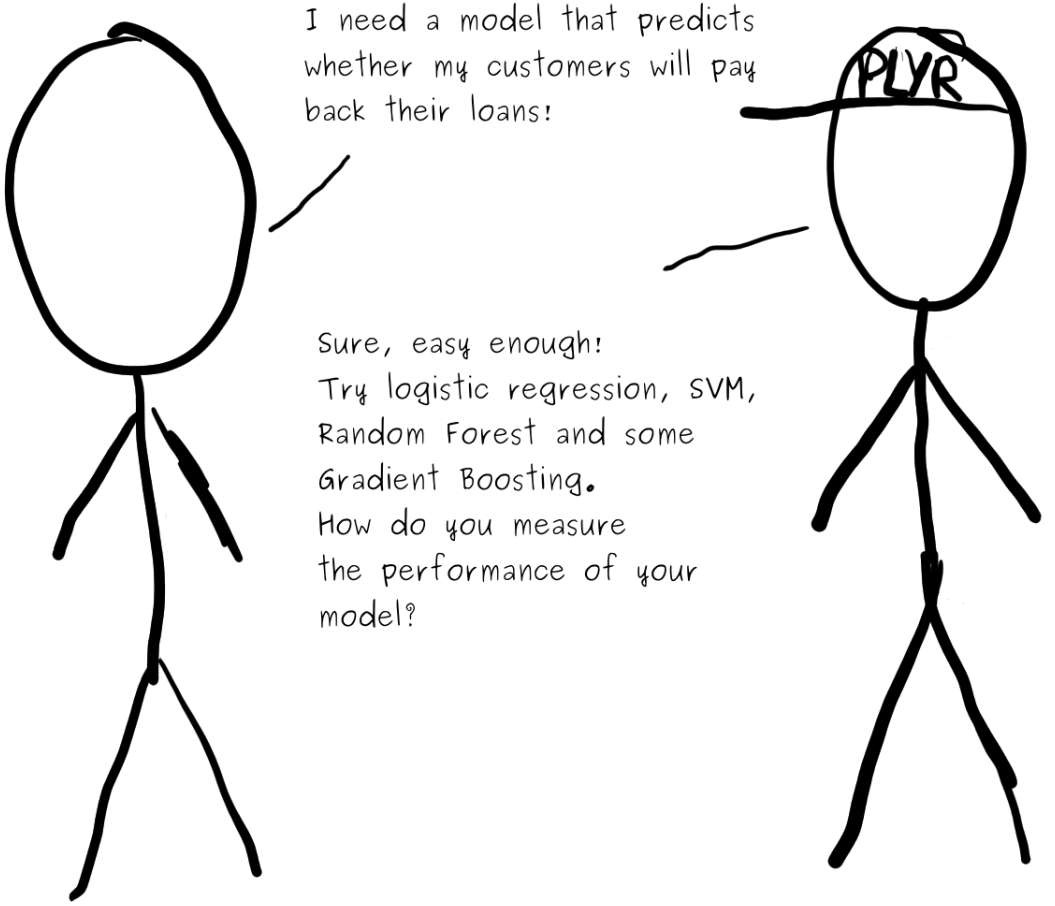
~~Towards human-centered AutoML~~

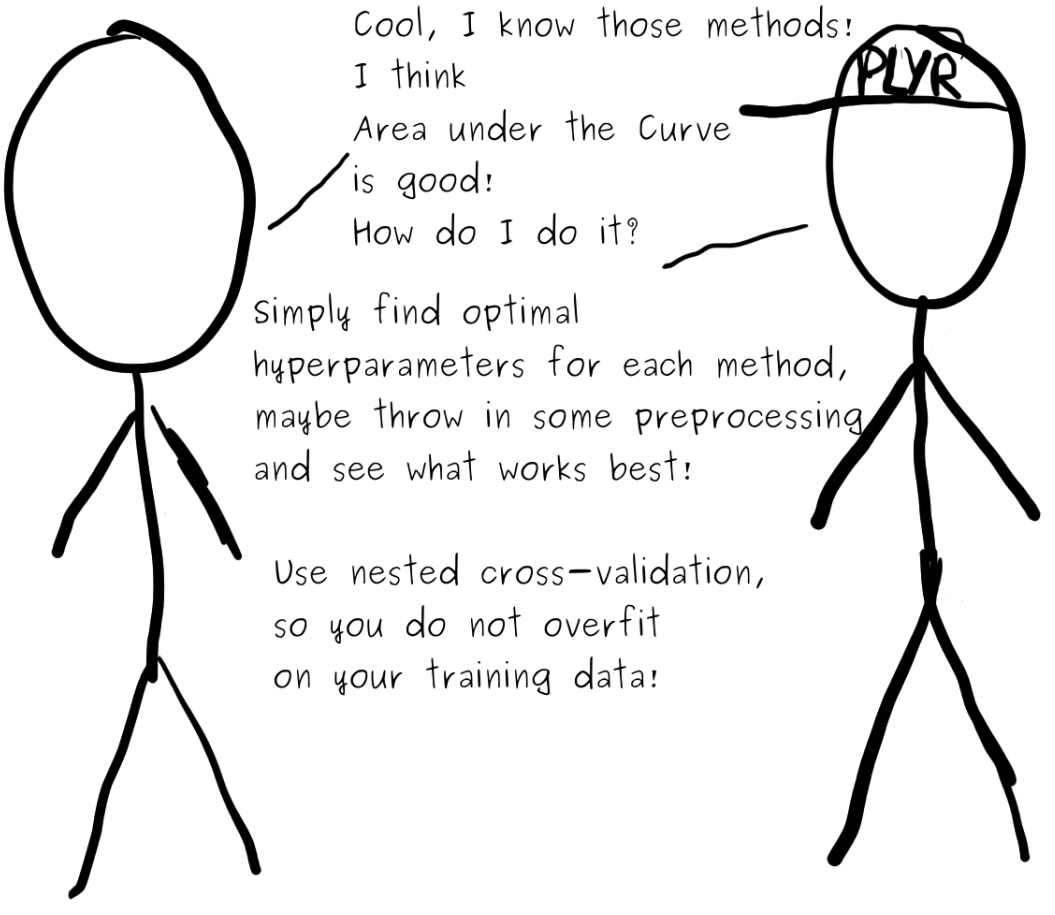
Multi-Objective AutoML

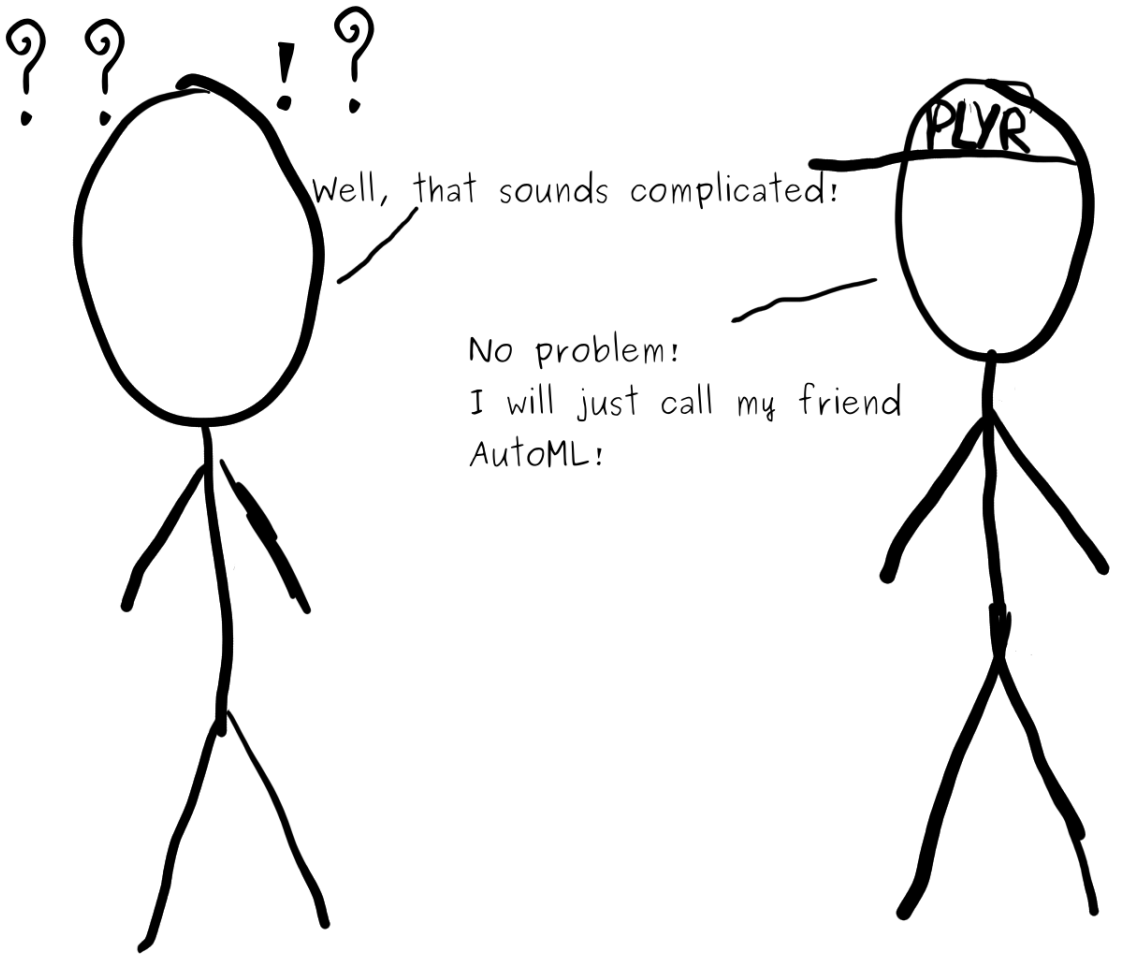
Florian Pfisterer, Stefan Coors, Janek Thomas, Bernd Bischl

LMU Munich

2019/07/02


I need a model that predicts whether my customers will pay back their loans!
PLYR
Sure, easy enough!
Try logistic regression, SVM, Random Forest and some Gradient Boosting.
How do you measure the performance of your model?


Cool, I know those methods!
I think
Area under the Curve
is good!
How do I do it?
PLYR
Simply find optimal
hyperparameters for each method,
maybe throw in some preprocessing
and see what works best!
Use nested cross-validation,
so you do not overfit
on your training data!

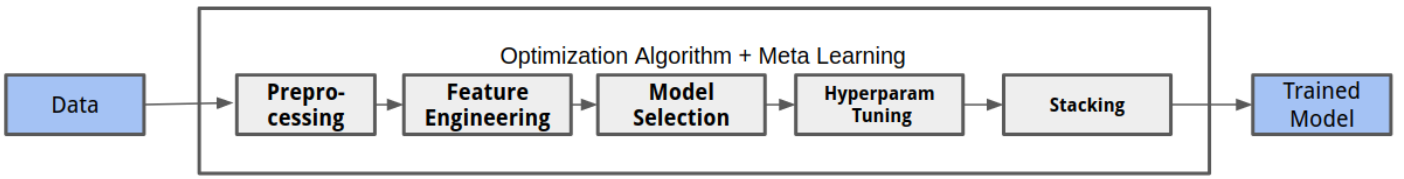

? ? ! ?
Well, that sounds complicated!
PLYR
No problem!
I will just call my friend
AutoML!


PLYR
Sure!
Give me your data
and I will get back
to you!


Cool!
The model also can't discriminate between men and women,
and
I need the model to be interpretable!
PLYR
Ahm ...
this is asking a lot!
I do not really know
how to help you there!

A short intro to AutoML

- Automatically obtain an *"optimal"* model for a dataset
- The system performs model selection, tuning, ...
- Many different flavours exist!



Why?

- Many steps in the typical ML pipeline can be easily automized!
- Computers are efficient in trying out many possibilities.
- Efficient search strategies exist!
- Humans are single-threaded and have little RAM!

Multi-Objective AutoML - Why?

- Current AutoML approaches are **very good** at optimizing predictive performance!
- **But:** Many applications require models that trade of or are *good* with respect to multiple objectives.

Problem:

To narrow focus on a single measure for predictive performance!

Users either use AutoML without considering other objectives, or do analysis manually!

Interesting Objectives:

Fairness

... usually means that our model f_θ trained on a dataset X and target y does not discriminate between a set of protected attributes A, such as ethnicity and gender.

There are many (often conflicting) definitions of fairness, to give two examples:

- Equalized Odds (Hardt, 2016)

  $$Pr\{\hat{Y} = 1 | A = 0, Y = y\} = Pr\{\hat{Y} = 1 | A = 1, Y = y\}, y \in \{0, 1\}$$

- Equal Opportunity (Hardt, 2016)

  $$Pr\{\hat{Y} = 1 | A = 0, Y = 1\} = Pr\{\hat{Y} = 1 | A = 1, Y = 1\}$$

- Further desideratum: Calibration

Interesting Objectives II:

Interpretability

Many post-hoc interpretability methods allow us to understand what our model learns. But: They mostly rely on **local** and **linear** explanations.

- Main Effect Complexity (Molnar, 2019)

  $\rightarrow$ How well can main effects be approximated by linear segments?

- Interaction Strength (Molnar, 2019)

  $\rightarrow$ How much of a model's prediction can **not** be explained by main effects?

- Sparsity

  Even simple models with $1000's$ of predictors are hard to grasp

Interesting Objectives III:

Robustness

- Robustness to adversarial examples, perturbations , distribution shift, ...

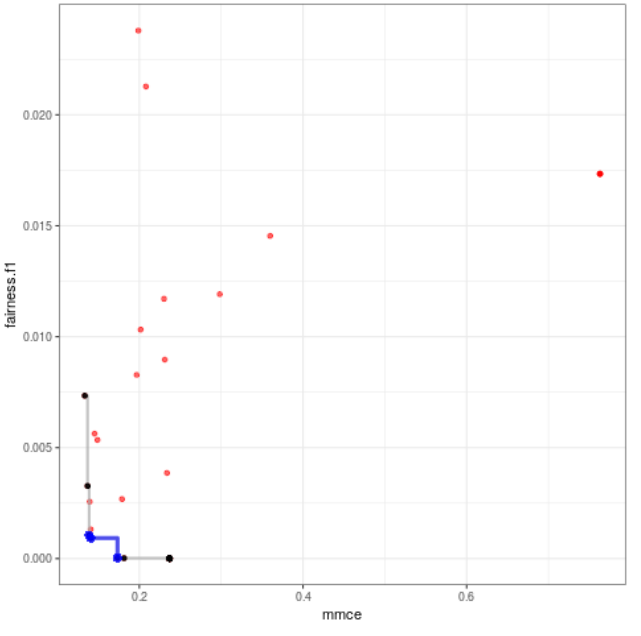
Memory and Inference Time

- Deploying on mobile devices, scoring *http* requests

...

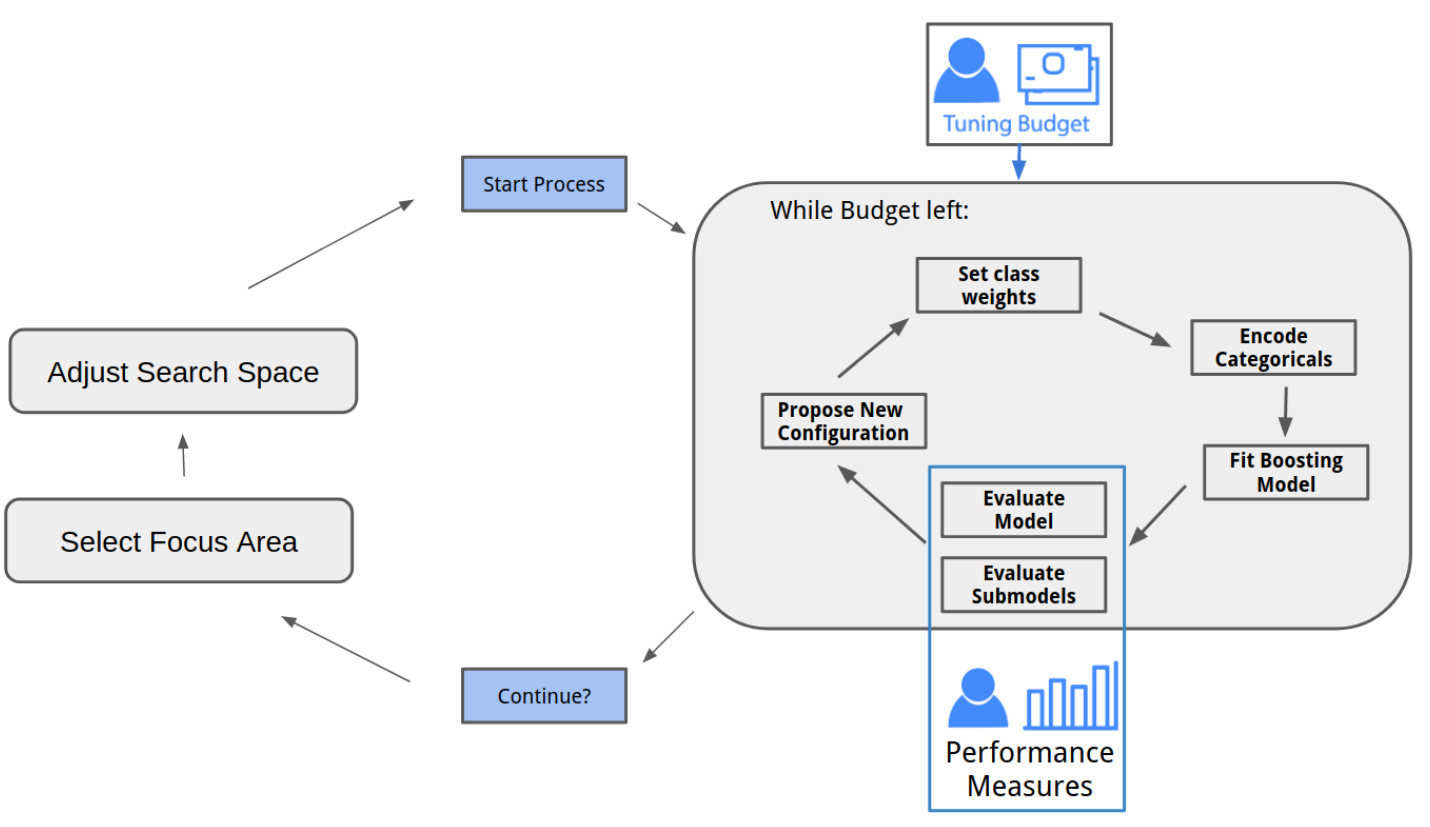
AutoXgboostMC

- We propose a simplified AutoML system (based on autoxgboost) in order to explore the setting
- Uses XGboost models, and a limited amount of preprocessing steps
- Optimize using Multi-Objective Bayesian Optimization
- Human-in-the-loop:
  - User can stop and restart the process, adjust parameters.
  - User specifies area, the optimization algorithm should focus in.

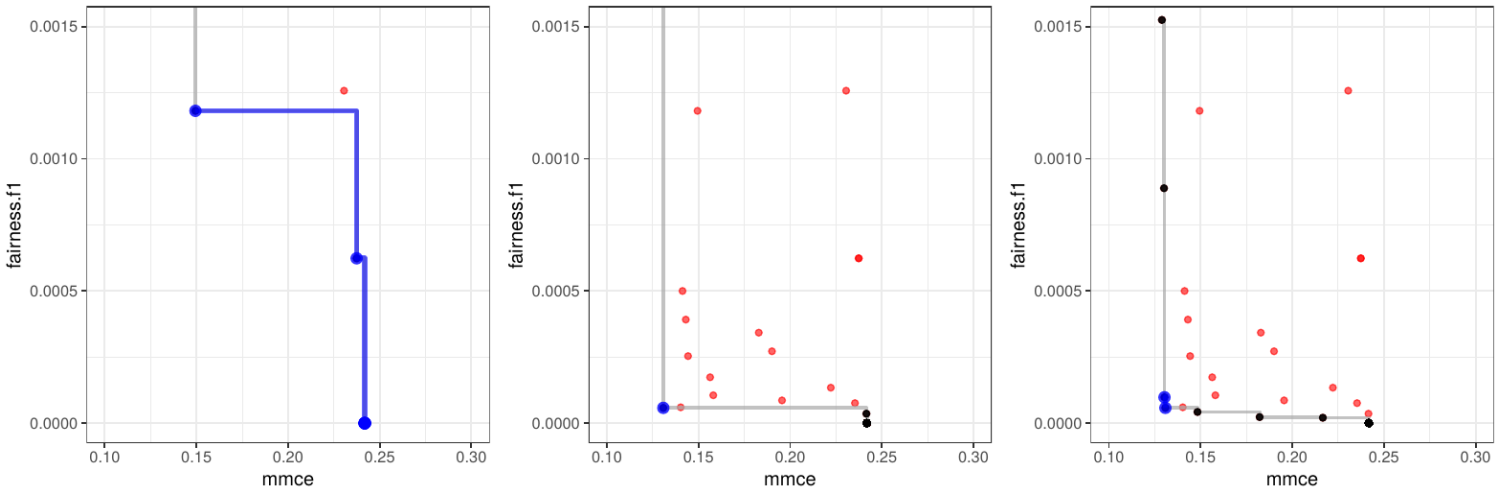


parEgo (Knowles, 2006) uses random projections in order to explore the pareto front. We can limit the range of random projections in order to focus on certain areas.

Workflow


Tuning Budget
Start Process
While Budget left:
Set class weights
Encode Categoricals
Fit Boosting Model
Evaluate Model
Evaluate Submodels
Propose New Configuration
Performance Measures
Continue?
Select Focus Area
Adjust Search Space

Pareto Front

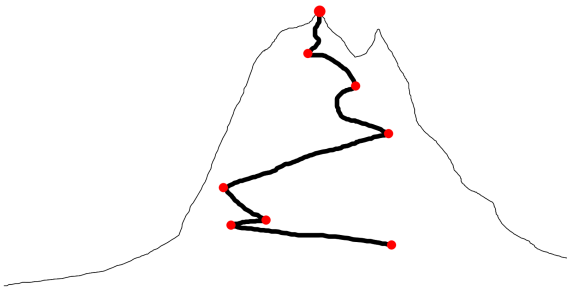


Pareto front for Fairness and MMCE after 20, 70 and 120 iterations.

- Limit the range of random projections (weights for the measures) in order to focus on specific areas.
- Grey line contains Pareto optimal points
- Blue segment: Pareto optimal for weights from $[0.1; 0.9]$ to $[0.9; 0.1]$.

Open Challenges

- **Awareness** for other objectives is often lacking. If they are not easily accessible users might just neglect them.
- **Fairness** measures are often not well-defined and highly depend on context
- Measures for **robustness** do not really exist and require more research.
- Research into **interpretability** measures has just started!
- New pre- and post-processing methods might be required.



- Several tools for multi-criteria optimization already exist, further research might be beneficial.
- Tools to increase **transparency** and **trust** in AutoML systems are important! Human-in-the-loop approaches can help here!

Thank you for your attention!

Check out the progress:

```
https://github.com/pfistfl/autoxgboostMC
```

Suggestions, Interesting applications?

florian.pfisterer@**stat.uni-muenchen.de**

References

- Hardt, M., Price, E., Srebro, N., et al. (2016). Equality of opportunity in supervised learning. In Advances in neural information processing systems
- Molnar, C., Casalicchio, G., and Bischl, B. (2019). Quantifying interpretability of arbitrary machine learning models through functional decomposition. arXiv preprintarXiv:1904.03867.
- Thomas, J., Coors, S., and Bischl, B. (2018). Automatic gradient boosting. International Workshop on Automatic Machine Learning at ICML.
- Knowles, J. (2006) ParEGO: a hybrid algorithm with on-line landscape approximation for expensive multiobjective optimization problems. IEEE Transactions on Evolutionary Computation (Volume: 10 , Issue: 1 , Feb. 2006)