

# On the role of (machine) learning in (mathematical) optimization

Andrea Lodi

Canada Excellence Research Chair  
École Polytechnique de Montréal, Québec, Canada  
`andrea.lodi@polymtl.ca`

CPAIOR 2017

@ Padova, (Italy), June 6, 2017

CANADA  
EXCELLENCE  
RESEARCH  
CHAIR



**DATA SCIENCE  
FOR REAL-TIME  
DECISION-MAKING**

- 1 Two of my favorite examples of **Big Data**
- 2 Something I do find interesting in **Big Data**:
  - 1 New (business) models
  - 2 Formulating and solving **integrated models**
- 3 The role of **learning**:
  - 1 An example in **Retail**
  - 2 **Machine Learning** paradigm
- 4 Machine **Learning** and Mathematical **Optimization**:
  - Q1: What can (Integer) Optimization do for Machine Learning?
  - Q2: **What can Machine Learning do for Optimization?**
  - Q3: What's new by the combination of Learning and Optimization?
- 5 Conclusions

## Ex. 1: automatic data collection (aka nowhere to hide)

A **face recognition system** has been put in place in a **mall** somewhere in the US.

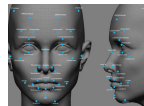
Main purpose of the system was **security**.

After collecting data for some time, it has been observed that the large **majority of the clients** entering in the mall around **lunch time** (11 AM - 3 PM) was composed by **Asian-American** people.

The company owning the mall implemented **two simple actions**:

- **revised the shifts** of the employees so as that (most of) the Asian-American ones were on duty in that time window;
- **hired** new Asian-American employees.

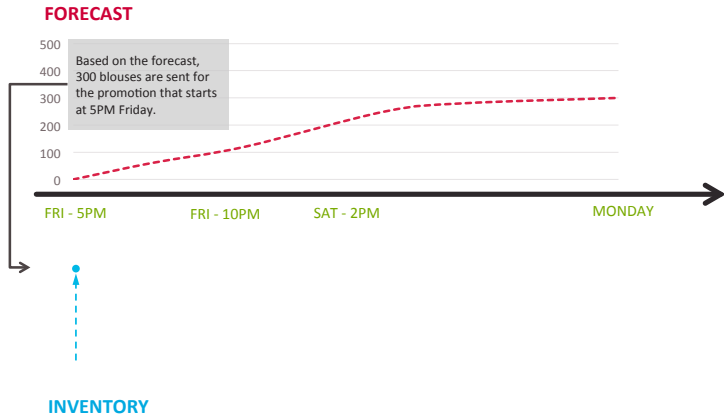
The overall effect has been a huge **increase in sales**.



# Ex. 2: integrated decision support

## Promotions Execution Integrated Real-time Decision Support

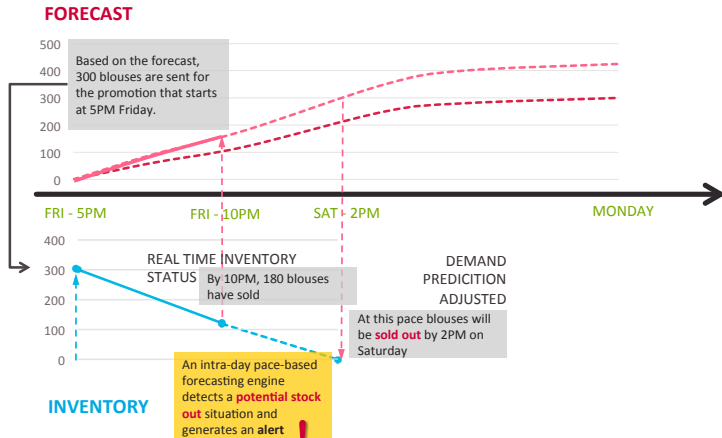
jda.



# Ex. 2: integrated decision support

## Promotions Execution Integrated Real-time Decision Support

jda.



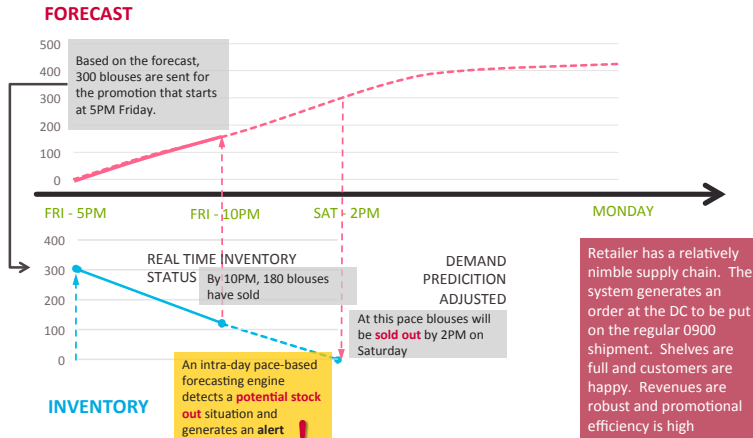
Copyright © 2014 JDA Software Group, Inc. Confidential

21

# Ex. 2: integrated decision support

## Promotions Execution Integrated Real-time Decision Support

jda.



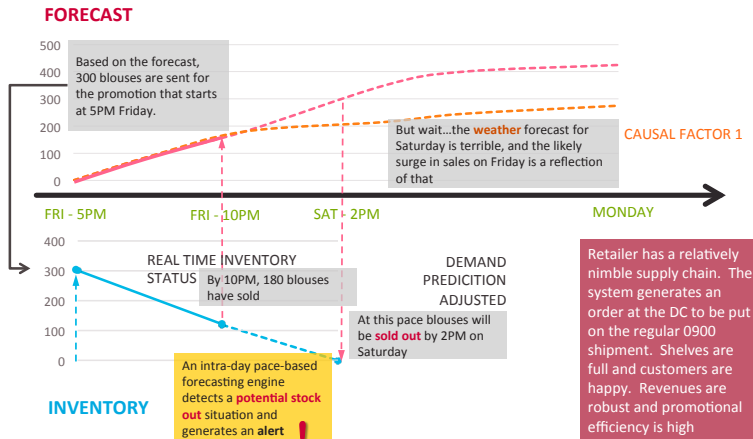
Copyright © 2014 JDA Software Group, Inc. Confidential

22

# Ex. 2: integrated decision support

## Promotions Execution Integrated Real-time Decision Support

jda.



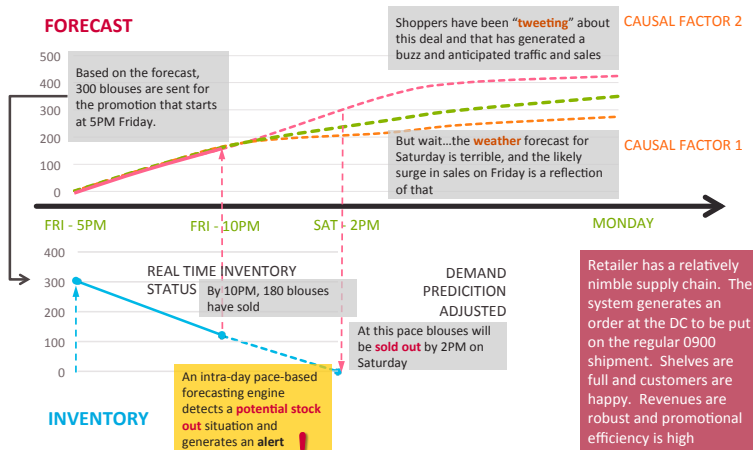
Copyright © 2014 JDA Software Group, Inc. Confidential

23

# Ex. 2: integrated decision support

## Promotions Execution Integrated Real-time Decision Support

jda.



Copyright © 2014 JDA Software Group, Inc. Confidential

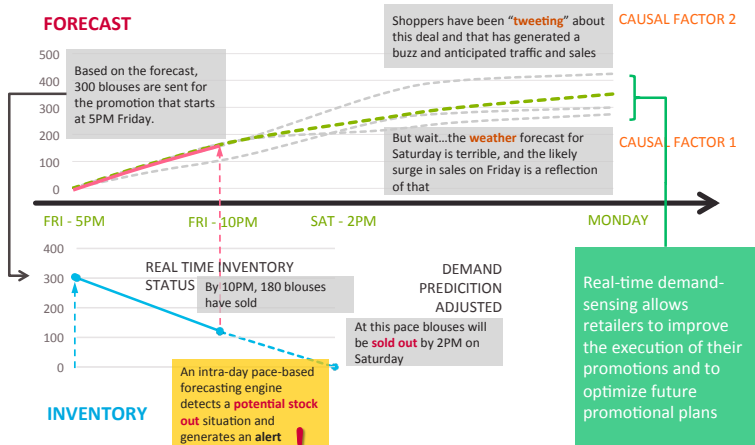
24



# Ex. 2: integrated decision support

## Promotions Execution Integrated Real-time Decision Support

jda.



Copyright © 2014 JDA Software Group, Inc. Confidential

25

[Côté, 2015]

# What I like of Big Data

The first example shows that **automatic collection of data** can lead to the definition of **new** (optimization) problems.

Disseminating **sensors** (including mobile devices) **everywhere** has become **cheap** (and **cool!**) but the real challenge is **taking decisions** over the collected (complex) data.

It is not completely clear if the (applied) **optimization problems** we were used to solve in contexts as diverse as routing, supply chain and logistics, energy, telecommunications, etc. are still there or, instead, **have radically changed**.

The spirit of **such a change** is shown by the second example: the **end-users behavior/preference** is putting more and more **pressure on the decision makers** and, by transitivity, **on the optimizers**. This is not true only in the retail industry but virtually in any other in which **a service is delivered**:

- **routing**, I can check with my mobile device where cabs/buses are located;
- **traffic management**, I am aware of congestions, accidents, etc. in the city;
- **cache allocation for video streaming**, complaints escalate in real time.

# What I like of Big Data (cont.d)

The most significant effect of considering the **end-users behavior** is that **complex systems** that have been traditionally **split into smaller parts**, optimized sequentially, now need to be tackled in an integrated fashion.

**Splitting** was happening **because of**

- 1 **difficulty and cost of collecting reliable data** for the entire system
- 2 **the size of the decision problems** associated with considering the entire system would have been **too large**
- 3 there was very **little perception** both among the industrial players and among the end-users **that splitting was avoidable**.

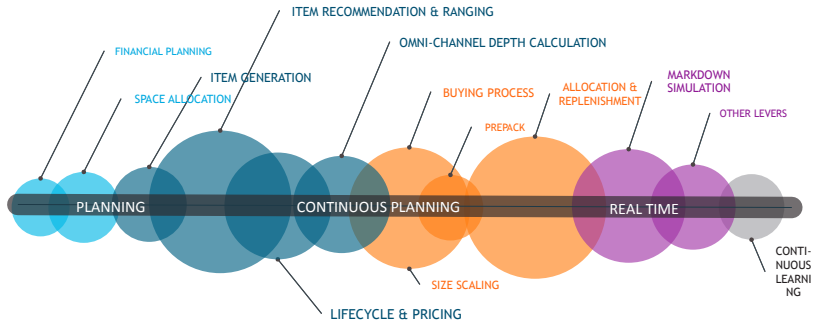
Lack of **technological communication**:

- the **different divisions** of, say, a firm, had **little data exchange**, and
- the end-user had **no mobile technology to be updated in real time**.

Mobile technology has **urged the request of integrated approaches** for decision making because of the **perception of missing opportunities**.

This is true in **energy** as well, where **smart meters** and **smart buildings** (producing energy as well as consuming it) are increasing **end-users' awareness** and pushing for more (**integrated**) **optimization**.

# Integrated models: (the dream of) big data in retail



# The role of learning

From an **optimization perspective**, formulating and solving those integrated models **is**, of course, **hard**.

This is because of

- 1 **volume**
- 2 **velocity**
- 3 **variety**

of the data, and also because **optimizers are not** – in general – **trained for that**.

One answer to this is introducing into the picture some **learning mechanisms** that allow to **treat data**, often **reducing their volume and variety**, and to take into account the **end-user perspective/behavior**.

In the retail context, one needs to **predict the sales** of a certain **product**, on a certain **shop location**, in a certain **season**, to a certain **segment of shoppers**.

**Learning from historical data** allows to compute a **score** associated with these choices and the **optimization** problem associated with the **assortment** can be **solved only after** these scores are computed.

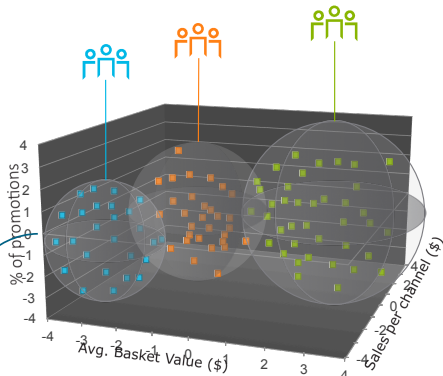
## Shopper Segmentation

jda.

- > Segments are created based on behaviors and preferences that bring value to the business
- > These variables must reveal opportunities for action, to be able to bring segmentation to tangible outcomes.

CLUSTERING ALGORITHM

FEATURES ENGINEERING



# Ex. 3: taking into account the end-user (cont.d)

## Attribute Based Forecasting

jda.

ITEMS  
ATTRIBUTES  
VALUES



LOCATIONS  
ATTRIBUTES  
VALUES



SEASONS  
ATTRIBUTES  
VALUES



SHOPPERS  
SEGMENTS



User judgment

Linear regressions on attributes

Neural networks

Random forests

Computerized adaptive testing

Support vector machine

...



Never seen product



|  |            |
|--|------------|
| Brand                                    | SuperClean |
| Fragrance                                | Fruits     |
| Price Band                               | Good       |
| Size                                     | Small      |
| Sales in Store A, for Segment A, in 2015 | ?          |

51

[Côté (2015)]

# Machine Learning

Generally speaking, **Machine Learning** is a collection of techniques for **learning patterns in or understanding the structure of data**, often with the aim of performing data mining, i.e., recovering **previously unknown, actionable information** from the learnt data.

Typically, in ML one has to “**learn**” from data (points in the so-called **training set**) a (nonlinear) **function** that **predicts a certain score** for new data points that are not in the training set.

Each data point is represented by a set of **features**, which define its characteristics, and **whose patterns should be learnt**.

The **techniques** used in ML **are diverse**, going from artificial neural networks, to first order methods like gradient descent, to convex optimization, etc.





# ML & Mathematical Optimization

I believe big data applications call for the **integration between** Machine Learning and Mathematical **Optimization**.

But, **how** such an integration should go?

And, what about **Mixed-Integer Programming** (MIP) specifically?

Of course, the **easiest integration** is already shown in the examples above, where **raw data** are “**crunched**” and “**prepared**” by Machine Learning to construct the decision model on which Mathematical Optimization is applied.

However, the integration is **not restricted** to let ML and MP work in **cascade**.

Modern ML paradigms like **deep learning** (essentially, learning by multiple layers) are facing more and **more complicated structures** in which the **features** (raw data observations) are **not kept fixed** but are “**transformed**” within the learning process.

Those **transformations** involve highly **nonconvex functions** and **discrete decisions**.

## March 2016: World Go Champion Beaten by Machine



# Q1: What can (integer) Optimization do for ML?

Discrete decisions have been disregarded so far in ML.

This is certainly due to the (negative) perception that were not affordable in practical computation (ML has always been concerned with large volumes of data) but it was also related to the fact that the parameters to be learnt were inherently continuous.

This might be less true in modern paradigms, those that led ML to contribute to the advances in computer vision, signal processing and speech recognition.

Moreover, there seems to be large room for using discrete variables to formulate nonconvexities that appear more and more to be crucial in ML.

# Q1: Discrete decisions in Support Vector Machine

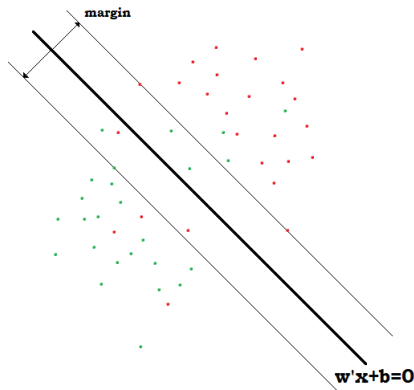
## Ramp Loss

$$\min \frac{\omega^\top \omega}{2} + \frac{C}{n} \sum_{i=1}^n \xi_i$$

$$y_i(\omega^\top x_i + b) \geq 1 - \xi_i \quad \forall i = 1, \dots, n$$

$$0 \leq \xi_i \quad \forall i = 1, \dots, n$$

$$\omega \in \mathbb{R}^d, b \in \mathbb{R}$$



# Q1: Discrete decisions in SVM (cont.d)

Ramp Loss  $g(\xi_i) = (\min\{\xi_i, 2\})^+$

$$\min \frac{\omega^\top \omega}{2} + \frac{C}{n} \left( \sum_{i=1}^n \xi_i + 2 \sum_{i=1}^n z_i \right)$$

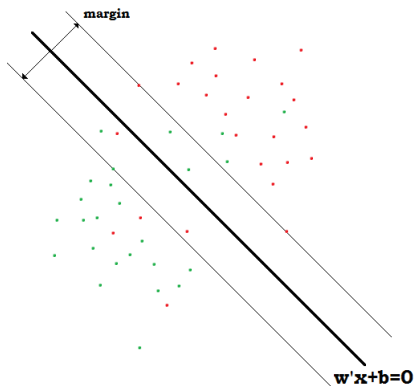
$$y_i(\omega^\top x_i + b) \geq 1 - \xi_i - Mz_i \quad \forall i = 1, \dots, n$$

$$0 \leq \xi_i \leq 2 \quad \forall i = 1, \dots, n$$

$$\omega \in \mathbb{R}^d, b \in \mathbb{R}$$

$$z \in \{0, 1\}^n$$

with  $M > 0$  big enough constant.



[Brooks (2011)]

Sophisticated methods for dealing with big- $M$  constraints in MIP have been recently devised and integrated within the IBM-Cplex solver, so as decent-size SVM instances above can now be routinely solved to optimality.

[Belotti, Bonami, Fischetti, Lodi, Monaci, Nogales & Salvagnin (2016)]

# Q1: What can (integer) Optimization do for ML? (cont.d)

The described one is **just one example** of a potential area of interaction:

- 1 there are ML problems that are **naturally casted as MIPs**,
- 2 there is a bunch of work to try to **solve them NOT as MIPs**,
- 3 maybe there is something to be **gained in treating them as MIPs!**

Other examples are in **semi-supervised SVM** and its **multi-category generalizations**.  
[Bennett & Demiriz (1998), Lodi & Pouliot (working paper)]

An additional area of interaction is the so-called **hyper-parameter optimization**, where the parameters of a (deep) **neural network** have to be **optimized** so as to make the learning effective.  
[Audet & Orban (2007, ...)]

MIP (mostly, **Combinatorial Optimization**) **sub-structure** are present in **Structured Prediction** problems. Namely, these are the ML problems in which some **constraints on the structure of the prediction** have to be satisfied.

A classical example is **word alignment** (a key step in **machine translation**), where **matching and transportation** structures can be effectively exploited.  
[Lacoste-Julien et al. (2006, 2013, ...)]

# Q1: Learning by Column Generation

Besides formulating learning / classification problems by IP, one can apply **sophisticated IP techniques** to the learning phase.

This is the case of **training a choice model** in assortment optimization, where given a subset of the **consumer's behaviors**, one has to find the **probability distribution** ( $\lambda_k$ ) that explains at best the training set, i.e., the **observed sales**.

This can be done in a very elegant way by **Column Generation**

$$\begin{aligned} \min_{\lambda, \epsilon^+, \epsilon^-} \quad & \mathbf{1}^T \epsilon^+ + \mathbf{1}^T \epsilon^- \\ \text{s.t.} \quad & A\lambda + \mathbf{1}^T \epsilon^+ - \mathbf{1}^T \epsilon^- = v \quad (\alpha) \\ & \mathbf{1}^T \lambda = 1 \quad (\nu) \\ & \lambda, \epsilon^+, \epsilon^- \geq 0 \end{aligned}$$

[Bertsimas and Misis (2015)]

and the challenge is to make it **practical for relevant sizes** of the number of products.

[Jena, Lodi and Palmer (2017)]



## Q2: What can ML do for (Integer) Optimization?

A fast growing literature has started to appear in the last **5 to 10 years** on the use of **Machine Learning techniques to help** Optimization, especially **MIP solvers**. Among the first in these series, the papers on **tuning MIP solvers**.  
[Hoos et al. (2010+)]

ML has, of course, started to be used within **Constraint Programming** as well, including Neural Networks and Decision Trees. [Lombardi & Milano (2015+)]

Learning when to use a decomposition.  
[Kruber, Lübbecke, Parmentier (2017): tomorrow!]

MIP solvers are **complex software** objects implementing a large variety of algorithmic approaches. **Strategic decisions** on how to **combine those approaches** in the most effective way have to be **taken over and over**. **Such decisions** are taken **heuristically**, often breaking ties in architecture-dependent ways, thus showing the **heuristic nature of MIP implementations**. [Lodi (2012)]

ML can help **systematize the process** that leads to take these decisions, especially when a **large quantity of data** can be collected.

## Q2: Variable selection in Branch and Bound

**Branch-and-Bound** algorithm (B&B):

- most **widely used** procedure for solving (Mixed-)Integer Programming problems
- **implicit enumeration** search, mapped into a decision tree
- leave (at least) two big choices:
  1. How to **split** a problem into subproblems (**variable selection**)
  2. Which **node/subproblem to select** for the next exploration

*... decisions play a key role for the algorithm efficiency!*

- as of today, **decisions** are made **heuristically** and **empirically evaluated**
- there are good branching strategies, but usually very costly

**Ultimate goal** (details to be discussed in slot #4)

---

Use ML to learn an **activation function** that can be adopted as approximation / prediction of a good B&B strategy, ideally with a **low computational cost**.

---

[Alvarez, Wehenkel & Louveaux (2016), Khalil, Le Bodic, Song, Nemhauser & Dilkina (2016)]

## Q2: MIQPs classification

We consider **Mixed-Integer Quadratic Programming** (MIQP)

$$\begin{aligned} \min \quad & \frac{1}{2}x^T Qx + c^T x \\ & Ax = b \\ & x_i \in \{0, 1\} \quad \forall i \in I \\ & l \leq x \leq u \end{aligned} \tag{1}$$

where  $Q = \{q_{ij}\}_{i,j=1\dots n} \in \mathbb{R}^{n \times n}$  is a real symmetric matrix, either convex or nonconvex, and all integer variables are binary.

Depending on the problems' structure, we can tackle them in different ways:

- $Q \succeq 0$ : perform **NLP based B&B** (or Outer Approximation algorithms)
- $Q \not\succeq 0$ : depending on variables' type,
  - pure 0-1: transform into either a **convex MIQP** or into a **MILP** (i.e., **linearize it**)
  - mixed: perform **Q-space reformulation/relaxation**, run Global Optimization algorithms (Spatial B&B)

## Q2: MIQPs classification (cont.d)

The **linearization approach** seems beneficial also for the convex case, both for pure 0-1 and mixed problems. However, **is linearizing always the best choice?**

*“[...] when one looks at a broader variety of test problems the decision to linearize (vs. not linearize) does not appear so clear-cut.”<sup>1</sup>”*

---

Exploit ML predictive machinery to understand whether it is favorable to linearize the quadratic part of the MIQP or not

---

- Learn an **offline classifier** predicting the most suited resolution approach within IBM-CPLEX framework (`qtoLin` linearization switch parameter)
- Gain **theoretical insights** about which features of the MIQPs most affect the prediction

[Bonami, Lodi, Zarpellon (working paper)]

---

<sup>1</sup>Fourer B. Quadratic Optimization Mysteries, Part 2: Two Formulations.

<http://bob4er.blogspot.com/2015/03/quadratic-optimization-mysteries-part-2.html>

## Q2: MIQPs classification - Dataset generation

... traditional benchmark sets are too small for learning!

We define and implement a **generator of MIQP instances**, spanning a variety of structural parameters and optimization components.

- (I) **Objective function data generation**: real symmetric matrices are generated via the `MATLAB` function

```
Q = sprandsym(size, density, eigenvalues)
```

- (II) **Variables' type definition**: binary / continuous variables are added to the problems with respect to the sign of  $Q$ , in different proportions
  - (III) **Constraints generation**: different constraints sets are added accordingly to the type of variables of the problem (e.g., cardinality, simplex, multi-dimensional knapsack)
- Dataset of 2300 instances, three types of MIQPs (0-1 convex, 0-1 nonconvex, mixed convex)
  - Plan to compare with traditional benchmark libraries for test / extensions

## Q2: MIQPs classification - Features design

We define a set of 23 features referring to an MIQP instance, and we divide them into two main blocks:

- **Static features** describe the **mathematical characteristics** of the instance, in terms of
  - variables - e.g., number, types, presence in constraints and objective
  - constraints - e.g., coefficients and variables presence
  - **quadratic objective function** - e.g., coefficients, variables presence, sparsity, spectral properties

They are extracted via `Cplex/Python` before any solving (pre)process takes place.

- **Dynamic features** describe the **initial behavior** with respect to different resolution methods.
  - e.g., bounds and solution times at the root node

They are extracted from the early stages of the optimization, after the preprocessing and the resolution of the root node relaxation.

## Q2: MIQPs classification - Labeling procedure

One of three different labels among  $\{L, NL, T\}$  can be assigned to a MIQP instance, describing the winner between *linearize*, *not-linearize* or the case of a *tie* of the two methods.

Each problem of the dataset is run with timelimit of 1h, for 5 different random seeds, with `qtolin` on and off.

To address solvability / consistency issues, we perform

- **Solvability check**, to discard never-solved instances
- **Seed consistency check** on each seed, to discard unstable instances w.r.t. the found upper and lower bounds
- **Global consistency check** on global best upper and lower bounds, to discard unstable instances

Running time is the ultimate compared measure, assessing the final label for each example.

## Q2: MIQPs classification - Learning experiments

Instances, features and labels give a dataset ready for supervised learning:

$$\{(x^i, y^i)\}_{i=1..N} \quad \text{where } x^i \in \mathbb{R}^d, y \in \{L, NL, T\} \quad \text{for } N \text{ MIQPs}$$

**Multiclass classifiers** such as

- Support Vector Machines (nonlinear RBF kernel) (SVM)

and ensemble methods based on Decision Trees (more interpretable than Neural Networks), such as

- Random Forests (RF)
- Extremely Randomized Trees (EXT)
- Gradient Tree Boosting (GTB)

**Methodology:** follow ML best practices to avoid overfitting

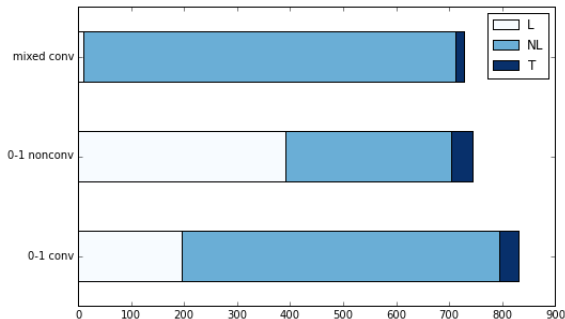
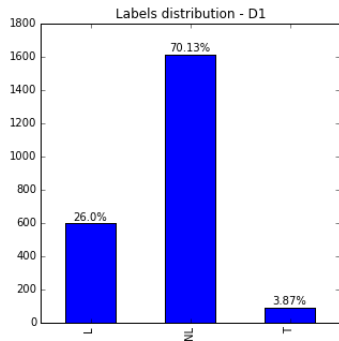
- **Training** phase to optimize parameters (1725 instances)
- $k$ -fold cross **validation** and grid search for hyper-parameters selection
- **Test** phase to assess classifiers' performance (575 instances)

Main implementation tool: `scikit-learn` library.



## Q2: MIQPs classification - Nutshell analysis

Before learning, look into the dataset! In a nutshell:



- Take care of **unbalanced data** in the learning procedure
- Can some **trends** already been recognized w.r.t. different problem types?
- More **(statistical) analyses** on features and data distribution

## Q2: MIQPs classification - Some results

Classifiers perform well with respect to **traditional classification measures**

|           | SVM  | RF   | EXT  | GTB  |
|-----------|------|------|------|------|
| Accuracy  | 0.85 | 0.89 | 0.85 | 0.87 |
| Precision | 0.82 | 0.87 | 0.82 | 0.85 |
| Recall    | 0.85 | 0.89 | 0.85 | 0.87 |
| F1 score  | 0.83 | 0.87 | 0.84 | 0.86 |

Are our predictors leading to a sensible **gain in running times**?

- For each example, depending on the predicted label, select the predicted mode (L, NL, T) running time. Take the shifted geometric mean of the prescribed times and normalize it w.r.t. the a posteriori best and worst labeling, to get a **timing score**  $\in [0, 1]$

|              | RF   | CPLEX default |
|--------------|------|---------------|
| Timing score | 0.99 | 0.48          |

## Q2: MIQPs classification - Going further

Deepen the **features analysis**:

- At a glance, **dynamic features** and static ones about **eigenvalues** are very important for the predictions

What about **other datasets**?

- First attempt on (part of) **CPLEX internal testbed** as new test set
- All **classifiers perform poorly** in terms of classification measures, but not so bad in terms of timing score

|              | RF   | EXT  | CPLEX default |
|--------------|------|------|---------------|
| Timing score | 0.89 | 0.91 | <b>0.96</b>   |

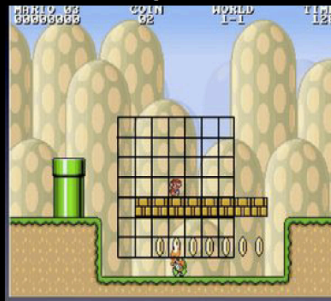
- Why? **Very different distribution** of features, problems types and labels w.r.t. the synthetic dataset, on which the predictors were trained

... there is much more to understand and test!

## Q2: Learning to Search

From Mario AI competition 2009

Input:



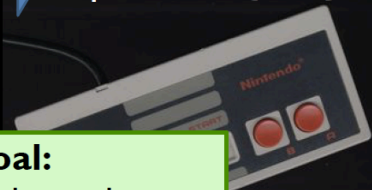
Output:

Jump in  $\{0,1\}$   
Right in  $\{0,1\}$   
Left in  $\{0,1\}$   
Speed in  $\{0,1\}$



**High level goal:**

Watch an expert play and  
learn to mimic her behavior



[Langford and Daumé III, 2015]

# Q3: The power of ML & Optimization together

Why are **learning** and **optimization** two faces of the same coin?

A nice example comes in **healthcare**, for the so-called **personalized medicine**.

ML could be used to **predict the medical outcome** that would follow from a **particular choice of combination and dosage of different drugs and treatments** for a patient over the course of a few months to come.

However, there could be an **exponential number of such combinations** to consider, and **constraints** to be satisfied (for example, because of known side-effects and resources).

**Exhaustively searching** in the space of such combinations is and will always be **unpractical** and mathematical optimization is likely to be the answer.

A **new methodology** integrating learning and optimization is **required**, and such a methodology is likely to be useful every time the **space of predictions** faces **combinatorial explosion**.

# Conclusions

We have discussed a **few important issues** arising in **big data (optimization)**, namely

- the change of perspective associated with dealing with the **end-users behavior**,
- the need of formulating and solving **integrated models**, and
- the **role of (machine) learning**.

I am an **optimistic person**, so I see **huge opportunities** through the interaction between Machine Learning and Mathematical Optimization, **including / especially on the Integer Programming side**.

There is plenty of room for **contributing** to the subject and ...

... getting on board in Montréal!

CANADA  
EXCELLENCE  
RESEARCH  
CHAIR

**DATA SCIENCE  
FOR REAL-TIME  
DECISION-MAKING**

MILA

**IVADO**  
INSTITUTE FOR DATA VALORISATION

The image features a black background with several logos. On the left, there is a logo consisting of a cluster of blue circles of varying sizes next to a grid of blue triangles. In the center, the word "MILA" is written in a light blue, sans-serif font. Above "MILA" is the text "CANADA EXCELLENCE RESEARCH CHAIR" in white. To the right of this text is a circular logo with a colorful geometric pattern of squares in shades of blue, green, and purple. Further right is the text "DATA SCIENCE FOR REAL-TIME DECISION-MAKING" in white, with "DATA SCIENCE" and "DECISION-MAKING" in a larger font. Below "MILA" is a colorful, multi-colored starburst logo. At the bottom right is the "IVADO" logo in white, with "INSTITUTE FOR DATA VALORISATION" written in smaller white text below it.