OpenML Use Cases

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March 23th, 2019

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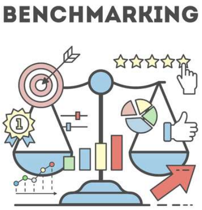
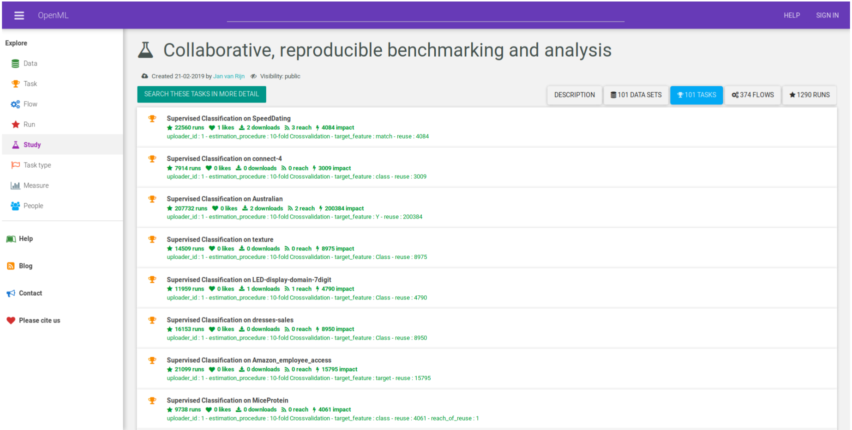


OpenML Benchmark Suites


OpenML
HELP
SIGN IN
Explore
Data
Task
Flow
Run
Study
Task type
Measure
People
Help
Blog
Contact
Please cite us
Collaborative, reproducible benchmarking and analysis
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SEARCH THESE TASKS IN MORE DETAIL
DESCRIPTION
101 DATA SETS
101 TASKS
374 FLOWS
1290 RUNS
Supervised Classification on SpeedDating
22560 runs 1 likes 2 downloads 3 reach 4084 impact
uploader_id : 1 - estimation_procedure : 10-fold Crossvalidation - target_feature : match - reuse : 4084
Supervised Classification on connect-4
7914 runs 0 likes 0 downloads 0 reach 3009 impact
uploader_id : 1 - estimation_procedure : 10-fold Crossvalidation - target_feature : class - reuse : 3009
Supervised Classification on Australian
207732 runs 0 likes 2 downloads 2 reach 200384 impact
uploader_id : 1 - estimation_procedure : 10-fold Crossvalidation - target_feature : Y - reuse : 200384
Supervised Classification on texture
14509 runs 0 likes 0 downloads 0 reach 8975 impact
uploader_id : 1 - estimation_procedure : 10-fold Crossvalidation - target_feature : Class - reuse : 8975
Supervised Classification on LED-display-domain-7digit
11959 runs 0 likes 1 downloads 1 reach 4790 impact
uploader_id : 1 - estimation_procedure : 10-fold Crossvalidation - target_feature : Class - reuse : 4790
Supervised Classification on dresses-sales
16153 runs 0 likes 0 downloads 0 reach 8950 impact
uploader_id : 1 - estimation_procedure : 10-fold Crossvalidation - target_feature : Class - reuse : 8950
Supervised Classification on Amazon_employee_access
21099 runs 0 likes 0 downloads 0 reach 15795 impact
uploader_id : 1 - estimation_procedure : 10-fold Crossvalidation - target_feature : target - reuse : 15795
Supervised Classification on MiceProtein
9738 runs 0 likes 0 downloads 0 reach 4061 impact
uploader_id : 1 - estimation_procedure : 10-fold Crossvalidation - target_feature : class - reuse : 4061 - reach_of_reuse : 1

OpenML Benchmark Suites

Common limitations of experimental evaluations:

- Often done on a small selection of datasets
  - Not sure about generalization to more datasets
  - 'Cherry picking'
- Publication bias
  - Every paper only reports good results
  - More useful to know WHEN (on what type of data) a new algorithm performs well
- Hard to compare conclusions across papers
- Abused datasets (example: liver-disorders)

OpenML Benchmark Suites

OpenML-100: A curated benchmark suite [Bischl et al., 2017].
Inclusion criteria:

- Basic data properties (500–100000 observations, < 5000 features, $>= 2$ classes)
- The ratio of the minority class and the majority class > 0.05
- Scientific publication introducing the dataset and learning task
- Pure classification tasks only (no data streams, multi-class tasks)
- No artificial data, binarized versions of regression datasets or sub-samples of bigger datasets
- Disadvantage: Very hard to get a good consensus about the inclusion criteria
- Next: The OpenML-CC18 (approx. 71 datasets)

OpenML Benchmark Suites

Benchmark suite:

- A collection of tasks
  - Terminology: A Study is a collection of runs
  - Collection of flows, datasets, ...
- Immutable (once closed)
- Standardized train-test splits are provided to ensure that results can be objectively compared
- results can be shared in a reproducible way through the APIs
- `https://docs.openml.org/benchmark/`

[B. Bischl, G. Casalicchio, M. Feurer, F. Hutter, M. Lang, R. G. Mantovani, J. N. van Rijn, and J. Vanschoren. Openml benchmarking suites and the openml100.

arXiv preprint arXiv:1708.03731, 2017]

Requirements

- A set of tasks
  - Upload dataset and create tasks (task creation soon available)
  - Use existing tasks
- Latest version of Python API (Development version)
  - `openml.dataset.list_datasets(...)`
  - `openml.study.create_benchmark_suite(...)`
- OpenML account and user id (needs to be configured)
- Also available for Java (see docs) and R (comming soon)

Create Benchmark Suite

```python
import openml

tasks = openml.tasks.list_tasks(
    number_instances='100..500',
    number_features='4..20',
    size=20)
# task is a Dict[int, OpenMLTask]

study = openml.study.create_benchmark_suite(
    alias=None,
    name="Benchmark Example",
    description="illustrates creating benchmark suites",
    task_ids=tasks.keys()
)
study_id = study.publish()
print('Uploaded study with id=%d' % study_id)
```

Find Benchmark Suite

```python
import openml

studies = openml.study.list_studies(
  main_entity_type='task',
  creator=1,
  status='all'
)
```

Lists all studies / benchmark suites that comply to a set of filters

- Legal filters: main_entity_type, uploader, status, ...
- `studies` is now a `Dict[int, OpenMLStudy]`
- Note: Recently created studies are 'in preparation'

Common operations

Attach additional tasks

```
tasks = openml.tasks.list_tasks(data_name='letter', size=1)
# tasks_new is Dict[int, OpenMLTask]
openml.study.attach_to_study(study_id, tasks.keys())
```

Common operations

Attach additional tasks

```
tasks = openml.tasks.list_tasks(data_name='letter', size=1)
# tasks_new is Dict[int, OpenMLTask]
openml.study.attach_to_study(study_id, tasks.keys())
```

Detach tasks

```
# given a variable study_id (int)
task_id = [2, 3, 4]
openml.study.detach_from_study(study_id, task_id)
```

Common operations

Attach additional tasks

```
tasks = openml.tasks.list_tasks(data_name='letter', size=1)
# tasks_new is Dict[int, OpenMLTask]
openml.study.attach_to_study(study_id, tasks.keys())
```

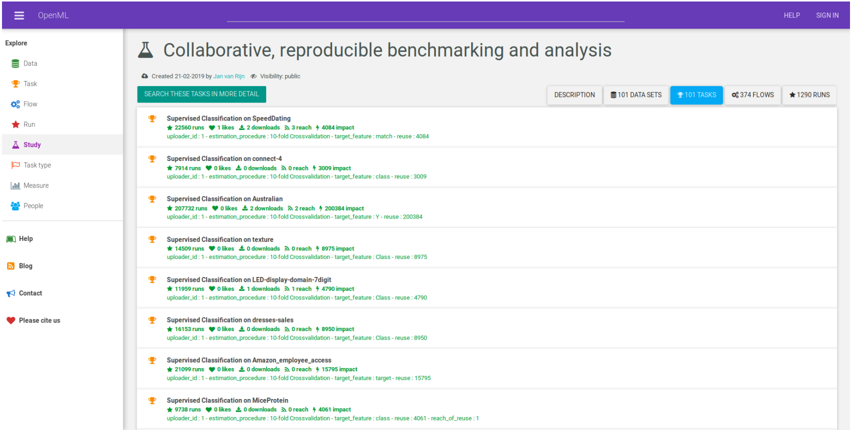
Detach tasks

```
# given a variable study_id (int)
task_id = [2, 3, 4]
openml.study.detach_from_study(study_id, task_id)
```

Activate benchmark suite (no mutations possible afterwards)

```
# given a variable study_id (int)
openml.study.status_update(study_id, 'active')
```

Benchmark Suite



Benchmark Suite

```
import openml  # development branch
import sklearn # version 0.20.0 and up

# given a variable study_id (int, str)
benchmark_suite = openml.study.get_study(study_id, 'tasks')
# build a sklearn classifier
clf = sklearn.pipeline.make_pipeline(
  sklearn.preprocessing.Imputer(),
  sklearn.tree.DecisionTreeClassifier()
)
# iterate over all tasks
for task_id in benchmark_suite.tasks:
  task = openml.tasks.get_task(task_id) # download the OpenML task
  X, y = task.get_X_and_y() # get the data (not used in this example)
  # run classifier on splits (requires API key)
  run = openml.runs.run_model_on_task(clf, task)
  # print accuracy score
  score = run.get_metric_score(sklearn.metrics.accuracy_score)
  print('Data set: %s; Accuracy: %0.2f' % (task.get_dataset().name,
                                          score.mean()))
  run.publish() # publish the experiment on OpenML (optional)
  print('URL for run: %s/run/%d' %(openml.config.server,run.run_id))
```


BUSTING THE
MYTHS

Myth Busting for Data Mining

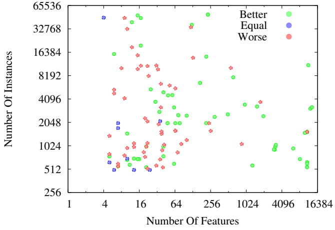
- Papers are generally build upon claims that are not well grounded, e.g.,
  - "We performed data transformation X because it is common practise."
  - "We set hyperparameter Y to value Z because the authors recommended these values."
- We can empirically analyze the validity of these claims on the meta-data from OpenML
- In this case: "The Importance of Feature Selection"

Effect of Feature Selection

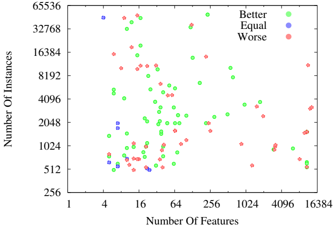
Experimental Setting by Post et al. [2016]:

- 400 binary classification datasets from OpenML
- 12 algorithms from Weka
- Correlation-based Feature Subset Selection
- We added runs that not existed on OpenML
- Recorded Area Under the ROC curve
- Limitation: Hyperparameter Optimization

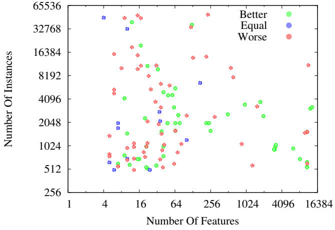
Effect of Feature Selection



k-NN



Naive Bayes



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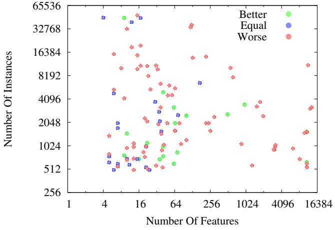


SMO

Effect of Feature Selection

Initial conclusions:

- Feature selection is often beneficial for the classifiers for which we expect it to be: k-NN and Naive Bayes
  - Surprisingly also for Decision Trees
- Feature selection is beneficial in 41% of the cases, only statistically significant in 10%
- Whether or not to use feature selection can be learned (see paper)
- Low amount of datasets on which feature selection significantly effects performance potentially indicates data bias
- Current Work: Linear vs. Non Linear classifiers

[M. J. Post, P. van der Putten, and J. N. van Rijn. Does Feature Selection Improve Classification? A Large Scale Experiment in OpenML.

In *Advances in Intelligent Data Analysis XV*, pages 158–170. Springer, 2016]

Linear vs. Non-linear

Reoccuring topic in literature, see [Strang et al., 2018] for several examples

	Linear	Non-linear
ease of tuning		
interpretability		
fit risk		
performance		

Linear vs. Non-linear

Reoccuring topic in literature, see [Strang et al., 2018] for several examples

	Linear	Non-linear
ease of tuning	+	-
interpretability		
fit risk		
performance		

Linear vs. Non-linear

Reoccuring topic in literature, see [Strang et al., 2018] for several examples

	Linear	Non-linear
ease of tuning	+	-
interpretability	+	-
fit risk		
performance		

Linear vs. Non-linear

Reoccuring topic in literature, see [Strang et al., 2018] for several examples

	Linear	Non-linear
ease of tuning	+	-
interpretability	+	-
fit risk	underfit	overfit
performance		

Linear vs. Non-linear

Reoccuring topic in literature, see [Strang et al., 2018] for several examples

	Linear	Non-linear
ease of tuning	+	-
interpretability	+	-
fit risk	underfit	overfit
performance	-	+

Linear vs. Non-linear

Reoccuring topic in literature, see [Strang et al., 2018] for several examples

	Linear	Non-linear
ease of tuning	+	-
interpretability	+	-
fit risk	underfit	overfit
performance	-	+
Tree	Decision Stump	Decision Tree

Universiteit Leiden

Linear vs. Non-linear

Reoccuring topic in literature, see [Strang et al., 2018] for several examples

	Linear	Non-linear
ease of tuning	+	-
interpretability	+	-
fit risk	underfit	overfit
performance	-	+
Tree	Decision Stump	Decision Tree
SVM	Linear Kernel	Gaussian Kernel

Linear vs. Non-linear

Reoccuring topic in literature, see [Strang et al., 2018] for several examples

	Linear	Non-linear
ease of tuning	+	-
interpretability	+	-
fit risk	underfit	overfit
performance	-	+
Tree	Decision Stump	Decision Tree
SVM	Linear Kernel	Gaussian Kernel
Neural Network	Perceptron	MLP

Requirements

- A Benchmark suite
  - This case: the OpenML-100
- Latest version of Python API (Development version)
- Run results of the linear and non-linear classifier
  - We will generate them
- Listing function `openml.evaluation.list_evaluations(...)`
- Plotting library (matplotlib)

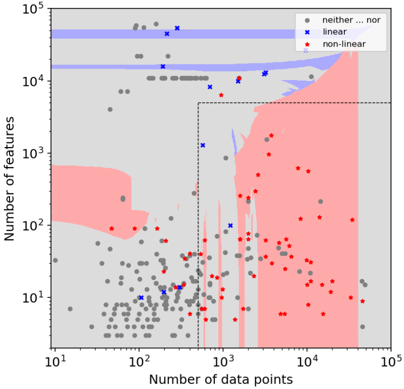
Generate Results

```python
import openml  # development branch
import sklearn # version 0.20.0 and up

# given a variable study_id (int, str)
benchmark_suite = openml.study.get_study('OpenML100', 'tasks')
# build a sklearn classifier
clfs = [
  sklearn.pipeline.make_pipeline( # non-linear
    sklearn.preprocessing.Imputer(),
    sklearn.svm.SVC()
  ),
  sklearn.pipeline.make_pipeline( # linear
    sklearn.preprocessing.Imputer(),
    sklearn.svm.LinearSVC()
  ),
]
run_ids = list()
for task_id in benchmark_suite.tasks:
  task = openml.tasks.get_task(task_id)
  for clf in clfs:
    run = openml.runs.run_model_on_task(clf, task)
    run.publish()
    print('URL for run: %s/run/%d' % (openml.config.server,
                                      run.run_id))
    run.push_tag('linear_vs_nonlinear')
```

Plot Results

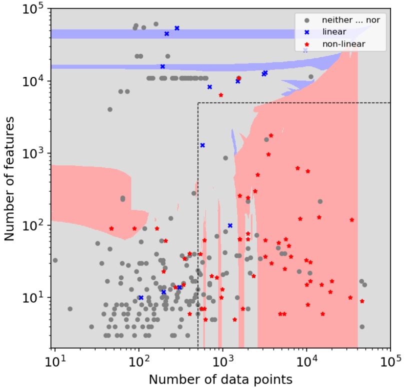
```
import openml  # development branch

# given a variable study_id (int, str)
suite = openml.study.get_study('OpenML100', 'tasks')
tasks = openml.tasks.list_tasks(task_ids=suite.tasks)
# given a variable uploader_id (int)
evals = openml.evaluation.evaluation_list(
  'predictive_accuracy',
  uploader=uploader_id,
  tag='linear_vs_nonlinear'
)

# organization
results = collections.defaultdict(dict)
for evaluation in evals.values():
    results[evaluation.setup_id][evaluation.task_id] = evaluation.value
# plot
for setup_id in results.keys():
  # find the tasks on which this evaluation is best
  res_x = []
  res_y = []
  for task_id in results[setup_id].keys():
    if results[setup_id][task_id] == [results[sid][task_id] for sid in results.keys()]:
      res_x.append(tasks[task_id]['NumberOfInstances'])
      res_y.append(tasks[task_id]['NumberOfFeatures'])
      plt.scatter(res_x, res_y)
# set labels, titles and (log-)scales
```

Linear vs. Non-Linear

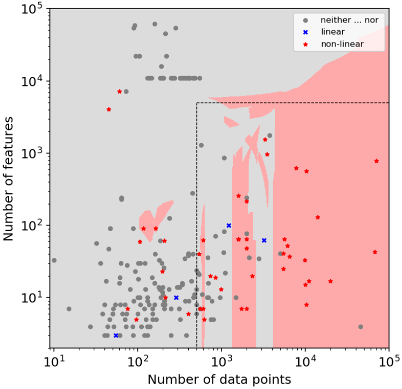


SVM

Linear vs. Non-Linear



SVM



Neural Networks

Linear vs. Non-Linear

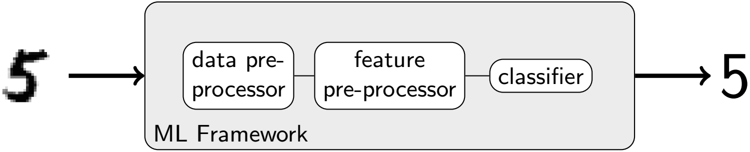
- Non-linear models are almost exclusively better than linear models (as expected)
- Statistical equivalent for low data regimes
- Limitation: Conservative statistical test
- benchmark suites such as OpenML-100 have limitations

[B. Strang, P. van der Putten, J. N. van Rijn, and F. Hutter. Don't rule out simple models prematurely: A large scale benchmark comparing linear and non-linear classifiers in openml.

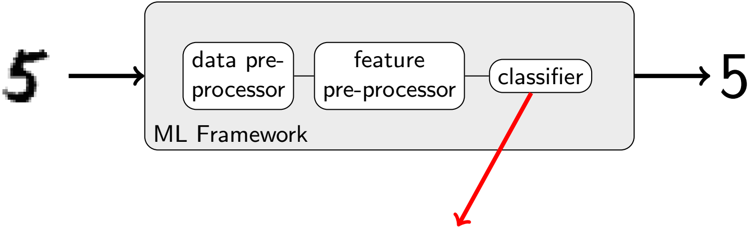
In *International Symposium on Intelligent Data Analysis*, pages 303–315. Springer, 2018]

Warm Starting Bayesian Optimization

The Machine Learning Pipeline

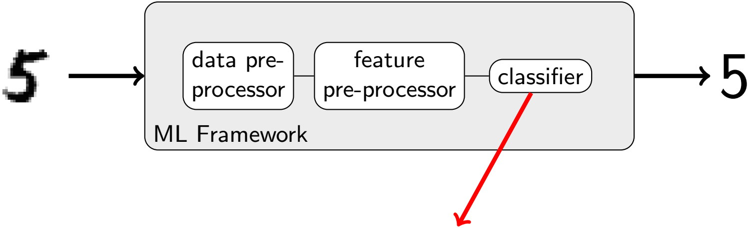


The Machine Learning Pipeline



classifier	$\#\lambda$
Adaboost	4
Bernoulli Naive Bayes	2
Decision Tree	4
Extra Trees	5
Gradient Boosting	6
k-NN	3
LDA	4
...	

The Machine Learning Pipeline



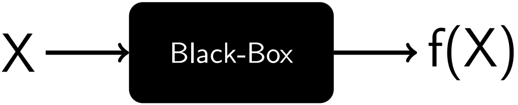
classifier	#λ
Adaboost	4
Bernoulli Naive Bayes	2
Decision Tree	4
Extra Trees	5
Gradient Boosting	6
k-NN	3
LDA	4
...	

The Problem Definition

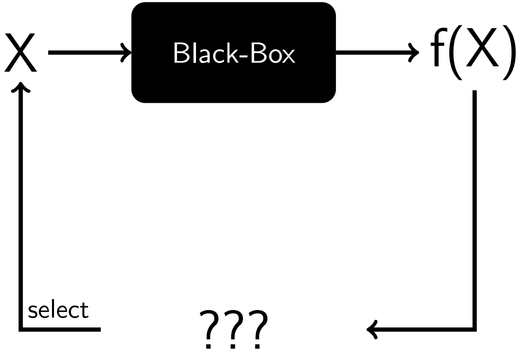
$$A^*, \lambda_* \in \underset{A \in \mathbf{A}, \lambda \in \Lambda}{\arg\min}\, L(A_{\lambda, D_{train}, D_{valid}})$$

Given a dataset D, find an algorithm A^* and its hyperparameters λ_* that minimizes a given loss function L

Black-Box Optimization



The Loop



The Human in the Loop

X → Black-Box → f(X)

select

+

. . .

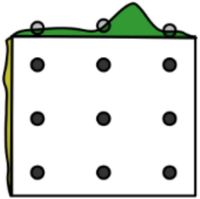
−

Not very efficient
Painful
Requires domain knowledge

Grid Search

X → Black-Box → f(X)

select



+

Very simple approach
Can be used to study the problem

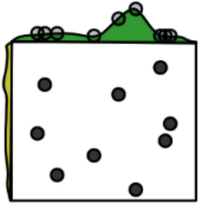
−

Does not scale to high dimensions
Grid needs to be defined

Random Search

X → Black-Box → f(X)

select



+

Even more simple
Easily parallelizable
Eventually converges to optimum

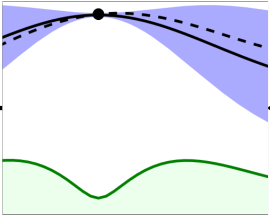
−

Not data efficient
Computationally expensive

Bayesian Optimization

X → Black-Box → f(X)

select



\+

Data efficient
State of the art

−

Not easy to parallelize

Requirements

- `sklearnbot` linrary
  - `https://github.com/openml/sklearn-bot`
- `openmlcontrib` library
  - Connects `openml` library with `pandas` and `ConfigSpace` library
  - `https://github.com/openml/openml-python-contrib`
- Both not on PyPI, installable from git
- Under active development (contributors welcome)

Plot Results

```python
import sklearnbot # requires openml and openmlcontib and ConfigSpace

# given a study_id (int)
tasks = openml.study.get_study(study_id, 'tasks').tasks

configuration_space = sklearnbot.config_spaces.get_config_space('svc', None)
output_dir = os.path.join(args.output_dir, args.classifier_name)

n_executions = 10
for i in range(n_executions):
    task_id = random.choice(tasks)
    success, run_id, folder = sklearnbot.bot.run_bot_on_task(task_id,
                                                             configuration_space,
                                                             output_dir,
                                                             args.upload_result)
```

Obtain Results

```
import openmlcontrib
import sklearnbot # requires openml and openmlcontib and ConfigSpace

# given a study_id (int)
suite = openml.study.get_study(study_id, 'tasks')
configuration_space = sklearnbot.config_spaces.get_config_space('svc', None)
# given a flow_id (int)
performance_data = openmlcontrib.meta.get_tasks_result_as_dataframe(
  task_ids=suite.tasks,
  flow_id=flow_id,
  num_runs=100,
  per_fold=False,
  configuration_space=config_space,
  evaluation_measures='predictive_accuracy',
  normalize=False
)

meta_features = openmlcontrib.meta.get_tasks_qualities_as_dataframe(
    study.tasks, False, -1, True)
setup_data_with_meta_features = performance_data.join(
    meta_features, on='task_id', how='inner')
```

Auto-sklearn

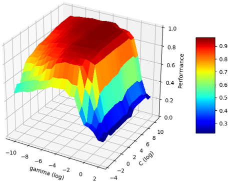
```
import autosklearn.classification
import sklearn.model_selection
import sklearn.datasets
import sklearn.metrics

# Load data and split into train and test data
X, y = sklearn.datasets.load_digits(return_X_y=True)
X_train, X_test, y_train, y_test = \
  sklearn.model_selection.train_test_split(X, y)
# Let auto-sklearn run for 1h
autosklearn.classification.AutoSklearnClassifier(
  time_left_for_this_task=3600)
automl.fit(X_train, y_train)
y_hat = automl.predict(X_test)
print("Accuracy score",
      sklearn.metrics.accuracy_score(y_test, y_hat))
```

[M. Feurer, A. Klein, K. Eggensperger, J. Springenberg, M. Blum, and F. Hutter. Efficient and robust automated machine learning.

In *Advances in neural information processing systems*, pages 2962–2970, 2015]

Hyperparameter Importance

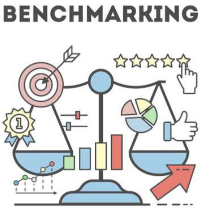
- Typically unanswered questions:
  - What is a good Configuration Space?
  - What are important hyperparameters?
  - How to sample over these?
- Hyperparameter Importance using OpenML: https://www.youtube.com/watch?v=mS4vL7_rSWQ



[J. N. van Rijn and F. Hutter. Hyperparameter importance across datasets.

In *Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, pages 2367–2376. ACM, 2018]

What have we learned



suites — effect of a component — warm starting AutoML

- `openml`, `openmlcontrib` and `sklearnbot`
- Also available on Java and R
- Under active development, contributors welcome :)
- This afternoon: Hands on session

References

B. Bischl, G. Casalicchio, M. Feurer, F. Hutter, M. Lang, R. G. Mantovani, J. N. van Rijn, and J. Vanschoren. Openml benchmarking suites and the openml100. *arXiv preprint arXiv:1708.03731*, 2017.

M. Feurer, A. Klein, K. Eggensperger, J. Springenberg, M. Blum, and F. Hutter. Efficient and robust automated machine learning. In *Advances in neural information processing systems*, pages 2962–2970, 2015.

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