scikit-learn new features

Tutorial

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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 0.20

Sept 26, 2018 - 13 months work

- 361 contributors
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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

Added in 0.20 by Andreas Müller, Joris Van den Bossche, Thomas Fan

OpenML fetcher

sklearn.datasets

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

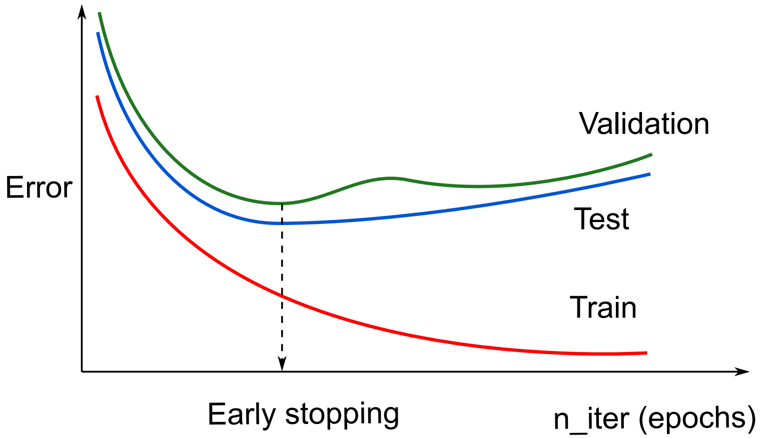
- ~20000 datasets available at www.openml.org

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)

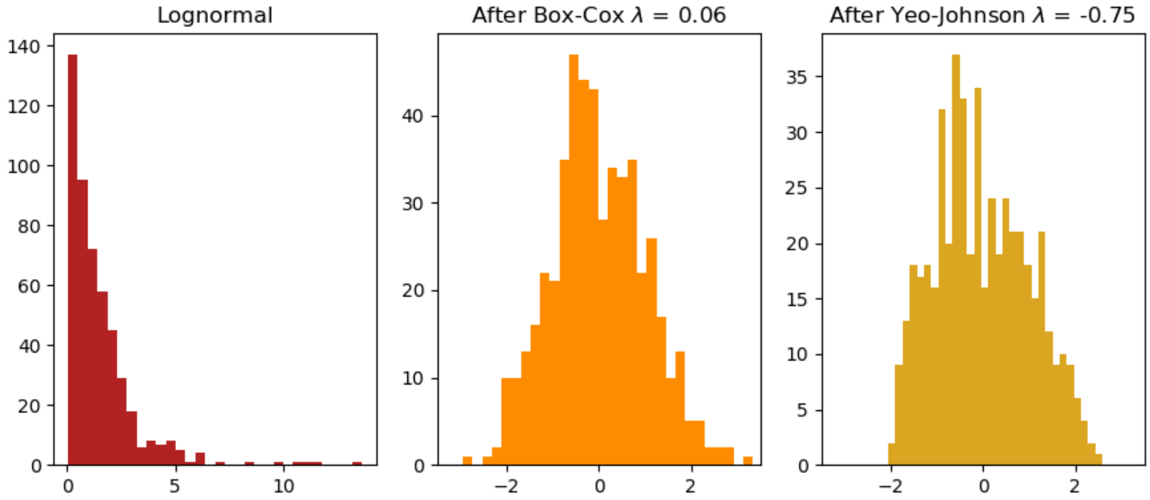
```
from sklearn.linear_model import SDGClassifier

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

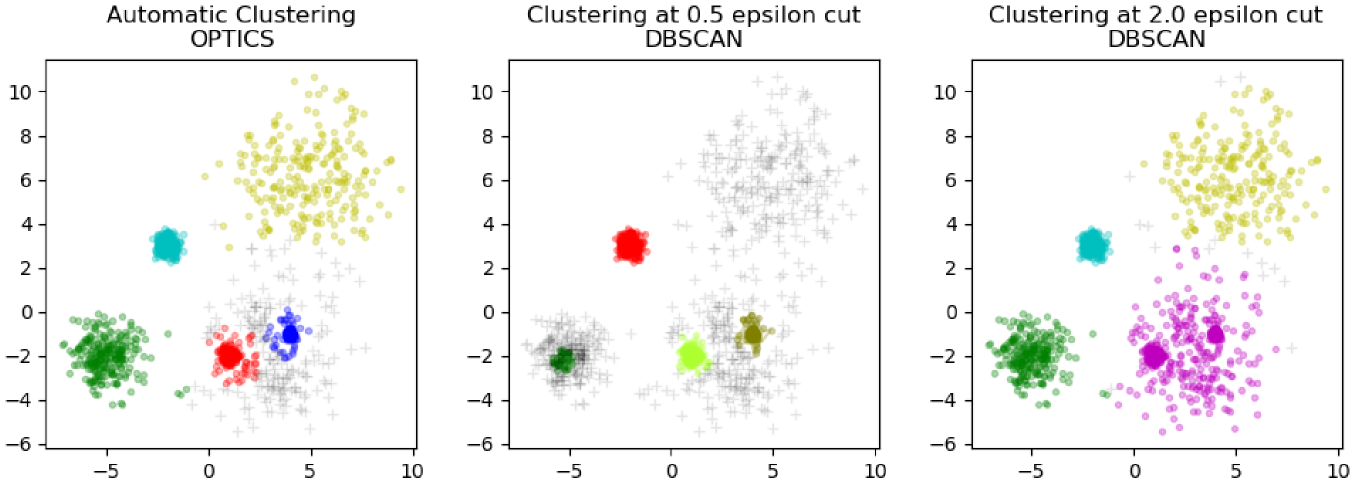
```
>>> import numpy as np
>>> from sklearn.experimental import enable_iterative_imputer
>>> from sklearn.impute import IterativeImputer
>>> imp = IterativeImputer(max_iter=10, random_state=0)
>>> imp.fit([[1, 2], [3, 6], [4, 8], [np.nan, 3], [7, np.nan]])
>>> X_test = [[np.nan, 2], [6, np.nan], [np.nan, 6]]
>>>
>>> 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 0.20

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
```

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
...
```

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