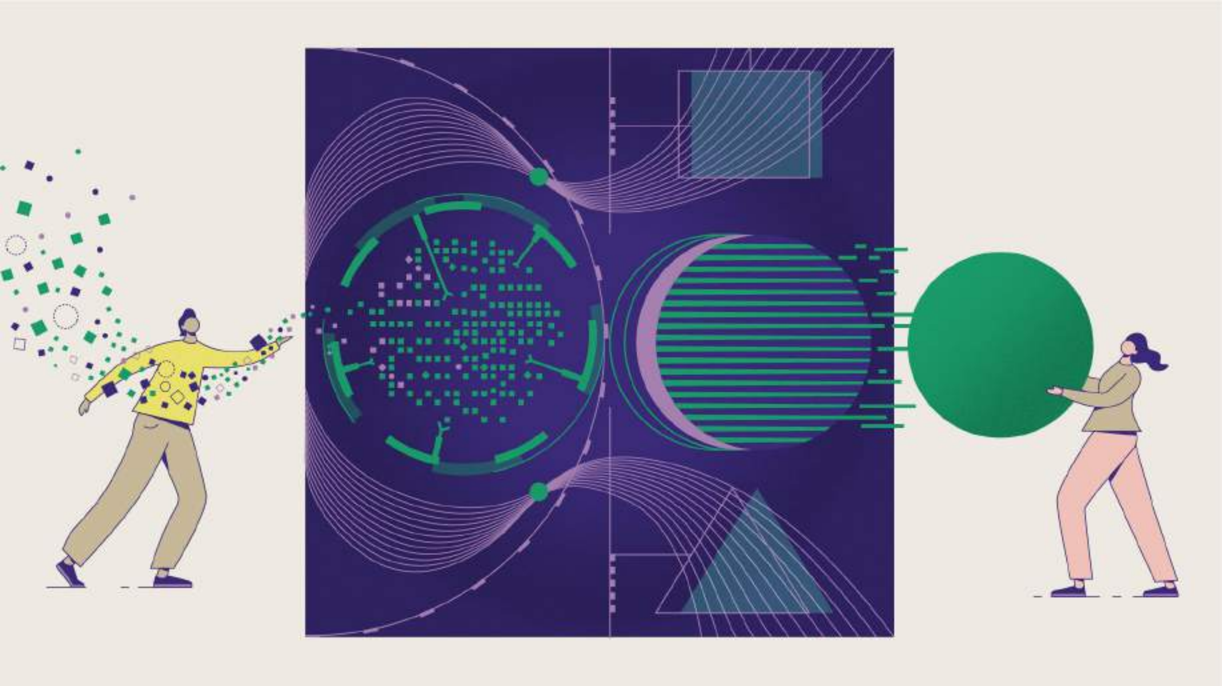

Efficient and Explainable AutoML

Marius Lindauer

Leibniz University Hannover

Big Success of AI in Recent Years

Images courtesy of Shutterstock

From Manual to Automated Machine Learning

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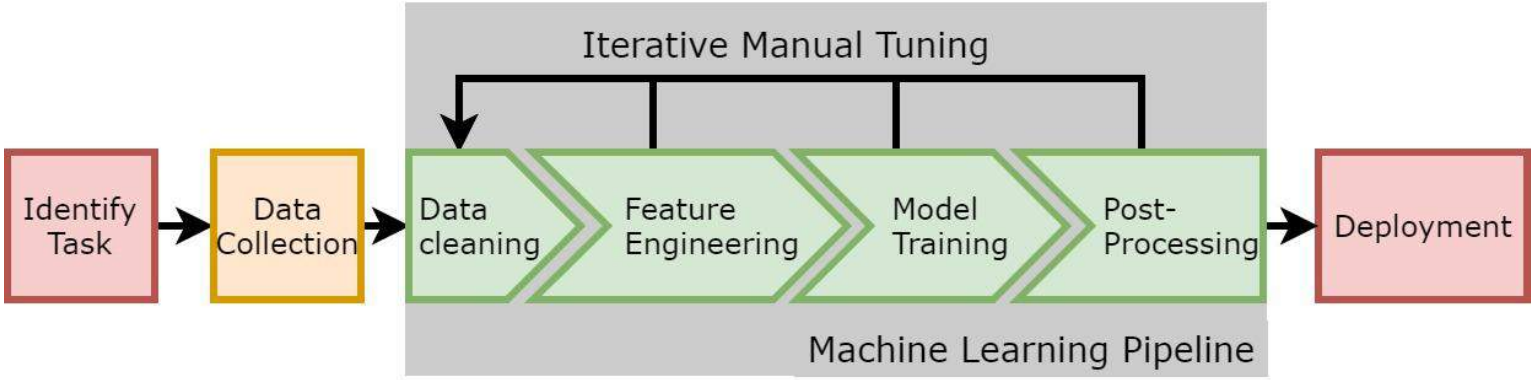

Mission Statement: Enabling users to efficiently apply ML!

Design Decisions taken care by AutoML

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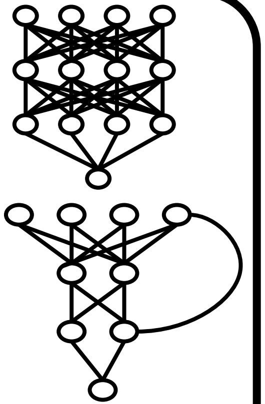
classifier	#λ
AdaBoost (AB)	4
Bernoulli naïve Bayes	2
decision tree (DT)	4
extreml. rand. trees	5
Gaussian naïve Bayes	-
gradient boosting (GB)	6
kNN	3
LDA	4
linear SVM	4
kernel SVM	7
multinomial naïve Bayes	2
passive aggressive	3
QDA	2
random forest (RF)	5
Linear Class. (SGD)	10

Algorithms



Architecture Design

preprocessor	#λ
extreml. rand. trees prepr.	5
fast ICA	4
feature agglomeration	4
kernel PCA	5
rand. kitchen sinks	2
linear SVM prepr.	3
no preprocessing	-
nystroem sampler	5
PCA	2
polynomial	3
random trees embed.	4
select percentile	2
select rates	3
one-hot encoding	2
imputation	1
balancing	1
rescaling	1

Pre-processing

Hyper-parameters

...

Using AutoML Matters! (example on a specific dataset)

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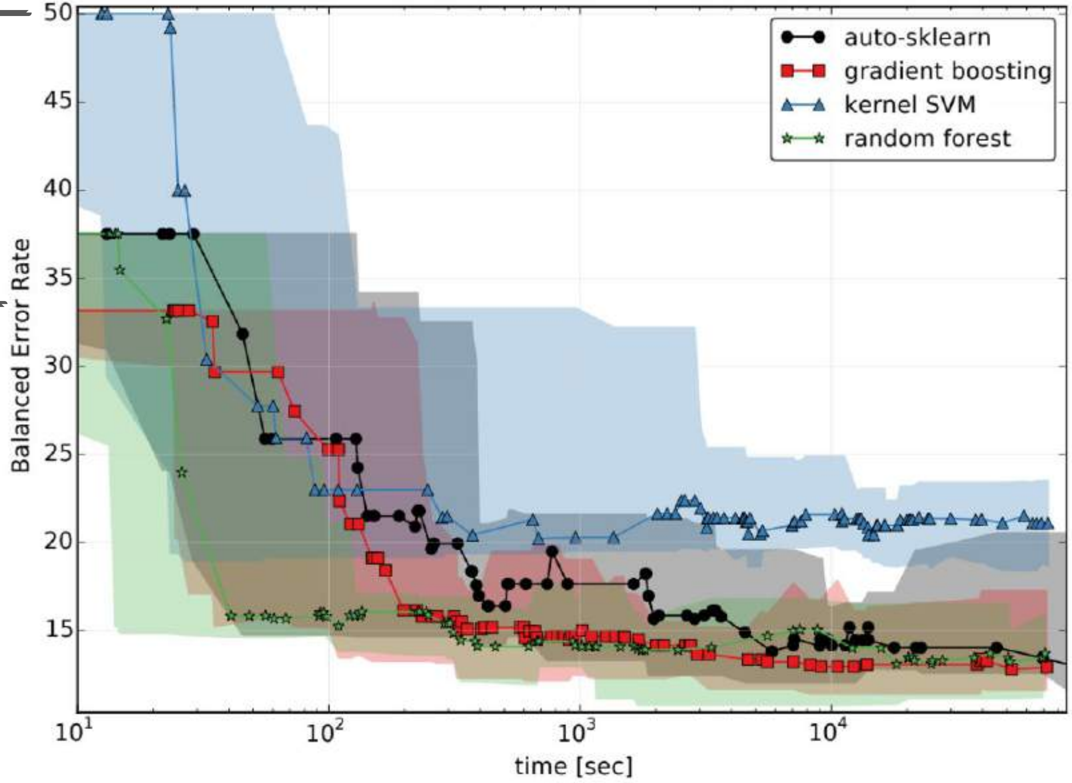
Choosing the correct algorithm
→ 17% improvement



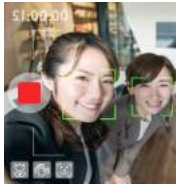
Optimized pipeline & hyperparameters
→ 20% - 29% improvement

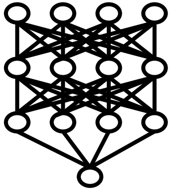
Exemplary Success Story:
Can DNNs outperform classical approaches on tabular data?

[Kadra et al. NeurIPS’21]

Previous Belief

1. Deep Neural Networks are especially well performing on high-dimensional data modalities (incl. images and text)

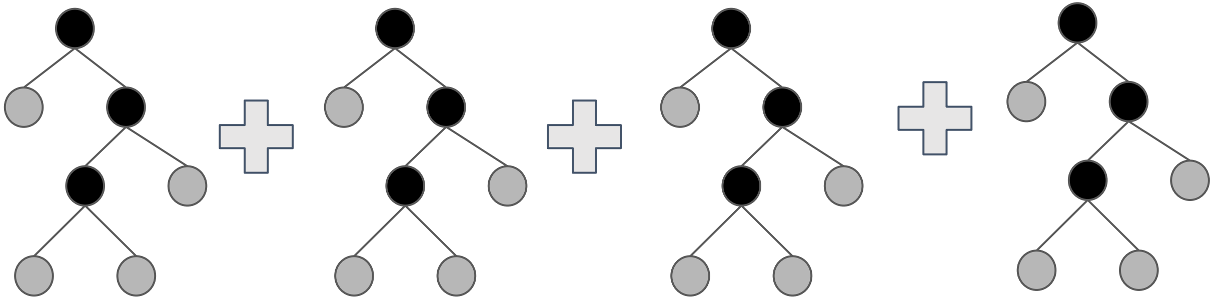




Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do eiusmod tempor incididunt ut labore et dolore magna aliqua.

2. Gradient-Boosted Decision Trees are state of the art on tabular data

	f_1	f_2	f_3	f_4	y
o_1	1	2	323	21	1
o_2	42	32	??	??	1
o_3	223	21	234	12	0
o_4	234	??	234	423	0
o_5	3	23	232	66	1



Idea I: Regularization against overfitting

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- DNNs are overparameterized and tabular datasets are often much smaller than image or text datasets
- → Sufficiently strong regularization could lead to better performance of DNNs?

- There are many regularization techniques for DNNs, incl.
  - Weight Decay [Krogh & Hertz 1991]
  - Dropout [Srivastava et al. 2014]
  - Batch Normalization [Ioffe & Szegedy 2015]
  - FGSM Adversarial Learning [Goodfellow et al. 2015]
  - Skip Connection [He et al. 2016]
  - Snapshot Ensembles [Loshchilov & Hutter 2017]
  - Shake-Shake [Gastaldi 2017]
  - Cut-Out [Devries & Taylor 2017]
  - Stochastic Weight Averaging [Izmailov et al. 2018]
  - Shake-Drop [Yamada et al. 2018]
  - Mix-Up [Zhang et al. 2018]
  - Lookahead Optimizer [Zhang et al. 2019]
  - Cut-Mix [Yun et al. 2019]

- Most of them developed for other data modalities (often computer vision)

Idea II: Use AutoML to find a Regularization Cocktail

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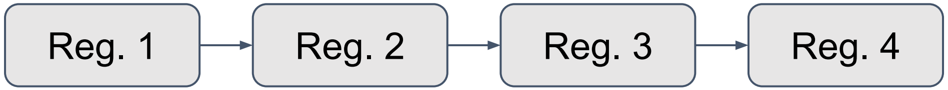
Group	Regularizer	Hyperparameter	Type	Range	Conditionality
Implicit	BN	BN-active	Boolean	$\{\text{True}, \text{False}\}$	–
	SWA	SWA-active	Boolean	$\{\text{True}, \text{False}\}$	-
	LA	LA-active	Boolean	$\{\text{True}, \text{False}\}$	–
		Step size	Continuous	$[0.5, 0.8]$	LA-active
		Num. steps	Integer	$[5, 10]$	LA-active
W. Decay	WD	WD-active	Boolean	$\{\text{True}, \text{False}\}$	–
		Decay factor	Continuous	$[10^{-5}, 0.1]$	WD-active
Ensemble	DO	DO-active	Boolean	$\{\text{True}, \text{False}\}$	–
		Dropout shape	Nominal	{funnel, long funnel, diamond, hexagon, brick, triangle, stairs}	DO-active
		Drop rate	Continuous	$[0.0, 0.8]$	DO-active
	SE	SE-active	Boolean	$\{\text{True}, \text{False}\}$	-
Structural	SC	SC-active	Boolean	$\{\text{True}, \text{False}\}$	–
		MB choice	Nominal	{SS, SD, Standard}	SC-active
	SD	Max. probability	Continuous	$[0.0, 1.0]$	SC-active $\wedge$ MB choice = SD
	SS	-	-	-	SC-active $\wedge$ MB choice = SS
Augmentation	–	Augment	Nominal	{MU, CM, CO, AT, None}	–
	MU	Mix. magnitude	Continuous	$[0.0, 1.0]$	Augment = MU
	CM	Probability	Continuous	$[0.0, 1.0]$	Augment = CM
	CO	Probability	Continuous	$[0.0, 1.0]$	Augment = CO
		Patch ratio	Continuous	$[0.0, 1.0]$	Augment = CO
	AT	-	-	-	Augment = AT

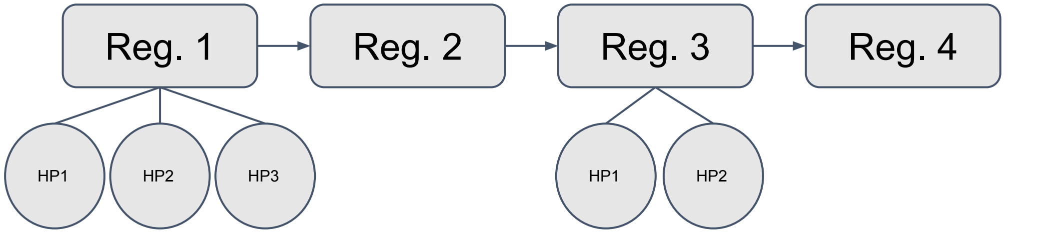
Challenges for AutoML

1. Training DNNs is fairly expensive

2. Pipeline of regularization techniques

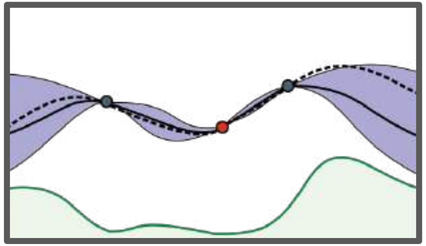


3. Each regularizer has its own hyperparameter → structured space



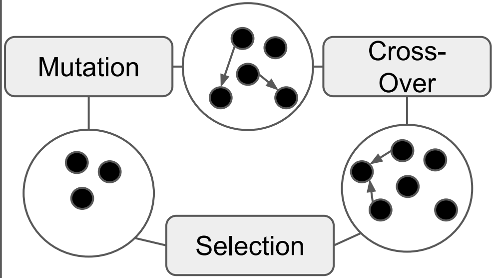
AutoML Techniques

Bayesian Optimization



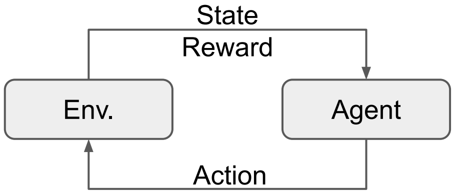
- Global optimization strategy
- Very sample efficient
- Very efficient for small/med. config. spaces

Evolutionary Algorithms



- Population based-approach
- Strong performance for longer budgets
- Easy to parallelize

Reinforcement Learning



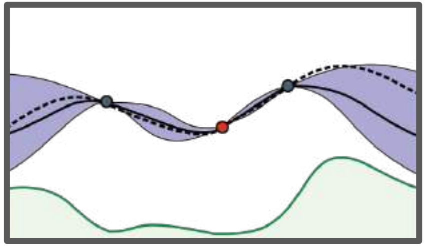
- Learning of a policy
- Can learn a generalizable policy
- Human-like approach

Planning

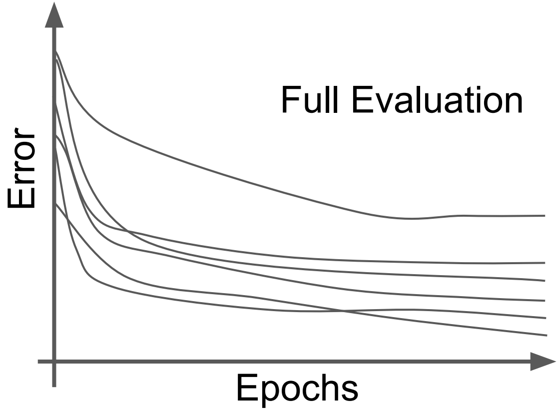
...

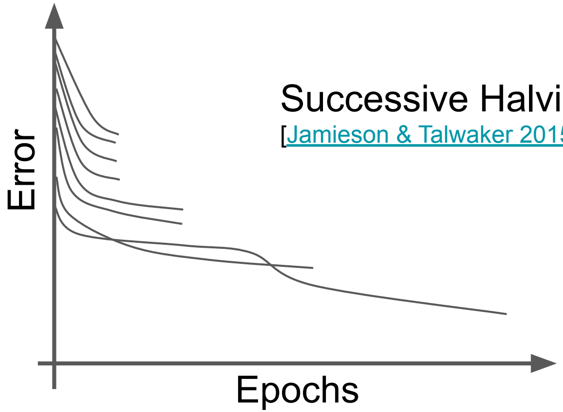
BOHB: Bayesian Optimization + Hyperband
[Falkner et al. 2018]

Bayesian Optimization



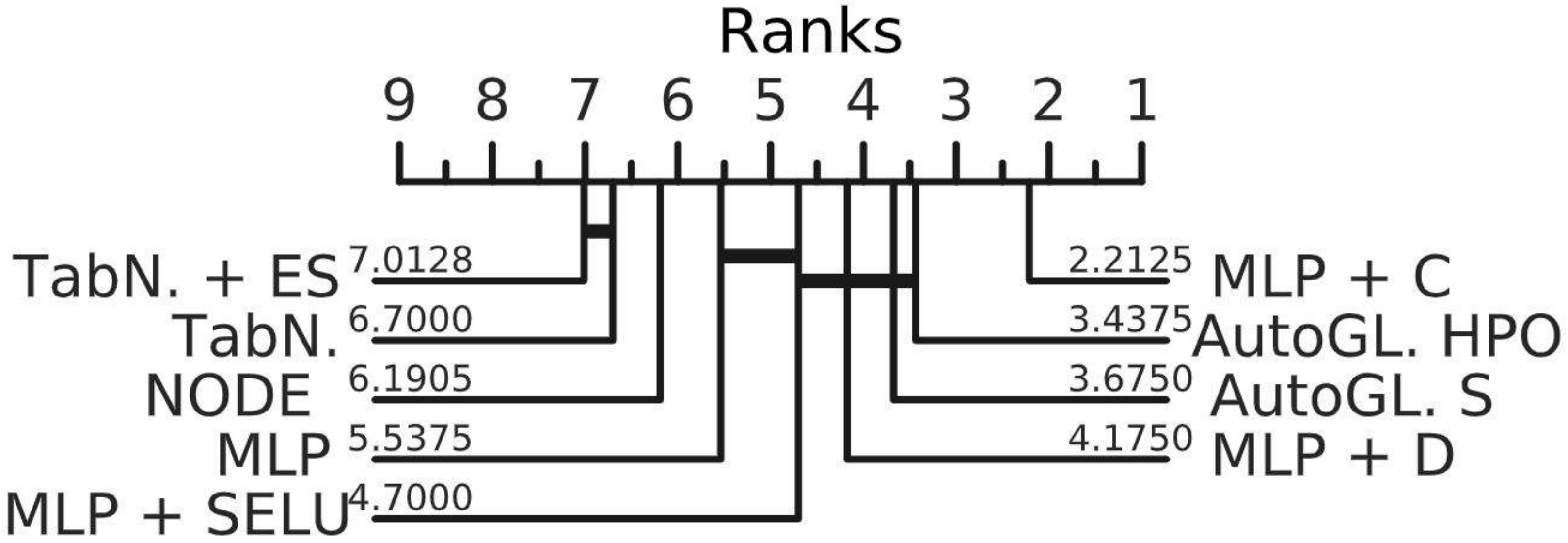
- Global optimization strategy
- Very sample efficient
- Very efficient for small/med. config. spaces



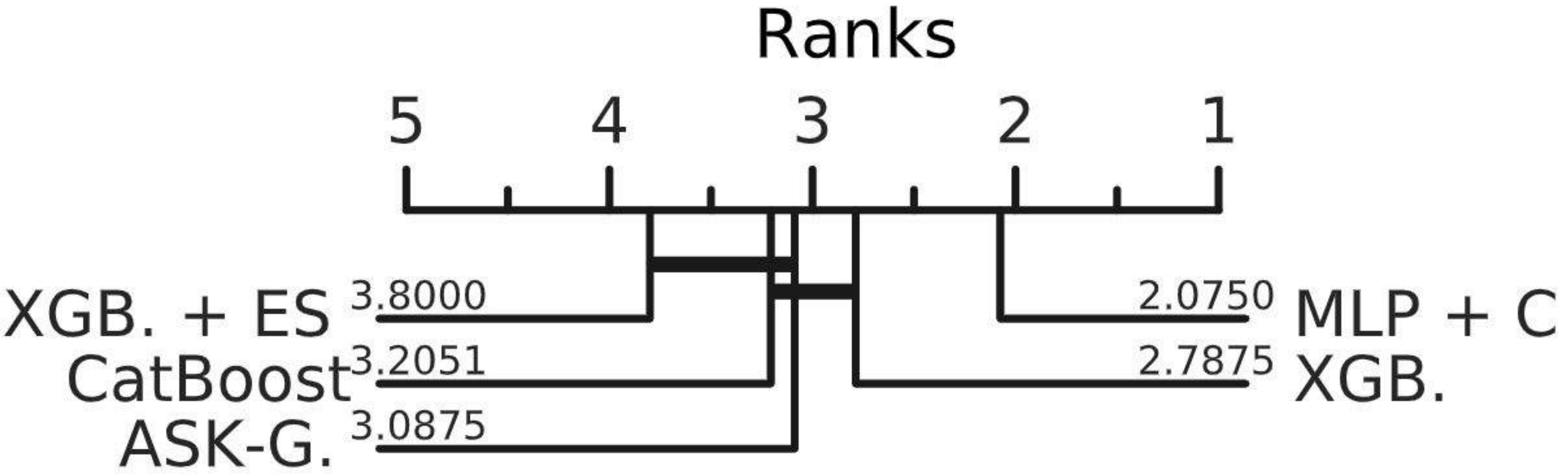


Successive Halving/Hyperband
[Jamieson & Talwaker 2015, Li et al. 2018]

Hypothesis 1: Regularization cocktails outperform state-of-the-art deep learning architectures on tabular datasets



Hypothesis 2: Regularization cocktails outperform Gradient-Boosted Decision Trees (GBDTs)



Hypothesis 3:
Regularization cocktails are time-efficient and achieve strong anytime results.

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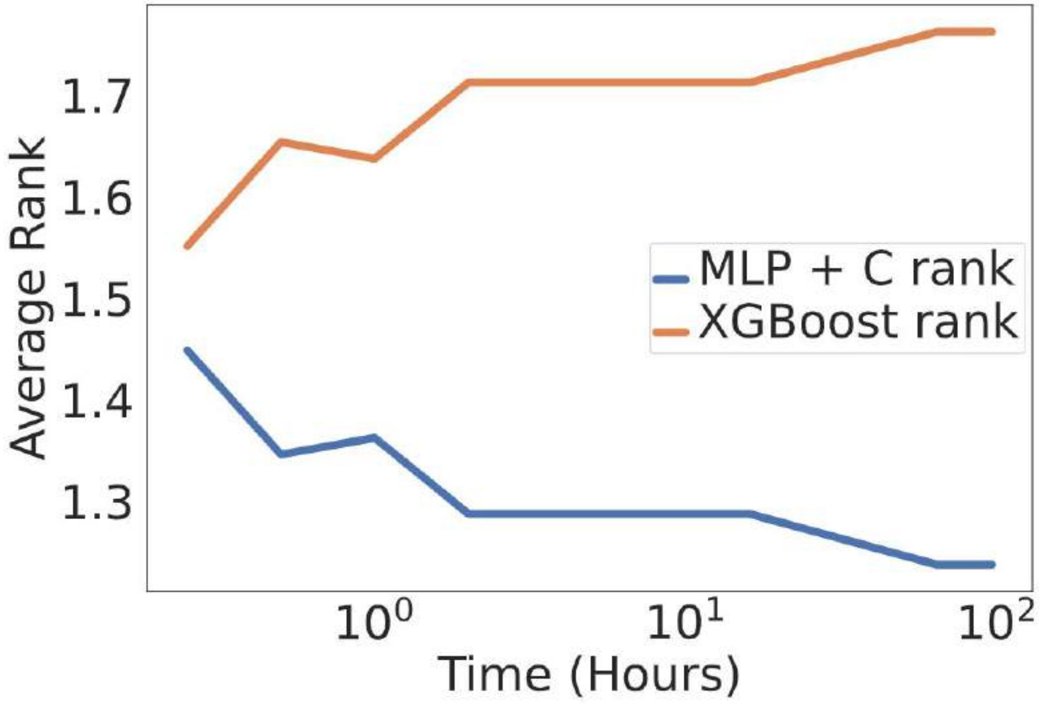


Limitations

1. **Only classification** and
   not regression, semi-supervised data or streaming data so far

2. We considered only somewhat **well-balanced datasets**

3. We used a fairly **simple DNN architecture and no general HPO**
   - simple multilayer perceptron (MLP)
   - fixed hyperparameters of the general training

4. There are **better AutoML frameworks** by now
   - e.g., we know that SMAC3 [Lindauer et al. 2021] performs often better than BOHB

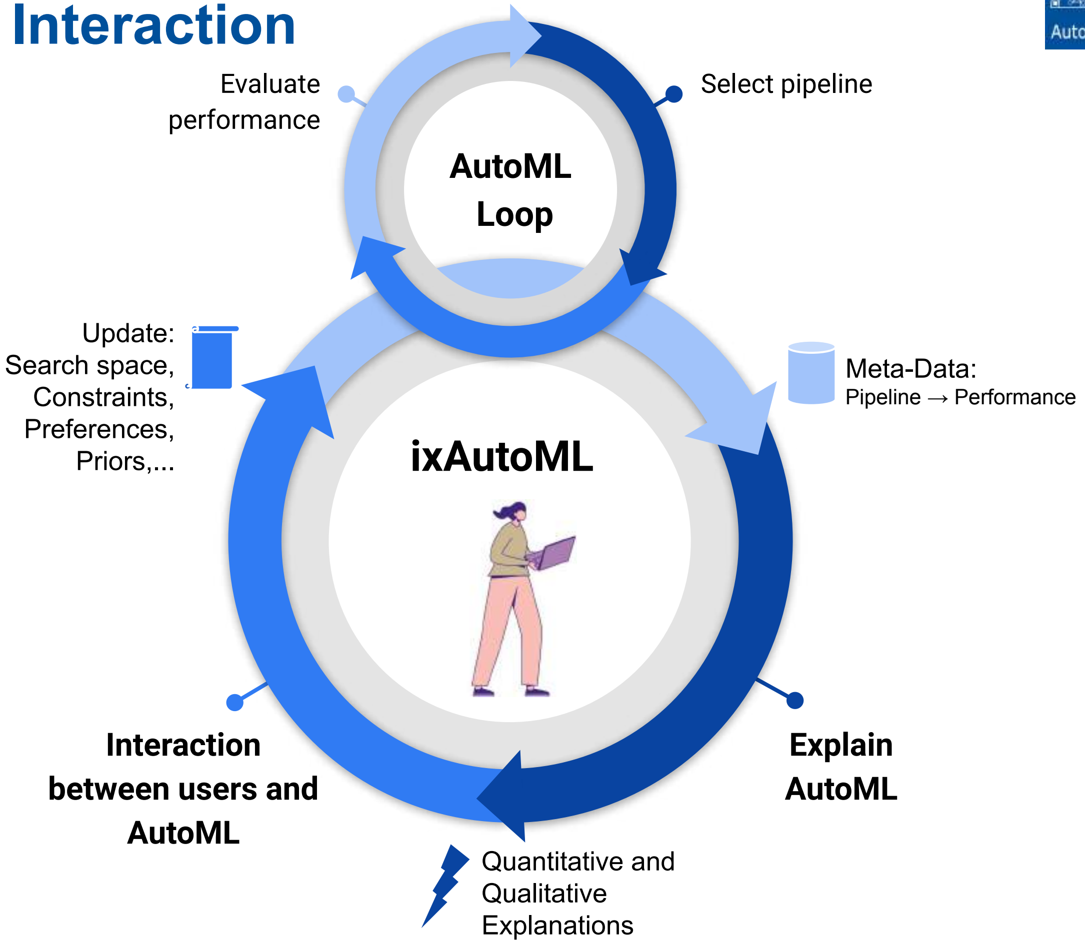
Humans and AutoML?

Towards Human-Centered AutoML

- Fully automated ML design can also receive pushback:
  - How to verify results (i.e., ML pipelines)?
  - How to bring in human expertise?
  - How to integrate into prototype-driven workflows?

- → Human-centered AutoML instead of fully automated ML

Explaining and Interaction



Can we explain what AutoML figured out?

[Moosbauer et al. NeurIPS'21]

Partial Dependence Plots [Friedman 2001]

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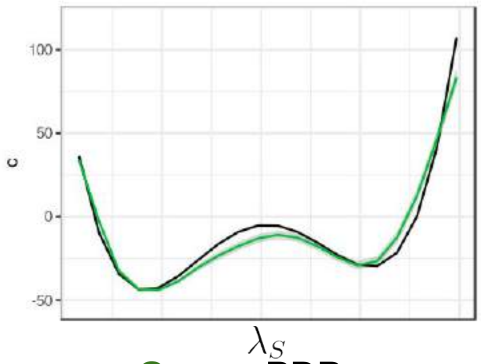
For, a subset S of the hyperparameters, the partial dependence function is:

$$c_S(\lambda_S) := \mathbb{E}_{\lambda_C}\left[c(\lambda)\right] = \int_{\Lambda_C} c(\lambda_S, \lambda_C) d\mathbb{P}(\lambda_C)$$

and can be approximated by Monte-Carlo integration on a surrogate model:

$$\hat{c}_S\left(\lambda_S\right) = \frac{1}{n}\sum_{i=1}^{n} \hat{m}\left(\lambda_S, \lambda_C^{(i)}\right)$$

where $\left(\lambda_C^{(i)}\right)_{i=1,\ldots,n} \sim \mathbb{P}(\lambda_C)$ and λ_S for a set of grid points.



Green: PDP
Black: Ground truth

→ Average of ICE curves.

Quantifying Uncertainties

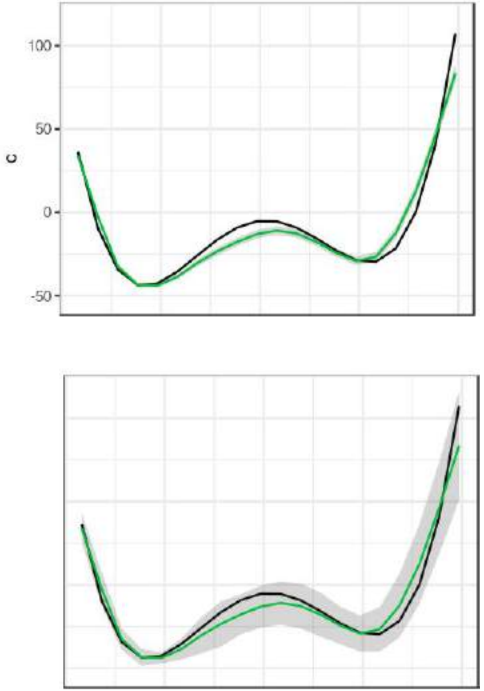
$$
\begin{aligned}
&\hat{s}_S^2(\lambda_S) \\
&= \mathbb{V}_{\hat{c}}\left[\hat{c}_S\left(\lambda_S\right)\right] \\
&= \mathbb{V}_{\hat{c}}\left[\frac{1}{n}\sum\nolimits_{i=1}^{n} \hat{c}\left(\lambda_S, \lambda_C^{(i)}\right)\right] \\
&= \frac{1}{n^2} 1^\top \hat{K}\left(\lambda_S\right)\ 1.
\end{aligned}
$$

→ requires a kernel correctly specifying the covariance structure (e.g., GPs).

Approximation:

$$
\hat{s}_S^2\left(\lambda_S\right) \approx \frac{1}{n}\sum\nolimits_{i=1}^{n} \hat{K}\left(\lambda_S\right)_{i,i}
$$

→ Model-agnostic (local) approximation



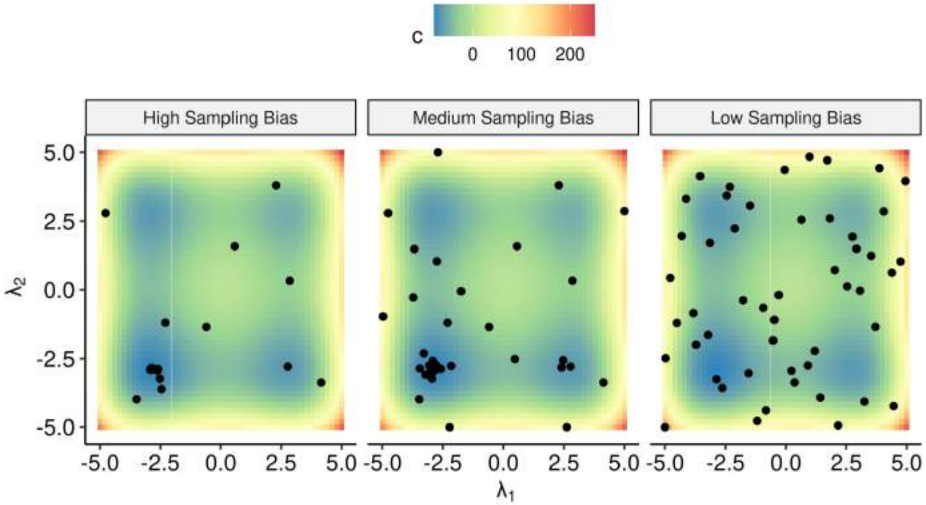
Ground truth
PDP
Uncertainty

Problem of Biased Sampling

- PDPs assume that the data is i.i.d.
- Obviously not the case for efficient AutoML tools with a focus on high-performance regions

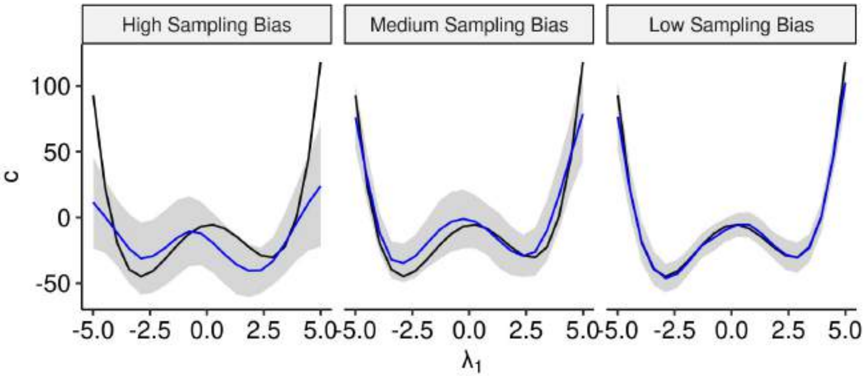
- Example:
  - BO with GPs and LCB
  - Different exploration rate for LCB to show different sampling bias

$$\mathrm{LCB}(\lambda) = \mu(\lambda) + \beta \cdot \sigma(\lambda)$$

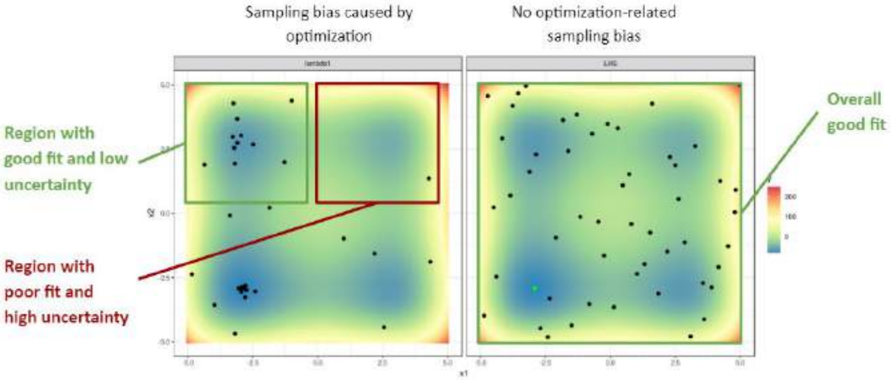


Impact of the Sampling Bias

- Simply using all observations from AutoML tools might lead to misleading PDPs
- Uncertainty estimates help to quantify the poor fits



→ of course, sampling bias is wanted and the solution cannot be to change the sampling behavior



Partitioning of Space

Partition space to obtain interpretable subspaces $\mathcal{N}'$.

Uncertainty variation across all ICE estimates:

$$L\left(\lambda_S, \mathcal{N}'\right) = \sum\nolimits_{i \in \mathcal{N}} \left(\hat{s}^2\left(\lambda_S, \lambda_C^{(i)}\right) - \hat{s}^2_{S|\mathcal{N}'}\left(\lambda_S\right)\right)^2$$

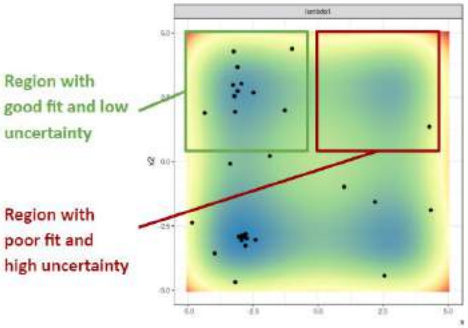
$$\hat{s}^2_{S|\mathcal{N}'}\left(\lambda_S\right) := \frac{1}{|\mathcal{N}'|} \sum_{i \in \mathcal{N}'} \hat{s}^2\left(\lambda_S, \lambda_C^{(i)}\right)$$

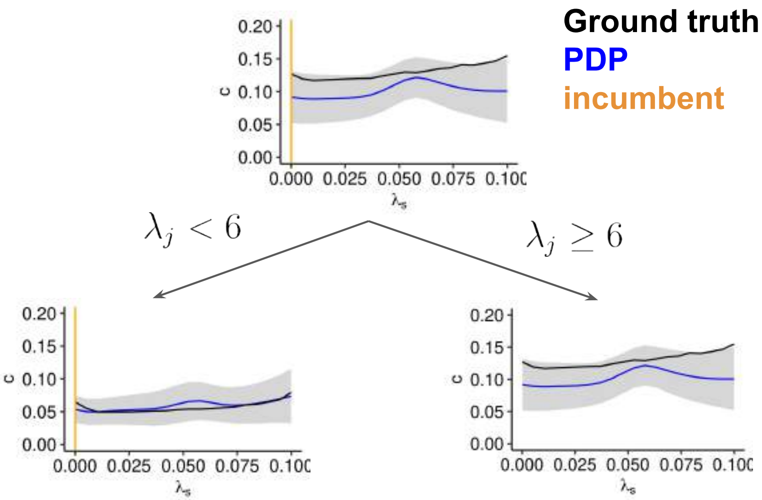
→ **Uncertainty structure of ICE curves should maximally agree**

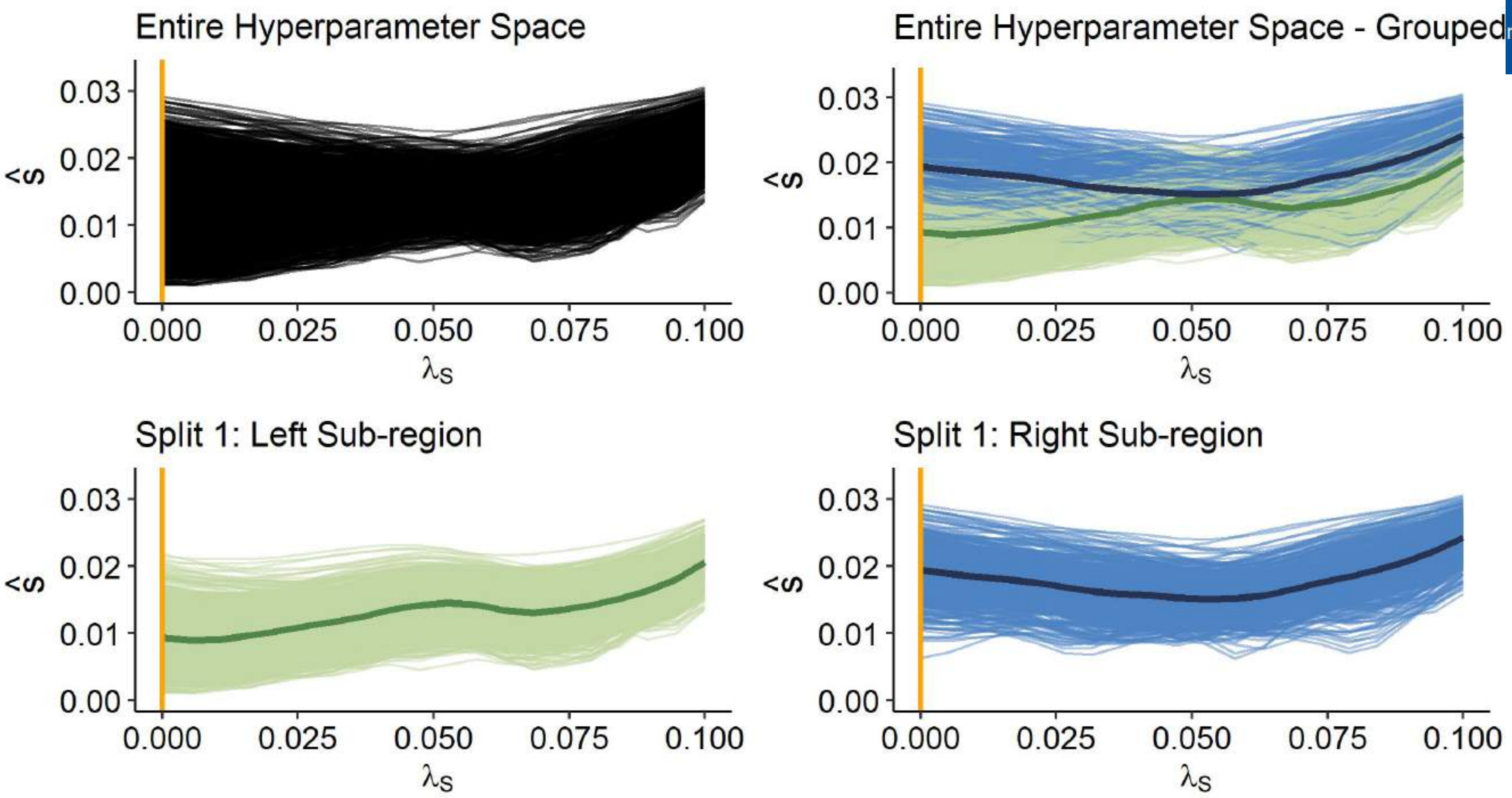
Split Loss = Aggregation over all grid points:

$$\mathcal{R}_{L2}(\mathcal{N}') = \sum\nolimits_{g=1}^{G} L(\lambda_S^{(g)}, \mathcal{N}')$$

Note (i): Partition only along the marginalized dimensions






Entire Hyperparameter Space
Entire Hyperparameter Space - Grouped
Split 1: Left Sub-region
Split 1: Right Sub-region
0.03
0.02
0.01
0.00
0.000
0.025
0.050
0.075
0.100
λ_S
$\hat{s}$

Explaining AutoML via PDPs

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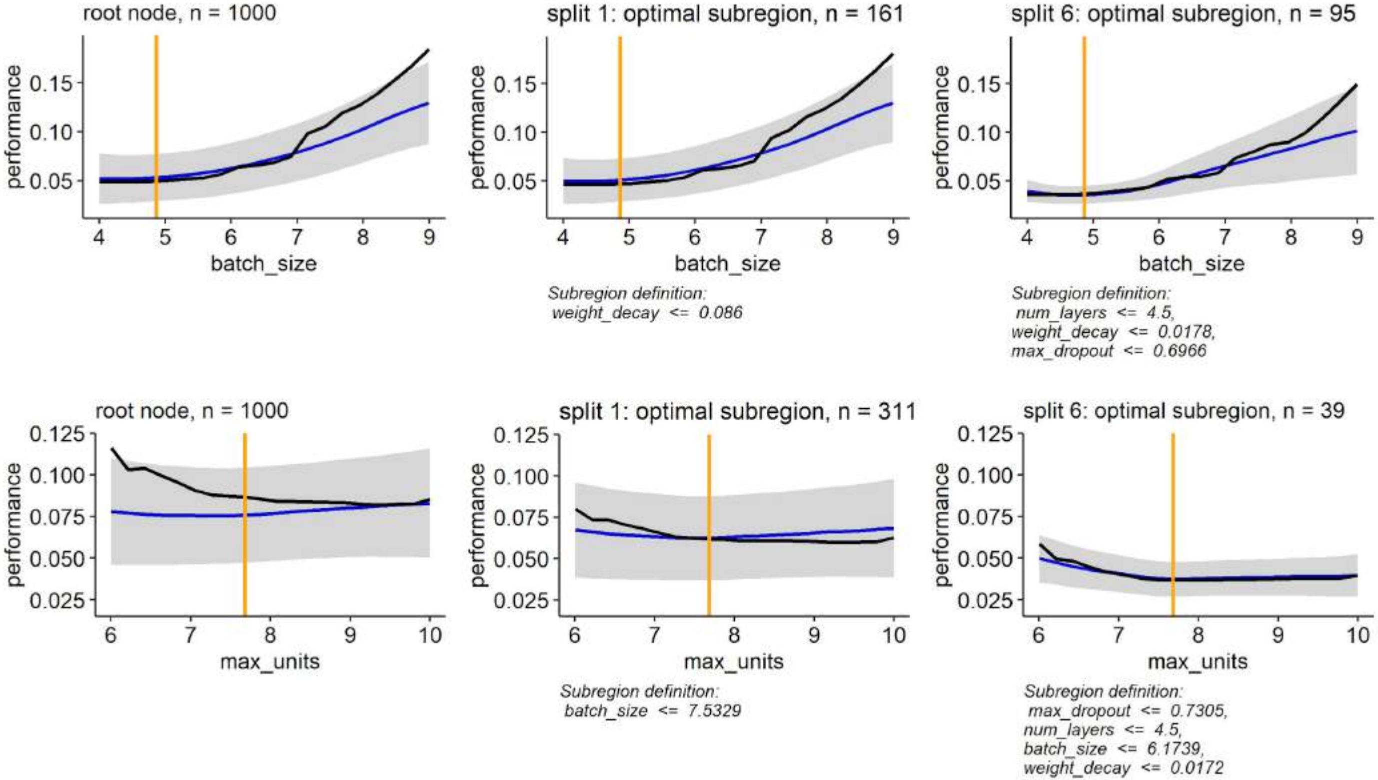
Ground truth
PDP
incumbent



Can Developers also Bring in their Expertise?

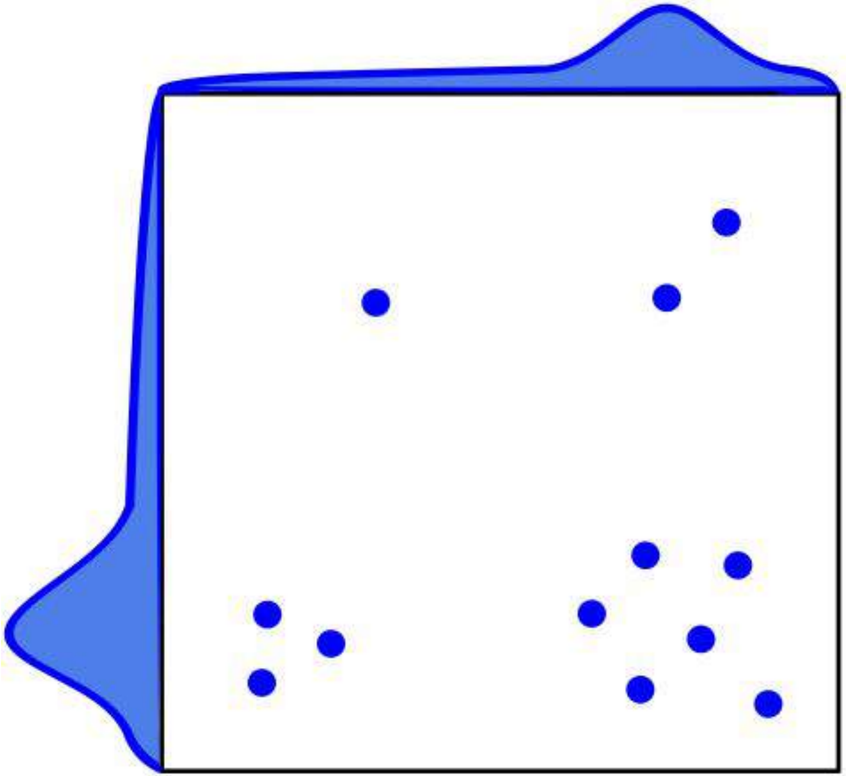
[Souza et al. ECML'21]



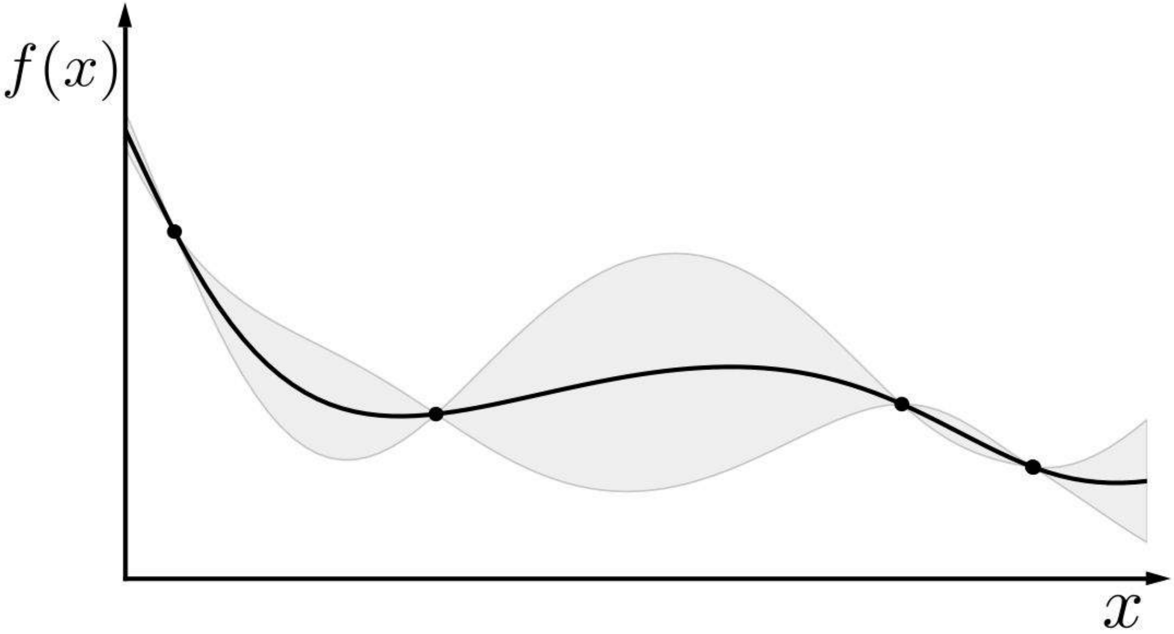

Integrating Human-Prior Knowledge

- ML practitioners often have an intuition for promising hyperparameter configurations
- → Sampling of configurations should focus in these regions

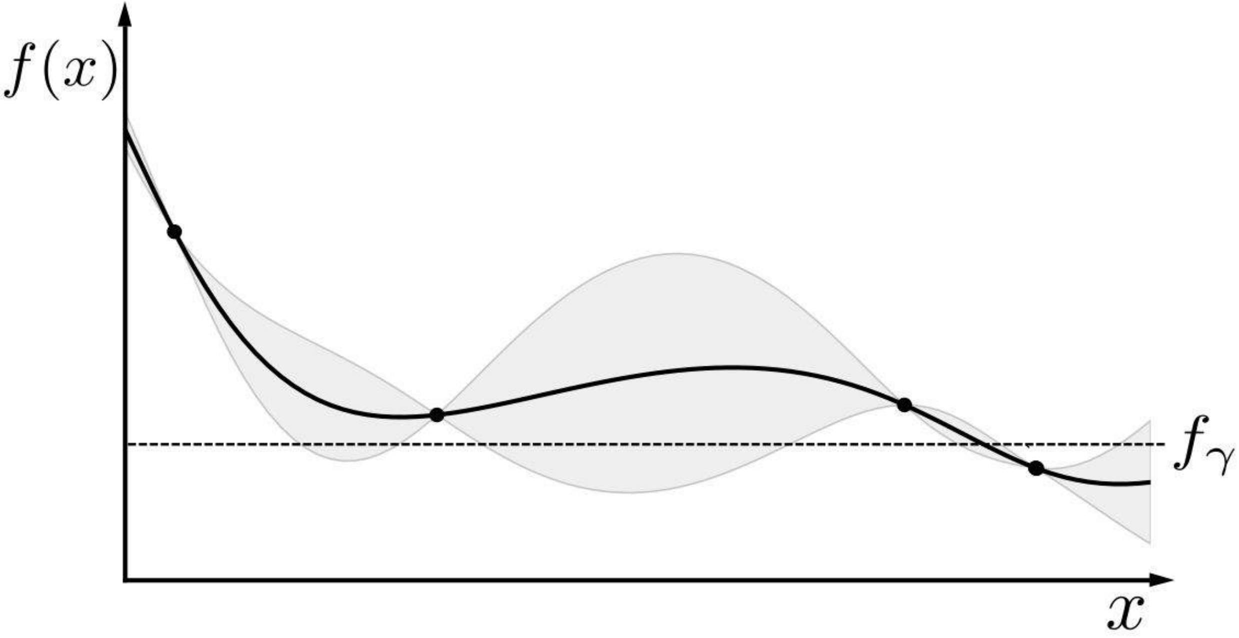
- However, practitioners can also be wrong with their intuition
- → Over time, we should trust the evaluated configurations and the surrogate more than the human expert



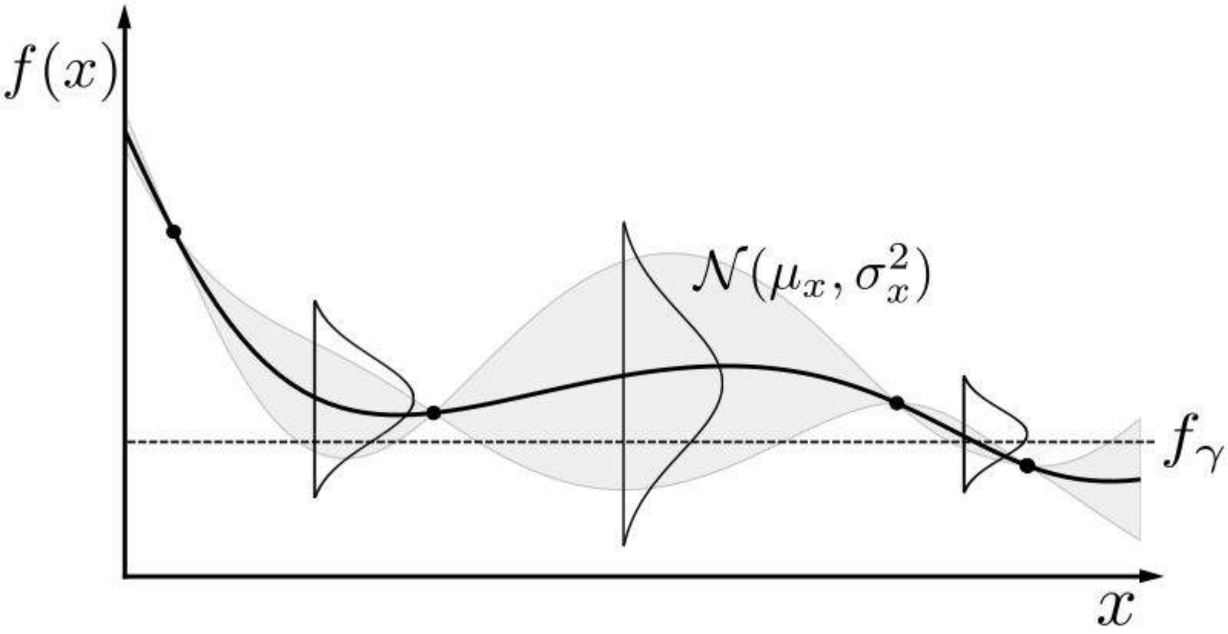
Human-Prior Knowledge -- BOPro



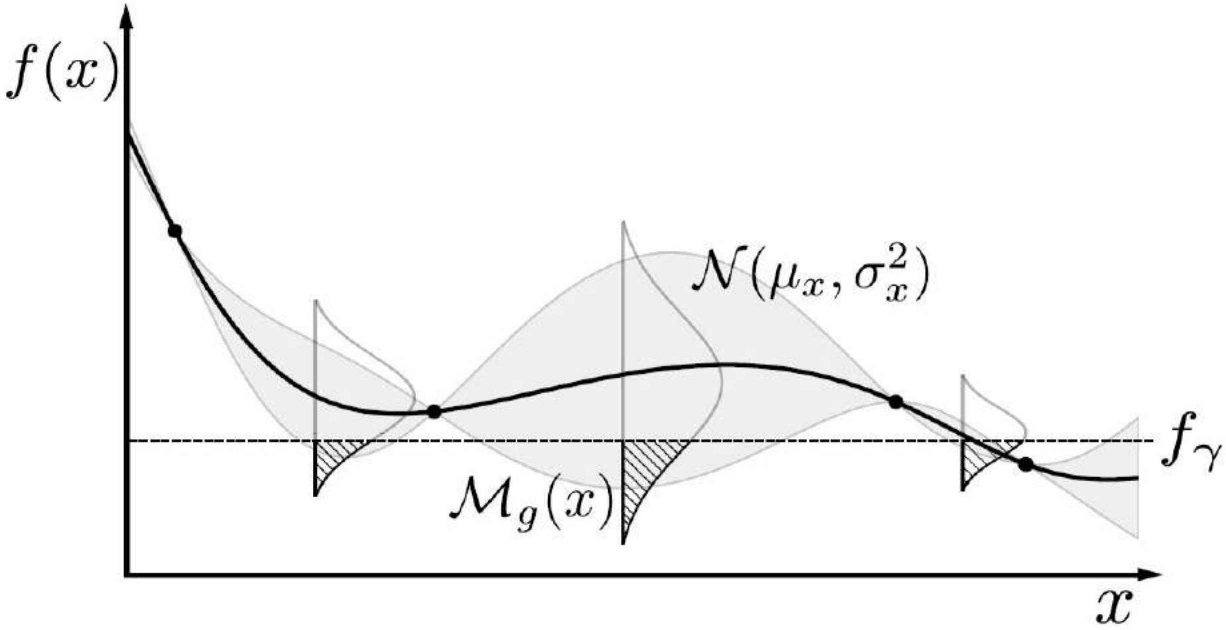
Human-Prior Knowledge -- BOPro



Human-Prior Knowledge -- BOPro



Human-Prior Knowledge -- BOPro



- Instead of modelling f(x), we model whether a configuration is "good" or "bad"
- Using the Gaussian distribution of a GP, we can determine the probability of being good

$$g(\boldsymbol{x}) \propto P_g(\boldsymbol{x}) \mathcal{M}_g(\boldsymbol{x})^{\frac{t}{\beta}}$$

Human-Prior Knowledge -- πBO [Hvarfner et al. 2021]

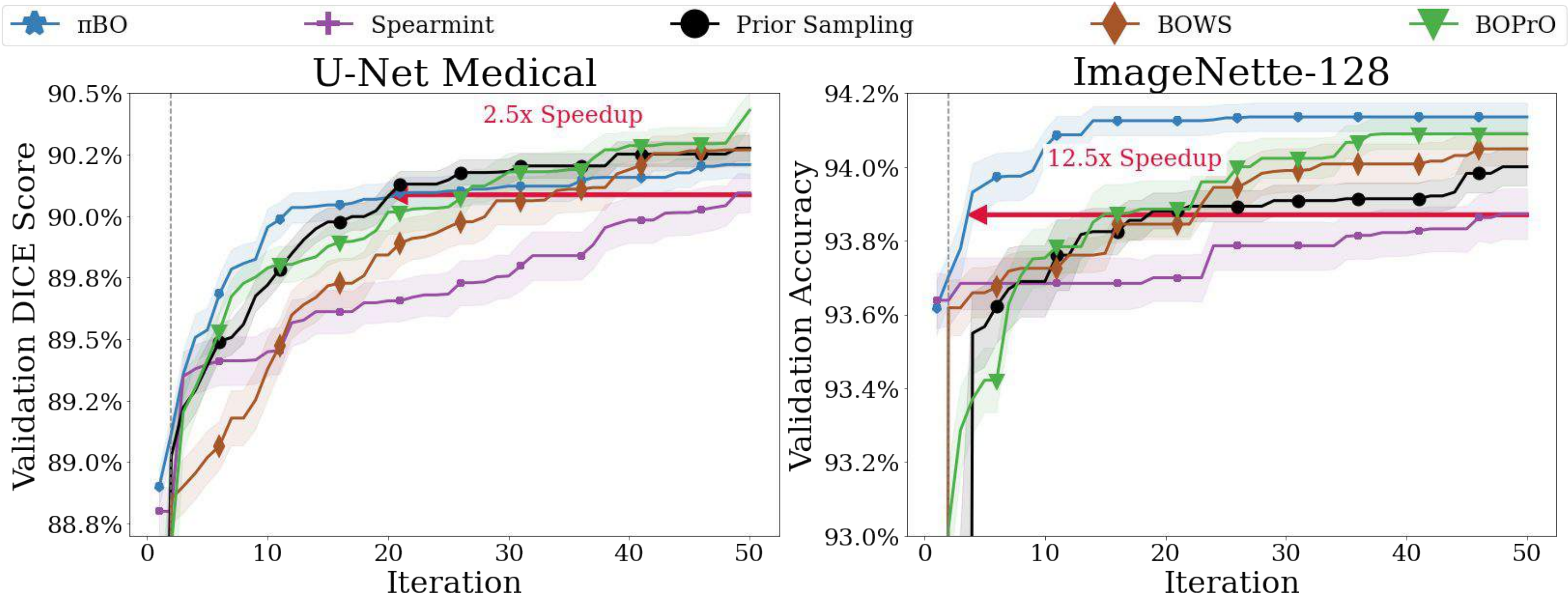
- BOPro has several assumptions on how to model the observations
- πBO is simpler: augment the the acquisition function of BO by a human prior preference

$$\alpha(x) = \hat{\mu}(x) + \kappa\hat{\sigma}(x)$$

$$\alpha_{\pi}(x) = \alpha(x)\pi(x)^{\frac{\beta}{t}}$$

- Advantages of πBO:
  - Can be combined with any acquisition function
  - Same convergence guarantees as with the original acquisition functions (e.g., EI)
  - Can again recover from misleading a-priori knowledge

Human-Prior Knowledge -- πBO [Hvarfner et al. 2021]



/AutoML_org/

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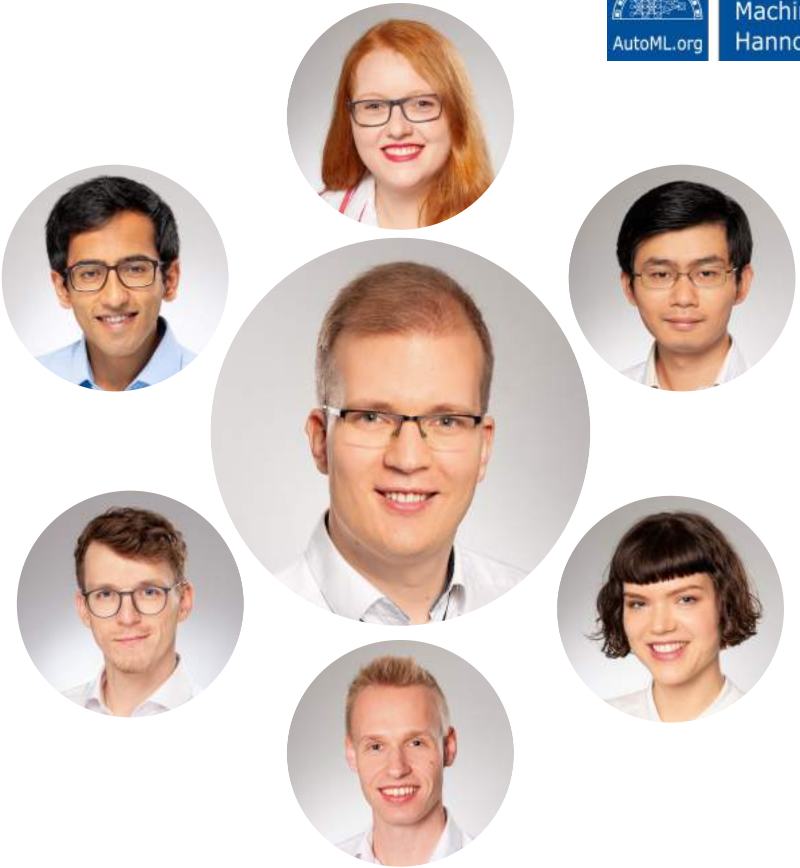
https://tinyurl.com/automlyt

Thank you!



Appendix

Cocktail Frequencies