# scikit-learn new features

## Tutorial

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*May 28, 2019*

## Agenda

1. Overview of new features in v0.20, v0.21
2. Tutorial: application examples

## Latest scikit-learn releases

**Version 0.20**

*Sept 26, 2018* - 13 months work

- 361 contributors
- 1130 commits, 63 new features (excl. bug fixes & enhancements)

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**Version 0.21**

*May 10, 2019* - 8 months work

- 221 contributors
- 795 commits, 24 new features (excl. bug fixes & enhancements)

scikit-learn.org/stable/whats_new.html

## ColumnTransformer
## sklearn.compose

Allows to apply different transformers to different columns of arrays or pandas DataFrames:

**Example**

# OpenML fetcher
## sklearn.datasets

Added a fetcher for OpenML, a free, open data sharing platform

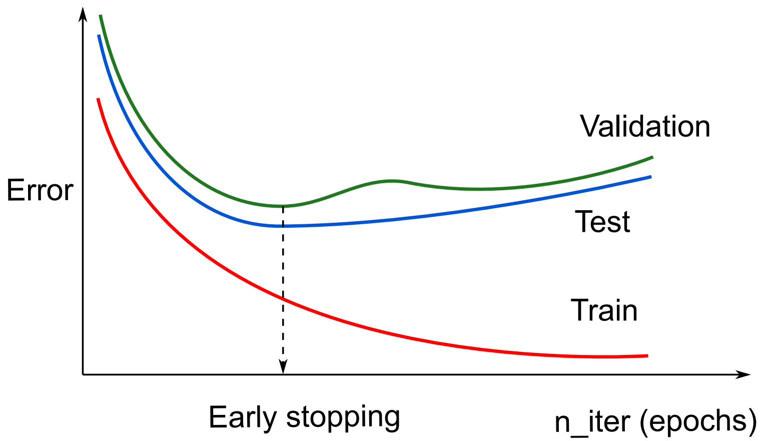
- ~20000 datasets available at www.openml.org

**Example**

*Added in v0.20 by Andreas Müller and Jan N. van Rijn.*

# Early stopping in models

Stop training earlier when the validation score no longer improves.



Supported in SDGClassifier, MLPClassifier, HistGradientBoostingClassifier (and corresponding regressors)

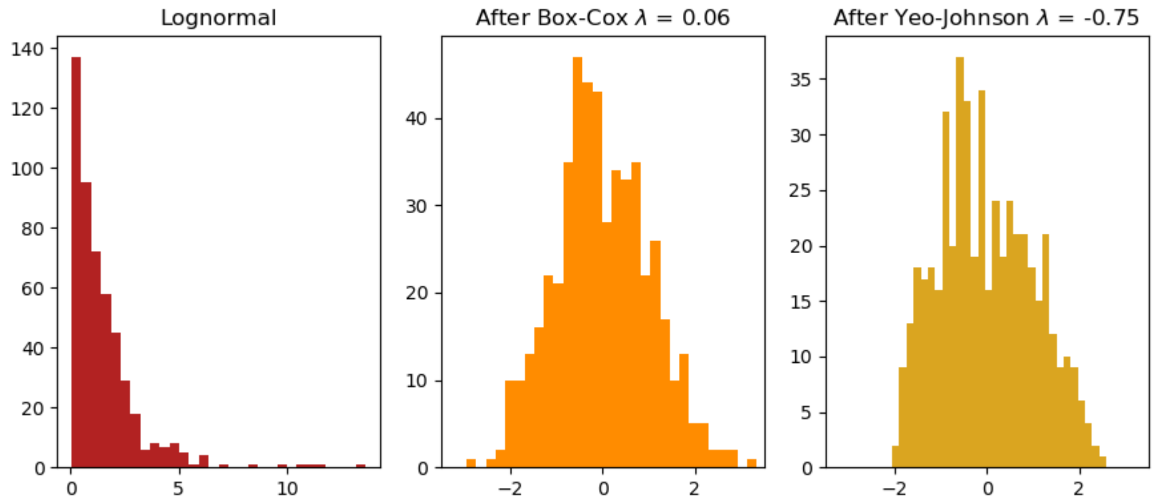
```
from sklearn.linear_model import SDGClassifier

SGDClassifier(early_stopping=True, n_iter_no_change=3,
              tol=0.0001, validation_fraction=0.2)
```

*Added in v0.20 by Tom Dupre la Tour.*

# PowerTransformer
## sklearn.preprocessing

Implements Yeo-Johnson and Box-Cox power transformations, that apply a power transform featurewise to make data more Gaussian-like.



Also see: QuantileTransform.

*Added in v0.20 by Eric Chang, Maniteja Nandana, Nicolas Hug.*

# IterativeImputer
sklearn.impute

Imputing missing values by modeling each feature with missing values as a function of other features in a round-robin fashion.

**Experimental**

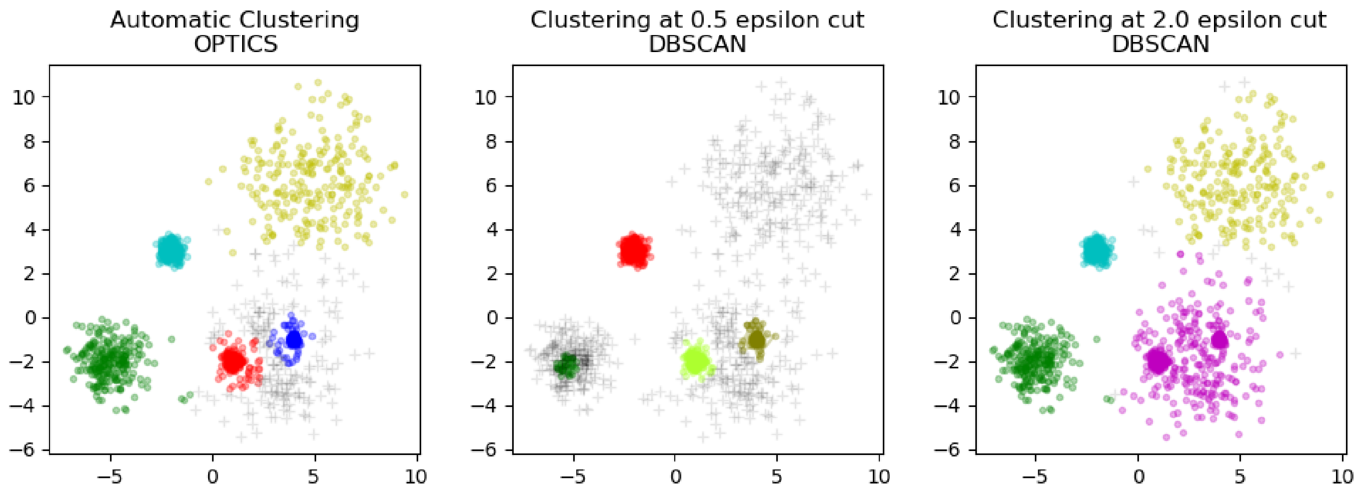
```
>>> import numpy as np
>>> from sklearn.experimental import enable_iterative_imputer
>>> from sklearn.impute import IterativeImputer
>>> imp = IterativeImputer(max_iter=10, random_state=0)
>>> imp.fit([[1, 2], [3, 6], [4, 8], [np.nan, 3], [7, np.nan]])
>>> X_test = [[np.nan, 2], [6, np.nan], [np.nan, 6]]
>>> # the model learns that the second feature is double the first
>>> print(np.round(imp.transform(X_test)))
[[ 1.  2.]
 [ 6. 12.]
 [ 3.  6.]]
```

*Added in v0.21 by Sergey Feldman and Ben Lawson.*

**Note**: NaN are ignored and handled in pre-processors as of v0.20.

# OPTICS
## sklearn.cluster

A new clustering algorithm related to DBSCAN, that has hyperparameters easier to set and that scales better



*Added in v0.21 by Shane, Adrin Jalali, Erich Schubert, Hanmin Qin, Assia Benbihi.*

# Histogram-based Gradient Boosting Trees

Gradient boosting trees inspired by LightGBM, significantly faster than `GradientBoostingClassifier` / `GradientBoostingRegressor`

**Experimental**

```
>>> # explicitly require this experimental feature
>>> from sklearn.experimental import enable_hist_gradient_boosting  # noqa
>>> from sklearn.ensemble import HistGradientBoostingClassifier
```

*Added in v0.21 by Nicolas Hug and Olivier Grisel.*

## NeighborhoodComponentsAnalysis sklearn.neighbors

A metric learning algorithm that learns a linear transformation to improve the classification accuracy in the transformed space.

```
from sklearn.neighbors.nca import NeighborhoodComponentsAnalysis
from sklearn.neighbors import KNeighborsClassifier
from sklearn.datasets import load_iris
from sklearn.model_selection import train_test_split
from sklearn.pipeline import make_pipeline

X, y = load_iris(return_X_y=True)
X_train, X_test, y_train, y_test = train_test_split(X, y,
     stratify=y, test_size=0.7, random_state=42)

knn = KNeighborsClassifier(n_neighbors=3)
knn.fit(X_train, y_train)

nca = make_pipeline(NeighborhoodComponentsAnalysis(random_state=42),
                    KNeighborsClassifier())
nca.fit(X_train, y_train)


print(knn.score(X_test, y_test))   # 0.93
print(nca.score(X_test, y_test))   # 0.96
```

*Added in v0.21 by William de Vazelhes.*

# Decision trees visualization

- Decision trees can be plotted with matplotlib without needing to install graphviz (`tree.plot_tree`)
- ASCII representation also available (`tree.export_text`)

```
>>> from sklearn.datasets import load_iris
>>> from sklearn.tree import DecisionTreeClassifier
>>> from sklearn.tree.export import export_text
>>> iris = load_iris()
>>> X = iris['data']
>>> y = iris['target']
>>> decision_tree = DecisionTreeClassifier(random_state=0, max_depth=2)
>>> decision_tree = decision_tree.fit(X, y)
>>> r = export_text(decision_tree, feature_names=iris['feature_names'])
>>> print(r)
|--- petal width (cm) <= 0.80
|   |--- class: 0
|--- petal width (cm) >  0.80
|   |--- petal width (cm) <= 1.75
|   |   |--- class: 1
|   |--- petal width (cm) >  1.75
|   |   |--- class: 2
...
```

*Added in v0.21 by Andreas Müller and Giuseppe Vettigli.*

## Estimator tags

- programmatic inspection of estimator capabilities (e.g. sparse or multilabel support)
- also determine the tests that are run by `check_estimator`

Useful when developing libraries that aim to comply with the scikit-learn API.

**Experimental**

```
class MyMultiOutputEstimator(BaseEstimator):

    def _more_tags(self):
        return {'multioutput_only': True,
                'non_deterministic': True}
```

*Added in v0.21 by Andreas Müller.*

## Tutorial

Requires

- scikit-learn 0.21.2
- pandas
- matplotlib

Tutorial notebook: github.com/glemaitre/scikit-learn-workshop-2019