Optimization meets Machine Learning

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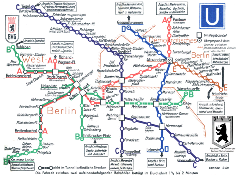
OR 2017 · Berlin · September 6, 2017

Optimization is Everywhere



Machine Learning is Everywhere

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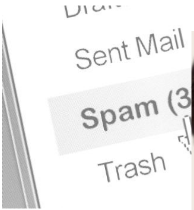

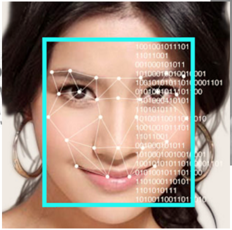

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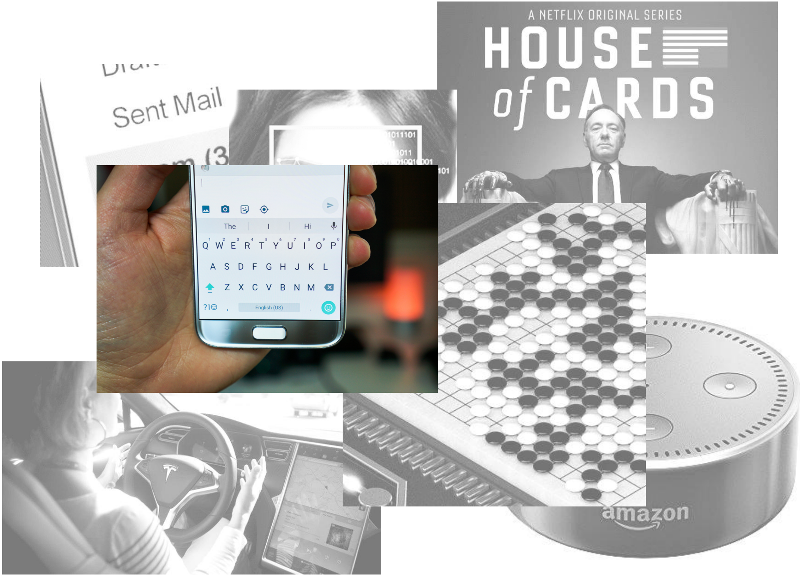

Machine Learning is Everywhere

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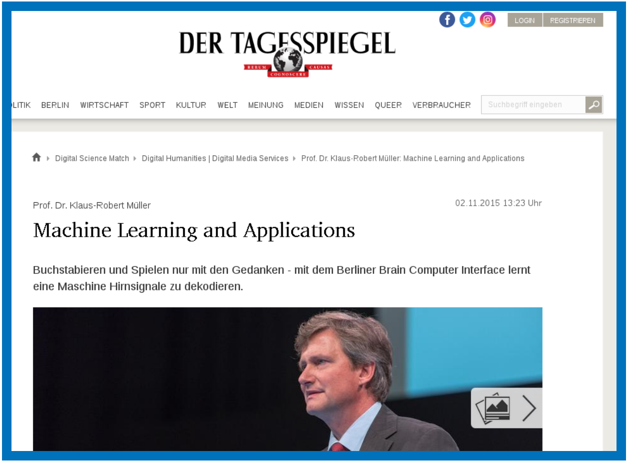
Literally *Everyone* speaks about Machine Learning



DER TAGESSPIEGEL

LOGIN REGISTRIEREN

LITIK BERLIN WIRTSCHAFT SPORT KULTUR WELT MEINUNG MEDIEN WISSEN QUEER VERBRAUCHER

Suchbegriff eingeben

Digital Science Match › Digital Humanities | Digital Media Services › Prof. Dr. Klaus-Robert Müller: Machine Learning and Applications

Prof. Dr. Klaus-Robert Müller

02.11.2015 13:23 Uhr

Machine Learning and Applications

Buchstabieren und Spielen nur mit den Gedanken - mit dem Berliner Brain Computer Interface lernt eine Maschine Hirnsignale zu dekodieren.

Literally *Everyone* speaks about Machine Learning

DER TAGESSPIEGEL
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Maschinelles Lernen

Künstlich, intelligent und frei

Firmen wie IBM, Facebook und Google investieren Millionen in künstliche Intelligenz. Teile ihrer Forschung stellen sie für alle frei zur Verfügung – aus gutem Grund.

Von **Eike Kühl**

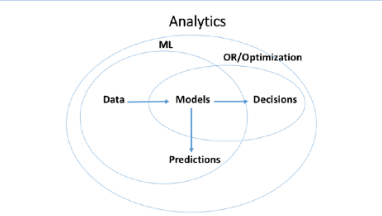
14. Dezember 2015, 19:28 Uhr / 19 Kommentare

Literally *Everyone* speaks about Machine Learning

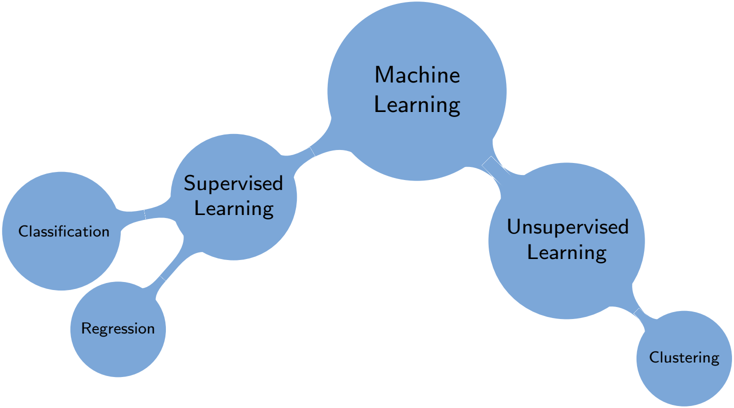
New INFORMS Journal on Optimization

> One of the largest opportunities of the field of optimization is to embrace data in a protagonist role and combine it with machine learning.
> — Dimitris Bertsimas, Editorial Statement

> My vision of the future for [. . .] optimization



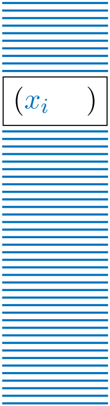
What *is* Machine Learning?



source: www.mathworks.com

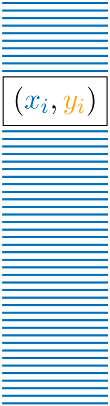
Supervised Learning: Classification

- data $\mathcal{X}$



Supervised Learning: Classification

- data $\mathcal{X}$ labels $\mathcal{Y}$



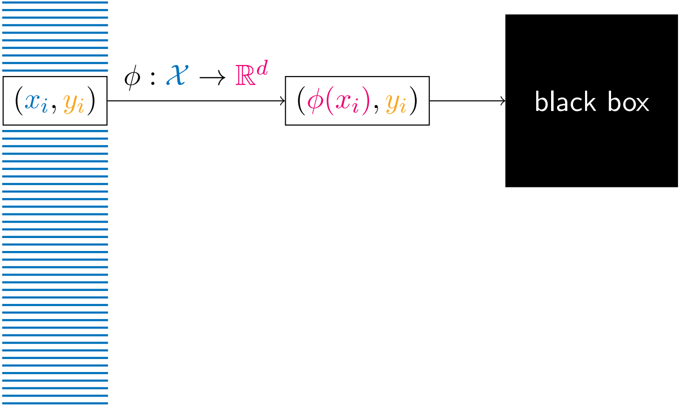
Supervised Learning: Classification

- data $\mathcal{X}$, d features, labels $\mathcal{Y}$

$$\boxed{(x_i, y_i)} \xrightarrow{\phi : \mathcal{X} \to \mathbb{R}^d} \boxed{(\phi(x_i), y_i)}$$

Supervised Learning: Classification

- data $\mathcal{X}$, d features, labels $\mathcal{Y}$



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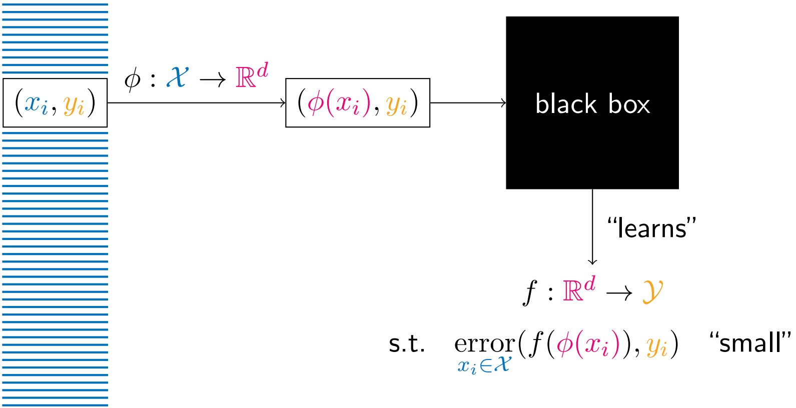

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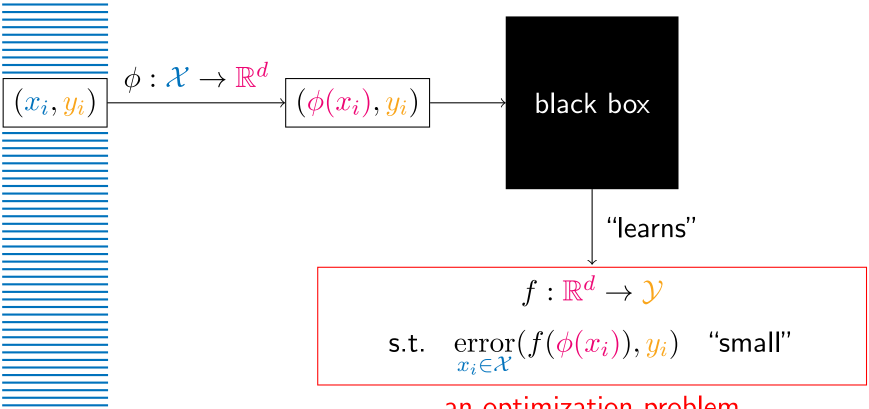
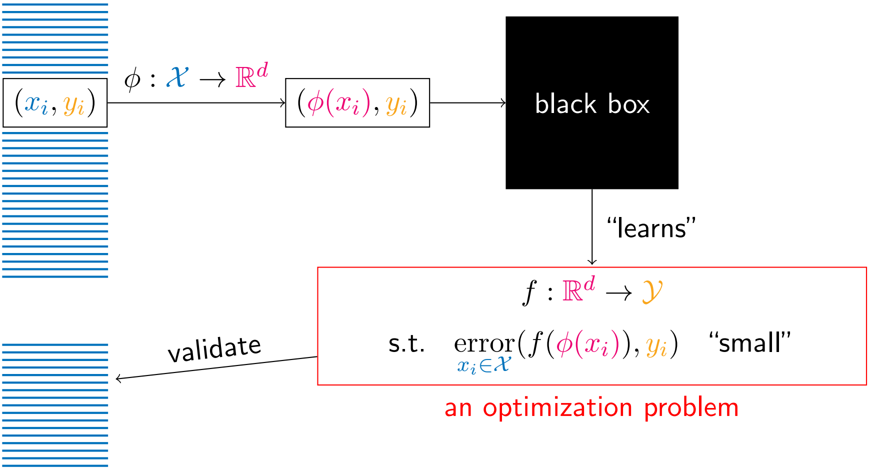


an optimization problem

Supervised Learning: Classification

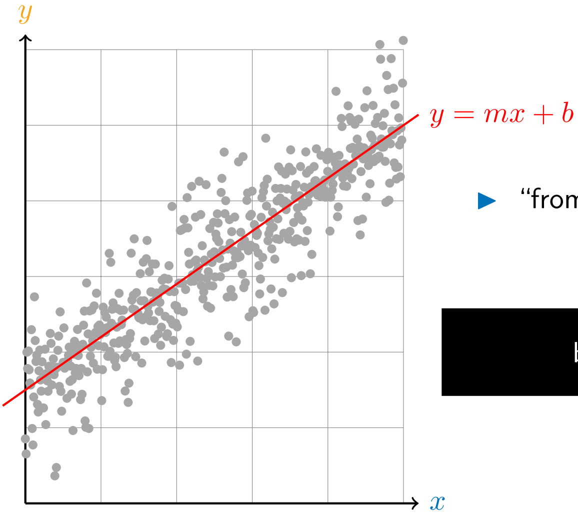
- data $\mathcal{X}$, d features, labels $\mathcal{Y}$



an optimization problem

Binary Classification: Dog or Muffin? Owl or Apple?

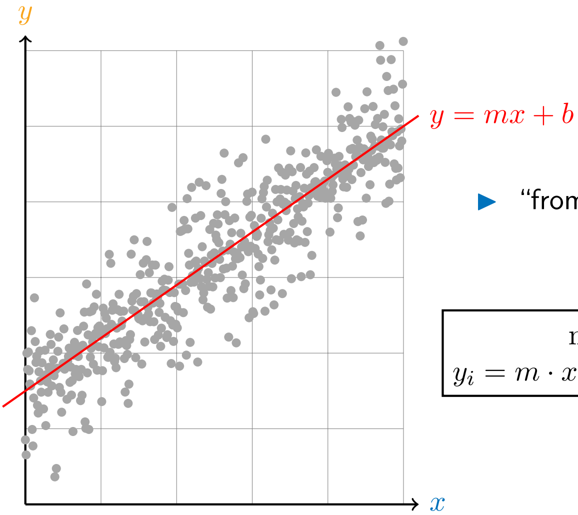
Supervised Learning: Regression



- “from $\{0,1\}$ to $[0,1]$”

black box

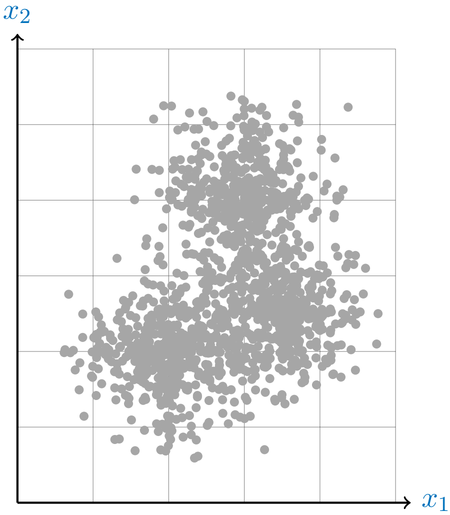
Supervised Learning: Regression

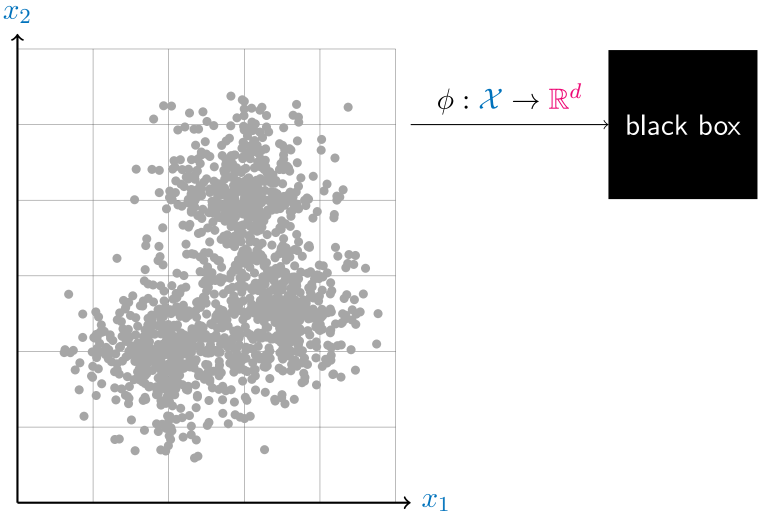


- "from $\{0, 1\}$ to $[0, 1]$"

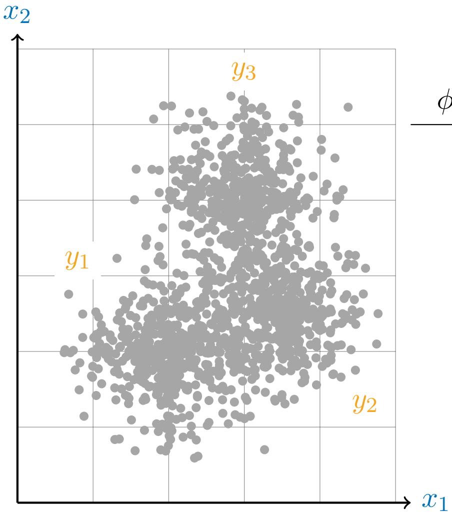
$$\boxed{\begin{array}{c} \min \sum_i \varepsilon_i^2 \\ y_i = m \cdot x_i + b + \varepsilon_i \quad x_i \in \mathcal{X} \end{array}}$$

Unsupervised Learning: Clustering




x_2
x_1
$\phi : \mathcal{X} \to \mathbb{R}^d$
black box

Unsupervised Learning: Clustering



$\phi : \mathcal{X} \to \mathbb{R}^d$

black box

"learns"

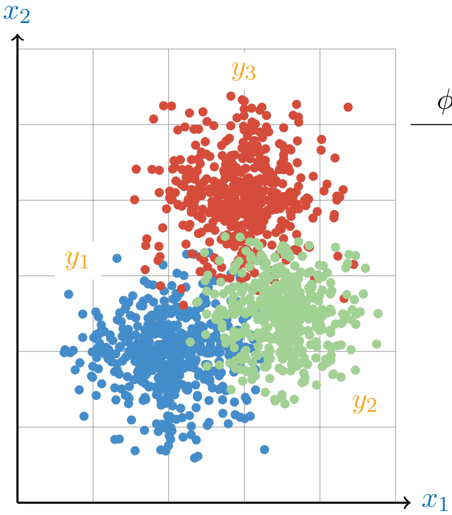
$f : \mathbb{R}^d \to \mathcal{Y}$

s.t. all

$x \in \mathcal{X} : f(\phi(x)) = y$

are "similar"

Unsupervised Learning: Clustering



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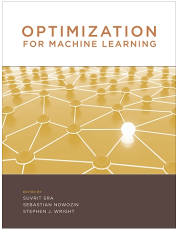
$x \in \mathcal{X} : f(\phi(x)) = y$

are "similar"

Optimization naturally appears in ML

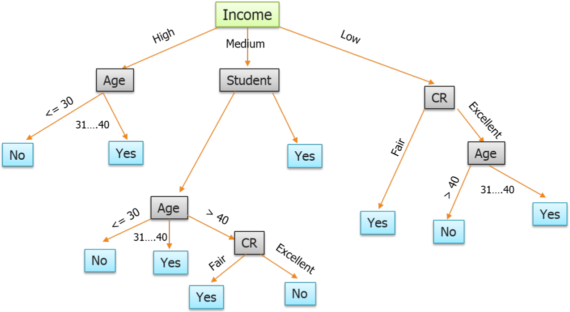
> Optimization lies at the heart of ML. Most ML problems reduce to optimization problems.
>
> — Bennett, Parrado-Hernández (2006)

- minimize e.g., prediction error
- continuous, convex optimization
- discrete, integer optimization



Example: A MIP in a black box : Classification Trees

- optimal classification trees Bertsimas & Dunn (2017)



source: www.edureka.co/blog/decision-trees

- use few nodes, shallow depth → formulated as MIP
- improves accuracy over classical CART method by 0.5–2%

Many Opportunities for Discrete Optimization in ML

- within black boxes to capture combinatorial explosion

→ see also Andrea's plenary on Friday

- feature selection
- outlier detection
- parameter tuning
- ...

How about the converse Direction?

- "emulating the expert" Bärmann, Pokutta & Schneider (2017)
- observe a decision maker $\max c_{\text{true}}^T x : x \in X(p)$
- learn their objective function given $(p_t, x_t^*)_{t=1,\dots,T}$
- *online learning*

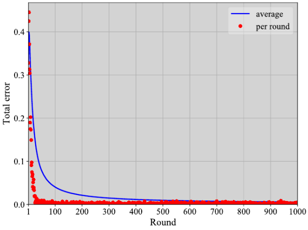


Figure 1. Linear Knapsack problem with $n = 100$ items over

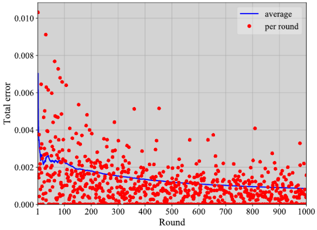


Figure 2. Resource-constrained shortest path problem on a grid

ML may help improving Optimization Algorithms

- e.g., branching in B&B
- *full strong branching* gives locally perfect information

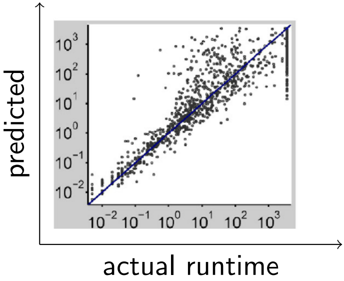
- predict the strong branching score of a variable
- features describe state of a variable
- supervised learning: regression

→ promising proof-of-concept
  Marcos Alvarez, Louveaux & Wehenkel (2017)

- survey on ML in branching/searching Lodi & Zarpellon (2017)

A Progress Bar for Branch-and-Bound?

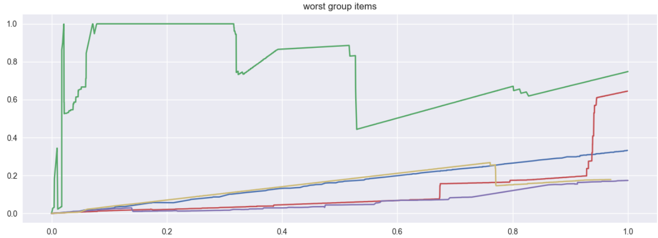
- predict the runtime of branch-and-bound algorithms
  Hutter, Xu, Hoos & Leyton-Brown (2014)
- CPLEX 12.1 on 1510 publicly available MIPs



A Progress Bar for Branch-and-Bound?

- very preliminary experiments with `gurobi` 7.5
- predict elapsed runtime percentage

  Kruber, L, Obeloer genannt Bregenhorn (2017)



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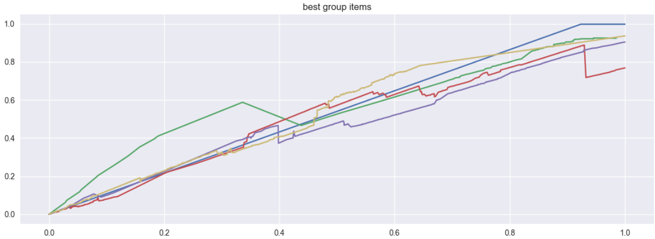


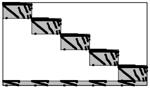
Learning when to solve a MIP by Branch-and-Price

- our MIP solver GCG detects many potential DW reformulations

⋮

MIP

+



CPU time

⋮

Kruber, L, Parmentier (2017)

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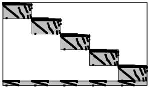
+



CPU time

⋮

$\xrightarrow{\phi}$

100+ features

#conss, #vars, %constype, %vartype, #blocks, . . .

Kruber, L, Parmentier (2017)

Learning when to solve a MIP by Branch-and-Price

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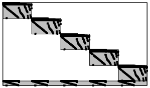


CPU time

⋮

ϕ →

100+ features

#conss, #vars, %constype, %vartype, #blocks, . . .

→ k-NN

learns ↓

binary classifier f

"run SCIP or GCG?"

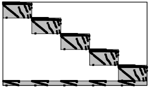
Kruber, L, Parmentier (2017)

- our MIP solver GCG detects many potential DW reformulations

⋮

MIP

+



CPU time

⋮

ϕ

100+ features
#conss, #vars, %constype, %vartype, #blocks, ...

k-NN

learns

binary classifier f

“run SCIP or GCG?”

faster

f		SCIP	GCG
	SCIP	69.5%	9.9%
	GCG	6.9%	13.7%

Kruber, L, Parmentier (2017)

What ML Answers can we (Optimizers) expect?

- we get statistical answers $\rightarrow$ not what we are used to see

- we have domain/expert knowledge: e.g., pseudo-costs
- ML may give a better predictor, but no *explanation*
- some info can be extracted from most influential features

$\rightarrow$ interpretability is a huge theoretical and practical topic

Decision Making: Machine Learning

> Machine Learning and Artificial Intelligence delivers the most value when you need to make lots of similar decisions quickly.
>
> — Ingo Mierswa, Rapidminer

- simple decisions: e.g., auto correct current word
- solution: often a single score $\rightarrow$ greedy
- keep/learn habits: extrapolate from the past (!)

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Typical Example: Predictive Maintenance

source: blog.capterra.com/should-you-invest-in-a-predictive-maintenance-strategy/

Exploit all Options: Prescriptive Maintenance

source: www.siemens.com/press/pool/de/pressebilder/photonews/pn200826/300dpi/pn200826-12_300dpi.jpg

Decision Making: Optimization

> How often can the result of an optimization model be captured in a single variable?
>
> — Ed Rothberg, Gurobi

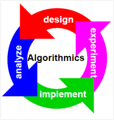
- solution: not only the objective value!
- complex decisions/plans: e.g., timetables, crew schedules, ...
- global scope: models all (reasonable) interdependencies

Perfect Partners

"Current Standard:" Predictive then Prescriptive Analytics

ML harnesses the bigness of data (the past and present);
Optimization captures the bigness of options (the future).

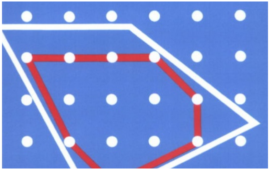
Learning (about) optimal Solutions

- in recurring complex decision situations
- learn how good (partial) solutions look like
- this may help finding good solutions faster
- learn spatio-temporal patterns to generate effective schedules
  Le, Liu, Lau (2016)
- 

Learning (about) Optimization Models

- ML can make sense of data
- optimization models are also “data”

→ (how) can ML help us make sense of optimization models?



- can ML learn good modeling?

Vision: Learning (about) Optimization Problems

- learn the *semantics* of a MIP model ("the problem")

$$
\begin{aligned}
\min \sum_{j=1}^{n} y_j & & \\
\text{s.t.} \sum_{j=1}^{n} x_{ij} &= 1 & i = 1,\dots,n \\
\sum_{i=1}^{n} a_i x_{ij} &\leq b & j = 1,\dots,n \\
x_{ij} &\leq y_j & i,j = 1,\dots,n \\
x_{ij},\, y_j &\in \{0,1\} & i,j = 1,\dots,n
\end{aligned}
$$

$\longrightarrow$

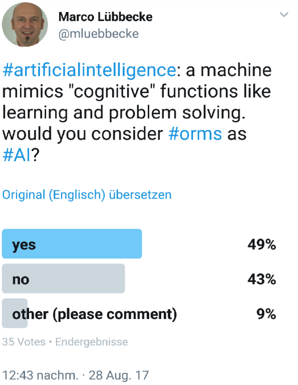
$\longrightarrow$

$$
\begin{aligned}
\min \sum_{p \in P} \nu_p & & \\
\text{s.t.} \sum_{p \in P : i \in p} \nu_p &= 1 & i = 1,\dots,n \\
\nu_p &\in \{0,1\} & p \in P
\end{aligned}
$$

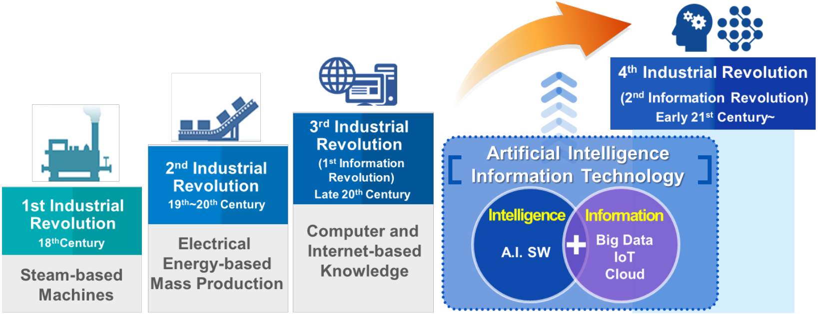
$\Rightarrow$ e.g., help the modeler find a better formulation

The AI Umbrella?

- OR vs. analytics discussion ✓
- OR vs. AI discussion ?



Why is this Relevant?



source: blogs.worldbank.org/category/tags/artificial-intelligence

- *if* the fourth industrial revolution is about AI, OR should be part of it

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