AutoML: Hyperparameter Optimization

Wrap Up

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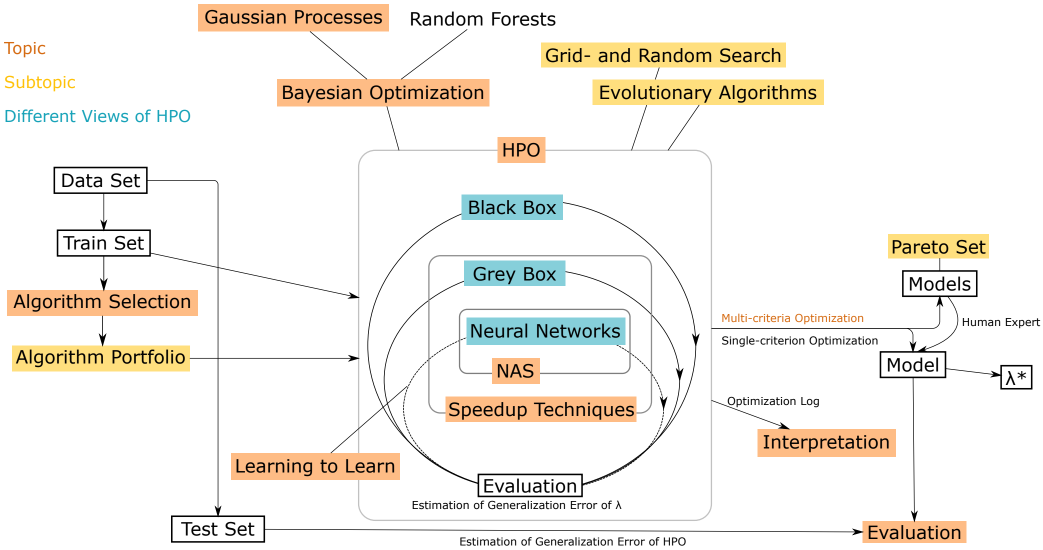
From HPO to AutoML

So far we covered

- Mechanisms to select ML algorithms for a data set (algorithm selection) SOLLTE DAS RAUS?
- HPO as black-box optimization
  - Grid- and random search, EAs, BO
- HPO as a grey box problem
  - Hyperband, BOHB
- Neural Architecture Search (NAS)
  - One-Shot approaches, DART
- Dynamic algorithm configuration (learning to learn)
  - Adapt configuration during training

From HPO to AutoML



Lecture Overview

What is missing?

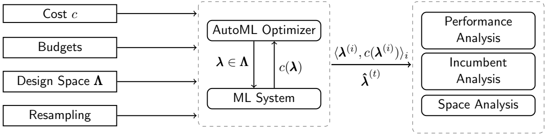
What do I need to know as an AutoML user?

- ~~Nothing, because it is automatic.~~
- Understand limitations of AutoML and framework.
- Know how to interpret the results.
- Maybe: Preprocessing and feature extraction.

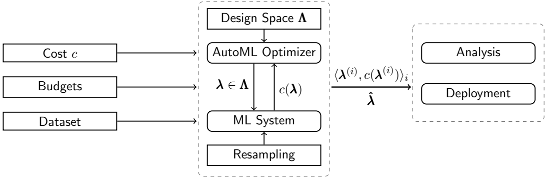
Ingredients to implement an AutoML?

- HPO algorithm
- ML / Pipeline framework
- Parallelization / Multifidelity
- Process encapsulation and time capping

Academic view:



Practitioners view:



Automate HPO

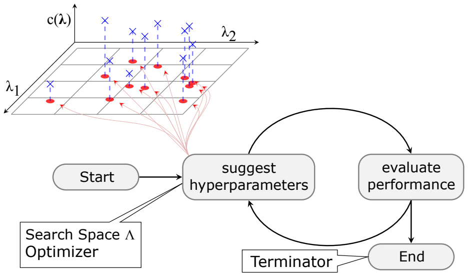
For AutoML the user only supplies ...

- dataset,
- performance measure and
- usually a time budget

To do HPO we need to ...

- preprocessing manually,
- decide on an optimization algorithm,
- an ML algorithm (to generate Inducer $\mathcal{I}$),
- a search space $\boldsymbol{\Lambda}$ and
- a resampling strategy to evaluate $c(\boldsymbol{\lambda})$.

To build an AutoML System we have to make these choices automatically $\rightarrow$ Following slides.



Choice of Learning Algorithm

- A plethora of learners exists, for different data sets different models are likely needed.
- Studies[Fernandez-Delgado et al. 2014] and experience have shown one the following is usually good – on tabular data:
  - Penalized regression, SVM, gradient boosting, random forests, neural networks
  - Random forests only beaten on few datasets by current AutoML frameworks [Gijsbers et al. 2019].
  - Example: Auto-Sklearn 2.0 [Feurer et al. 2020] uses: extra trees, gradient boosting, passive aggressive, random forest, linear model

Choice of Search Space for a Learning Algorithm

- Ranges often selected based on experience
  - Compare to other AutoML Frameworks: e.g. Auto-Sklearn 2.0 [Feurer et al. 2020] WAS SOLL DAS HEISSEN
- Sensitivity analysis often does not exist for learners
- Solution: Analysis of previous HPO runs and learn mapping $\mathbf{D} \rightarrow \mathcal{P}(\mathbf{\Lambda})$ is risky (leaving out important ranges) and complicated.
- Instead: Use big search space $\mathbf{\Lambda}$ and try to predict good initial design (e.g. for Bayesian Optimization). NAJA WEISS NICHT OB ICH DEM SO ZUSTIMME

Algorithm	Hyperparameter	Type	Lower	Upper	Trafo
glmnet					
(Elastic net)	alpha	numeric	0	1	-
	lambda	numeric	-10	10	2^x
rpart					
(Decision tree)	cp	numeric	0	1	-
	maxdepth	integer	1	30	-
	minbucket	integer	1	60	-
	minsplit	integer	1	60	-
kknn					
(k-nearest neighbor)	k	integer	1	30	-
svm					
(Support vector machine)	kernel	discrete	-	-	-
	cost	numeric	-10	10	2^x
	gamma	numeric	-10	10	2^x
	degree	integer	2	5	-
ranger					
(Random forest)	num.trees	integer	1	2000	-
	replace	logical	-	-	-
	sample.fraction	numeric	0.1	1	-
	mtry	numeric	0	1	$x \cdot p$
	respect.unordered.factors	logical	-	-	-
	min.node.size	numeric	0	1	n^x
xgboost					
(Gradient boosting)	nrounds	integer	1	5000	-
	eta	numeric	-10	0	2^x
	subsample	numeric	0.1	1	-
	booster	discrete	-	-	-
	max_depth	integer	1	15	-
	min_child_weight	numeric	0	7	2^x
	colsample_bytree	numeric	0	1	-
	colsample_bylevel	numeric	0	1	-
	lambda	numeric	-10	10	2^x
	alpha	numeric	-10	10	2^x

Taken from [Probst et al. 2019].

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Parameter	Def.P	Def.O	Tun.P	Tun.O	$q_{0.05}$	$q_{0.95}$
glmnet			0.069	0.024		
alpha	1	0.403	0.038	0.006	0.009	0.981
lambda	0	0.004	0.034	0.021	0.001	0.147
rpart			0.038	0.012		
cp	0.01	0	0.025	0.002	0	0.008
maxdepth	30	21	0.004	0.002	12.1	27
minbucket	7	12	0.005	0.006	3.85	41.6
minsplit	20	24	0.004	0.004	5	49.15
kknn			0.031	0.006		
k	7	30	0.031	0.006	9.95	30
svm			0.056	0.042		
kernel	radial	radial	0.030	0.024		
cost	1	682.478	0.016	0.006	0.002	920.582
gamma	$1/p$	0.005	0.030	0.022	0.003	18.195
degree	3	3	0.008	0.014	2	4
ranger			0.010	0.006		
num.trees	500	983	0.001	0.001	206.35	1740.15
replace	TRUE	FALSE	0.002	0.001		
sample.fraction	1	0.703	0.004	0.002	0.323	0.974
mtry	$\sqrt{p}$	$p \cdot 0.257$	0.006	0.003	0.035	0.692
respect.unordered.factors	TRUE	FALSE	0.000	0.000		
min.node.size	1	1	0.001	0.001	0.007	0.513
xgboost			0.043	0.014		
nrounds	500	4168	0.004	0.002	920.7	4550.95
eta	0.3	0.018	0.006	0.005	0.002	0.355
subsample	1	0.839	0.004	0.002	0.545	0.958
booster	gbtree	gbtree	0.015	0.008		
max_depth	6	13	0.001	0.001	5.6	14
min_child_weight	1	2.06	0.008	0.002	1.295	6.984
colsample_bytree	1	0.752	0.006	0.001	0.419	0.864
colsample_bylevel	1	0.585	0.008	0.001	0.335	0.886
lambda	1	0.982	0.003	0.002	0.008	29.755
alpha	1	1.113	0.003	0.002	0.002	6.105

Table 3: Defaults (package defaults (Def.P) and optimal defaults (Def.O)), tunability of the hyperparameters with the package defaults (Tun.P) and our optimal defaults (Tun.O) as reference and tuning space quantiles ($q_{0.05}$ and $q_{0.95}$) for different parameters of the algorithms.

Taken from [Probst et al. 2019].

Choice of Resampling Strategy

For computation of generalization error / cost:

$$c(\boldsymbol{\lambda}) = \frac{1}{k} \sum_{i=1}^{k} \widehat{GE}_{\mathcal{D}^i_{\text{val}}} \left(\mathcal{I}(\mathcal{D}^i_{\text{train}}, \boldsymbol{\lambda})\right) \tag{1}$$

Rules of thumb:

- Default: 10-fold CV ($R = 10$)
- Huge datasets: Holdout
- Tiny datasets: 10x10 repeated CV
- Stratification for imbalanced classes

Watch out for this:

- Small sample size situation because of imbalancies
- Leave-one-object out
- Time dependencies
- A good AutoML system should let you customize resampling

Choice of Optimization Algorithm

Choose optimization algorithm based on ...

- complexity of search space / budget
- time-costs of evals

Complex search space

$\rightarrow$ Random Search, TPE, BO with RF

Numerical (lower-dim) search space and tight budget

$\rightarrow$ BO with GP

Expensive evals

$\rightarrow$ Hyperband, BOHB

Deep Learning

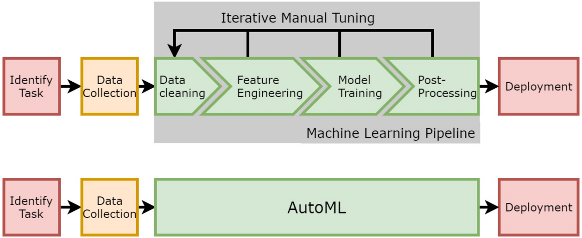
$\rightarrow$ Parametrize architectures, then HPO, see above

$\rightarrow$ NAS

Preprocessing

Ideal AutoML systems should also optimize:

- ✗ Data preprocessing
- ✗ Feature engineering
- ✗ Feature selection
- ✓ Model training



Lecture Overview

1. The Missing Building Blocks
2. Common Preprocessing Steps
3. Combined Preprocessing and Model Building: Pipelining

Preprocessing capabilities differ heavily

Tool	Platform	Input data sources		Data pre-processing	Data types detected					Feature engineering				ML Tasks		Model selection and Hyperparameter optimization					Quick start / early stop			Model evaluation / Result analysis/ Visualization		
		Spreadsheet datasets	Image, text		Numerical	Categorical	Datetime	Time-series	Other (Hierarchical types) (7*)	Datetime, categorical processing	Imbalance, missing values	Feature selection, reduction	Advanced feature extraction (8*)	Supervised learning (9*)	Unsupervised learning (10*)	Ensemble	Genetic algorithm	Random search	Bayesian search	Neural architecture search	Quick finding of starting model	Allow maximum limit search time	Restrict time consuming combination of components	Model dashboard	Feature importance	Model explainability and interpretation, and reason code (11*)
TransmogrifAI	Apache Spark	Y	N	Y(*)	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	N	Y	N	Y	Y	N	N			Y	Y	
H2O-AutoML	H2O clusters	Y	N	Y	Y	Y	Y	Y	N	Y	Y	Y	N	Y	N	Y	N	Y	N	N	N	Y	Y	Y	Y	Y
Darwin (+)	GCP	Y	N	Y	Y	Y	Y	Y	N	Y	Y	Y	Y	Y	Y	Y	Y	N	N	Y	Y	Y	N	Y	Y	Y
DataRobot (+)	Datarobot & AWS	Y	Y	Y	Y	Y	N	Y	N	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	N	N	Y		Y	Y	Y
Google AutoML (+)	Google Cloud	N	Y	Y						N	Y	Y	Y	Y	Y		Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Auto-sklearn		Y	N	N	N	N	N	N	N	Y(2*)	Y	Y	Y	Y	N	Y	N	Y	Y	N	Y	Y	Y	Y	Y	Y
MLjar (+)	MLJAR Cloud	Y(3*)	N	Y	Y	Y	N	N	N	Y	Y(4*)	N	N	Y(5*)	N	Y	N	Y	N	N	N	N	N	Y	Y	N
Auto_ml		Y	N	N	N	N	N	N	N	Y	Y	Y	Y	Y	N	Y	N	Y	Y	N	N	N	N	Y	Y	Y
TPOT		Y	N	N	N	N	N	N	N	N	Y	N	Y	Y	N	Y	Y	N	N	N	N	Y	N	Y	Y	N
Auto-keras		Y	Y	N	N	N	N	N	N	N	Y	Y	N	Y	N	N	N	Y	Y	Y	Y	Y	N	Y	N	Y
Ludwig		Y	Y	Y(*)	Y	Y	N	Y	Y	N	Y	Y	Y	Y	N	Y	N	Y	Y	Y	Y	N	N	Y	Y	N
Auto-Weka		Y	N	N	Y	Y	N	N	N	N	Y	Y	N	Y	N	Y	N	Y	Y	N	N	Y	Y	Y	N	N
Azure ML (+)	Azure	Y	Y	Y(6*)	Y	Y	Y	Y	N	Y	Y	Y	Y	Y	N	Y	N	Y	Y	N		Y	Y	Y	Y	
Sagemaker (+)	AWS	Y	Y	Y	Y	Y	Y	Y	N	Y	Y	Y	Y	Y	Y	N	Y	Y	Y	N		Y	N	Y	Y	Y
H2O-Driverless AI (+)	H2O clusters	Y(3*)	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	N	N	N	Y	Y	Y	Y

Fig. 2. Comparison table of functionality for AutoML tools. (+): commercialized tools; (∗): the function is not very stable, it fails for some datasets; (2∗): categorical input must be converted into integers; (3∗): datasets have to include headers; (4∗): missing values must be represented as NA; (5∗): multiclass classification not provided; (6∗): need some users' input for dataset description such as column types; (7∗): ability to detect primitive data types and rich data types such as: text (id, url, phone), numerical (integer, real); (8∗): advanced feature processing: bucketing of values, removing features with zero variance or features with drift over time; (9∗): supervised learning includes binary classification, multiclass classification, regression; (10∗): unsupervised learning includes clustering and anomaly detection; (11∗): model interpretation and explainability refers to techniques such as LIME, Shapley, Decision Tree Surrogate, Partial Dependence, Individual Conditional Expectation, Lift chart, feature fit, prediction distribution plot, accuracy over time, hot spot and reason codes; In a few empty cells, it is not clear that the functionality is provided from documentations of the tools, to the best of our knowledge.

Taken from Truong et al., 2019 ICTAI.

Highlighted: Non-commercial AutoML Frameworks

- detection of feature types: some
- preprocess categorical values: some
- missing values: all
- imbalances: all

Cleaning

Data cleaning can hardly be automatized but a few heuristics exist:

- Remove ID Columns, Columns with mostly unique values.
- Outlier detection (in the feature space)
- Detect time series or spatial data $\rightarrow$ randomized validation might be flawed.

Categorical Features: Dummy Encoding

ML algorithm does not support categorical features + few unique values → use dummy encoding.

SalePrice	Central.Air	Bldg.Type
189900	Y	1Fam
195500	Y	1Fam
213500	Y	TwnhsE
191500	Y	TwnhsE
236500	Y	TwnhsE

SalePrice	Y	Bldg.Type.2fmCon	Bldg.Type.Duplex	Bldg.Type.Twnhs	Bldg.Type.TwnhsE
189900	1	0	0	0	0
195500	1	0	0	0	0
213500	1	0	0	0	1
191500	1	0	0	0	1
236500	1	0	0	0	1

Categorical Features: Target Encoding

Avoid high cardinality categorical features because they are problematic for all ML algorithms
$\rightarrow$ use Target Encoding (also Impact Encoding).

Goal: Each categorical feature $\boldsymbol{x}$ should be encoded in a single numeric feature $\tilde{\boldsymbol{x}}$

$$\text{Regression: } \mathrm{Impact}(x) = \mathbb{E}(\boldsymbol{y}|x) - \mathbb{E}(\boldsymbol{y})$$

$$\text{Classification: } \mathrm{Impact}(x) = \mathrm{logit}(P(y = \text{target}|x)) - \mathrm{logit}(P(y = \text{target}))$$

- Needs regularization (through CV) to prevent target leakage [Zumel et al. 2019]
- Advantage: Handles unknown categorical levels on test data.

Alternatives: Factorization Machines, clustering feature levels, feature hashing

D_{train}

x	y
A	10
A	20
B	30

Encoding

x	$\tilde{x}$
A	-5
B	10

D_{test}

x	$\tilde{x}$
A	-5
B	10
C	0

Common Preprocessing Steps: Missing Values

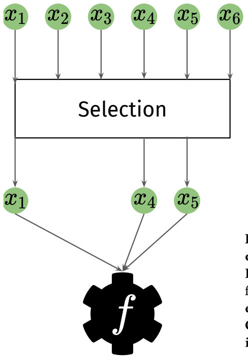
Missing values:

- Additional factor column indicating missingness
- Replace missing values with <u>out of range</u> or median/mode
- Advanced imputation strategies seldom advantageous (also because data mostly not missing at random)

Feature Selection

Feature selection:

- Filter
- Stepwise selection methods: Needs to be applied on the whole pipeline (impractical!)
- Seldom increases performance but decreases computational costs $\rightarrow$ Multi-criteria optimization.
  - Combined Feature Selection and HPO: [Binder et al. 2020]
- Happens indirectly in learning algorithm: random forest, lasso regression, ...



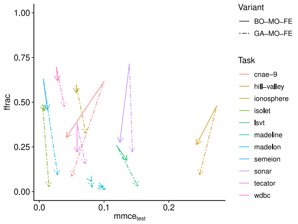


Figure 3: Comparison of multi-objective and single-objective methods applied to the SVM learning algorithm: Performance $\mathrm{mmce}_{\mathrm{test}}$ and the fraction of included features ffrac found after 2000 evaluations by baseline BO-SO (tail end of arrows), BO-MO-FE (head of solid arrows) and GA-MO-FE (head of dashed arrows). Each dataset (Table 1) is shown, values are averaged over 10 outer CV runs. Choice of individuals for MO methods described in Section 6.2.

Taken from [Binder et al. 2020].

Common Feature Construction Methods

Reduction:

- PCA, ICA, autoencoder

Feature extraction:

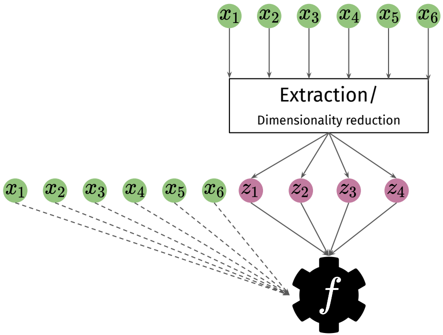
- Polynomial Features: $x_j \longrightarrow x_j, x_j^2, x_j^3, \ldots$
- Interactions: $x_j, x_k \longrightarrow x_j, x_k, x_j \cdot x_k$

Feature generation:

- Transform to "circular" features (year, month, day)
  e.g. $\tilde{x}_1 = sin(2\pi \cdot x/24)$ and $\tilde{x}_2 = cos(2\pi \cdot x/24)$

Combine with external data:

- names $\longrightarrow$ gender, ethnicity, age
- home address $\longrightarrow$ household income
- location + date $\longrightarrow$ weather



Imbalanced Classes

Imbalanced classes:

- over-sampling of minority class
- seldom: under-sampling of majority class
- Influence of more advanced methods (e.g. SMOTE) on the predictive accuracy questionable.

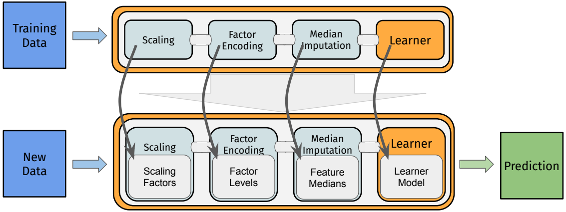
Lecture Overview

Pipelining

Most preprocessing steps have parameters or can be switched on/off in the pipeline.

Goal: Find optimal preprocessing parameters $\rightarrow$ HPO

- Most preprocessing methods have states similar to the model of an inducer.
- Applying preprocessing to the whole dataset leads to overfitting.
- Pipeline has to be optimized as a whole: $\mathbf{\Lambda} = \mathbf{\Lambda}_{\text{pipeline}} \times \mathbf{\Lambda}_{\mathcal{I}}$ within the resampling procedure.



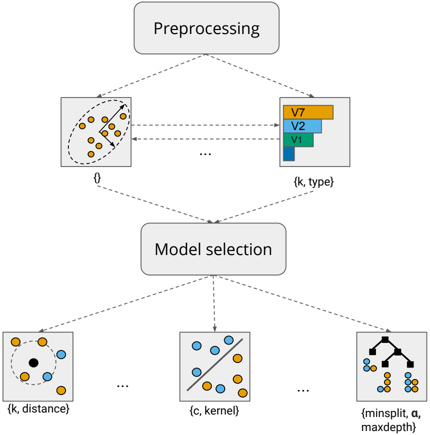
Optimizing Pipelines

- Introducing different choices for preprocessing.
- Tuning over multiple learning algorithms.

$\rightarrow$ $\boldsymbol{\Lambda}$ becomes hierarchical search space!

Suitable optimizers:

- Random Search, TPE, Hyperband
- BO with RF surrogate
- Evolutionary approaches (similar to NAS)



Obtaining Final Model

Options:

- Choose the optimal path as linear pipeline.
- Build ensemble of best configurations (e.g. [LeDell and Poirier, 2020]).