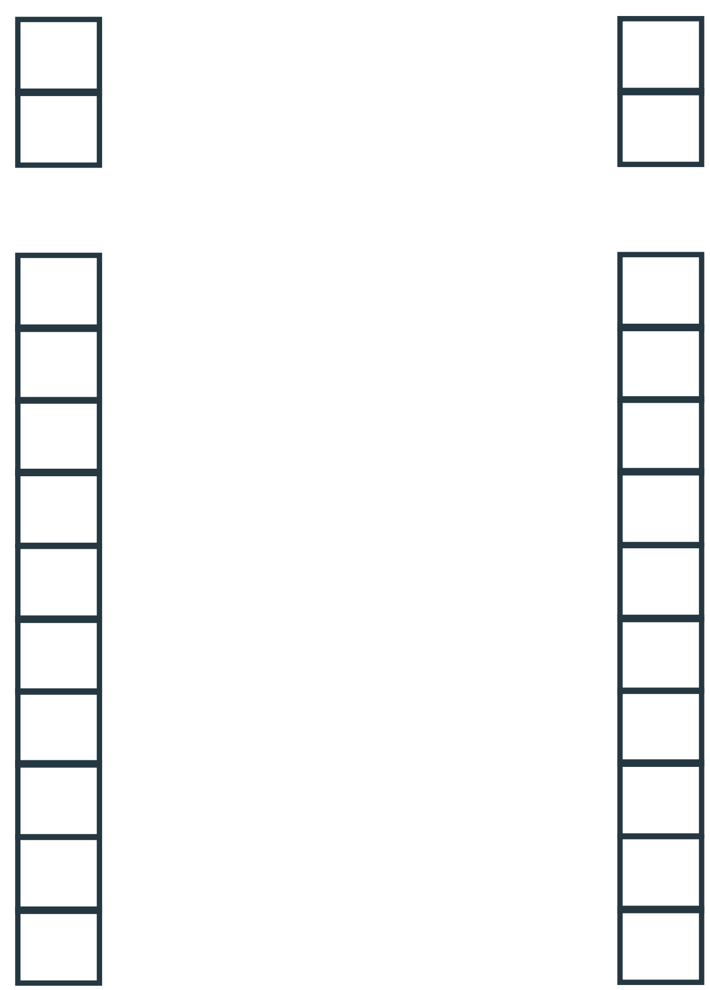
$\bar{\mathbf{y}}^*$

Nb of assignable containers of each type

Nb of containers of each type in the solution

Nb of of assignable railcars of each type

Nb of railcars of each type in the solution



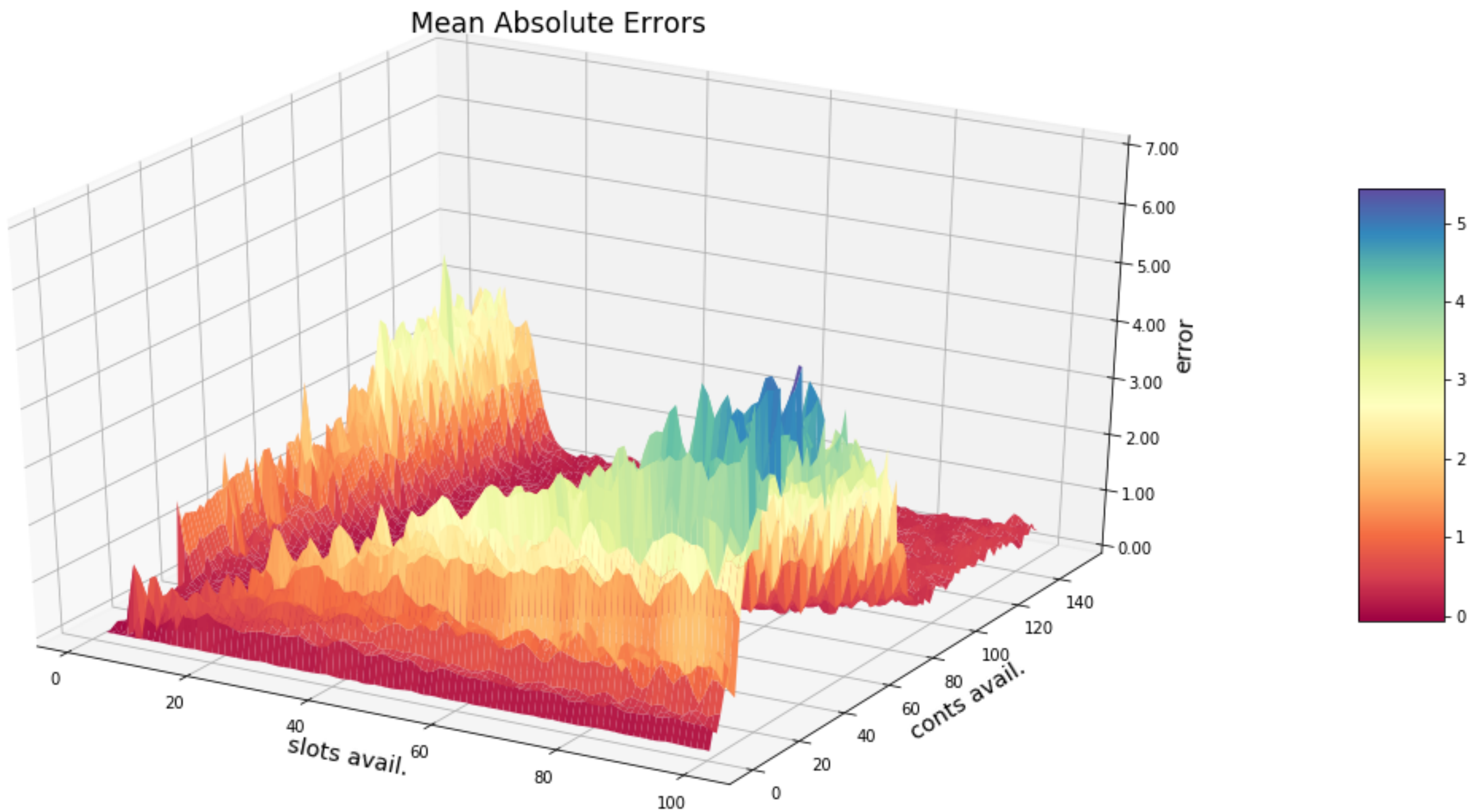
TACTICAL 1: MULTILAYER PERCEPTRON

- Multilayer perceptron (MLP): approximately 7 layers and 500 rectified linear units (ReLU) per layer (hyper parameters)
- Classification / Regression (linear units in output layer and rounding to the nearest integer)
- **Training** and **validation**
  - Minimization of neg. likelihood function / sum of absolute errors
  - Mini-batch stochastic gradient descent and learning rate adaptation by the adaptive moment estimation (Adam) method
  - Regularization: early stopping
  - Random search for hyper parameter selection
- Mean Absolute Error (MAE) over slots and containers

TACTICAL 1: MULTILAYER PERCEPTRON

- Average performance of the MLP model is very good
  - **MAE** of only **2.1 containers/slots** for classes A, B and C (up to 100 platforms and 300 containers) with very small standard deviation (0.01)
- MLP results are considerably **better than benchmarks**
- The marginal value of using 100 times more observations is fairly small: modest increase in MAE from 0.985 to 1.304 on class A instances)
- **Prediction times are negligible**, milliseconds or less and with very little variation

TACTICAL 1: MULTILAYER PERCEPTRON



TACTICAL 1: MULTILAYER PERCEPTRON

- The models trained and validated on simpler instances (A, B and C) generalize well to harder instances (D)
  - MAE of 2.85 (training on class A)
  - MAE of 0.32 (training on classes A, B and C)
  - Important variability across models with different hyper parameters when only trained on class A (MAE varies between 0.74 and 9.05)
- Numerical analysis of **feasibility**: there exists a feasible operational solution for a given predicted tactical solution in 96.6% of the instances (the share is much lower for the benchmarks)

TACTICAL 1: MULTILAYER PERCEPTRON

What if we solve a sample average approximation (SAA) of the two stage stochastic program?

- Class A instances
- The average absolute error of the SAA solution is similar to that of the ML algorithm: 0.82 compared to 0.985
- The computing times for SAA vary between 1 second to 4 minutes with an average of 1 minute

TACTICAL 2: NMT MODEL

PLEASE CONTACT EMMA FREJINGER IF YOU'RE INTERESTED IN THIS TOPIC.
THESE SLIDES ARE LEFT OUT FROM THE PUBLICLY SHARED VERSION OF THE PRESENTATION BECAUSE THE RESULTS HAVE NOT BEEN PUBLISHED.
EMMA.FREJINGER@CIRRELT.CA

Conclusion and perspectives

Novel combinations of **machine learning** and **operations research** methodologies have potential to solve hard decision-making problems under imperfect information.

We presented such a **methodology** that allows to predict solutions to a decision-making problem in very **short computing time**.

A lot of **research** left to be done and numerous **applications** to explore.

Thank you!

emma.frejinger@cirrelt.ca