Learning a classification of Mixed-Integer Quadratic Programming problems

CERMICS 2018 – June 29, 2018, Fréjus

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About Mixed-Integer Quadratic Programming problems

Mixed-Integer Quadratic Programming problems

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

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

- Modeling of practical applications (e.g., portfolio optimization)
- First extension of linear algorithms into nonlinear ones

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We say an MIQP is ***convex*** (resp. ***nonconvex***) if and only if the matrix Q is positive semi-definite, $Q \succeq 0$ (resp. indefinite, $Q \not\succeq 0$).

⟶ `IBM-CPLEX` solver can solve both convex and nonconvex MIQPs to proven optimality

Solving MIQPs with CPLEX

Convex 0-1

NLP B&B

Convex mixed

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Nonconvex 0-1

convexify + NLP B&B

Convexification: **augment diagonal** of Q, using $x_i = x_i^2$ for $x_i \in \{0, 1\}$:
$x^T Q x \to x^T (Q + \rho \mathbb{I}_n) x - \rho e^T x$, where $Q + \rho \mathbb{I}_n \succeq 0$ for some $\rho > 0$

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Linearization: replace $q_{ij} x_i x_j$ where $x_i \in \{0,1\}$ and $l_j \leq x_j \leq u_j$ with a new variable y_{ij} and **McCormick inequalities**

$\longrightarrow$ Linearization is always full in 0-1 case

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Convexification is relaxation - Spatial B&B

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NL: NLP B&B
L: linearize + MILP B&B

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$\longrightarrow$ Linearization is always full in 0-1 MIQP *(may not for mixed ones)*

Linearize vs. not linearize

The linearization approach seems beneficial also for the convex case, but **is linearizing always the best choice?**

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Example[1]: convex 0-1 MIQP, $n = 200$

Linearize

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Total (root+branch&cut) = 2112.63 sec.

CPLEX 12.6.0.0: optimal integer solution;
objective 29576.27517
474330 MIP simplex iterations
294 branch-and-bound nodes
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Not linearize

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Total (root+branch&cut) = 0.42 sec.

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```
MIP Presolve added 39800 rows and 19900
columns.
Reduced MIP has 39801 rows, 20100
columns, and 79800 nonzeros.
Reduced MIP has 20100 binaries, 0
general, and 0 indicators.
```

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"[. . .] when one looks at a broader variety of test problems the decision to ***linearize (vs. not linearize)*** *does not appear so clear-cut.[2]"*

[1] Fourer R. Quadratic Optimization Mysteries, Part 1: Two Versions.
[2] Fourer R. Quadratic Optimization Mysteries, Part 2: Two Formulations.
http://bob4er.blogspot.com/2015/03/quadratic-optimization-mysteries-part-2.html

Linearize vs. not linearize - Goal

Goal

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

- Learn an offline classifier predicting the most suited resolution approach within `CPLEX` framework, in an instance-specific way

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- Parameter `qtolin` controls the linearization switch

L	**on**	`CPLEX` linearizes (*all?*) quadratic terms
NL	**off**	`CPLEX` does *not* linearize quadratic terms
`DEF`	**auto**	Let `CPLEX` decide (default)

Data and experiments

Steps to apply supervised learning

Dataset generation

- Generator of MIQPs, spanning over various parameters
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  (variables, constraints, objective, spectrum, ...)
- Dynamic features (2) · Early behavior in optimization process
  (bounds and times at root node)

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- 1h, 5 seeds · Solvability and consistency checks
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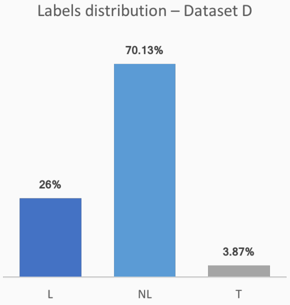
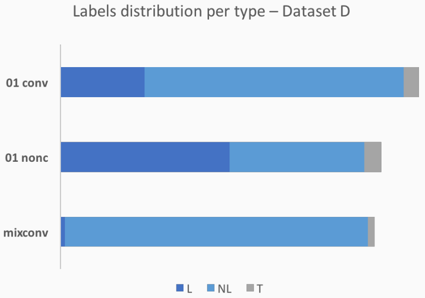
$\{(\mathbf{x}^k, \mathbf{y}^k)\}_{k=1..N}$ where $\mathbf{x}^k \in \mathbb{R}^d$, $\mathbf{y}^k \in \{\mathrm{L}, \mathrm{NL}, \mathrm{T}\}$ for N MIQPs

Dataset $\mathcal{D}$ (nutshell) analysis

- **2300** instances, $n \in \{25, 50, \ldots, 200\}$, density $d \in \{0.2, 0.4, \ldots, 1\}$





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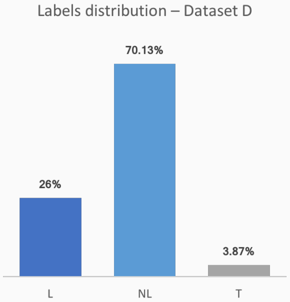

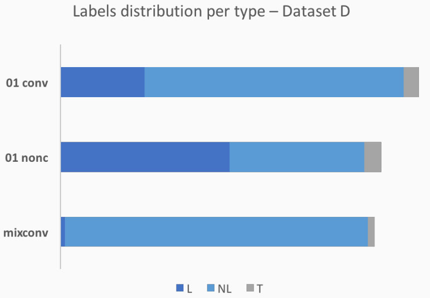

- **Multiclass classifiers**: SVM and Decision Tree based methods (Random Forests (RF) · Extremely Randomized Trees (EXT) · Gradient Tree Boosting (GTB))
- Avoid overfitting with **ML best practices**
- **Tool**: `scikit-learn` library

Learning results on $\mathcal{D}_{test}$

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

$\mathcal{D}_{test}$ - *Multiclass - All features*				
	SVM	RF	EXT	GTB
Accuracy	0.85	0.89	0.84	0.87
Precision	0.82	0.85	0.81	0.85
Recall	0.85	0.89	0.84	0.87
F1 score	0.83	0.87	0.82	0.86

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⟶ **Binary setting**: remove all tie cases · performance improved
How relevant are ties with respect to the question L vs. NL?

Hints of features importance

Ensemble methods based on Decision Trees provide an **importance score** for each feature.

Top scoring ones are dynamic ft.s and those about eigenvalues:

(dyn. ft.)
- Difference of lower bounds for L and NL at root node

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$\longrightarrow$ **Static features setting**: remove dynamic features · performance slightly deteriorated

How does the prediction change without information at root node?

Measure the optimization gain

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Evaluate classifiers' performance in optimization terms, and quantify the gain with respect to `CPLEX` *default strategy*.

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- For each classifier *clf* and DEF, build a **times vector $\mathbf{t_{clf}}$**: for every test example, select the runtime corresponding to its label $\in \{L, NL, T\}$, as predicted by *clf*

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- Build also t_{best} (t_{worst}) containing times corresponding to the correct (wrong) labels

Complementary optimization measures

Using times vectors $\mathbf{t}_{\mathbf{clf}}$ define

- $\sigma_{\mathbf{clf}}$ **Sum of predicted runtimes**: sum over times in t_{clf}
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$\sigma_{\mathtt{DEF}}/\sigma_{clf}$	3.88	4.40	4.04	4.26	–
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- DEF could take up to 4x more time to run MIQPs of $\mathcal{D}_{test}$, compared to a trained classifier
- Measures are better for classifiers hitting **timelimit** less frequently (and both L and NL reach timelimit multiple times!)

Ongoing questions

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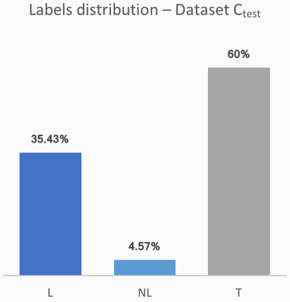
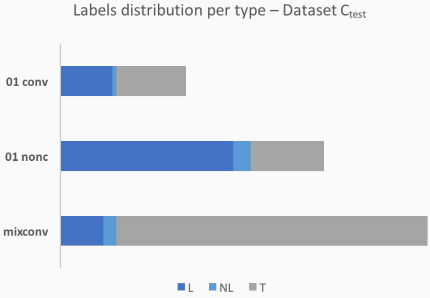
- Selection from QPLIB · **24 instances**
- Part of `CPLEX` internal testbed · **175 instances**, used as new test set $\mathcal{C}_{test}$ for classifiers trained on the synthetic data. Again **unbalanced**, but with majority of ties and few NL.





Results on $\mathcal{C}_{test}$

- $\mathcal{C}_{test}$ is dominated by few structured combinatorial instances
- **Very different distribution** of features

All classifiers perform very poorly in terms of classification measures (most often T is predicted as NL), **but** . . .

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All classifiers perform very poorly in terms of classification measures (most often T is predicted as NL), **but** ...

... performance is not bad in optimization terms:

	SVM	RF	EXT	GTB	**DEF**
$\sigma_{\texttt{DEF}}/\sigma_{clf}$	0.48	0.53	0.71	0.42	–
$N\sigma_{clf}$	0.75	0.90	0.91	0.74	**0.96**

Given the high **presence of ties**, runtimes for L and NL are most often comparable, so **the loss in performance is not dramatic**.

Why those predictions?

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- The **bound at the root** node seems to decide the label!
- **Convexification** and **linearization** clearly affect

  • **formulation size** • **formulation strength** • **implementation efficacy** • ...

  ...each problem type might have its own decision function for the question *L vs. NL*

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More experiments to come:

- Employ a **larger** and **heterogeneous dataset**
- Go beyond preliminary **features evaluation**
- Define a custom **loss/scoring function**

Thanks! Questions?