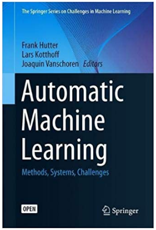
Automated Machine Learning

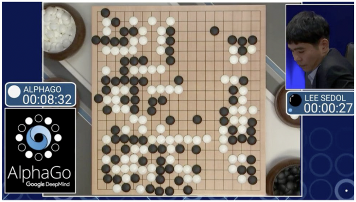
Stéphane Canu
asi.insa-rouen.fr/enseignants/~scanu
scanu@insa-rouen.fr



INSA Rouen Normandie

Motivation

The importance of Hyperparameter optimization (HPO)



AlphaGo: tuning 10 hyperparameters improved win rate from 50% to 65% before playing Lee Sedol

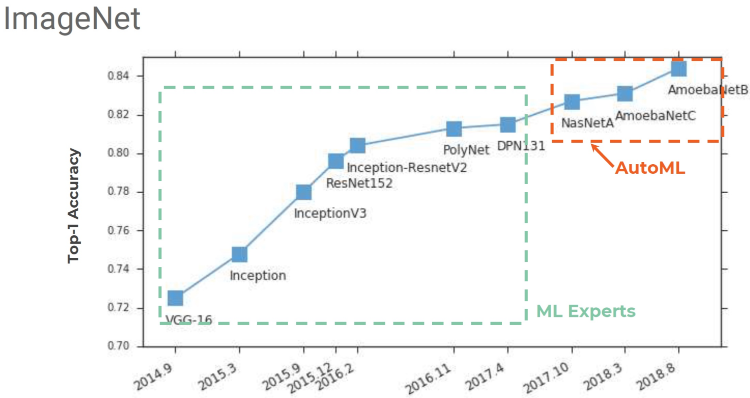
Hyperparameter Group	Hyperparameters
Finetuning Strategies	Percentage of the Model to Freeze, Layer Decay, Linear Probing, Stochastic Norm, SP-Regularization, DELTA Regularization, BSS Regularization, Co-Tuning
Regularization Techniques	MixUp, MixUp Probability*, CutMix, Drop-Out, Label Smoothing, Gradient Clipping
Data Augmentation	Data Augmentation Type (Trivial Augment, Random Augment, Auto-Augment), Auto-Augment Policy*, Number of operations*, Magnitude*
Optimization	Optimizer type (SGD, SGD+Momentum, Adam, AdamW, Adamp), Beta-s*, Momentum*, Learning Rate, Warm-up Learning Rate, Weight Decay, Batch Size
Learning Rate Scheduling	Scheduler Type (Cosine, Step, Multi-Step, Plateau), Patience*, Decay Rate*, Decay Epochs*

Hyperparameters for fine-tuning foundation models

Too many choices [Pineda et al, 2023]

Motivation

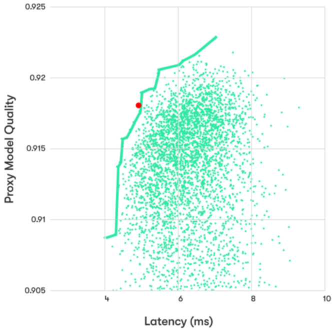
Quoc Le from Google « *AI Frontiers Conference* »nov 2018 « *Using Machine Learning to Automate Machine Learning* »

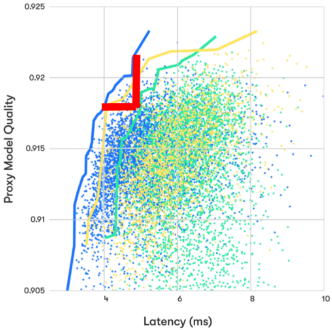


slideshare.net/AIFrontiers/quoc-le-at-ai-frontiers-using-machine-learning-to-automate-machine-learning

Motivation

How to build Waymo auto pilot (semantic segmentation task)?

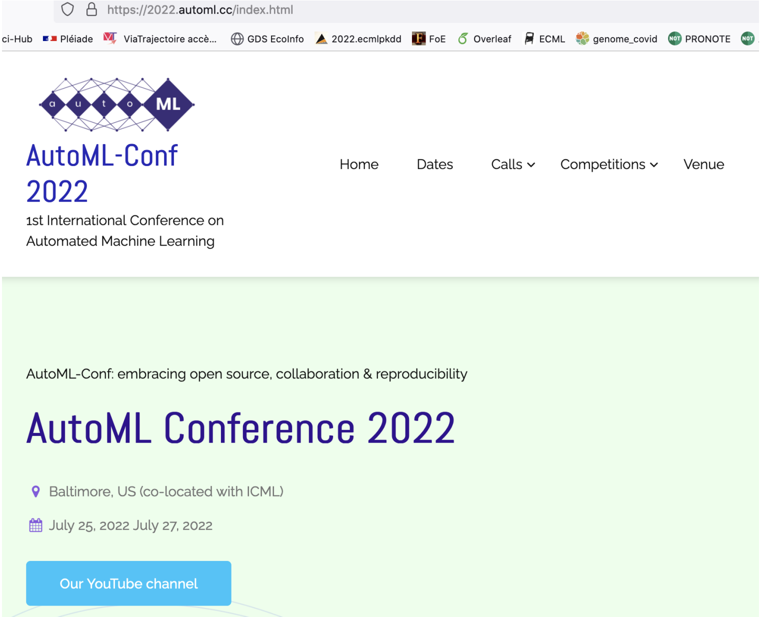




random search Auto ML .

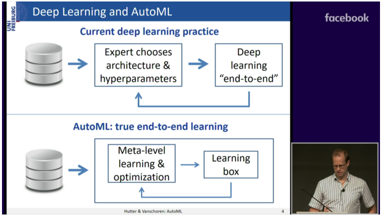
https://blog.waymo.com/2019/07/automl-automating-design-of-machine.html

Motivation


https://2022.automl.cc/index.html
ci-Hub Pléiade ViaTrajectoire accè... GDS EcoInfo 2022.ecmlpkdd FoE Overleaf ECML genome_covid PRONOTE
a u t o ML
AutoML-Conf 2022
1st International Conference on Automated Machine Learning
Home
Dates
Calls
Competitions
Venue
AutoML-Conf: embracing open source, collaboration & reproducibility
AutoML Conference 2022
Baltimore, US (co-located with ICML)
July 25, 2022 July 27, 2022
Our YouTube channel

Lecture road map

1. AutoML and the machine learning process
2. Dataset
3. Preprocessing
4. Hyperparameter tuning
5. Post processing – Model agregation
6. Auto ML frameworks



http://www.automl.org/

AutoML = Learning to learn

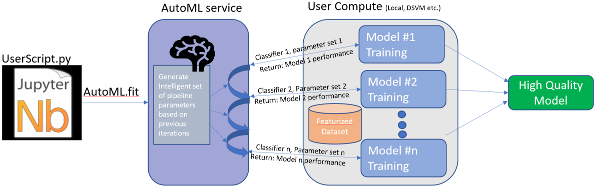
- input:
  1. data $\mathcal{S} = (x_i, y_i), i = 1, \ldots, n$
  2. ML algorithm(s) $f_\ell(x, \theta, h)$

     x input

     θ parameters

     h hyperparameters
  3. other datasets with solutions $(S_j, f_{\ell_j}(x, \theta_j, h_j)), j = 1, \ldots, m$

- output: a decision function f combining $f_{\ell_k}(x, \theta_k, h_k), k = 1, \ldots, K$



Microsoft's automated machine learning

A simple example

Learning to learn?

- input:
  1. data $\mathcal{S} = (x_i, y_i), i = 1, \dots, n$ classification y$\in \{0, 1\}$
  2. ML algorithm(s) $f_\ell(x, \theta, h)$

     SVM $f_1(x, \theta = (\alpha, b), h = (C, \sigma, \varepsilon))$

     RF $f_2(x, \theta, h = (t, p, d, \dots))$

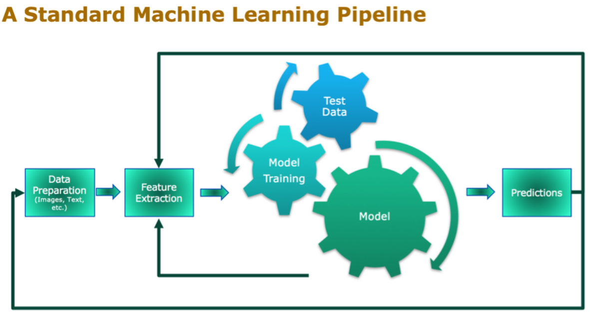
     kNN $f_3(x, \theta = \sim, h = k)$

     ...
  3. other datasets with solutions: Iris, glass, cover type,... (UCI)

- output: $K = 3$ models were selected

$$f(x) = \frac{1}{2} f_1(x, (\alpha^\star, b^\star), (1, .1, = 0)) + \frac{1}{3} f_3(x, k = 3) + \frac{1}{6} f_3(x, k = 5)$$

The ML pipeline



ML algorithm(s) $\rightarrow$ ML Pipeline

- coding/normalization/missing values...
- preprosessing
  - feature generation
  - representation (PCA...)
  - feature selection
  - ...

Easily 20 to 50 design decisions: Time budget issues

Auto ML research fields

- hyperparameter optimization (HPO)
  GridSearchCV

```
parameters = {'kernel':('linear', 'rbf'), 'C':[1, 10]}
svc = svm.SVC(gamma="scale")
clf = GridSearchCV(estimator=svc, param_grid=parameters, cv=5)
```

- NAS = neural architecture search (specific hyper parameter)
- combining models
- meta learning (long term goal)
  sklearn.pipeline

```
from sklearn.pipeline import Pipeline

logistic = SGDClassifier(loss='log', penalty='l2',
early_stopping=True, max_iter=10000, tol=1e-5, random_state=0)
pca = PCA()
pipe = Pipeline(steps=[('pca', pca), ('logistic', logistic)])
```

Problem statement: automated machine learning

Define a search space $\mathcal{A}$

$$
\begin{aligned}
\min_{a \in \mathcal{A}} \quad & \mathcal{L}_{val}(w^\star(a), a) \\
\text{avec} \quad & w^\star(a) = \arg\min_{w} \mathcal{L}_{\text{train}}(w, a)
\end{aligned}
$$

2 Problem Statement: Automated Machine Learning

Let $P(\mathcal{D})$ be a distribution of datasets from which we can sample an individual dataset's distribution $P_d = P(\mathbf{X}, \mathbf{y})$. The AutoML problem is to generate a trained pipeline $\mathcal{M}_{\boldsymbol{\lambda}} : \mathbf{x} \mapsto y$, hyper-parameterized by $\boldsymbol{\lambda} \in \boldsymbol{\Lambda}$ that automatically produces predictions for samples from the distribution P_d minimizing the generalization error:

$$GE(\mathcal{M}_{\boldsymbol{\lambda}}) = \int \mathcal{L}(\mathcal{M}_{\boldsymbol{\lambda}}(\mathbf{x}), y) P_d(\mathbf{x}, y) d\mathbf{x} dy. \qquad (1)$$

Since a dataset can only be observed through a set of n independent observations $\mathcal{D}_d = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\} \sim P_d$, we can only empirically approximate the generalization error on sample data:

$$\widehat{GE}(\mathcal{M}_{\boldsymbol{\lambda}}, \mathcal{D}_d) = \frac{1}{|\mathcal{D}_d|} \sum_{(\mathbf{x}_i, y_i) \in \mathcal{D}_d} \mathcal{L}(\mathcal{M}_{\boldsymbol{\lambda}}(\mathbf{x}_i), y_i). \qquad (2)$$

AutoML systems automatically search for the best $\mathcal{M}_{\boldsymbol{\lambda}^*}$:

$$\mathcal{M}_{\boldsymbol{\lambda}^*} \in \operatorname*{argmin}_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} \widehat{GE}(\mathcal{M}_{\boldsymbol{\lambda}}, \mathcal{D}_{\text{train}}) \qquad (3)$$

and estimate GE, e.g., by a k-fold cross validation:

$$\widehat{GE}_{\text{CV}}(\mathcal{M}_{\boldsymbol{\lambda}}, \mathcal{D}_{\text{train}}) = \frac{1}{k} \sum_{i=1}^{k} \widehat{GE}(\mathcal{M}_{\boldsymbol{\lambda}}^{\mathcal{D}_{\text{train}}^{(\text{train},i)}}, \mathcal{D}_{\text{train}}^{(\text{val},i)}) \qquad (4)$$

where $\mathcal{M}_{\boldsymbol{\lambda}}^{\mathcal{D}_{\text{train}}^{(\text{train},i)}}$ denotes that $\mathcal{M}_{\boldsymbol{\lambda}}$ was trained on the i-th training fold $\mathcal{D}_{\text{train}}^{(\text{train},i)}$. Assuming that an AutoML system can select via $\boldsymbol{\lambda}$ both, the algorithm and its hyperparameter settings, this definition using $\widehat{GE}_{\text{CV}}$ is equivalent to the definition of the CASH problem [2], [4].

2.1 Time-bounded AutoML

In practice, users are not only interested to obtain an optimal pipeline $\mathcal{M}_{\boldsymbol{\lambda}^*}$ eventually, but have constraints on how much time and compute resources they are willing to invest. We denote the time it takes to evaluate $\widehat{GE}(\boldsymbol{\lambda}, \mathcal{D}_{\text{train}})$ as $t_{\boldsymbol{\lambda}}$ and the overall optimization budget by T. Our goal is to find

$$\mathcal{M}_{\boldsymbol{\lambda}^*} \in \operatorname*{argmin}_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} \widehat{GE}(\boldsymbol{\lambda}, \mathcal{D}_{\text{train}}) \text{ s.t. } \left(\sum t_{\boldsymbol{\lambda}}\right) < T \qquad (5)$$

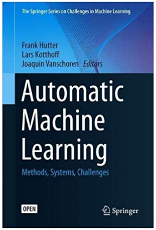
where the sum is over all pipelines evaluated, explicitly honouring the optimization budget T.

2.2 Generalization of AutoML

Ultimately, a well performing and robust optimization policy $\pi : \mathcal{D} \mapsto \mathcal{M}_{\boldsymbol{\lambda}}^{\mathcal{D}}$ of an AutoML system should not only perform well on a single dataset but on the entire distribution over datasets $P(\mathcal{D})$. Therefore, the meta-problem of

Lecture road map

1. AutoML and the machine learning process
2. Dataset
3. Preprocessing
4. Hyperparameter tuning
5. Post processing – Model agregation
6. Auto ML frameworks



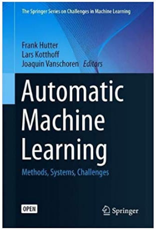
Real-world benchmark datasets for ML

- UCI Machine Learning Archive: 488 Data Sets
  `https://archive.ics.uci.edu/ml/datasets.php`

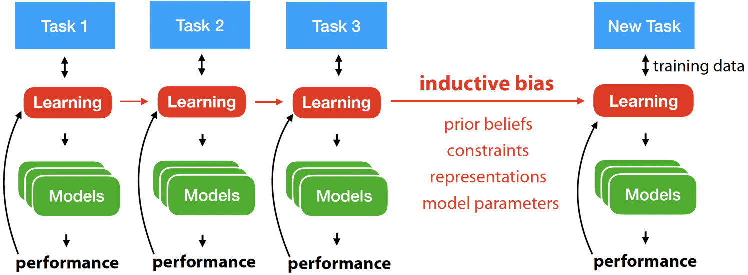
- OpenML: 2972 results
  `https://www.openml.org/search?type=data`
- Kaggle: 24171 dataset
  `https://www.kaggle.com/datasets`
- Wikipadia List of datasets for machine-learning research
  `https://en.wikipedia.org/wiki/List_of_datasets_for_machine-learning_research`
- PMLB: A large, curated repository of benchmark datasets for evaluating supervised machine learning algorithms
  `https://github.com/EpistasisLab/penn-ml-benchmarks`

Lecture road map

1. AutoML and the machine learning process
2. Dataset
3. Preprocessing
4. Hyperparameter tuning
5. Post processing – Model agregation
6. Auto ML frameworks



Preprocessing: Meta-learning



Toward meta-data: use 144 UCI data sets

- Represent the problems: X
- Find similar problems: $d(new, X)$
- Adapt the configuration: algorithm, pipeline, hyper-parameters...

How to represent a problem?

Use meta-feature

- Data D:
  - Number of instances, features, classes, missing values, outliers...
  - Statistical: skewness, kurtosis, corr., sparsity, entropy, mutual info...
- Model-based T: properties of simple a decision tree trained the data
- Landmarkers P: performance of fast algorithms trained on the task

Equiv. nr. feats	$\frac{H(C)}{MI(C,X)}$	Intrinsic dimensionality (Michie et al., 1994)	
Noise-signal ratio	$\frac{H(X)-MI(C,X)}{MI(C,X)}$	Noisiness of data (Michie et al., 1994)	
Fisher's discrimin.	$\frac{(\mu_{c1}-\mu_{c2})^2}{\sigma_{c1}^2-\sigma_{c2}^2}$	Separability classes c_1, c_2 (Ho and Basu, 2002)	See Ho:2002
Volume of overlap		Class distribution overlap (Ho and Basu, 2002)	See Ho and Basu (2002)
Concept variation		Task complexity (Vilalta and Drissi, 2002)	See Vilalta (1999)
Data consistency		Data quality (Köpf and Iglezakis, 2002)	See Köpf and Iglezakis (2002)
Nr nodes, leaves	$\lvert\eta\rvert, \lvert\psi\rvert$	Concept complexity (Peng et al., 2002)	Tree depth
Branch length		Concept complexity (Peng et al., 2002)	min,max,μ,σ
Nodes per feature	$\lvert\eta_X\rvert$	Feature importance (Peng et al., 2002)	min,max,μ,σ
Leaves per class	$\frac{\lvert\psi_c\rvert}{\lvert\psi\rvert}$	Class complexity (Filchenkov and Pendryak, 2015)	min,max,μ,σ
Leaves agreement	$\frac{n_{\psi_i}}{n}$	Class separability (Bensusan et al., 2000)	min,max,μ,σ
Information gain		Feature importance (Bensusan et al., 2000)	min,max,μ,σ, gini
Landmarker(1NN)	$P(\theta_{1NN}, t_j)$	Data sparsity (Pfahringer et al., 2000)	See Pfahringer et al. (2000)
Landmarker(Tree)	$P(\theta_{Tree}, t_j)$	Data separability (Pfahringer et al., 2000)	Stump,RandomTree
Landmarker(Lin)	$P(\theta_{Lin}, t_j)$	Linear separability (Pfahringer et al., 2000)	Lin.Disciminant
Landmarker(NB)	$P(\theta_{NB}, t_j)$	Feature independence (Pfahringer et al., 2000)	See Ler et al. (2005)

$X = (D, T, P)$

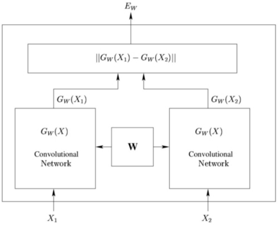
2018 J. Vanschoren, "Meta-Learning: A Survey"

Find similar problems

Compute a distance between problems:

- k-NN
- Deep metric learning: e.g. Siamese Network
  Output (Target): A label, 0 for similar, 1else.
  - Similar: loss $= \min_W \|G_W(X_1) - G_W(X_2)\|^2$
  - Else: loss =

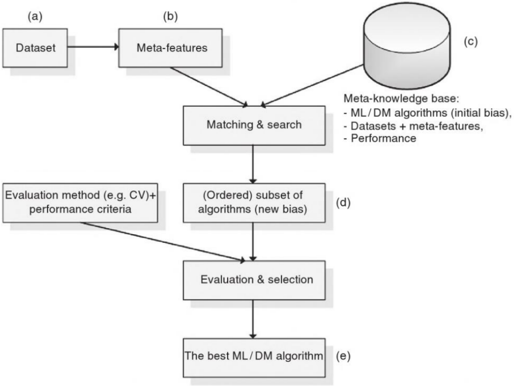
$$\min_W max(m - \|G_W(X_1) - G_W(X_2)\|, 0)^2$$



NeurIPS 1994 Bromley et al. "Signature verification using a" siamese" time delay neural network"

Recommend and adapt configurations

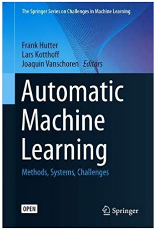
- Zero-shot meta-models: take the best
- Ranking weighted models
- Randomly pick, tune and adapt



Brazdil et al. "Metalearning: Applications to Data Mining", 2008

Lecture road map

1. AutoML and the machine learning process
2. Dataset
3. Preprocessing
4. Hyperparameter tuning
5. Post processing – Model agregation
6. Auto ML frameworks



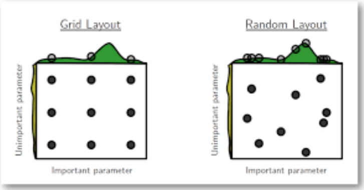
Hyperparameter tunning

Different types of hyperparameters

- continuous (SVM's C, learning rate)
- integer (kNN's k, number of layer)
- categorical
  - algorithm choice
  - activation function
  - ...

Easily 20 to 50 design decisions: Time budget issues

Hyperparameter tunning



Use preprocessing to find out the domain

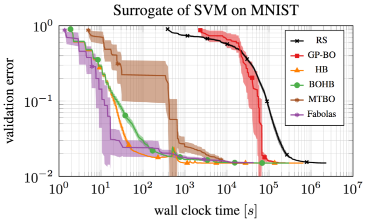
- grid search
- random search
- reinforcement learning
- evolutionary strategy
- Hyperparameter Gradient Descent [Franceschi et al, ICML 2018]
- Bayesian search

J. Bergstra and Y. Bengio. "Random search for hyper-parameter optimization.", JMLR 2012

how to manage the time budget to scale

- Brute force (time out)

- Many cheap evaluations on small data
  Few expensive evaluations on all data



- Successive Halving (SH) [Jamieson & Talwalkar, AISTATS 2016]
  - begin with traininng m models
  - at each time step keep half of them

- Hyperband, [Li et al, ICLR 2017] a bandit strategy that dynamically allocates resources to a set of random configurations and uses successive halving

- Bayesian optim. [Falkner, Kleil, ICML 2018]

Falkner et al.. "BOHB: Robust and Efficient Hyperparameter Optimization at Scale", JMLR 2018

Hyperparameter auto tuning tools

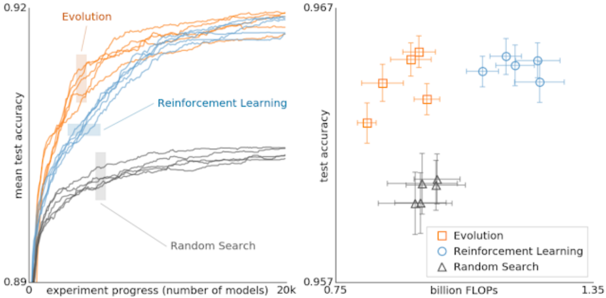
Package	Complex Hyperparameter Spaces	Multi-Objective	Multi-Fidelity	Instances	CLI	Parallelism
HyperMapper	✅	✅	❌	❌	❌	❌
Optuna	✅	✅	✅	❌	✅	✅
Hyperopt	✅	❌	❌	❌	✅	✅
BoTorch	❌	✅	✅	❌	❌	✅
OpenBox	✅	✅	❌	❌	❌	✅
HpBandSter	✅	❌	✅	❌	❌	✅
SMAC	✅	✅	✅	✅	✅	✅

last update of table in 2021

https://github.com/automl/HpBandSter
https://github.com/automl/SMAC3

by M. Lindauer and F. Hutter, Lecture at AutoML Fall School 2022: The AutoML Landscape

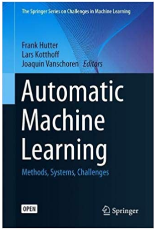
Results on the neural architecture search



Regularized Evolution for Image Classifier Architecture Search E. Real et al, 2018

Lecture road map

1. AutoML and the machine learning process
2. Dataset
3. Preprocessing
4. Hyperparameter tuning
5. Post processing – Model agregation
6. Auto ML frameworks



Post processing: Model agregation (Stacking)

Model construction

- Predictor generation: $f_1(X), \ldots, f_K(X)$
- Feature: $\Phi(X) = (f_1(X), \ldots, f_K(X))^T \ldots$

Penalized Loss

- Minimization of

$$\operatorname*{arg\,min}_{\beta \in \Theta} \frac{1}{n} \sum_{i=1}^{n} \ell(Y_i, < \Phi(X_i), \beta >) + pen(\beta)$$

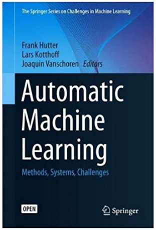
  where $pen(\theta)$ is a penalty.
- Predictor selection if β is sparse.

Classical Penalties

- AIC / Ridge / Lasso / Elastic Net

Lecture road map

1. AutoML and the machine learning process
2. Dataset
3. Preprocessing
4. Hyperparameter tuning
5. Post processing – Model agregation
6. Auto ML frameworks

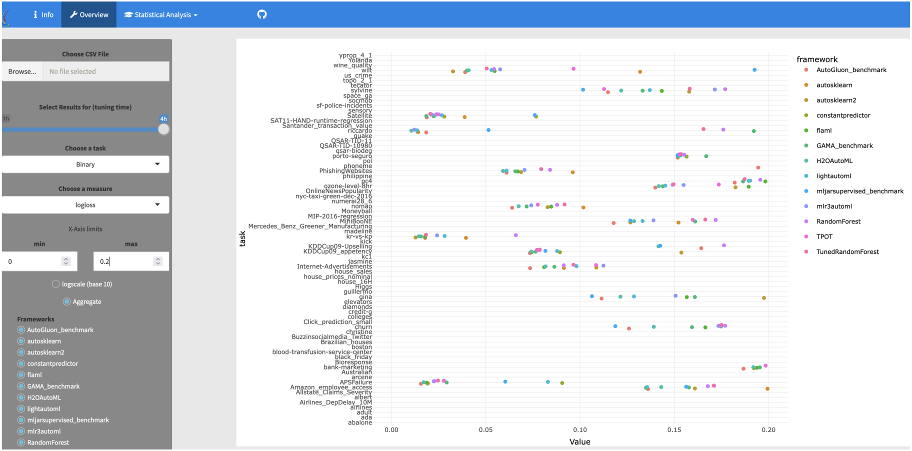


Auto ML frameworks

- based on frameworks
  - H2O `docs.h2o.ai/h2o/latest-stable/h2o-docs/automl.html` build on H2O framework
  - Auto Sklearn `automl.github.io/auto-sklearn/master/` build on SKLearn framework
  - Auto-WEKA `www.automl.org/automl/autoweka/` build on WEKA framework
- commercial:
  - Google (Vizier, automlvision, automl NLP), Azure, FBLearner...
- research (other)
  - TPOT `github.com/EpistasisLab/tpot` Tree-Based Pipeline Opti.
  - MLJar `github.com/mljar/mljar-supervised`
  - AutoGluon (Amazon) `github.com/awslabs/autogluon`
  - http://news.mit.edu/2019/nonprogrammers-data-science-0115

  ...
- AutoML Frameworks
  `openml.github.io/automlbenchmark/frameworks.html`

Auto ML Benchmark



https://compstat-lmu.shinyapps.io/AutoML-Benchmark-Analysis/

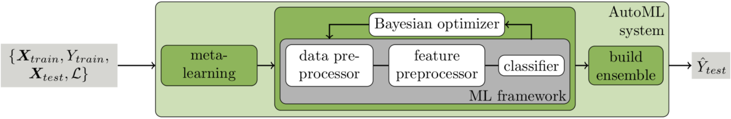
Auto ML tools

- Auto WEKA [Thornton et al, KDD 2013]
  - Based on WEKA and SMAC Hyperopt sklearn [Komer et al, 2014]
- Auto sklearn [Feurer al, NIPS 2015]
  - Based on scikit learn & SMAC / BOHB
  - Won AutoML competitions 2015-2016 & 2017-2018
- Auto pytorch [Zimmer et al., IEEE PAMI 2021]
  - optimizes the network architecture (NAS) and the hyperparameters
- TPOT [Olson et al, EvoApplications 2016]
  - Based on scikit learn and evolutionary algorithms
- H2O AutoML
  - Based on random search and stacking

https://www.automl.org/

Auto ML at work: Auto Sklearn

auto-sklearn in one image



auto-sklearn in four lines of code

```
import autosklearn.classification
cls = autosklearn.classification.AutoSklearnClassifier()
cls.fit(X_train, y_train)
predictions = cls.predict(X_test)
```

Auto ML at work: Auto Sklearn

6. AutoML

https://papers.nips.cc/paper/5872-efficient-and-robust-automated-machine-learning
https://automl.github.io/auto-sklearn/stable/

and for the doc https://automl.github.io/auto-sklearn/stable/api.html

In [19]:
```python
import warnings
warnings.filterwarnings("ignore")

import autosklearn.classification
import sklearn.model_selection
import sklearn.datasets
import sklearn.metrics

from autosklearn.metrics import make_scorer

automl = autosklearn.classification.AutoSklearnClassifier(
     time_left_for_this_task=7200,
         per_run_time_limit=600,
     exclude_estimators=None,
#     include_preprocessors=["no_preprocessing", ],
     exclude_preprocessors=None)

scorer = autosklearn.metrics.make_scorer(
        'f1_score',
        sklearn.metrics.f1_score,
        pos_label=1,
    )

automl.fit(X_train, y_train, metric=scorer)

y_pred = automl.predict(X_test)
cf_auto = confusion_matrix(y_test, y_pred)*100/len(y_test)
```

```
[WARNING] [2019-03-18 23:05:40,546:AutoMLSMBO(1)::afcbe3320b92b2a2a9cf1cd0de64b65c] Could not find meta-data director
y /Users/stephane/.local/lib/python3.6/site-packages/autosklearn/metalearning/files/f1_score_binary.classification_de
nse
[WARNING] [2019-03-18 23:05:40,589:EnsembleBuilder(1):afcbe3320b92b2a2a9cf1cd0de64b65c] No models better than random
- using Dummy Score!
[WARNING] [2019-03-18 23:05:40,667:EnsembleBuilder(1):afcbe3320b92b2a2a9cf1cd0de64b65c] No models better than random
```

In [21]:
```python
(automl.get_models_with_weights())
```

Out[21]:
```
[(0.2,
  SimpleClassificationPipeline({'balancing:strategy': 'none', 'categorical_encoding:__choice__': 'one_hot_encoding',
'classifier:__choice__': 'random_forest', 'imputation:strategy': 'mean', 'preprocessor:__choice__': 'no_preprocessing
', 'rescaling:__choice__': 'standardize', 'categorical_encoding:one_hot_encoding:use_minimum_fraction': 'True', 'clas
sifier:random_forest:bootstrap': 'True', 'classifier:random_forest:criterion': 'gini', 'classifier:random_forest:max_
depth': 'None', 'classifier:random_forest:max_features': 0.5, 'classifier:random_forest:max_leaf_nodes': 'None', 'cla
ssifier:random_forest:min_impurity_decrease': 0.0, 'classifier:random_forest:min_samples_leaf': 1, 'classifier:random
_forest:min_samples_split': 2, 'classifier:random_forest:min_weight_fraction_leaf': 0.0, 'classifier:random_forest:n_
estimators': 100, 'categorical_encoding:one_hot_encoding:minimum_fraction': 0.01},
  dataset_properties={
    'task': 1,
    'sparse': False,
    'multilabel': False,
    'multiclass': False,
    'target_type': 'classification',
    'signed': False})),
 (0.18,
  SimpleClassificationPipeline({'balancing:strategy': 'none', 'categorical_encoding:__choice__': 'one_hot_encoding',
'classifier:__choice__': 'random_forest', 'imputation:strategy': 'mean', 'preprocessor:__choice__': 'no_preprocessing
```

Conclusion

- How to explore?
- How to evaluate?
- How to combine?