pyod Documentation

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Yue Zhao

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Getting Started

Deployment & Documentation & Stats

Build Status & Coverage & Maintainability & License

PyOD is a comprehensive and scalable **Python toolkit** for **detecting outlying objects** in multivariate data. This exciting yet challenging field is commonly referred as Outlier Detection or Anomaly Detection. Since 2017, PyOD [AZNL19] has been successfully used in various academic researches and commercial products [ARSLS19][AKW19][AZH18b][AZNHL19]. It is also well acknowledged by the machine learning community with various dedicated posts/tutorials, including Analytics Vidhya, Towards Data Science, KDnuggets, Computer Vision News, and awesome-machine-learning.

PyOD is featured for:

- **Unified APIs, detailed documentation, and interactive examples** across various algorithms.
- **Advanced models**, including **Neural Networks/Deep Learning** and **Outlier Ensembles**.
- **Optimized performance with JIT and parallelization** when possible, using numba and joblib.
- **Compatible with both Python 2 & 3**.

Note on Python 2.7: The maintenance of Python 2.7 will be stopped by January 1, 2020 (see official announcement) To be consistent with the Python change and PyOD's dependent libraries, e.g., scikit-learn, we will stop supporting Python 2.7 in the near future (dates are still to be decided). We encourage you to use Python 3.5 or newer for the latest functions and bug fixes. More information can be found at Moving to require Python 3.

API Demo:

```
# train the KNN detector
from pyod.models.knn import KNN
clf = KNN()
clf.fit(X_train)

# get outlier scores
y_train_scores = clf.decision_scores_  # raw outlier scores
y_test_scores = clf.decision_function(X_test)  # outlier scores
```

Citing PyOD:

PyOD paper is published in JMLR (machine learning open-source software track). If you use PyOD in a scientific publication, we would appreciate citations to the following paper:

```
@article{zhao2019pyod,
  author  = {Zhao, Yue and Nasrullah, Zain and Li, Zheng},
  title   = {PyOD: A Python Toolbox for Scalable Outlier Detection},
  journal = {Journal of Machine Learning Research},
  year    = {2019},
  volume  = {20},
  number  = {96},
  pages   = {1-7},
  url     = {http://jmlr.org/papers/v20/19-011.html}
}
```

or:

```
Zhao, Y., Nasrullah, Z. and Li, Z., 2019. PyOD: A Python Toolbox for Scalable Outlier␣
↪Detection. Journal of machine learning research (JMLR), 20(96), pp.1-7.
```

Key Links and Resources:

- View the latest codes on Github
- Execute Interactive Jupyter Notebooks
- Anomaly Detection Resources

CHAPTER 1

Implemented Algorithms

PyOD toolkit consists of three major functional groups:

(i) Individual Detection Algorithms :

1. Linear Models for Outlier Detection:

Type	Abbr	Algorithm	Year	Class	Ref
Linear Model	PCA	Principal Component Analysis (the sum of weighted projected distances to the eigenvector hyperplanes)	2003	*pyod.models.pca.PCA*	[ASCSC03]
Linear Model	MCD	Minimum Covariance Determinant (use the mahalanobis distances as the outlier scores)	1999	*pyod.models.mcd.MCD*	[ARD99][AHR04]
Linear Model	OCSVM	One-Class Support Vector Machines	2001	*pyod.models.ocsvm.OCSVM*	[AScholkopfPST+01]
Proximity-Based	LOF	Local Outlier Factor	2000	*pyod.models.lof.LOF*	[ABKNS00]
Proximity-Based	COF	Connectivity-Based Outlier Factor	2002	*pyod.models.cof.COF*	[ATCFC02]
Proximity-Based	CBLOF	Clustering-Based Local Outlier Factor	2003	*pyod.models.cblof.CBLOF*	[AHXD03]
Proximity-Based	LOCI	LOCI: Fast outlier detection using the local correlation integral	2003	*pyod.models.loci.LOCI*	[APKGF03]
Proximity-Based	HBOS	Histogram-based Outlier Score	2012	*pyod.models.hbos.HBOS*	[AGD12]
Proximity-Based	kNN	k Nearest Neighbors (use the distance to the kth nearest neighbor as the outlier score	2000	*pyod.models.knn.KNN*	[ARRS00][AAP02]
Proximity-Based	AvgKNN	Average kNN (use the average distance to k nearest neighbors as the outlier score)	2002	*pyod.models.knn.KNN*	[ARRS00][AAP02]
Proximity-Based	MedKNN	Median kNN (use the median distance to k nearest neighbors as the outlier score)	2002	*pyod.models.knn.KNN*	[ARRS00][AAP02]
Proximity-Based	SOD	Subspace Outlier Detection	2009	*pyod.models.sod.SOD*	[BKKrogerSZ09]
Probabilistic	ABOD	Angle-Based Outlier Detection	2008	*pyod.models.abod.ABOD*	[AKZ+08]
Probabilistic	FastABOD	Fast Angle-Based Outlier Detection using approximation	2008	*pyod.models.abod.ABOD*	[AKZ+08]
Probabilistic	SOS	Stochastic Outlier Selection	2012	*pyod.models.sos.SOS*	[AJHuszarPvdH12]
Outlier Ensembles	IForest	Isolation Forest	2008	*pyod.models.iforest.IForest*	[ALTZ08][ALTZ12]
Outlier Ensembles		Feature Bagging	2005	*pyod.models.feature_bagging.FeatureBagging*	[ALK05]
Outlier Ensembles	LSCP	LSCP: Locally Selective Combination of Parallel Outlier Ensembles	2019	*pyod.models.lscp.LSCP*	[AZNHL19]
Outlier Ensembles	XGBOD	Extreme Boosting Based Outlier Detection **(Supervised)**	2018	*pyod.models.xgbod.XGBOD*	[AZH18a]
Neural Networks	AutoEncoder	Fully connected AutoEncoder (use reconstruction error as the outlier score)	2015	*pyod.models.auto_encoder.AutoEncoder*	[AAgg15]
Neural Networks	SO_GAAL	Single-Objective Generative Adversarial Active Learning	2019	*pyod.models.so_gaal.SO_GAAL*	[ALLZ+19]
Neural Networks	MO_GAAL	Multiple-Objective Generative Adversarial Active Learning	2019	*pyod.models.mo_gaal.MO_GAAL*	[ALLZ+19]

(ii) Outlier Ensembles & Outlier Detector Combination Frameworks:

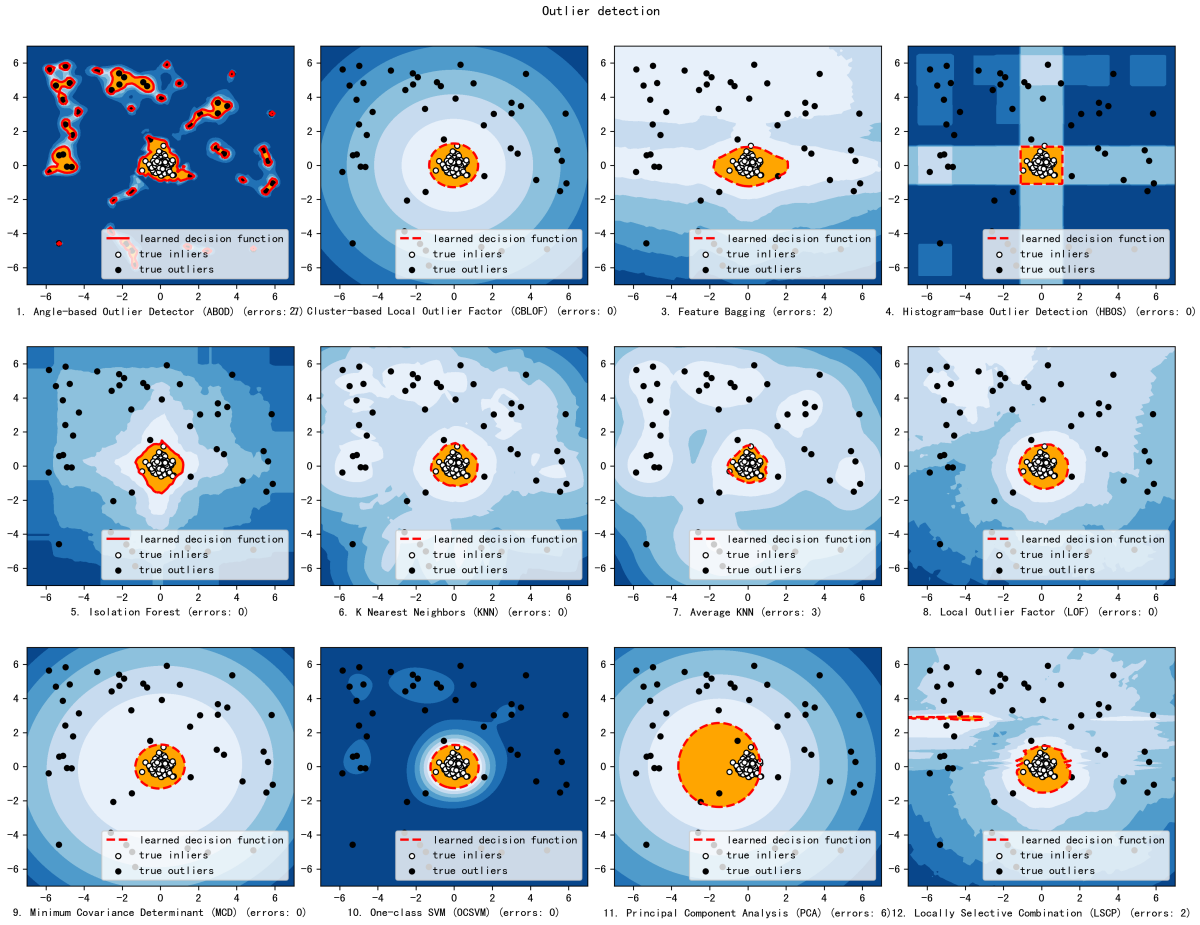
Type	Abbr	Algorithm	Year	Ref	
Outlier Ensembles		Feature Bagging	2005	*pyod.models.feature_bagging.FeatureBagging*	[ALK05]
Outlier Ensembles	LSCP	LSCP: Locally Selective Combination of Parallel Outlier Ensembles	2019	*pyod.models.lscp.LSCP*	[AZNHL19]
Combination	Average	Simple combination by averaging the scores	2015	*pyod.models.combination.average()*	[AAS15]
Combination	Weighted Average	Simple combination by averaging the scores with detector weights	2015	*pyod.models.combination.average()*	[AAS15]
Combination	Maximization	Simple combination by taking the maximum scores	2015	*pyod.models.combination.maximization()*	[AAS15]
Combination	AOM	Average of Maximum	2015	*pyod.models.combination.aom()*	[AAS15]
Combination	MOA	Maximum of Average	2015	*pyod.models.combination.moa()*	[AAS15]

(iii) Utility Functions:

Type	Name	Function
Data	*pyod.utils.data.generate_data()*	Synthesized data generation; normal data is generated by a multivariate Gaussian and outliers are generated by a uniform distribution
Data	*pyod.utils.data.generate_data_clusters()*	Synthesized data generation in clusters; more complex data patterns can be created with multiple clusters
Stat	*pyod.utils.stat_models.wpearsonr()*	Calculate the weighted Pearson correlation of two samples
Utility	*pyod.utils.utility.get_label_n()*	Turn raw outlier scores into binary labels by assign 1 to top n outlier scores
Utility	*pyod.utils.utility.precision_n_scores()*	calculate precision @ rank n

The comparison among of implemented models is made available below (Figure, compare_all_models.py, Interactive Jupyter Notebooks). For Jupyter Notebooks, please navigate to **"/notebooks/Compare All Models.ipynb"**.

Check the latest benchmark. You could replicate this process by running benchmark.py.


Outlier detection
learned decision function
true inliers
true outliers
1. Angle-based Outlier Detector (ABOD) (errors: 27)
2. Cluster-based Local Outlier Factor (CBLOF) (errors: 0)
3. Feature Bagging (errors: 2)
4. Histogram-base Outlier Detection (HBOS) (errors: 0)
5. Isolation Forest (errors: 0)
6. K Nearest Neighbors (KNN) (errors: 0)
7. Average KNN (errors: 3)
8. Local Outlier Factor (LOF) (errors: 0)
9. Minimum Covariance Determinant (MCD) (errors: 0)
10. One-class SVM (OCSVM) (errors: 0)
11. Principal Component Analysis (PCA) (errors: 6)
12. Locally Selective Combination (LSCP) (errors: 2)

CHAPTER 2

API Cheatsheet & Reference

The following APIs are applicable for all detector models for easy use.

- *pyod.models.base.BaseDetector.fit()*: Fit detector. y is optional for unsupervised methods.
- *pyod.models.base.BaseDetector.decision_function()*: Predict raw anomaly score of X using the fitted detector.
- *pyod.models.base.BaseDetector.predict()*: Predict if a particular sample is an outlier or not using the fitted detector.
- *pyod.models.base.BaseDetector.predict_proba()*: Predict the probability of a sample being outlier using the fitted detector.
- *pyod.models.base.BaseDetector.fit_predict()*: **[Deprecated in V0.6.9]** Fit detector first and then predict whether a particular sample is an outlier or not.
- *pyod.models.base.BaseDetector.fit_predict_score()*: **[Deprecated in V0.6.9]** Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

Key Attributes of a fitted model:

- *pyod.models.base.BaseDetector.decision_scores_*: The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores.
- *pyod.models.base.BaseDetector.labels_*: The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies.

Note : fit_predict() and fit_predict_score() are deprecated in V0.6.9 due to consistency issue and will be removed in V0.8.0. To get the binary labels of the training data X_train, one should call clf.fit(X_train) and use *pyod.models.base.BaseDetector.labels_*, instead of calling clf.predict(X_train).

2.1 Installation

It is recommended to use **pip** for installation. Please make sure **the latest version** is installed, as PyOD is updated frequently:

```
pip install pyod            # normal install
pip install --upgrade pyod  # or update if needed
pip install --pre pyod      # or include pre-release version for new features
```

Alternatively, you could clone and run setup.py file:

```
git clone https://github.com/yzhao062/pyod.git
cd pyod
pip install .
```

Warning: The maintenance of Python 2.7 will be stopped by January 1, 2020 (see official announcement). To be consistent with the Python change and PyOD's dependent libraries, e.g., scikit-learn, we will stop supporting Python 2.7 in the near future (dates are still to be decided). We encourage you to use Python 3.5 or newer for the latest functions and bug fixes. More information can be found at Moving to require Python 3.

Required Dependencies:

- Python 2.7, 3.5, 3.6, or 3.7
- numpy>=1.13
- numba>=0.35
- scipy>=0.19.1
- scikit_learn>=0.19.1

Optional Dependencies (see details below):

- keras (optional, required for AutoEncoder)
- matplotlib (optional, required for running examples)
- pandas (optional, required for running benchmark)
- tensorflow (optional, required for AutoEncoder, other backend works)
- xgboost (optional, required for XGBOD)

Warning: PyOD has multiple neural network based models, e.g., AutoEncoders, which are implemented in Keras. However, PyOD does **NOT** install **keras** and/or **tensorFlow** for you. This reduces the risk of interfering with your local copies. If you want to use neural-net based models, please make sure Keras and a backend library, e.g., TensorFlow, are installed. Instructions are provided: neural-net FAQ. Similarly, models depending on **xgboost**, e.g., XGBOD, would **NOT** enforce xgboost installation by default.

Warning: Running examples needs **matplotlib**, which may throw errors in conda virtual environment on mac OS. See reasons and solutions mac_matplotlib.

Warning: PyOD contains multiple models that also exist in scikit-learn. However, these two libraries' API is not exactly the same–it is recommended to use only one of them for consistency but not mix the results. Refer sckit-learn and PyOD for more information.

2.2 Examples

2.2.1 Featured Tutorials

PyOD has been well acknowledged by the machine learning community with a few featured posts and tutorials.

Analytics Vidhya: An Awesome Tutorial to Learn Outlier Detection in Python using PyOD Library

KDnuggets: Intuitive Visualization of Outlier Detection Methods

Towards Data Science: Anomaly Detection for Dummies

Computer Vision News (March 2019): Python Open Source Toolbox for Outlier Detection

awesome-machine-learning: General-Purpose Machine Learning

2.2.2 kNN Example

Full example: knn_example.py

1. Import models

```
from pyod.models.knn import KNN   # kNN detector
```

2. Generate sample data with *pyod.utils.data.generate_data()*:

```
contamination = 0.1  # percentage of outliers
n_train = 200  # number of training points
n_test = 100  # number of testing points

X_train, y_train, X_test, y_test = generate_data(
    n_train=n_train, n_test=n_test, contamination=contamination)
```

3. Initialize a *pyod.models.knn.KNN* detector, fit the model, and make the prediction.

```
# train kNN detector
clf_name = 'KNN'
clf = KNN()
clf.fit(X_train)

# get the prediction labels and outlier scores of the training data
y_train_pred = clf.labels_  # binary labels (0: inliers, 1: outliers)
y_train_scores = clf.decision_scores_  # raw outlier scores

# get the prediction on the test data
y_test_pred = clf.predict(X_test)  # outlier labels (0 or 1)
y_test_scores = clf.decision_function(X_test)  # outlier scores
```

4. Evaluate the prediction using ROC and Precision @ Rank n *pyod.utils.data.evaluate_print()*.

```
# evaluate and print the results
print("\nOn Training Data:")
evaluate_print(clf_name, y_train, y_train_scores)
print("\nOn Test Data:")
evaluate_print(clf_name, y_test, y_test_scores)
```

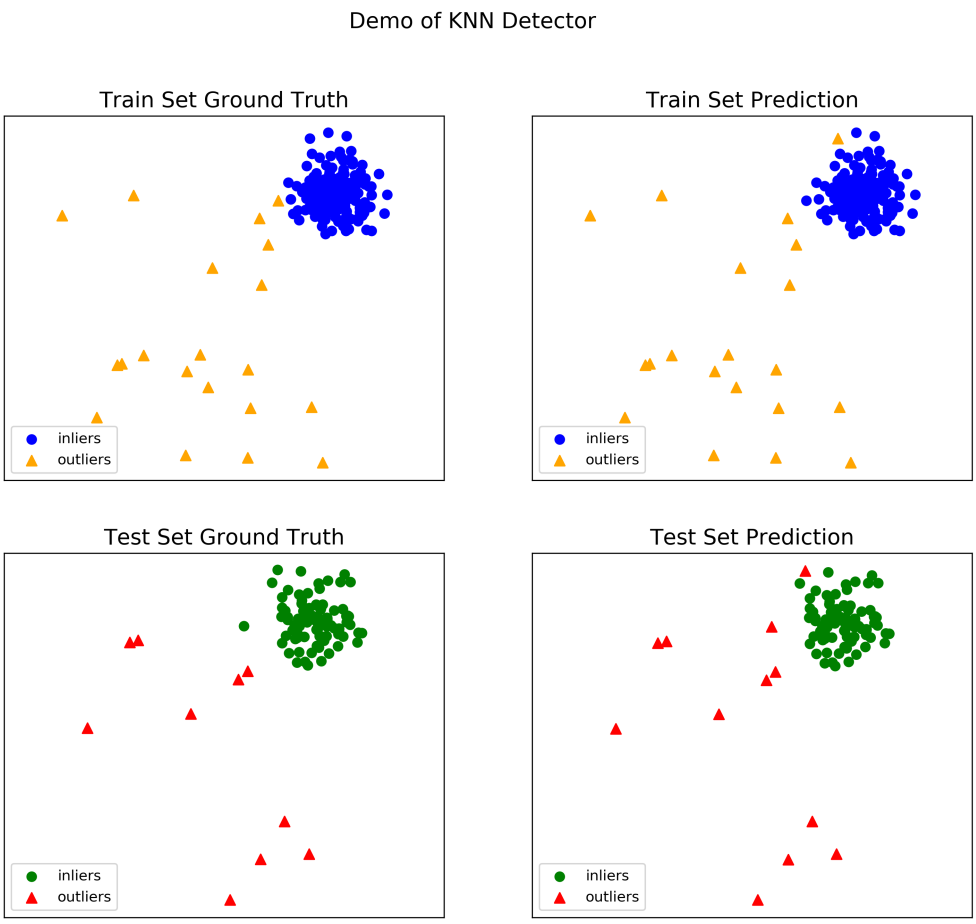
5. See sample outputs on both training and test data.

```
On Training Data:
KNN ROC:1.0, precision @ rank n:1.0

On Test Data:
KNN ROC:0.9989, precision @ rank n:0.9
```

6. Generate the visualizations by visualize function included in all examples.

```
visualize(clf_name, X_train, y_train, X_test, y_test, y_train_pred,
          y_test_pred, show_figure=True, save_figure=False)
```



2.2.3 Model Combination Example

Outlier detection often suffers from model instability due to its unsupervised nature. Thus, it is recommended to combine various detector outputs, e.g., by averaging, to improve its robustness. Detector combination is a subfield of outlier ensembles; refer [BKalayciE18] for more information.

Four score combination mechanisms are shown in this demo:

1. **Average**: average scores of all detectors.
2. **maximization**: maximum score across all detectors.
3. **Average of Maximum (AOM)**: divide base detectors into subgroups and take the maximum score for each subgroup. The final score is the average of all subgroup scores.
4. **Maximum of Average (MOA)**: divide base detectors into subgroups and take the average score for each subgroup. The final score is the maximum of all subgroup scores.

"examples/comb_example.py" illustrates the API for combining the output of multiple base detectors (comb_example.py, Jupyter Notebooks). For Jupyter Notebooks, please navigate to **"/notebooks/Model Combination.ipynb"**

1. Import models and generate sample data.

```
from pyod.models.knn import KNN   # kNN detector
from pyod.models.combination import aom, moa, average, maximization
from pyod.utils.data import generate_data

X, y= generate_data(train_only=True)  # load data
```

2. Initialize 20 kNN outlier detectors with different k (10 to 200), and get the outlier scores.

```
# initialize 20 base detectors for combination
k_list = [10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 110, 120, 130, 140,
          150, 160, 170, 180, 190, 200]

train_scores = np.zeros([X_train.shape[0], n_clf])
test_scores = np.zeros([X_test.shape[0], n_clf])

for i in range(n_clf):
    k = k_list[i]

    clf = KNN(n_neighbors=k, method='largest')
    clf.fit(X_train_norm)

    train_scores[:, i] = clf.decision_scores_
    test_scores[:, i] = clf.decision_function(X_test_norm)
```

3. Then the output scores are standardized into zero average and unit std before combination. This step is crucial to adjust the detector outputs to the same scale.

```
from pyod.utils.utility import standardizer

# scores have to be normalized before combination
train_scores_norm, test_scores_norm = standardizer(train_scores, test_
↪scores)
```

4. Four different combination algorithms are applied as described above:

```
comb_by_average = average(test_scores_norm)
comb_by_maximization = maximization(test_scores_norm)
comb_by_aom = aom(test_scores_norm, 5) # 5 groups
comb_by_moa = moa(test_scores_norm, 5)) # 5 groups
```

5. Finally, all four combination methods are evaluated by ROC and Precision @ Rank n:

```
Combining 20 kNN detectors
Combination by Average ROC:0.9194, precision @ rank n:0.4531
Combination by Maximization ROC:0.9198, precision @ rank n:0.4688
Combination by AOM ROC:0.9257, precision @ rank n:0.4844
Combination by MOA ROC:0.9263, precision @ rank n:0.4688
```

References

2.3 Benchmarks

2.3.1 Introduction

A benchmark is supplied for select algorithms to provide an overview of the implemented models. In total, 17 benchmark datasets are used for comparison, which can be downloaded at ODDS.

For each dataset, it is first split into 60% for training and 40% for testing. All experiments are repeated 10 times independently with random splits. The mean of 10 trials is regarded as the final result. Three evaluation metrics are provided:

- The area under receiver operating characteristic (ROC) curve
- Precision @ rank n (P@N)
- Execution time

You could replicate this process by running benchmark.py.

We also provide the hardware specification for reference.

Specification	Value
Platform	PC
OS	Microsoft Windows 10 Enterprise
CPU	Intel i7-6820HQ @ 2.70GHz
RAM	32GB
Software	PyCharm 2018.02
Python	Python 3.6.2
Core	Single core (no parallelization)

2.3.2 ROC Performance

Table 1: ROC Performances (average of 10 independent trials)

Data	#Samples	# Dimensions	Outlier Perc	ABOD	CBLOF	FB	HBOS	IForest	KNN	LOF	MCD	OCSVM	PCA
arrhythmia	452	274	14.6018	0.7688	0.7835	0.7781	0.8219	0.8005	0.7861	0.7787	0.7790	0.7812	0.7815
cardio	1831	21	9.6122	0.5692	0.9276	0.5867	0.8351	0.9213	0.7236	0.5736	0.8135	0.9348	0.9504
glass	214	9	4.2056	0.7951	0.8504	0.8726	0.7389	0.7569	0.8508	0.8644	0.7901	0.6324	0.6747
ionosphere	351	33	35.8974	0.9248	0.8134	0.8730	0.5614	0.8499	0.9267	0.8753	0.9557	0.8419	0.7962
letter	1600	32	6.2500	0.8783	0.5070	0.8660	0.5927	0.6420	0.8766	0.8594	0.8074	0.6118	0.5283
lympho	148	18	4.0541	0.9110	0.9728	0.9753	0.9957	0.9941	0.9745	0.9771	0.9000	0.9759	0.9847
mnist	7603	100	9.2069	0.7815	0.8009	0.7205	0.5742	0.8159	0.8481	0.7161	0.8666	0.8529	0.8527
musk	3062	166	3.1679	0.1844	0.9879	0.5263	1.0000	0.9999	0.7986	0.5287	0.9998	1.0000	1.0000
optdigits	5216	64	2.8758	0.4667	0.5089	0.4434	0.8732	0.7253	0.3708	0.4500	0.3979	0.4997	0.5086
pendigits	6870	16	2.2707	0.6878	0.9486	0.4595	0.9238	0.9435	0.7486	0.4698	0.8344	0.9303	0.9352
pima	768	8	34.8958	0.6794	0.7348	0.6235	0.7000	0.6806	0.7078	0.6271	0.6753	0.6215	0.6481
satellite	6435	36	31.6395	0.5714	0.6693	0.5572	0.7581	0.7022	0.6836	0.5573	0.8030	0.6622	0.5988
satimage-2	5803	36	1.2235	0.8190	0.9917	0.4570	0.9804	0.9947	0.9536	0.4577	0.9959	0.9978	0.9822
shuttle	49097	9	7.1511	0.6234	0.6272	0.4724	0.9855	0.9971	0.6537	0.5264	0.9903	0.9917	0.9898
vertebral	240	6	12.5000	0.4262	0.3486	0.4166	0.3263	0.3905	0.3817	0.4081	0.3906	0.4431	0.4027
vowels	1456	12	3.4341	0.9606	0.5856	0.9425	0.6727	0.7585	0.9680	0.9410	0.8076	0.7802	0.6027
wbc	378	30	5.5556	0.9047	0.9227	0.9325	0.9516	0.9310	0.9366	0.9349	0.9210	0.9319	0.9159

2.3.3 P@N Performance

Table 2: Precision @ N Performances (average of 10 independent trials)

Data	#Samples	# Dimensions	Outlier Perc	ABOD	CBLOF	FB	HBOS	IForest	KNN	LOF	MCD	OCSVM	PCA
arrhythmia	452	274	14.6018	0.3808	0.4539	0.4230	0.5111	0.4961	0.4464	0.4334	0.3995	0.4614	0.4613
cardio	1831	21	9.6122	0.2374	0.5876	0.1690	0.4476	0.5041	0.3323	0.1541	0.4317	0.5011	0.6090
glass	214	9	4.2056	0.1702	0.0726	0.1476	0.0000	0.0726	0.0726	0.1476	0.0000	0.1726	0.0726
ionosphere	351	33	35.8974	0.8442	0.6088	0.7056	0.3295	0.6369	0.8602	0.7063	0.8806	0.7000	0.5729
letter	1600	32	6.2500	0.3801	0.0749	0.3642	0.0715	0.1003	0.3312	0.3641	0.1933	0.1510	0.0875
lympho	148	18	4.0541	0.4483	0.7517	0.7517	0.8467	0.9267	0.7517	0.7517	0.5183	0.7517	0.7517
mnist	7603	100	9.2069	0.3555	0.3348	0.3299	0.1188	0.3135	0.4204	0.3343	0.3462	0.3962	0.3846
musk	3062	166	3.1679	0.0507	0.7766	0.2230	0.9783	0.9680	0.2733	0.1695	0.9742	1.0000	0.9799
optdigits	5216	64	2.8758	0.0060	0.0000	0.0244	0.2194	0.0301	0.0000	0.0234	0.0000	0.0000	0.0000
pendigits	6870	16	2.2707	0.0812	0.2768	0.0658	0.2979	0.3422	0.0984	0.0653	0.0893	0.3287	0.3187
pima	768	8	34.8958	0.5193	0.5413	0.4480	0.5424	0.5111	0.5413	0.4555	0.4962	0.4704	0.4943
satellite	6435	36	31.6395	0.3902	0.4152	0.3902	0.5690	0.5676	0.4994	0.3893	0.6845	0.5346	0.4784
satimage-2	5803	36	1.2235	0.2130	0.8846	0.0555	0.6939	0.8754	0.3809	0.0555	0.6481	0.9356	0.8041
shuttle	49097	9	7.1511	0.1977	0.2943	0.0695	0.9551	0.9546	0.2184	0.1424	0.7506	0.9542	0.9501
vertebral	240	6	12.5000	0.0601	0.0000	0.0644	0.0071	0.0343	0.0238	0.0506	0.0071	0.0238	0.0226
vowels	1456	12	3.4341	0.5710	0.0831	0.3224	0.1297	0.1875	0.5093	0.3551	0.2186	0.2791	0.1364
wbc	378	30	5.5556	0.3060	0.5055	0.5188	0.5817	0.5088	0.4952	0.5188	0.4577	0.5125	0.4767

2.3.4 Execution Time

Table 3: Time Elapsed in Seconds (average of 10 independent trials)

Data	#Samples	# Dimensions	Outlier Perc	ABOD	CBLOF	FB	HBOS	IForest	KNN	LOF	MCD	OCSVM	PCA
arrhythmia	452	274	14.6018	0.3667	0.2123	0.5651	0.1383	0.2669	0.1075	0.0743	1.4165	0.0473	0.0596
cardio	1831	21	9.6122	0.3824	0.1255	0.7741	0.0053	0.2672	0.2249	0.0993	0.5418	0.0883	0.0035
glass	214	9	4.2056	0.0352	0.0359	0.0317	0.0022	0.1724	0.0173	0.0025	0.0325	0.0010	0.0011
ionosphere	351	33	35.8974	0.0645	0.0459	0.0728	0.0082	0.1864	0.0302	0.0070	0.0718	0.0048	0.0018
letter	1600	32	6.2500	0.3435	0.1014	0.7361	0.0080	0.2617	0.1882	0.0935	1.1942	0.0888	0.0041
lympho	148	18	4.0541	0.0277	0.0353	0.0266	0.0037	0.1712	0.0111	0.0021	0.0327	0.0014	0.0012
mnist	7603	100	9.2069	7.4192	1.1339	48.2750	0.0480	1.9314	7.3431	6.7901	4.7448	5.0203	0.1569
musk	3062	166	3.1679	2.3860	0.4134	13.8610	0.0587	1.2736	2.2057	1.9835	25.5501	1.3774	0.1637
optdigits	5216	64	2.8758	2.7279	0.4977	14.2399	0.0303	0.7783	2.1205	1.7799	1.8599	1.5618	0.0519
pendigits	6870	16	2.2707	1.4339	0.2847	3.8185	0.0090	0.5879	0.8659	0.5936	2.2209	0.9666	0.0062
pima	768	8	34.8958	0.1357	0.0698	0.0908	0.0019	0.1923	0.0590	0.0102	0.0474	0.0087	0.0013
satellite	6435	36	31.6395	1.7970	0.4269	7.5566	0.0161	0.6449	1.2578	0.9868	2.6916	1.3697	0.0245
satimage-2	5803	36	1.2235	1.5209	0.3705	5.6561	0.0148	0.5529	1.0587	0.7525	2.3935	1.1114	0.0151
shuttle	49097	9	7.1511	14.3611	1.2524	59.2131	0.0953	3.3906	9.4958	11.1500	12.1449	44.6830	0.0378
vertebral	240	6	12.5000	0.0529	0.0444	0.0339	0.0014	0.1786	0.0161	0.0025	0.0446	0.0015	0.0010
vowels	1456	12	3.4341	0.3380	0.0889	0.3125	0.0044	0.2751	0.1125	0.0367	0.9745	0.0469	0.0023
wbc	378	30	5.5556	0.1014	0.0691	0.0771	0.0063	0.2030	0.0287	0.0078	0.0864	0.0062	0.0035

2.4 API CheatSheet

The following APIs are applicable for all detector models for easy use.

- *pyod.models.base.BaseDetector.fit()*: Fit detector. y is optional for unsupervised methods.
- *pyod.models.base.BaseDetector.decision_function()*: Predict raw anomaly score of X using the fitted detector.
- *pyod.models.base.BaseDetector.predict()*: Predict if a particular sample is an outlier or not using the fitted detector.
- *pyod.models.base.BaseDetector.predict_proba()*: Predict the probability of a sample being outlier using the fitted detector.
- *pyod.models.base.BaseDetector.fit_predict()*: **[Deprecated in V0.6.9]** Fit detector first and then predict whether a particular sample is an outlier or not.

- *pyod.models.base.BaseDetector.fit_predict_score()*: **[Deprecated in V0.6.9]** Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

Key Attributes of a fitted model:

- *pyod.models.base.BaseDetector.decision_scores_*: The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores.
- *pyod.models.base.BaseDetector.labels_*: The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies.

Note : fit_predict() and fit_predict_score() are deprecated in V0.6.9 due to consistency issue and will be removed in V0.8.0. To get the binary labels of the training data X_train, one should call clf.fit(X_train) and use *pyod.models.base.BaseDetector.labels_*, instead of calling clf.predict(X_train).

See base class definition below:

2.4.1 pyod.models.base module

Base class for all outlier detector models

class pyod.models.base.**BaseDetector**(*contamination=0.1*)
Bases: object

Abstract class for all outlier detection algorithms.

pyod would stop supporting Python 2 in the future. Consider move to Python 3.5+.

Parameters **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set. Used when fitting to define the threshold on the decision function.

decision_scores_
The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores. This value is available once the detector is fitted.

Type numpy array of shape (n_samples,)

threshold_
The threshold is based on contamination. It is the n_samples * contamination most abnormal samples in decision_scores_. The threshold is calculated for generating binary outlier labels.

Type float

labels_
The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies. It is generated by applying threshold_ on decision_scores_.

Type int, either 0 or 1

decision_function(*X*)
Predict raw anomaly scores of X using the fitted detector.

The anomaly score of an input sample is computed based on the fitted detector. For consistency, outliers are assigned with higher anomaly scores.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples. Sparse matrices are accepted only if they are supported by the base estimator.

Returns **anomaly_scores** – The anomaly score of the input samples.

Return type numpy array of shape (n_samples,)

fit(*X*, *y=None*)
Fit detector. y is optional for unsupervised methods.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **y** (*numpy array of shape (n_samples,), optional (default=None)*) – The ground truth of the input samples (labels).

fit_predict(*X*, *y=None*)
DEPRECATED

Fit detector first and then predict whether a particular sample is an outlier or not.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

outlier_labels [numpy array of shape (n_samples,)] For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Deprecated since version 0.6.9: *fit_predict* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency.

fit_predict_score(*X*, *y*, *scoring='roc_auc_score'*)
DEPRECATED

Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

scoring [str, optional (default='roc_auc_score')] Evaluation metric:

- 'roc_auc_score': ROC score
- 'prc_n_score': Precision @ rank n score

score : float

Deprecated since version 0.6.9: *fit_predict_score* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency. Scoring could be done by calling an evaluation method, e.g., AUC ROC.

get_params(*deep=True*)
Get parameters for this estimator.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Parameters **deep** (*boolean, optional*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns **params** – Parameter names mapped to their values.

Return type mapping of string to any

predict(*X*)
Predict if a particular sample is an outlier or not.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Return type numpy array of shape (n_samples,)

predict_proba(*X*, *method='linear'*)

Predict the probability of a sample being outlier. Two approaches are possible:

1. simply use Min-max conversion to linearly transform the outlier scores into the range of [0,1]. The model must be fitted first.
2. use unifying scores, see [BKKSZ11].

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **method** (*str, optional (default='linear')*) – probability conversion method. It must be one of 'linear' or 'unify'.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

set_params(***params*)

Set the parameters of this estimator. The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Returns **self**

Return type object

2.5 API Reference

2.5.1 All Models

pyod.models.abod module

Angle-based Outlier Detector (ABOD)

class pyod.models.abod.**ABOD**(*contamination=0.1*, *n_neighbors=5*, *method='fast'*)

Bases: *pyod.models.base.BaseDetector*

ABOD class for Angle-base Outlier Detection. For an observation, the variance of its weighted cosine scores to all neighbors could be viewed as the outlying score. See [BKZ+08] for details.

Two version of ABOD are supported:

- Fast ABOD: use k nearest neighbors to approximate.
- Original ABOD: consider all training points with high time complexity at O(n^3).

Parameters

- **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set. Used when fitting to define the threshold on the decision function.
- **n_neighbors** (*int, optional (default=10)*) – Number of neighbors to use by default for k neighbors queries.
- **method** (*str, optional (default='fast')*) – Valid values for metric are:
  - 'fast': fast ABOD. Only consider n_neighbors of training points
  - 'default': original ABOD with all training points, which could be slow

decision_scores_
The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores. This value is available once the detector is fitted.

Type numpy array of shape (n_samples,)

threshold_
The threshold is based on `contamination`. It is the `n_samples * contamination` most abnormal samples in `decision_scores_`. The threshold is calculated for generating binary outlier labels.

Type float

labels_
The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies. It is generated by applying `threshold_` on `decision_scores_`.

Type int, either 0 or 1

decision_function(*X*)
Predict raw anomaly score of X using the fitted detector.

The anomaly score of an input sample is computed based on different detector algorithms. For consistency, outliers are assigned with larger anomaly scores.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The training input samples. Sparse matrices are accepted only if they are supported by the base estimator.

Returns **anomaly_scores** – The anomaly score of the input samples.

Return type numpy array of shape (n_samples,)

fit(*X*, *y=None*)
Fit detector. y is optional for unsupervised methods.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **y** (*numpy array of shape (n_samples,), optional (default=None)*) – The ground truth of the input samples (labels).

fit_predict(*X*, *y=None*)
DEPRECATED

Fit detector first and then predict whether a particular sample is an outlier or not.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

outlier_labels [numpy array of shape (n_samples,)] For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Deprecated since version 0.6.9: *fit_predict* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency.

fit_predict_score(*X*, *y*, *scoring='roc_auc_score'*)
DEPRECATED

Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

scoring [str, optional (default='roc_auc_score')] Evaluation metric:

- 'roc_auc_score': ROC score
- 'prc_n_score': Precision @ rank n score

score : float

Deprecated since version 0.6.9: *fit_predict_score* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency. Scoring could be done by calling an evaluation method, e.g., AUC ROC.

get_params(*deep=True*)
Get parameters for this estimator.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Parameters **deep** (*boolean, optional*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns **params** – Parameter names mapped to their values.

Return type mapping of string to any

predict(*X*)
Predict if a particular sample is an outlier or not.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Return type numpy array of shape (n_samples,)

predict_proba(*X*, *method='linear'*)
Predict the probability of a sample being outlier. Two approaches are possible:

1. simply use Min-max conversion to linearly transform the outlier scores into the range of [0,1]. The model must be fitted first.
2. use unifying scores, see [BKKSZ11].

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **method** (*str, optional (default='linear')*) – probability conversion method. It must be one of 'linear' or 'unify'.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

set_params(***params*)

Set the parameters of this estimator. The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Returns **self**

Return type object

pyod.models.auto_encoder module

Using Auto Encoder with Outlier Detection

class pyod.models.auto_encoder.**AutoEncoder**(*hidden_neurons=None*, *hidden_activation='relu'*, *output_activation='sigmoid'*, *loss=<function mean_squared_error>*, *optimizer='adam'*, *epochs=100*, *batch_size=32*, *dropout_rate=0.2*, *l2_regularizer=0.1*, *validation_size=0.1*, *preprocessing=True*, *verbose=1*, *random_state=None*, *contamination=0.1*)

Bases: *pyod.models.base.BaseDetector*

Auto Encoder (AE) is a type of neural networks for learning useful data representations unsupervisedly. Similar to PCA, AE could be used to detect outlying objects in the data by calculating the reconstruction errors. See [BAgg15] Chapter 3 for details.

Parameters

- **hidden_neurons** (*list, optional (default=[64, 32, 32, 64])*) – The number of neurons per hidden layers.
- **hidden_activation** (*str, optional (default='relu')*) – Activation function to use for hidden layers. All hidden layers are forced to use the same type of activation. See https://keras.io/activations/
- **output_activation** (*str, optional (default='sigmoid')*) – Activation function to use for output layer. See https://keras.io/activations/
- **loss** (*str or obj, optional (default=keras.losses.mean_squared_error)*) – String (name of objective function) or objective function. See https://keras.io/losses/

- **optimizer** (*str, optional (default='adam')*) – String (name of optimizer) or optimizer instance. See https://keras.io/optimizers/
- **epochs** (*int, optional (default=100)*) – Number of epochs to train the model.
- **batch_size** (*int, optional (default=32)*) – Number of samples per gradient update.
- **dropout_rate** (*float in (0., 1), optional (default=0.2)*) – The dropout to be used across all layers.
- **l2_regularizer** (*float in (0., 1), optional (default=0.1)*) – The regularization strength of activity_regularizer applied on each layer. By default, l2 regularizer is used. See https://keras.io/regularizers/
- **validation_size** (*float in (0., 1), optional (default=0.1)*) – The percentage of data to be used for validation.
- **preprocessing** (*bool, optional (default=True)*) – If True, apply standardization on the data.
- **verbose** (*int, optional (default=1)*) – Verbosity mode.
  - 0 = silent
  - 1 = progress bar
  - 2 = one line per epoch.

  For verbosity >= 1, model summary may be printed.
- **random_state** (*random_state: int, RandomState instance or None, optional*) – (default=None) If int, random_state is the seed used by the random number generator; If RandomState instance, random_state is the random number generator; If None, the random number generator is the RandomState instance used by *np.random*.
- **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set. When fitting this is used to define the threshold on the decision function.

encoding_dim_
The number of neurons in the encoding layer.

Type int

compression_rate_
The ratio between the original feature and the number of neurons in the encoding layer.

Type float

model_
The underlying AutoEncoder in Keras.

Type Keras Object

history_
The AutoEncoder training history.

Type Keras Object

decision_scores_
The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores. This value is available once the detector is fitted.

Type numpy array of shape (n_samples,)

threshold_
The threshold is based on `contamination`. It is the `n_samples * contamination` most abnormal samples in `decision_scores_`. The threshold is calculated for generating binary outlier labels.

Type float

labels_
The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies. It is generated by applying `threshold_` on `decision_scores_`.

Type int, either 0 or 1

decision_function(*X*)
Predict raw anomaly score of X using the fitted detector.

The anomaly score of an input sample is computed based on different detector algorithms. For consistency, outliers are assigned with larger anomaly scores.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The training input samples. Sparse matrices are accepted only if they are supported by the base estimator.

Returns **anomaly_scores** – The anomaly score of the input samples.

Return type numpy array of shape (n_samples,)

fit(*X*, *y=None*)
Fit detector. y is optional for unsupervised methods.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **y** (*numpy array of shape (n_samples,), optional (default=None)*) – The ground truth of the input samples (labels).

fit_predict(*X*, *y=None*)
DEPRECATED

Fit detector first and then predict whether a particular sample is an outlier or not.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

outlier_labels [numpy array of shape (n_samples,)] For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Deprecated since version 0.6.9: *fit_predict* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency.

fit_predict_score(*X*, *y*, *scoring='roc_auc_score'*)
DEPRECATED

Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

scoring [str, optional (default='roc_auc_score')] Evaluation metric:

- 'roc_auc_score': ROC score
- 'prc_n_score': Precision @ rank n score

score : float

Deprecated since version 0.6.9: *fit_predict_score* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency. Scoring could be done by calling an evaluation method, e.g., AUC ROC.

get_params(*deep=True*)

Get parameters for this estimator.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Parameters **deep** (*boolean, optional*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns **params** – Parameter names mapped to their values.

Return type mapping of string to any

predict(*X*)

Predict if a particular sample is an outlier or not.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Return type numpy array of shape (n_samples,)

predict_proba(*X*, *method='linear'*)

Predict the probability of a sample being outlier. Two approaches are possible:

1. simply use Min-max conversion to linearly transform the outlier scores into the range of [0,1]. The model must be fitted first.
2. use unifying scores, see [BKKSZ11].

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **method** (*str, optional (default='linear')*) – probability conversion method. It must be one of 'linear' or 'unify'.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

set_params(***params*)

Set the parameters of this estimator. The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Returns self

Return type object

pyod.models.cblof module

Clustering Based Local Outlier Factor (CBLOF)

class pyod.models.cblof.**CBLOF**(*n_clusters=8*, *contamination=0.1*, *clustering_estimator=None*, *alpha=0.9*, *beta=5*, *use_weights=False*, *check_estimator=False*, *random_state=None*, *n_jobs=1*)

Bases: *pyod.models.base.BaseDetector*

The CBLOF operator calculates the outlier score based on cluster-based local outlier factor.

CBLOF takes as an input the data set and the cluster model that was generated by a clustering algorithm. It classifies the clusters into small clusters and large clusters using the parameters alpha and beta. The anomaly score is then calculated based on the size of the cluster the point belongs to as well as the distance to the nearest large cluster.

Use weighting for outlier factor based on the sizes of the clusters as proposed in the original publication. Since this might lead to unexpected behavior (outliers close to small clusters are not found), it is disabled by default.Outliers scores are solely computed based on their distance to the closest large cluster center.

By default, kMeans is used for clustering algorithm instead of Squeezer algorithm mentioned in the original paper for multiple reasons.

See [BHXD03] for details.

Parameters

- **n_clusters** (*int, optional (default=8)*) – The number of clusters to form as well as the number of centroids to generate.
- **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set. Used when fitting to define the threshold on the decision function.
- **clustering_estimator** (*Estimator, optional (default=None)*) – The base clustering algorithm for performing data clustering. A valid clustering algorithm should be passed in. The estimator should have standard sklearn APIs, fit() and predict(). The estimator should have attributes `labels_` and `cluster_centers_`. If `cluster_centers_` is not in the attributes once the model is fit, it is calculated as the mean of the samples in a cluster.

  If not set, CBLOF uses KMeans for scalability. See https://scikit-learn.org/stable/modules/generated/sklearn.cluster.KMeans.html
- **alpha** (*float in (0.5, 1), optional (default=0.9)*) – Coefficient for deciding small and large clusters. The ratio of the number of samples in large clusters to the number of samples in small clusters.
- **beta** (*int or float in (1,), optional (default=5)*) – Coefficient for deciding small and large clusters. For a list sorted clusters by size *|C1|, |C2|, ..., |Cn|, beta = |Ck|/|Ck-1|*
- **use_weights** (*bool, optional (default=False)*) – If set to True, the size of clusters are used as weights in outlier score calculation.
- **check_estimator** (*bool, optional (default=False)*) – If set to True, check whether the base estimator is consistent with sklearn standard.

> **Warning:** check_estimator may throw errors with scikit-learn 0.20 above.

- **random_state** (*int, RandomState or None, optional (default=None)*) – If int, random_state is the seed used by the random number generator; If RandomState instance, random_state is the random number generator; If None, the random number generator is the RandomState instance used by *np.random*.
- **n_jobs** (*integer, optional (default=1)*) – The number of jobs to run in parallel for both *fit* and *predict*. If -1, then the number of jobs is set to the number of cores.

clustering_estimator_
Base estimator for clustering.

Type Estimator, sklearn instance

cluster_labels_
Cluster assignment for the training samples.

Type list of shape (n_samples,)

n_clusters_
Actual number of clusters (possibly different from n_clusters).

Type int

cluster_sizes_
The size of each cluster once fitted with the training data.

Type list of shape (**n_clusters_**,)

decision_scores_
The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores. This value is available once the detector is fitted.

Type numpy array of shape (n_samples,)

cluster_centers_
The center of each cluster.

Type numpy array of shape (**n_clusters_**, n_features)

small_cluster_labels_
The cluster assignments belonging to small clusters.

Type list of clusters numbers

large_cluster_labels_
The cluster assignments belonging to large clusters.

Type list of clusters numbers

threshold_
The threshold is based on `contamination`. It is the `n_samples * contamination` most abnormal samples in `decision_scores_`. The threshold is calculated for generating binary outlier labels.

Type float

labels_
The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies. It is generated by applying `threshold_` on `decision_scores_`.

Type int, either 0 or 1

decision_function(*X*)
Predict raw anomaly score of X using the fitted detector.

The anomaly score of an input sample is computed based on different detector algorithms. For consistency, outliers are assigned with larger anomaly scores.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The training input samples. Sparse matrices are accepted only if they are supported by the base estimator.

Returns **anomaly_scores** – The anomaly score of the input samples.

Return type numpy array of shape (n_samples,)

fit(*X*, *y=None*)
Fit detector. y is optional for unsupervised methods.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **y** (*numpy array of shape (n_samples,), optional (default=None)*) – The ground truth of the input samples (labels).

fit_predict(*X*, *y=None*)
DEPRECATED

Fit detector first and then predict whether a particular sample is an outlier or not.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

outlier_labels [numpy array of shape (n_samples,)] For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Deprecated since version 0.6.9: *fit_predict* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency.

fit_predict_score(*X*, *y*, *scoring='roc_auc_score'*)
DEPRECATED

Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

scoring [str, optional (default='roc_auc_score')] Evaluation metric:

- 'roc_auc_score': ROC score
- 'prc_n_score': Precision @ rank n score

score : float

Deprecated since version 0.6.9: *fit_predict_score* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency. Scoring could be done by calling an evaluation method, e.g., AUC ROC.

get_params(*deep=True*)
Get parameters for this estimator.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Parameters **deep** (*boolean, optional*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns **params** – Parameter names mapped to their values.

Return type mapping of string to any

predict(*X*)
Predict if a particular sample is an outlier or not.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Return type numpy array of shape (n_samples,)

predict_proba(*X*, *method='linear'*)
Predict the probability of a sample being outlier. Two approaches are possible:

1. simply use Min-max conversion to linearly transform the outlier scores into the range of [0,1]. The model must be fitted first.
2. use unifying scores, see [BKKSZ11].

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **method** (*str, optional (default='linear')*) – probability conversion method. It must be one of 'linear' or 'unify'.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

set_params(***params*)
Set the parameters of this estimator. The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Returns **self**

Return type object

pyod.models.cof module

Connectivity-Based Outlier Factor (COF) Algorithm

class pyod.models.cof.**COF**(*contamination=0.1*, *n_neighbors=20*)
Bases: *pyod.models.base.BaseDetector*

Connectivity-Based Outlier Factor (COF) COF uses the ratio of average chaining distance of data point and the average of average chaining distance of k nearest neighbor of the data point, as the outlier score for observations.

See [BTCFC02] for details.

Parameters

- **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set. Used when fitting to define the threshold on the decision function.
- **n_neighbors** (*int, optional (default=20)*) – Number of neighbors to use by default for k neighbors queries. Note that n_neighbors should be less than the number of samples. If n_neighbors is larger than the number of samples provided, all samples will be used.

decision_scores_
The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores. This value is available once the detector is fitted.

Type numpy array of shape (n_samples,)

threshold_
The threshold is based on `contamination`. It is the `n_samples * contamination` most abnormal samples in `decision_scores_`. The threshold is calculated for generating binary outlier labels.

Type float

labels_
The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies. It is generated by applying `threshold_` on `decision_scores_`.

Type int, either 0 or 1

n_neighbors_
Number of neighbors to use by default for k neighbors queries.

Type int

decision_function(*X*)
Predict raw anomaly score of X using the fitted detector. The anomaly score of an input sample is computed based on different detector algorithms. For consistency, outliers are assigned with larger anomaly scores.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The training input samples. Sparse matrices are accepted only if they are supported by the base estimator.

Returns **anomaly_scores** – The anomaly score of the input samples.

Return type numpy array of shape (n_samples,)

fit(*X*, *y=None*)
Fit detector. y is optional for unsupervised methods.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **y** (*numpy array of shape (n_samples,), optional (default=None)*) – The ground truth of the input samples (labels).

fit_predict(*X*, *y=None*)
DEPRECATED

Fit detector first and then predict whether a particular sample is an outlier or not.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

outlier_labels [numpy array of shape (n_samples,)] For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Deprecated since version 0.6.9: *fit_predict* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency.

fit_predict_score(*X*, *y*, *scoring='roc_auc_score'*)
DEPRECATED

Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

scoring [str, optional (default='roc_auc_score')] Evaluation metric:

- 'roc_auc_score': ROC score
- 'prc_n_score': Precision @ rank n score

score : float

Deprecated since version 0.6.9: *fit_predict_score* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency. Scoring could be done by calling an evaluation method, e.g., AUC ROC.

get_params(*deep=True*)
Get parameters for this estimator.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Parameters **deep** (*boolean, optional*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns **params** – Parameter names mapped to their values.

Return type mapping of string to any

predict(*X*)
Predict if a particular sample is an outlier or not.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Return type numpy array of shape (n_samples,)

predict_proba(*X*, *method='linear'*)
Predict the probability of a sample being outlier. Two approaches are possible:

1. simply use Min-max conversion to linearly transform the outlier scores into the range of [0,1]. The model must be fitted first.
2. use unifying scores, see [BKKSZ11].

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **method** (*str, optional (default='linear')*) – probability conversion method. It must be one of 'linear' or 'unify'.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

set_params(***params*)

Set the parameters of this estimator. The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Returns **self**

Return type object

pyod.models.combination module

A collection of model combination functionalities.

pyod.models.combination.**aom**(*scores*, *n_buckets=5*, *method='static'*, *bootstrap_estimators=False*, *random_state=None*)

Average of Maximum - An ensemble method for combining multiple estimators. See [BAS15] for details.

First dividing estimators into subgroups, take the maximum score as the subgroup score. Finally, take the average of all subgroup outlier scores.

Parameters

- **scores** (*numpy array of shape (n_samples, n_estimators)*) – The score matrix outputted from various estimators
- **n_buckets** (*int, optional (default=5)*) – The number of subgroups to build
- **method** (*str, optional (default='static')*) – {'static', 'dynamic'}, if 'dynamic', build subgroups randomly with dynamic bucket size.
- **bootstrap_estimators** (*bool, optional (default=False)*) – Whether estimators are drawn with replacement.
- **random_state** (*int, RandomState instance or None, optional (default=None)*) – If int, random_state is the seed used by the random number generator; If RandomState instance, random_state is the random number generator; If None, the random number generator is the RandomState instance used by *np.random*.

Returns **combined_scores** – The combined outlier scores.

Return type Numpy array of shape (n_samples,)

pyod.models.combination.**average**(*scores*, *estimator_weights=None*)
Combination method to merge the outlier scores from multiple estimators by taking the average.

Parameters

- **scores** (*numpy array of shape (n_samples, n_estimators)*) – Score matrix from multiple estimators on the same samples.
- **estimator_weights** (*list of shape (1, n_estimators)*) – If specified, using weighted average

Returns **combined_scores** – The combined outlier scores.

Return type numpy array of shape (n_samples,)

pyod.models.combination.**maximization**(*scores*)
Combination method to merge the outlier scores from multiple estimators by taking the maximum.

Parameters **scores** (*numpy array of shape (n_samples, n_estimators)*) – Score matrix from multiple estimators on the same samples.

Returns **combined_scores** – The combined outlier scores.

Return type numpy array of shape (n_samples,)

pyod.models.combination.**moa**(*scores*, *n_buckets=5*, *method='static'*, *bootstrap_estimators=False*, *random_state=None*)
Maximization of Average - An ensemble method for combining multiple estimators. See [BAS15] for details.

First dividing estimators into subgroups, take the average score as the subgroup score. Finally, take the maximization of all subgroup outlier scores.

Parameters

- **scores** (*numpy array of shape (n_samples, n_estimators)*) – The score matrix outputted from various estimators
- **n_buckets** (*int, optional (default=5)*) – The number of subgroups to build
- **method** (*str, optional (default='static')*) – {'static', 'dynamic'}, if 'dynamic', build subgroups randomly with dynamic bucket size.
- **bootstrap_estimators** (*bool, optional (default=False)*) – Whether estimators are drawn with replacement.
- **random_state** (*int, RandomState instance or None, optional (default=None)*) – If int, random_state is the seed used by the random number generator; If RandomState instance, random_state is the random number generator; If None, the random number generator is the RandomState instance used by *np.random*.

Returns **combined_scores** – The combined outlier scores.

Return type Numpy array of shape (n_samples,)

pyod.models.feature_bagging module

Feature bagging detector

class pyod.models.feature_bagging.**FeatureBagging**(*base_estimator=None*, *n_estimators=10*, *contamination=0.1*, *max_features=1.0*, *bootstrap_features=False*, *check_detector=True*, *check_estimator=False*, *n_jobs=1*, *random_state=None*, *combination='average'*, *verbose=0*, *estimator_params=None*)

Bases: *pyod.models.base.BaseDetector*

A feature bagging detector is a meta estimator that fits a number of base detectors on various sub-samples of the dataset and use averaging or other combination methods to improve the predictive accuracy and control over-fitting.

The sub-sample size is always the same as the original input sample size but the features are randomly sampled from half of the features to all features.

By default, LOF is used as the base estimator. However, any estimator could be used as the base estimator, such as kNN and ABOD.

Feature bagging first construct n subsamples by random selecting a subset of features, which induces the diversity of base estimators.

Finally, the prediction score is generated by averaging/taking the maximum of all base detectors. See [BLK05] for details.

Parameters

- **base_estimator** (*object or None, optional (default=None)*) – The base estimator to fit on random subsets of the dataset. If None, then the base estimator is a LOF detector.
- **n_estimators** (*int, optional (default=10)*) – The number of base estimators in the ensemble.
- **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set. Used when fitting to define the threshold on the decision function.
- **max_features** (*int or float, optional (default=1.0)*) – The number of features to draw from X to train each base estimator.
  - If int, then draw *max_features* features.
  - If float, then draw *max_features * X.shape[1]* features.
- **bootstrap_features** (*bool, optional (default=False)*) – Whether features are drawn with replacement.
- **check_detector** (*bool, optional (default=True)*) – If set to True, check whether the base estimator is consistent with pyod standard.
- **check_estimator** (*bool, optional (default=False)*) – If set to True, check whether the base estimator is consistent with sklearn standard.

  Deprecated since version 0.6.9: *check_estimator* will be removed in pyod 0.8.0.; it will be replaced by *check_detector*.
- **n_jobs** (*optional (default=1)*) – The number of jobs to run in parallel for both *fit* and *predict*. If -1, then the number of jobs is set to the number of cores.

- **random_state** (*int, RandomState or None, optional (default=None)*) – If int, random_state is the seed used by the random number generator; If RandomState instance, random_state is the random number generator; If None, the random number generator is the RandomState instance used by *np.random*.
- **combination** (*str, optional (default='average')*) – the method of combination:
  - if 'average': take the average of all detectors
  - if 'max': take the maximum scores of all detectors
- **verbose** (*int, optional (default=0)*) – Controls the verbosity of the building process.
- **estimator_params** (*dict, optional (default=None)*) – The list of attributes to use as parameters when instantiating a new base estimator. If none are given, default parameters are used.

decision_scores_
The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores. This value is available once the detector is fitted.

Type numpy array of shape (n_samples,)

threshold_
The threshold is based on `contamination`. It is the `n_samples * contamination` most abnormal samples in `decision_scores_`. The threshold is calculated for generating binary outlier labels.

Type float

labels_
The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies. It is generated by applying `threshold_` on `decision_scores_`.

Type int, either 0 or 1

decision_function(*X*)
Predict raw anomaly score of X using the fitted detector.

The anomaly score of an input sample is computed based on different detector algorithms. For consistency, outliers are assigned with larger anomaly scores.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The training input samples. Sparse matrices are accepted only if they are supported by the base estimator.

Returns **anomaly_scores** – The anomaly score of the input samples.

Return type numpy array of shape (n_samples,)

fit(*X*, *y=None*)
Fit detector. y is optional for unsupervised methods.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **y** (*numpy array of shape (n_samples,), optional (default=None)*) – The ground truth of the input samples (labels).

fit_predict(*X*, *y=None*)
DEPRECATED

Fit detector first and then predict whether a particular sample is an outlier or not.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

outlier_labels [numpy array of shape (n_samples,)] For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Deprecated since version 0.6.9: *fit_predict* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency.

fit_predict_score(*X*, *y*, *scoring='roc_auc_score'*)
DEPRECATED

Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

scoring [str, optional (default='roc_auc_score')] Evaluation metric:

- 'roc_auc_score': ROC score
- 'prc_n_score': Precision @ rank n score

score : float

Deprecated since version 0.6.9: *fit_predict_score* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency. Scoring could be done by calling an evaluation method, e.g., AUC ROC.

get_params(*deep=True*)
Get parameters for this estimator.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Parameters **deep** (*boolean, optional*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns **params** – Parameter names mapped to their values.

Return type mapping of string to any

predict(*X*)
Predict if a particular sample is an outlier or not.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Return type numpy array of shape (n_samples,)

predict_proba(*X*, *method='linear'*)
Predict the probability of a sample being outlier. Two approaches are possible:

1. simply use Min-max conversion to linearly transform the outlier scores into the range of [0,1]. The model must be fitted first.

2. use unifying scores, see [BKKSZ11].

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **method** (*str, optional (default='linear')*) – probability conversion method. It must be one of 'linear' or 'unify'.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

set_params(***params*)

Set the parameters of this estimator. The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Returns **self**

Return type object

pyod.models.hbos module

Histogram-based Outlier Detection (HBOS)

class pyod.models.hbos.**HBOS**(*n_bins=10*, *alpha=0.1*, *tol=0.5*, *contamination=0.1*)

Bases: *pyod.models.base.BaseDetector*

Histogram- based outlier detection (HBOS) is an efficient unsupervised method. It assumes the feature independence and calculates the degree of outlyingness by building histograms. See [BGD12] for details.

Parameters

- **n_bins** (*int, optional (default=10)*) – The number of bins.
- **alpha** (*float in (0, 1), optional (default=0.1)*) – The regularizer for preventing overflow.
- **tol** (*float in (0, 1), optional (default=0.1)*) – The parameter to decide the flexibility while dealing the samples falling outside the bins.
- **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set. Used when fitting to define the threshold on the decision function.

bin_edges_

The edges of the bins.

Type numpy array of shape (n_bins + 1, n_features)

hist_

The density of each histogram.

Type numpy array of shape (n_bins, n_features)

decision_scores_
The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores. This value is available once the detector is fitted.

Type numpy array of shape (n_samples,)

threshold_
The threshold is based on `contamination`. It is the `n_samples * contamination` most abnormal samples in `decision_scores_`. The threshold is calculated for generating binary outlier labels.

Type float

labels_
The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies. It is generated by applying `threshold_` on `decision_scores_`.

Type int, either 0 or 1

decision_function(*X*)
Predict raw anomaly score of X using the fitted detector.

The anomaly score of an input sample is computed based on different detector algorithms. For consistency, outliers are assigned with larger anomaly scores.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The training input samples. Sparse matrices are accepted only if they are supported by the base estimator.

Returns **anomaly_scores** – The anomaly score of the input samples.

Return type numpy array of shape (n_samples,)

fit(*X*, *y=None*)
Fit detector. y is optional for unsupervised methods.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **y** (*numpy array of shape (n_samples,), optional (default=None)*) – The ground truth of the input samples (labels).

fit_predict(*X*, *y=None*)
DEPRECATED

Fit detector first and then predict whether a particular sample is an outlier or not.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

outlier_labels [numpy array of shape (n_samples,)] For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Deprecated since version 0.6.9: *fit_predict* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency.

fit_predict_score(*X*, *y*, *scoring='roc_auc_score'*)
DEPRECATED

Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

scoring [str, optional (default='roc_auc_score')] Evaluation metric:

- 'roc_auc_score': ROC score
- 'prc_n_score': Precision @ rank n score

score : float

Deprecated since version 0.6.9: *fit_predict_score* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency. Scoring could be done by calling an evaluation method, e.g., AUC ROC.

get_params(*deep=True*)

Get parameters for this estimator.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Parameters **deep** (*boolean, optional*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns **params** – Parameter names mapped to their values.

Return type mapping of string to any

predict(*X*)

Predict if a particular sample is an outlier or not.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Return type numpy array of shape (n_samples,)

predict_proba(*X*, *method='linear'*)

Predict the probability of a sample being outlier. Two approaches are possible:

1. simply use Min-max conversion to linearly transform the outlier scores into the range of [0,1]. The model must be fitted first.
2. use unifying scores, see [BKKSZ11].

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **method** (*str, optional (default='linear')*) – probability conversion method. It must be one of 'linear' or 'unify'.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

set_params(***params*)

Set the parameters of this estimator. The method works on simple estimators as well as on nested objects

(such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Returns self

Return type object

pyod.models.iforest module

IsolationForest Outlier Detector. Implemented on scikit-learn library.

class pyod.models.iforest.**IForest**(*n_estimators=100*, *max_samples='auto'*, *contamination=0.1*, *max_features=1.0*, *bootstrap=False*, *n_jobs=1*, *behaviour='old'*, *random_state=None*, *verbose=0*)

Bases: *pyod.models.base.BaseDetector*

Wrapper of scikit-learn Isolation Forest with more functionalities.

The IsolationForest 'isolates' observations by randomly selecting a feature and then randomly selecting a split value between the maximum and minimum values of the selected feature. See [BLTZ08][BLTZ12] for details.

Since recursive partitioning can be represented by a tree structure, the number of splittings required to isolate a sample is equivalent to the path length from the root node to the terminating node.

This path length, averaged over a forest of such random trees, is a measure of normality and our decision function.

Random partitioning produces noticeably shorter paths for anomalies. Hence, when a forest of random trees collectively produce shorter path lengths for particular samples, they are highly likely to be anomalies.

Parameters

- **n_estimators** (*int, optional (default=100)*) – The number of base estimators in the ensemble.
- **max_samples** (*int or float, optional (default="auto")*) – The number of samples to draw from X to train each base estimator.
  - If int, then draw *max_samples* samples.
  - If float, then draw *max_samples * X.shape[0]* samples.
  - If "auto", then *max_samples=min(256, n_samples)*.

  If max_samples is larger than the number of samples provided, all samples will be used for all trees (no sampling).
- **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set. Used when fitting to define the threshold on the decision function.
- **max_features** (*int or float, optional (default=1.0)*) – The number of features to draw from X to train each base estimator.
  - If int, then draw *max_features* features.
  - If float, then draw *max_features * X.shape[1]* features.
- **bootstrap** (*boolean, optional (default=False)*) – If True, individual trees are fit on random subsets of the training data sampled with replacement. If False, sampling without replacement is performed.

- **n_jobs** (*integer, optional (default=1)*) – The number of jobs to run in parallel for both *fit* and *predict*. If -1, then the number of jobs is set to the number of cores.
- **behaviour** (*str, default='old'*) – Behaviour of the `decision_function` which can be either 'old' or 'new'. Passing `behaviour='new'` makes the `decision_function` change to match other anomaly detection algorithm API which will be the default behaviour in the future. As explained in details in the `offset_` attribute documentation, the `decision_function` becomes dependent on the contamination parameter, in such a way that 0 becomes its natural threshold to detect outliers.

  New in version 0.7.0: `behaviour` is added in 0.7.0 for back-compatibility purpose.

  Deprecated since version 0.20: `behaviour='old'` is deprecated in sklearn 0.20 and will not be possible in 0.22.

  Deprecated since version 0.22: `behaviour` parameter will be deprecated in sklearn 0.22 and removed in 0.24.

  Warning: Only applicable for sklearn 0.20 above.

- **random_state** (*int, RandomState instance or None, optional (default=None)*) – If int, random_state is the seed used by the random number generator; If RandomState instance, random_state is the random number generator; If None, the random number generator is the RandomState instance used by *np.random*.
- **verbose** (*int, optional (default=0)*) – Controls the verbosity of the tree building process.

estimators_
The collection of fitted sub-estimators.

Type list of DecisionTreeClassifier

estimators_samples_
The subset of drawn samples (i.e., the in-bag samples) for each base estimator.

Type list of arrays

max_samples_
The actual number of samples

Type integer

decision_scores_
The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores. This value is available once the detector is fitted.

Type numpy array of shape (n_samples,)

threshold_
The threshold is based on `contamination`. It is the `n_samples * contamination` most abnormal samples in `decision_scores_`. The threshold is calculated for generating binary outlier labels.

Type float

labels_
The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies. It is generated by applying `threshold_` on `decision_scores_`.

Type int, either 0 or 1

decision_function(*X*)
Predict raw anomaly score of X using the fitted detector.

The anomaly score of an input sample is computed based on different detector algorithms. For consistency, outliers are assigned with larger anomaly scores.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The training input samples. Sparse matrices are accepted only if they are supported by the base estimator.

Returns **anomaly_scores** – The anomaly score of the input samples.

Return type numpy array of shape (n_samples,)

fit(*X*, *y=None*)
Fit detector. y is optional for unsupervised methods.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **y** (*numpy array of shape (n_samples,), optional (default=None)*) – The ground truth of the input samples (labels).

fit_predict(*X*, *y=None*)
DEPRECATED

Fit detector first and then predict whether a particular sample is an outlier or not.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

outlier_labels [numpy array of shape (n_samples,)] For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Deprecated since version 0.6.9: *fit_predict* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency.

fit_predict_score(*X*, *y*, *scoring='roc_auc_score'*)
DEPRECATED

Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

scoring [str, optional (default='roc_auc_score')] Evaluation metric:

- 'roc_auc_score': ROC score
- 'prc_n_score': Precision @ rank n score

score : float

Deprecated since version 0.6.9: *fit_predict_score* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency. Scoring could be done by calling an evaluation method, e.g., AUC ROC.

get_params(*deep=True*)
Get parameters for this estimator.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Parameters **deep** (*boolean, optional*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns **params** – Parameter names mapped to their values.

Return type mapping of string to any

predict(*X*)
Predict if a particular sample is an outlier or not.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Return type numpy array of shape (n_samples,)

predict_proba(*X*, *method='linear'*)
Predict the probability of a sample being outlier. Two approaches are possible:

1. simply use Min-max conversion to linearly transform the outlier scores into the range of [0,1]. The model must be fitted first.
2. use unifying scores, see [BKKSZ11].

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **method** (*str, optional (default='linear')*) – probability conversion method. It must be one of 'linear' or 'unify'.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

set_params(***params*)
Set the parameters of this estimator. The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Returns **self**

Return type object

pyod.models.knn module

k-Nearest Neighbors Detector (kNN)

class pyod.models.knn.**KNN**(*contamination=0.1*, *n_neighbors=5*, *method='largest'*, *radius=1.0*, *algorithm='auto'*, *leaf_size=30*, *metric='minkowski'*, *p=2*, *metric_params=None*, *n_jobs=1*, ***kwargs*)

Bases: *pyod.models.base.BaseDetector*

kNN class for outlier detection. For an observation, its distance to its kth nearest neighbor could be viewed as the outlying score. It could be viewed as a way to measure the density. See [BRRS00][BAP02] for details.

Three kNN detectors are supported: largest: use the distance to the kth neighbor as the outlier score mean: use the average of all k neighbors as the outlier score median: use the median of the distance to k neighbors as the outlier score

Parameters

- **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set. Used when fitting to define the threshold on the decision function.
- **n_neighbors** (*int, optional (default = 5)*) – Number of neighbors to use by default for k neighbors queries.
- **method** (*str, optional (default='largest')*) – {'largest', 'mean', 'median'}
  - 'largest': use the distance to the kth neighbor as the outlier score
  - 'mean': use the average of all k neighbors as the outlier score
  - 'median': use the median of the distance to k neighbors as the outlier score
- **radius** (*float, optional (default = 1.0)*) – Range of parameter space to use by default for *radius_neighbors* queries.
- **algorithm** (*{'auto', 'ball_tree', 'kd_tree', 'brute'}, optional*) – Algorithm used to compute the nearest neighbors:
  - 'ball_tree' will use BallTree
  - 'kd_tree' will use KDTree
  - 'brute' will use a brute-force search.
  - 'auto' will attempt to decide the most appropriate algorithm based on the values passed to *fit()* method.

  Note: fitting on sparse input will override the setting of this parameter, using brute force.
- **leaf_size** (*int, optional (default = 30)*) – Leaf size passed to BallTree or KDTree. This can affect the speed of the construction and query, as well as the memory required to store the tree. The optimal value depends on the nature of the problem.
- **metric** (*string or callable, default 'minkowski'*) – metric to use for distance computation. Any metric from scikit-learn or scipy.spatial.distance can be used.

  If metric is a callable function, it is called on each pair of instances (rows) and the resulting value recorded. The callable should take two arrays as input and return one value indicating the distance between them. This works for Scipy's metrics, but is less efficient than passing the metric name as a string.

  Distance matrices are not supported.

  Valid values for metric are:
  - from scikit-learn: ['cityblock', 'cosine', 'euclidean', 'l1', 'l2', 'manhattan']

– from scipy.spatial.distance: ['braycurtis', 'canberra', 'chebyshev', 'correlation', 'dice', 'hamming', 'jaccard', 'kulsinski', 'mahalanobis', 'matching', 'minkowski', 'rogerstanimoto', 'russellrao', 'seuclidean', 'sokalmichener', 'sokalsneath', 'sqeuclidean', 'yule']

See the documentation for scipy.spatial.distance for details on these metrics.

- **p** (*integer, optional (default = 2)*) – Parameter for the Minkowski metric from sklearn.metrics.pairwise.pairwise_distances. When p = 1, this is equivalent to using manhattan_distance (l1), and euclidean_distance (l2) for p = 2. For arbitrary p, minkowski_distance (l_p) is used. See http://scikit-learn.org/stable/modules/generated/sklearn.metrics.pairwise.pairwise_distances
- **metric_params** (*dict, optional (default = None)*) – Additional keyword arguments for the metric function.
- **n_jobs** (*int, optional (default = 1)*) – The number of parallel jobs to run for neighbors search. If -1, then the number of jobs is set to the number of CPU cores. Affects only kneighbors and kneighbors_graph methods.

decision_scores_
The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores. This value is available once the detector is fitted.

Type numpy array of shape (n_samples,)

threshold_
The threshold is based on `contamination`. It is the `n_samples * contamination` most abnormal samples in `decision_scores_`. The threshold is calculated for generating binary outlier labels.

Type float

labels_
The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies. It is generated by applying `threshold_` on `decision_scores_`.

Type int, either 0 or 1

decision_function(*X*)
Predict raw anomaly score of X using the fitted detector.

The anomaly score of an input sample is computed based on different detector algorithms. For consistency, outliers are assigned with larger anomaly scores.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The training input samples. Sparse matrices are accepted only if they are supported by the base estimator.

Returns **anomaly_scores** – The anomaly score of the input samples.

Return type numpy array of shape (n_samples,)

fit(*X*, *y=None*)
Fit detector. y is optional for unsupervised methods.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **y** (*numpy array of shape (n_samples,), optional (default=None)*) – The ground truth of the input samples (labels).

fit_predict(*X*, *y=None*)
DEPRECATED

Fit detector first and then predict whether a particular sample is an outlier or not.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

outlier_labels [numpy array of shape (n_samples,)] For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Deprecated since version 0.6.9: *fit_predict* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency.

fit_predict_score(*X*, *y*, *scoring='roc_auc_score'*)
DEPRECATED

Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

scoring [str, optional (default='roc_auc_score')] Evaluation metric:

- 'roc_auc_score': ROC score
- 'prc_n_score': Precision @ rank n score

score : float

Deprecated since version 0.6.9: *fit_predict_score* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency. Scoring could be done by calling an evaluation method, e.g., AUC ROC.

get_params(*deep=True*)
Get parameters for this estimator.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Parameters **deep** (*boolean, optional*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns **params** – Parameter names mapped to their values.

Return type mapping of string to any

predict(*X*)
Predict if a particular sample is an outlier or not.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Return type numpy array of shape (n_samples,)

predict_proba(*X*, *method='linear'*)
Predict the probability of a sample being outlier. Two approaches are possible:

1. simply use Min-max conversion to linearly transform the outlier scores into the range of [0,1]. The model must be fitted first.

2. use unifying scores, see [BKKSZ11].

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **method** (*str, optional (default='linear')*) – probability conversion method. It must be one of 'linear' or 'unify'.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

set_params(***params*)

Set the parameters of this estimator. The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Returns **self**

Return type object

pyod.models.lof module

Local Outlier Factor (LOF). Implemented on scikit-learn library.

class pyod.models.lof.**LOF**(*n_neighbors=20*, *algorithm='auto'*, *leaf_size=30*, *metric='minkowski'*, *p=2*, *metric_params=None*, *contamination=0.1*, *n_jobs=1*)

Bases: *pyod.models.base.BaseDetector*

Wrapper of scikit-learn LOF Class with more functionalities. Unsupervised Outlier Detection using Local Outlier Factor (LOF).

The anomaly score of each sample is called Local Outlier Factor. It measures the local deviation of density of a given sample with respect to its neighbors. It is local in that the anomaly score depends on how isolated the object is with respect to the surrounding neighborhood. More precisely, locality is given by k-nearest neighbors, whose distance is used to estimate the local density. By comparing the local density of a sample to the local densities of its neighbors, one can identify samples that have a substantially lower density than their neighbors. These are considered outliers. See [BBKNS00] for details.

Parameters

- **n_neighbors** (*int, optional (default=20)*) – Number of neighbors to use by default for *kneighbors* queries. If n_neighbors is larger than the number of samples provided, all samples will be used.
- **algorithm** (*{'auto', 'ball_tree', 'kd_tree', 'brute'}, optional*) – Algorithm used to compute the nearest neighbors:
  - 'ball_tree' will use BallTree
  - 'kd_tree' will use KDTree
  - 'brute' will use a brute-force search.
  - 'auto' will attempt to decide the most appropriate algorithm based on the values passed to *fit()* method.

Note: fitting on sparse input will override the setting of this parameter, using brute force.

- **leaf_size** (*int, optional (default=30)*) – Leaf size passed to *BallTree* or *KDTree*. This can affect the speed of the construction and query, as well as the memory required to store the tree. The optimal value depends on the nature of the problem.
- **metric** (*string or callable, default 'minkowski'*) – metric used for the distance computation. Any metric from scikit-learn or scipy.spatial.distance can be used.

  If 'precomputed', the training input X is expected to be a distance matrix.

  If metric is a callable function, it is called on each pair of instances (rows) and the resulting value recorded. The callable should take two arrays as input and return one value indicating the distance between them. This works for Scipy's metrics, but is less efficient than passing the metric name as a string.

  Valid values for metric are:

  – from scikit-learn: ['cityblock', 'cosine', 'euclidean', 'l1', 'l2', 'manhattan']

  – from scipy.spatial.distance: ['braycurtis', 'canberra', 'chebyshev', 'correlation', 'dice', 'hamming', 'jaccard', 'kulsinski', 'mahalanobis', 'matching', 'minkowski', 'rogerstanimoto', 'russellrao', 'seuclidean', 'sokalmichener', 'sokalsneath', 'sqeuclidean', 'yule']

  See the documentation for scipy.spatial.distance for details on these metrics: http://docs.scipy.org/doc/scipy/reference/spatial.distance.html
- **p** (*integer, optional (default = 2)*) – Parameter for the Minkowski metric from sklearn.metrics.pairwise.pairwise_distances. When p = 1, this is equivalent to using manhattan_distance (l1), and euclidean_distance (l2) for p = 2. For arbitrary p, minkowski_distance (l_p) is used. See http://scikit-learn.org/stable/modules/generated/sklearn.metrics.pairwise.pairwise_distances
- **metric_params** (*dict, optional (default = None)*) – Additional keyword arguments for the metric function.
- **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set. When fitting this is used to define the threshold on the decision function.
- **n_jobs** (*int, optional (default = 1)*) – The number of parallel jobs to run for neighbors search. If `-1`, then the number of jobs is set to the number of CPU cores. Affects only kneighbors and kneighbors_graph methods.

n_neighbors_
The actual number of neighbors used for *kneighbors* queries.

Type int

decision_scores_
The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores. This value is available once the detector is fitted.

Type numpy array of shape (n_samples,)

threshold_
The threshold is based on `contamination`. It is the `n_samples * contamination` most abnormal samples in `decision_scores_`. The threshold is calculated for generating binary outlier labels.

Type float

labels_
The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies. It is generated by applying `threshold_` on `decision_scores_`.

Type int, either 0 or 1

decision_function(*X*)
Predict raw anomaly score of X using the fitted detector.

The anomaly score of an input sample is computed based on different detector algorithms. For consistency, outliers are assigned with larger anomaly scores.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The training input samples. Sparse matrices are accepted only if they are supported by the base estimator.

Returns **anomaly_scores** – The anomaly score of the input samples.

Return type numpy array of shape (n_samples,)

fit(*X*, *y=None*)
Fit detector. y is optional for unsupervised methods.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **y** (*numpy array of shape (n_samples,), optional (default=None)*) – The ground truth of the input samples (labels).

fit_predict(*X*, *y=None*)
DEPRECATED

Fit detector first and then predict whether a particular sample is an outlier or not.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

outlier_labels [numpy array of shape (n_samples,)] For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Deprecated since version 0.6.9: *fit_predict* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency.

fit_predict_score(*X*, *y*, *scoring='roc_auc_score'*)
DEPRECATED

Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

scoring [str, optional (default='roc_auc_score')] Evaluation metric:

- 'roc_auc_score': ROC score
- 'prc_n_score': Precision @ rank n score

score : float

Deprecated since version 0.6.9: *fit_predict_score* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency. Scoring could be done by calling an evaluation method, e.g., AUC ROC.

get_params(*deep=True*)
Get parameters for this estimator.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Parameters **deep** (*boolean, optional*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns **params** – Parameter names mapped to their values.

Return type mapping of string to any

predict(*X*)
Predict if a particular sample is an outlier or not.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Return type numpy array of shape (n_samples,)

predict_proba(*X*, *method='linear'*)
Predict the probability of a sample being outlier. Two approaches are possible:

1. simply use Min-max conversion to linearly transform the outlier scores into the range of [0,1]. The model must be fitted first.
2. use unifying scores, see [BKKSZ11].

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **method** (*str, optional (default='linear')*) – probability conversion method. It must be one of 'linear' or 'unify'.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

set_params(***params*)
Set the parameters of this estimator. The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Returns **self**

Return type object

pyod.models.loci module

Local Correlation Integral (LOCI). Part of the codes are adapted from https://github.com/Cloudy10/loci

class pyod.models.loci.**LOCI**(*contamination=0.1*, *alpha=0.5*, *k=3*)

Bases: *pyod.models.base.BaseDetector*

Local Correlation Integral.

LOCI is highly effective for detecting outliers and groups of outliers (a.k.a.micro-clusters), which offers the following advantages and novelties: (a) It provides an automatic, data-dictated cut-off to determine whether a point is an outlier—in contrast, previous methods force users to pick cut-offs, without any hints as to what cut-off value is best for a given dataset. (b) It can provide a LOCI plot for each point; this plot summarizes a wealth of information about the data in the vicinity of the point, determining clusters, micro-clusters, their diameters and their inter-cluster distances. None of the existing outlier-detection methods can match this feature, because they output only a single number for each point: its outlierness score.(c) It can be computed as quickly as the best previous methods Read more in the [BPKGF03].

Parameters

- **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set. Used when fitting to define the threshold on the decision function.
- **alpha** (*int, default = 0.5*) – The neighbourhood parameter measures how large of a neighbourhood should be considered "local".
- **k** (*int, default = 3*) – An outlier cutoff threshold for determine whether or not a point should be considered an outlier.

decision_scores_

The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores. This value is available once the detector is fitted.

Type numpy array of shape (n_samples,)

threshold_

The threshold is based on `contamination`. It is the `n_samples * contamination` most abnormal samples in `decision_scores_`. The threshold is calculated for generating binary outlier labels.

Type float

labels_

The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies. It is generated by applying `threshold_` on `decision_scores_`.

Type int, either 0 or 1

Examples

```
>>> from pyod.models.loci import LOCI
>>> from pyod.utils.data import generate_data
>>> n_train = 50
>>> n_test = 50
>>> contamination = 0.1
>>> X_train, y_train, X_test, y_test = generate_data(
...     n_train=n_train, n_test=n_test,
...     contamination=contamination, random_state=42)
>>> clf = LOCI()
```

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```
>>> clf.fit(X_train)
LOCI(alpha=0.5, contamination=0.1, k=None)
```

decision_function(*X*)
Predict raw anomaly scores of X using the fitted detector.

The anomaly score of an input sample is computed based on the fitted detector. For consistency, outliers are assigned with higher anomaly scores.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples. Sparse matrices are accepted only if they are supported by the base estimator.

Returns **anomaly_scores** – The anomaly score of the input samples.

Return type numpy array of shape (n_samples,)

fit(*X*, *y=None*)
Fit the model using X as training data.

Parameters **X** (*array, shape (n_samples, n_features)*) – Training data.

Returns **self**

Return type object

fit_predict(*X*, *y=None*)
DEPRECATED

Fit detector first and then predict whether a particular sample is an outlier or not.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

outlier_labels [numpy array of shape (n_samples,)] For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Deprecated since version 0.6.9: *fit_predict* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency.

fit_predict_score(*X*, *y*, *scoring='roc_auc_score'*)
DEPRECATED

Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

scoring [str, optional (default='roc_auc_score')] Evaluation metric:

- 'roc_auc_score': ROC score
- 'prc_n_score': Precision @ rank n score

score : float

Deprecated since version 0.6.9: *fit_predict_score* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency. Scoring could be done by calling an evaluation method, e.g., AUC ROC.

get_params(*deep=True*)
Get parameters for this estimator.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Parameters **deep** (*boolean, optional*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns **params** – Parameter names mapped to their values.

Return type mapping of string to any

predict(*X*)
Predict if a particular sample is an outlier or not.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Return type numpy array of shape (n_samples,)

predict_proba(*X*, *method='linear'*)
Predict the probability of a sample being outlier. Two approaches are possible:

1. simply use Min-max conversion to linearly transform the outlier scores into the range of [0,1]. The model must be fitted first.
2. use unifying scores, see [BKKSZ11].

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **method** (*str, optional (default='linear')*) – probability conversion method. It must be one of 'linear' or 'unify'.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

set_params(***params*)
Set the parameters of this estimator. The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Returns **self**

Return type object

pyod.models.lscp module

Locally Selective Combination of Parallel Outlier Ensembles (LSCP). Adapted from the original implementation.

class pyod.models.lscp.**LSCP**(*detector_list*, *local_region_size=30*, *local_max_features=1.0*, *n_bins=10*, *random_state=None*, *contamination=0.1*)

Bases: *pyod.models.base.BaseDetector*

Locally Selection Combination in Parallel Outlier Ensembles

LSCP is an unsupervised parallel outlier detection ensemble which selects competent detectors in the local region of a test instance. This implementation uses an Average of Maximum strategy. First, a heterogeneous list of base detectors is fit to the training data and then generates a pseudo ground truth for each train instance is generated by taking the maximum outlier score.

For each test instance: 1) The local region is defined to be the set of nearest training points in randomly sampled feature subspaces which occur more frequently than a defined threshold over multiple iterations.

2) Using the local region, a local pseudo ground truth is defined and the pearson correlation is calculated between each base detector's training outlier scores and the pseudo ground truth.

3) A histogram is built out of pearson correlation scores; detectors in the largest bin are selected as competent base detectors for the given test instance.

4) The average outlier score of the selected competent detectors is taken to be the final score.

See [BZNHL19] for details.

Parameters

- **detector_list** (*list, length must be greater than 1*) – Base unsupervised outlier detectors from PyOD. (Note: requires fit and decision_function methods)
- **local_region_size** (*int, optional (default=30)*) – Number of training points to consider in each iteration of the local region generation process (30 by default).
- **local_max_features** (*float in (0.5, 1.), optional (default=1.0)*) – Maximum proportion of number of features to consider when defining the local region (1.0 by default).
- **n_bins** (*int, optional (default=10)*) – Number of bins to use when selecting the local region
- **random_state** (*RandomState, optional (default=None)*) – A random number generator instance to define the state of the random permutations generator.
- **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set. Used when fitting to define the threshold on the decision function (0.1 by default).

decision_scores_
The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores. This value is available once the detector is fitted.

Type numpy array of shape (n_samples,)

threshold_
The threshold is based on `contamination`. It is the `n_samples * contamination` most abnormal samples in `decision_scores_`. The threshold is calculated for generating binary outlier labels.

Type float

labels_
The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies. It is generated by applying `threshold_` on `decision_scores_`.

Type int, either 0 or 1

Examples

```
>>> from pyod.utils.data import generate_data
>>> from pyod.utils.utility import standardizer
>>> from pyod.models.lscp import LSCP
>>> from pyod.models.lof import LOF
>>> X_train, y_train, X_test, y_test = generate_data(
...     n_train=50, n_test=50,
...     contamination=0.1, random_state=42)
>>> X_train, X_test = standardizer(X_train, X_test)
>>> detector_list = [LOF(), LOF()]
>>> clf = LSCP(detector_list)
>>> clf.fit(X_train)
LSCP(...)
```

decision_function(*X*)
Predict raw anomaly score of X using the fitted detector.

The anomaly score of an input sample is computed based on different detector algorithms. For consistency, outliers are assigned with larger anomaly scores.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The training input samples. Sparse matrices are accepted only if they are supported by the base estimator.

Returns **anomaly_scores** – The anomaly score of the input samples.

Return type numpy array of shape (n_samples,)

fit(*X*, *y=None*)
Fit detector. y is optional for unsupervised methods.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **y** (*numpy array of shape (n_samples,), optional (default=None)*) – The ground truth of the input samples (labels).

fit_predict(*X*, *y=None*)
DEPRECATED

Fit detector first and then predict whether a particular sample is an outlier or not.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

outlier_labels [numpy array of shape (n_samples,)] For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Deprecated since version 0.6.9: *fit_predict* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency.

fit_predict_score(*X*, *y*, *scoring='roc_auc_score'*)
DEPRECATED

Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

scoring [str, optional (default='roc_auc_score')] Evaluation metric:

- 'roc_auc_score': ROC score
- 'prc_n_score': Precision @ rank n score

score : float

Deprecated since version 0.6.9: *fit_predict_score* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency. Scoring could be done by calling an evaluation method, e.g., AUC ROC.

get_params(*deep=True*)

Get parameters for this estimator.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Parameters **deep** (*boolean, optional*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns **params** – Parameter names mapped to their values.

Return type mapping of string to any

predict(*X*)

Predict if a particular sample is an outlier or not.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Return type numpy array of shape (n_samples,)

predict_proba(*X*, *method='linear'*)

Predict the probability of a sample being outlier. Two approaches are possible:

1. simply use Min-max conversion to linearly transform the outlier scores into the range of [0,1]. The model must be fitted first.
2. use unifying scores, see [BKKSZ11].

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **method** (*str, optional (default='linear')*) – probability conversion method. It must be one of 'linear' or 'unify'.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

set_params(***params*)

Set the parameters of this estimator. The method works on simple estimators as well as on nested objects

(such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Returns self

Return type object

pyod.models.mcd module

Outlier Detection with Minimum Covariance Determinant (MCD)

class pyod.models.mcd.**MCD**(*contamination=0.1*, *store_precision=True*, *assume_centered=False*, *support_fraction=None*, *random_state=None*)

Bases: *pyod.models.base.BaseDetector*

Detecting outliers in a Gaussian distributed dataset using Minimum Covariance Determinant (MCD): robust estimator of covariance.

The Minimum Covariance Determinant covariance estimator is to be applied on Gaussian-distributed data, but could still be relevant on data drawn from a unimodal, symmetric distribution. It is not meant to be used with multi-modal data (the algorithm used to fit a MinCovDet object is likely to fail in such a case). One should consider projection pursuit methods to deal with multi-modal datasets.

First fit a minimum covariance determinant model and then compute the Mahalanobis distance as the outlier degree of the data

See [BRD99][BHR04] for details.

Parameters

- **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set. Used when fitting to define the threshold on the decision function.
- **store_precision** (*bool*) – Specify if the estimated precision is stored.
- **assume_centered** (*Boolean*) – If True, the support of the robust location and the covariance estimates is computed, and a covariance estimate is recomputed from it, without centering the data. Useful to work with data whose mean is significantly equal to zero but is not exactly zero. If False, the robust location and covariance are directly computed with the FastMCD algorithm without additional treatment.
- **support_fraction** (*float, 0 < support_fraction < 1*) – The proportion of points to be included in the support of the raw MCD estimate. Default is None, which implies that the minimum value of support_fraction will be used within the algorithm: [n_sample + n_features + 1] / 2
- **random_state** (*int, RandomState instance or None, optional (default=None)*) – If int, random_state is the seed used by the random number generator; If RandomState instance, random_state is the random number generator; If None, the random number generator is the RandomState instance used by *np.random*.

raw_location_
The raw robust estimated location before correction and re-weighting.

Type array-like, shape (n_features,)

raw_covariance_
The raw robust estimated covariance before correction and re-weighting.

Type array-like, shape (n_features, n_features)

raw_support_
A mask of the observations that have been used to compute the raw robust estimates of location and shape, before correction and re-weighting.

Type array-like, shape (n_samples,)

location_
Estimated robust location

Type array-like, shape (n_features,)

covariance_
Estimated robust covariance matrix

Type array-like, shape (n_features, n_features)

precision_
Estimated pseudo inverse matrix. (stored only if store_precision is True)

Type array-like, shape (n_features, n_features)

support_
A mask of the observations that have been used to compute the robust estimates of location and shape.

Type array-like, shape (n_samples,)

decision_scores_
The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores. This value is available once the detector is fitted. Mahalanobis distances of the training set (on which *:meth:'fit* is called) observations.

Type numpy array of shape (n_samples,)

threshold_
The threshold is based on `contamination`. It is the `n_samples * contamination` most abnormal samples in `decision_scores_`. The threshold is calculated for generating binary outlier labels.

Type float

labels_
The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies. It is generated by applying `threshold_` on `decision_scores_`.

Type int, either 0 or 1

decision_function(*X*)
Predict raw anomaly score of X using the fitted detector.

The anomaly score of an input sample is computed based on different detector algorithms. For consistency, outliers are assigned with larger anomaly scores.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The training input samples. Sparse matrices are accepted only if they are supported by the base estimator.

Returns **anomaly_scores** – The anomaly score of the input samples.

Return type numpy array of shape (n_samples,)

fit(*X*, *y=None*)
Fit detector. y is optional for unsupervised methods.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **y** (*numpy array of shape (n_samples,), optional (default=None)*) – The ground truth of the input samples (labels).

fit_predict(*X*, *y=None*)
DEPRECATED

Fit detector first and then predict whether a particular sample is an outlier or not.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

outlier_labels [numpy array of shape (n_samples,)] For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Deprecated since version 0.6.9: *fit_predict* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency.

fit_predict_score(*X*, *y*, *scoring='roc_auc_score'*)
DEPRECATED

Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

scoring [str, optional (default='roc_auc_score')] Evaluation metric:

- 'roc_auc_score': ROC score
- 'prc_n_score': Precision @ rank n score

score : float

Deprecated since version 0.6.9: *fit_predict_score* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency. Scoring could be done by calling an evaluation method, e.g., AUC ROC.

get_params(*deep=True*)
Get parameters for this estimator.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Parameters **deep** (*boolean, optional*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns **params** – Parameter names mapped to their values.

Return type mapping of string to any

predict(*X*)
Predict if a particular sample is an outlier or not.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Return type numpy array of shape (n_samples,)

predict_proba(*X*, *method='linear'*)

Predict the probability of a sample being outlier. Two approaches are possible:

1. simply use Min-max conversion to linearly transform the outlier scores into the range of [0,1]. The model must be fitted first.
2. use unifying scores, see [BKKSZ11].

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **method** (*str, optional (default='linear')*) – probability conversion method. It must be one of 'linear' or 'unify'.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

set_params(***params*)

Set the parameters of this estimator. The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Returns **self**

Return type object

pyod.models.mo_gaal module

Multiple-Objective Generative Adversarial Active Learning. Part of the codes are adapted from https://github.com/leibinghe/GAAL-based-outlier-detection

class pyod.models.mo_gaal.**MO_GAAL**(*k=10*, *stop_epochs=20*, *lr_d=0.01*, *lr_g=0.0001*, *decay=1e-06*, *momentum=0.9*, *contamination=0.1*)

Bases: *pyod.models.base.BaseDetector*

Multi-Objective Generative Adversarial Active Learning.

MO_GAAL directly generates informative potential outliers to assist the classifier in describing a boundary that can separate outliers from normal data effectively. Moreover, to prevent the generator from falling into the mode collapsing problem, the network structure of SO-GAAL is expanded from a single generator (SO-GAAL) to multiple generators with different objectives (MO-GAAL) to generate a reasonable reference distribution for the whole dataset. Read more in the [BLLZ+19].

Parameters

- **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set. Used when fitting to define the threshold on the decision function.
- **k** (*int, optional (default=10)*) – The number of sub generators.

- **stop_epochs** (*int, optional (default=20)*) – The number of epochs of training.
- **lr_d** (*float, optional (default=0.01)*) – The learn rate of the discriminator.
- **lr_g** (*float, optional (default=0.0001)*) – The learn rate of the generator.
- **decay** (*float, optional (default=1e-6)*) – The decay parameter for SGD.
- **momentum** (*float, optional (default=0.9)*) – The momentum parameter for SGD.

decision_scores_
The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores. This value is available once the detector is fitted.

Type numpy array of shape (n_samples,)

threshold_
The threshold is based on `contamination`. It is the `n_samples * contamination` most abnormal samples in `decision_scores_`. The threshold is calculated for generating binary outlier labels.

Type float

labels_
The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies. It is generated by applying `threshold_` on `decision_scores_`.

Type int, either 0 or 1

decision_function(*X*)
Predict raw anomaly score of X using the fitted detector.

The anomaly score of an input sample is computed based on different detector algorithms. For consistency, outliers are assigned with larger anomaly scores.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The training input samples. Sparse matrices are accepted only if they are supported by the base estimator.

Returns **anomaly_scores** – The anomaly score of the input samples.

Return type numpy array of shape (n_samples,)

fit(*X*, *y=None*)
Fit detector. y is optional for unsupervised methods.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **y** (*numpy array of shape (n_samples,), optional (default=None)*) – The ground truth of the input samples (labels).

fit_predict(*X*, *y=None*)
DEPRECATED

Fit detector first and then predict whether a particular sample is an outlier or not.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

outlier_labels [numpy array of shape (n_samples,)] For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Deprecated since version 0.6.9: *fit_predict* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency.

fit_predict_score(*X*, *y*, *scoring='roc_auc_score'*)
DEPRECATED

Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

scoring [str, optional (default='roc_auc_score')] Evaluation metric:

- 'roc_auc_score': ROC score
- 'prc_n_score': Precision @ rank n score

score : float

Deprecated since version 0.6.9: *fit_predict_score* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency. Scoring could be done by calling an evaluation method, e.g., AUC ROC.

get_params(*deep=True*)
Get parameters for this estimator.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Parameters **deep** (*boolean, optional*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns **params** – Parameter names mapped to their values.

Return type mapping of string to any

predict(*X*)
Predict if a particular sample is an outlier or not.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Return type numpy array of shape (n_samples,)

predict_proba(*X*, *method='linear'*)
Predict the probability of a sample being outlier. Two approaches are possible:

1. simply use Min-max conversion to linearly transform the outlier scores into the range of [0,1]. The model must be fitted first.
2. use unifying scores, see [BKKSZ11].

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

- **method** (*str, optional (default='linear')*) – probability conversion method. It must be one of 'linear' or 'unify'.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

set_params(***params*)

Set the parameters of this estimator. The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Returns **self**

Return type object

pyod.models.ocsvm module

One-class SVM detector. Implemented on scikit-learn library.

class pyod.models.ocsvm.**OCSVM**(*kernel='rbf'*, *degree=3*, *gamma='auto'*, *coef0=0.0*, *tol=0.001*, *nu=0.5*, *shrinking=True*, *cache_size=200*, *verbose=False*, *max_iter=-1*, *contamination=0.1*)

Bases: *pyod.models.base.BaseDetector*

Wrapper of scikit-learn one-class SVM Class with more functionalities. Unsupervised Outlier Detection.

Estimate the support of a high-dimensional distribution.

The implementation is based on libsvm. See http://scikit-learn.org/stable/modules/svm.html#svm-outlier-detection and [BScholkopfPST+01].

Parameters

- **kernel** (*string, optional (default='rbf')*) – Specifies the kernel type to be used in the algorithm. It must be one of 'linear', 'poly', 'rbf', 'sigmoid', 'precomputed' or a callable. If none is given, 'rbf' will be used. If a callable is given it is used to precompute the kernel matrix.
- **nu** (*float, optional*) – An upper bound on the fraction of training errors and a lower bound of the fraction of support vectors. Should be in the interval (0, 1]. By default 0.5 will be taken.
- **degree** (*int, optional (default=3)*) – Degree of the polynomial kernel function ('poly'). Ignored by all other kernels.
- **gamma** (*float, optional (default='auto')*) – Kernel coefficient for 'rbf', 'poly' and 'sigmoid'. If gamma is 'auto' then 1/n_features will be used instead.
- **coef0** (*float, optional (default=0.0)*) – Independent term in kernel function. It is only significant in 'poly' and 'sigmoid'.
- **tol** (*float, optional*) – Tolerance for stopping criterion.
- **shrinking** (*boolean, optional*) – Whether to use the shrinking heuristic.
- **cache_size** (*float, optional*) – Specify the size of the kernel cache (in MB).

- **verbose** (*bool, default: False*) – Enable verbose output. Note that this setting takes advantage of a per-process runtime setting in libsvm that, if enabled, may not work properly in a multithreaded context.
- **max_iter** (*int, optional (default=-1)*) – Hard limit on iterations within solver, or -1 for no limit.
- **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set. Used when fitting to define the threshold on the decision function.

support_
Indices of support vectors.

Type array-like, shape = [n_SV]

support_vectors_
Support vectors.

Type array-like, shape = [nSV, n_features]

dual_coef_
Coefficients of the support vectors in the decision function.

Type array, shape = [1, n_SV]

coef_
Weights assigned to the features (coefficients in the primal problem). This is only available in the case of a linear kernel.

*coef_* is readonly property derived from *dual_coef_* and *support_vectors_*

Type array, shape = [1, n_features]

intercept_
Constant in the decision function.

Type array, shape = [1,]

decision_scores_
The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores. This value is available once the detector is fitted.

Type numpy array of shape (n_samples,)

threshold_
The threshold is based on `contamination`. It is the `n_samples * contamination` most abnormal samples in `decision_scores_`. The threshold is calculated for generating binary outlier labels.

Type float

labels_
The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies. It is generated by applying `threshold_` on `decision_scores_`.

Type int, either 0 or 1

decision_function(*X*)
Predict raw anomaly score of X using the fitted detector.

The anomaly score of an input sample is computed based on different detector algorithms. For consistency, outliers are assigned with larger anomaly scores.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The training input samples. Sparse matrices are accepted only if they are supported by the base estimator.

Returns **anomaly_scores** – The anomaly score of the input samples.

Return type numpy array of shape (n_samples,)

fit (*X*, *y=None*, *sample_weight=None*, ***params*)
Fit detector. y is optional for unsupervised methods.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **y** (*numpy array of shape (n_samples,), optional (default=None)*) – The ground truth of the input samples (labels).

fit_predict (*X*, *y=None*)
DEPRECATED

Fit detector first and then predict whether a particular sample is an outlier or not.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

outlier_labels [numpy array of shape (n_samples,)] For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Deprecated since version 0.6.9: *fit_predict* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency.

fit_predict_score (*X*, *y*, *scoring='roc_auc_score'*)
DEPRECATED

Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

scoring [str, optional (default='roc_auc_score')] Evaluation metric:

- 'roc_auc_score': ROC score
- 'prc_n_score': Precision @ rank n score

score : float

Deprecated since version 0.6.9: *fit_predict_score* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency. Scoring could be done by calling an evaluation method, e.g., AUC ROC.

get_params (*deep=True*)
Get parameters for this estimator.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Parameters **deep** (*boolean, optional*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns **params** – Parameter names mapped to their values.

Return type mapping of string to any

predict(*X*)

Predict if a particular sample is an outlier or not.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Return type numpy array of shape (n_samples,)

predict_proba(*X*, *method='linear'*)

Predict the probability of a sample being outlier. Two approaches are possible:

1. simply use Min-max conversion to linearly transform the outlier scores into the range of [0,1]. The model must be fitted first.
2. use unifying scores, see [BKKSZ11].

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **method** (*str, optional (default='linear')*) – probability conversion method. It must be one of 'linear' or 'unify'.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

set_params(***params*)

Set the parameters of this estimator. The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Returns **self**

Return type object

pyod.models.pca module

Principal Component Analysis (PCA) Outlier Detector

class pyod.models.pca.**PCA**(*n_components=None*, *n_selected_components=None*, *contamination=0.1*, *copy=True*, *whiten=False*, *svd_solver='auto'*, *tol=0.0*, *iterated_power='auto'*, *random_state=None*, *weighted=True*, *standardization=True*)

Bases: *pyod.models.base.BaseDetector*

Principal component analysis (PCA) can be used in detecting outliers. PCA is a linear dimensionality reduction using Singular Value Decomposition of the data to project it to a lower dimensional space.

In this procedure, covariance matrix of the data can be decomposed to orthogonal vectors, called eigenvectors, associated with eigenvalues. The eigenvectors with high eigenvalues capture most of the variance in the data.

Therefore, a low dimensional hyperplane constructed by k eigenvectors can capture most of the variance in the data. However, outliers are different from normal data points, which is more obvious on the hyperplane constructed by the eigenvectors with small eigenvalues.

Therefore, outlier scores can be obtained as the sum of the projected distance of a sample on all eigenvectors. See [BSCSC03][BAgg15] for details.

Score(X) = Sum of weighted euclidean distance between each sample to the hyperplane constructed by the selected eigenvectors

Parameters

- **n_components** (*int, float, None or string*) – Number of components to keep. if n_components is not set all components are kept:

```
n_components == min(n_samples, n_features)
```

  if n_components == 'mle' and svd_solver == 'full', Minka's MLE is used to guess the dimension if `0 < n_components < 1` and svd_solver == 'full', select the number of components such that the amount of variance that needs to be explained is greater than the percentage specified by n_components n_components cannot be equal to n_features for svd_solver == 'arpack'.

- **n_selected_components** (*int, optional (default=None)*) – Number of selected principal components for calculating the outlier scores. It is not necessarily equal to the total number of the principal components. If not set, use all principal components.

- **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set. Used when fitting to define the threshold on the decision function.

- **copy** (*bool (default True)*) – If False, data passed to fit are overwritten and running fit(X).transform(X) will not yield the expected results, use fit_transform(X) instead.

- **whiten** (*bool, optional (default False)*) – When True (False by default) the *components_* vectors are multiplied by the square root of n_samples and then divided by the singular values to ensure uncorrelated outputs with unit component-wise variances.

  Whitening will remove some information from the transformed signal (the relative variance scales of the components) but can sometime improve the predictive accuracy of the downstream estimators by making their data respect some hard-wired assumptions.

- **svd_solver** (*string {'auto', 'full', 'arpack', 'randomized'}*) –

  auto : the solver is selected by a default policy based on *X.shape* and *n_components*: if the input data is larger than 500x500 and the number of components to extract is lower than 80% of the smallest dimension of the data, then the more efficient 'randomized' method is enabled. Otherwise the exact full SVD is computed and optionally truncated afterwards.

  full : run exact full SVD calling the standard LAPACK solver via *scipy.linalg.svd* and select the components by postprocessing

  arpack : run SVD truncated to n_components calling ARPACK solver via *scipy.sparse.linalg.svds*. It requires strictly 0 < n_components < X.shape[1]

  randomized : run randomized SVD by the method of Halko et al.

- **tol** (*float >= 0, optional (default .0)*) – Tolerance for singular values computed by svd_solver == 'arpack'.
- **iterated_power** (*int >= 0, or 'auto', (default 'auto')*) – Number of iterations for the power method computed by svd_solver == 'randomized'.
- **random_state** (*int, RandomState instance or None, optional (default None)*) – If int, random_state is the seed used by the random number generator; If RandomState instance, random_state is the random number generator; If None, the random number generator is the RandomState instance used by *np.random*. Used when `svd_solver` == 'arpack' or 'randomized'.
- **weighted** (*bool, optional (default=True)*) – If True, the eigenvalues are used in score computation. The eigenvectors with small eigenvalues comes with more importance in outlier score calculation.
- **standardization** (*bool, optional (default=True)*) – If True, perform standardization first to convert data to zero mean and unit variance. See http://scikit-learn.org/stable/auto_examples/preprocessing/plot_scaling_importance.html

components_
Principal axes in feature space, representing the directions of maximum variance in the data. The components are sorted by `explained_variance_`.

Type array, shape (n_components, n_features)

explained_variance_
The amount of variance explained by each of the selected components.

Equal to n_components largest eigenvalues of the covariance matrix of X.

Type array, shape (n_components,)

explained_variance_ratio_
Percentage of variance explained by each of the selected components.

If `n_components` is not set then all components are stored and the sum of explained variances is equal to 1.0.

Type array, shape (n_components,)

singular_values_
The singular values corresponding to each of the selected components. The singular values are equal to the 2-norms of the `n_components` variables in the lower-dimensional space.

Type array, shape (n_components,)

mean_
Per-feature empirical mean, estimated from the training set.

Equal to *X.mean(axis=0)*.

Type array, shape (n_features,)

n_components_
The estimated number of components. When n_components is set to 'mle' or a number between 0 and 1 (with svd_solver == 'full') this number is estimated from input data. Otherwise it equals the parameter n_components, or n_features if n_components is None.

Type int

noise_variance_
The estimated noise covariance following the Probabilistic PCA model from Tipping and Bishop 1999.

See "Pattern Recognition and Machine Learning" by C. Bishop, 12.2.1 p. 574 or http://www.miketipping.com/papers/met-mppca.pdf. It is required to computed the estimated data covariance and score samples.

Equal to the average of (min(n_features, n_samples) - n_components) smallest eigenvalues of the covariance matrix of X.

Type float

decision_scores_
The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores. This value is available once the detector is fitted.

Type numpy array of shape (n_samples,)

threshold_
The threshold is based on `contamination`. It is the `n_samples * contamination` most abnormal samples in `decision_scores_`. The threshold is calculated for generating binary outlier labels.

Type float

labels_
The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies. It is generated by applying `threshold_` on `decision_scores_`.

Type int, either 0 or 1

decision_function(*X*)
Predict raw anomaly score of X using the fitted detector.

The anomaly score of an input sample is computed based on different detector algorithms. For consistency, outliers are assigned with larger anomaly scores.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The training input samples. Sparse matrices are accepted only if they are supported by the base estimator.

Returns **anomaly_scores** – The anomaly score of the input samples.

Return type numpy array of shape (n_samples,)

explained_variance_
The amount of variance explained by each of the selected components.

Equal to n_components largest eigenvalues of the covariance matrix of X.

Decorator for scikit-learn PCA attributes.

fit(*X*, *y=None*)
Fit detector. y is optional for unsupervised methods.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **y** (*numpy array of shape (n_samples,), optional (default=None)*) – The ground truth of the input samples (labels).

fit_predict(*X*, *y=None*)
DEPRECATED

Fit detector first and then predict whether a particular sample is an outlier or not.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

outlier_labels [numpy array of shape (n_samples,)] For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Deprecated since version 0.6.9: *fit_predict* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency.

fit_predict_score(*X*, *y*, *scoring='roc_auc_score'*)
DEPRECATED

Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

scoring [str, optional (default='roc_auc_score')] Evaluation metric:

- 'roc_auc_score': ROC score
- 'prc_n_score': Precision @ rank n score

score : float

Deprecated since version 0.6.9: *fit_predict_score* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency. Scoring could be done by calling an evaluation method, e.g., AUC ROC.

get_params(*deep=True*)
Get parameters for this estimator.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Parameters **deep** (*boolean, optional*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns **params** – Parameter names mapped to their values.

Return type mapping of string to any

noise_variance_
The estimated noise covariance following the Probabilistic PCA model from Tipping and Bishop 1999. See "Pattern Recognition and Machine Learning" by C. Bishop, 12.2.1 p. 574 or http://www.miketipping.com/papers/met-mppca.pdf. It is required to computed the estimated data covariance and score samples.

Equal to the average of (min(n_features, n_samples) - n_components) smallest eigenvalues of the covariance matrix of X.

Decorator for scikit-learn PCA attributes.

predict(*X*)
Predict if a particular sample is an outlier or not.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Return type numpy array of shape (n_samples,)

predict_proba(*X*, *method='linear'*)

Predict the probability of a sample being outlier. Two approaches are possible:

1. simply use Min-max conversion to linearly transform the outlier scores into the range of [0,1]. The model must be fitted first.
2. use unifying scores, see [BKKSZ11].

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **method** (*str, optional (default='linear')*) – probability conversion method. It must be one of 'linear' or 'unify'.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

set_params(***params*)

Set the parameters of this estimator. The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Returns **self**

Return type object

pyod.models.sod module

Subspace Outlier Detection (SOD)

class pyod.models.sod.**SOD**(*contamination=0.1*, *n_neighbors=20*, *ref_set=10*, *alpha=0.8*)

Bases: *pyod.models.base.BaseDetector*

Subspace outlier detection (SOD) schema aims to detect outlier in varying subspaces of a high dimensional feature space. For each data object, SOD explores the axis-parallel subspace spanned by the data object's neighbors and determines how much the object deviates from the neighbors in this subspace.

See [BKKrogerSZ09] for details.

Parameters

- **n_neighbors** (*int, optional (default=20)*) – Number of neighbors to use by default for k neighbors queries.
- **ref_set** (*int, optional (default=10)*) – specifies the number of shared nearest neighbors to create the reference set. Note that ref_set must be smaller than n_neighbors.
- **alpha** (*float in (0., 1.), optional (default=0.8)*) – specifies the lower limit for selecting subspace. 0.8 is set as default as suggested in the original paper.
- **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set. Used when fitting to define the threshold on the decision function.

decision_scores_
The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores. This value is available once the detector is fitted.

Type numpy array of shape (n_samples,)

threshold_
The threshold is based on `contamination`. It is the `n_samples * contamination` most abnormal samples in `decision_scores_`. The threshold is calculated for generating binary outlier labels.

Type float

labels_
The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies. It is generated by applying `threshold_` on `decision_scores_`.

Type int, either 0 or 1

decision_function(*X*)
Predict raw anomaly score of X using the fitted detector. The anomaly score of an input sample is computed based on different detector algorithms. For consistency, outliers are assigned with larger anomaly scores.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The training input samples. Sparse matrices are accepted only if they are supported by the base estimator.

Returns **anomaly_scores** – The anomaly score of the input samples.

Return type numpy array of shape (n_samples,)

fit(*X*, *y=None*)
Fit detector. y is optional for unsupervised methods.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **y** (*numpy array of shape (n_samples,), optional (default=None)*) – The ground truth of the input samples (labels).

fit_predict(*X*, *y=None*)
DEPRECATED

Fit detector first and then predict whether a particular sample is an outlier or not.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

outlier_labels [numpy array of shape (n_samples,)] For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Deprecated since version 0.6.9: *fit_predict* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency.

fit_predict_score(*X*, *y*, *scoring='roc_auc_score'*)
DEPRECATED

Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

scoring [str, optional (default='roc_auc_score')] Evaluation metric:

- 'roc_auc_score': ROC score
- 'prc_n_score': Precision @ rank n score

score : float

Deprecated since version 0.6.9: *fit_predict_score* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency. Scoring could be done by calling an evaluation method, e.g., AUC ROC.

get_params(*deep=True*)

Get parameters for this estimator.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Parameters **deep** (*boolean, optional*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns **params** – Parameter names mapped to their values.

Return type mapping of string to any

predict(*X*)

Predict if a particular sample is an outlier or not.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Return type numpy array of shape (n_samples,)

predict_proba(*X*, *method='linear'*)

Predict the probability of a sample being outlier. Two approaches are possible:

1. simply use Min-max conversion to linearly transform the outlier scores into the range of [0,1]. The model must be fitted first.
2. use unifying scores, see [BKKSZ11].

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **method** (*str, optional (default='linear')*) – probability conversion method. It must be one of 'linear' or 'unify'.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

set_params(***params*)

Set the parameters of this estimator. The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Returns self

Return type object

pyod.models.so_gaal module

Single-Objective Generative Adversarial Active Learning. Part of the codes are adapted from https://github.com/leibinghe/GAAL-based-outlier-detection

class pyod.models.so_gaal.**SO_GAAL**(*stop_epochs=20*, *lr_d=0.01*, *lr_g=0.0001*, *decay=1e-06*, *momentum=0.9*, *contamination=0.1*)

Bases: *pyod.models.base.BaseDetector*

Single-Objective Generative Adversarial Active Learning.

SO-GAAL directly generates informative potential outliers to assist the classifier in describing a boundary that can separate outliers from normal data effectively. Moreover, to prevent the generator from falling into the mode collapsing problem, the network structure of SO-GAAL is expanded from a single generator (SO-GAAL) to multiple generators with different objectives (MO-GAAL) to generate a reasonable reference distribution for the whole dataset. Read more in the [BLLZ+19].

Parameters

- **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set. Used when fitting to define the threshold on the decision function.
- **stop_epochs** (*int, optional (default=20)*) – The number of epochs of training.
- **lr_d** (*float, optional (default=0.01)*) – The learn rate of the discriminator.
- **lr_g** (*float, optional (default=0.0001)*) – The learn rate of the generator.
- **decay** (*float, optional (default=1e-6)*) – The decay parameter for SGD.
- **momentum** (*float, optional (default=0.9)*) – The momentum parameter for SGD.

decision_scores_
The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores. This value is available once the detector is fitted.

Type numpy array of shape (n_samples,)

threshold_
The threshold is based on `contamination`. It is the `n_samples * contamination` most abnormal samples in `decision_scores_`. The threshold is calculated for generating binary outlier labels.

Type float

labels_
The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies. It is generated by applying `threshold_` on `decision_scores_`.

Type int, either 0 or 1

decision_function(*X*)
Predict raw anomaly score of X using the fitted detector.

The anomaly score of an input sample is computed based on different detector algorithms. For consistency, outliers are assigned with larger anomaly scores.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The training input samples. Sparse matrices are accepted only if they are supported by the base estimator.

Returns **anomaly_scores** – The anomaly score of the input samples.

Return type numpy array of shape (n_samples,)

fit(*X*, *y=None*)
Fit detector. y is optional for unsupervised methods.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **y** (*numpy array of shape (n_samples,), optional (default=None)*) – The ground truth of the input samples (labels).

fit_predict(*X*, *y=None*)
DEPRECATED

Fit detector first and then predict whether a particular sample is an outlier or not.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

outlier_labels [numpy array of shape (n_samples,)] For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Deprecated since version 0.6.9: *fit_predict* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency.

fit_predict_score(*X*, *y*, *scoring='roc_auc_score'*)
DEPRECATED

Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

scoring [str, optional (default='roc_auc_score')] Evaluation metric:

- 'roc_auc_score': ROC score
- 'prc_n_score': Precision @ rank n score

score : float

Deprecated since version 0.6.9: *fit_predict_score* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency. Scoring could be done by calling an evaluation method, e.g., AUC ROC.

get_params(*deep=True*)
Get parameters for this estimator.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Parameters **deep** (*boolean, optional*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns **params** – Parameter names mapped to their values.

Return type mapping of string to any

predict(*X*)

Predict if a particular sample is an outlier or not.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Return type numpy array of shape (n_samples,)

predict_proba(*X*, *method='linear'*)

Predict the probability of a sample being outlier. Two approaches are possible:

1. simply use Min-max conversion to linearly transform the outlier scores into the range of [0,1]. The model must be fitted first.
2. use unifying scores, see [BKKSZ11].

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **method** (*str, optional (default='linear')*) – probability conversion method. It must be one of 'linear' or 'unify'.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

set_params(***params*)

Set the parameters of this estimator. The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Returns **self**

Return type object

pyod.models.sos module

Stochastic Outlier Selection (SOS). Part of the codes are adapted from https://github.com/jeroenjanssens/scikit-sos

class pyod.models.sos.**SOS**(*contamination=0.1*, *perplexity=4.5*, *metric='euclidean'*, *eps=1e-05*)

Bases: *pyod.models.base.BaseDetector*

Stochastic Outlier Selection.

SOS employs the concept of affinity to quantify the relationship from one data point to another data point. Affinity is proportional to the similarity between two data points. So, a data point has little affinity with a dissimilar data point. A data point is selected as an outlier when all the other data points have insufficient affinity with it. Read more in the [BJHuszarPvdH12].

Parameters

- **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set. Used when fitting to define the threshold on the decision function.
- **perplexity** (*float, optional (default=4.5)*) – A smooth measure of the effective number of neighbours. The perplexity parameter is similar to the parameter k in kNN algorithm (the number of nearest neighbors). The range of perplexity can be any real number between 1 and n-1, where n is the number of samples.
- **metric** (*str, default 'euclidean'*) – Metric used for the distance computation. Any metric from scipy.spatial.distance can be used.

  Valid values for metric are:

  – 'euclidean'

  – from scipy.spatial.distance: ['braycurtis', 'canberra', 'chebyshev', 'correlation', 'dice', 'hamming', 'jaccard', 'kulsinski', 'mahalanobis', 'matching', 'minkowski', 'rogerstanimoto', 'russellrao', 'seuclidean', 'sokalmichener', 'sokalsneath', 'sqeuclidean', 'yule']

  See the documentation for scipy.spatial.distance for details on these metrics: http://docs.scipy.org/doc/scipy/reference/spatial.distance.html
- **eps** (*float, optional (default = 1e-5)*) – Tolerance threshold for floating point errors.

decision_scores_
The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores. This value is available once the detector is fitted.

Type numpy array of shape (n_samples,)

threshold_
The threshold is based on `contamination`. It is the `n_samples * contamination` most abnormal samples in `decision_scores_`. The threshold is calculated for generating binary outlier labels.

Type float

labels_
The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies. It is generated by applying `threshold_` on `decision_scores_`.

Type int, either 0 or 1

Examples

```
>>> from pyod.models.sos import SOS
>>> from pyod.utils.data import generate_data
>>> n_train = 50
>>> n_test = 50
>>> contamination = 0.1
>>> X_train, y_train, X_test, y_test = generate_data(
...     n_train=n_train, n_test=n_test,
```

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(continued from previous page)

```
...     contamination=contamination, random_state=42)
>>>
>>> clf = SOS()
>>> clf.fit(X_train)
SOS(contamination=0.1, eps=1e-05, metric='euclidean', perplexity=4.5)
```

decision_function(*X*)
Predict raw anomaly score of X using the fitted detector.

The anomaly score of an input sample is computed based on different detector algorithms. For consistency, outliers are assigned with larger anomaly scores.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The training input samples. Sparse matrices are accepted only if they are supported by the base estimator.

Returns **anomaly_scores** – The anomaly score of the input samples.

Return type numpy array of shape (n_samples,)

fit(*X*, *y=None*)
Fit detector. y is optional for unsupervised methods.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **y** (*numpy array of shape (n_samples,), optional (default=None)*) – The ground truth of the input samples (labels).

fit_predict(*X*, *y=None*)
DEPRECATED

Fit detector first and then predict whether a particular sample is an outlier or not.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

outlier_labels [numpy array of shape (n_samples,)] For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Deprecated since version 0.6.9: *fit_predict* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency.

fit_predict_score(*X*, *y*, *scoring='roc_auc_score'*)
DEPRECATED

Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

scoring [str, optional (default='roc_auc_score')] Evaluation metric:

- 'roc_auc_score': ROC score
- 'prc_n_score': Precision @ rank n score

score : float

Deprecated since version 0.6.9: *fit_predict_score* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency. Scoring could be done by calling an evaluation method, e.g., AUC ROC.

get_params(*deep=True*)

Get parameters for this estimator.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Parameters **deep** (*boolean, optional*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns **params** – Parameter names mapped to their values.

Return type mapping of string to any

predict(*X*)

Predict if a particular sample is an outlier or not.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Return type numpy array of shape (n_samples,)

predict_proba(*X*, *method='linear'*)

Predict the probability of a sample being outlier. Two approaches are possible:

1. simply use Min-max conversion to linearly transform the outlier scores into the range of [0,1]. The model must be fitted first.
2. use unifying scores, see [BKKSZ11].

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **method** (*str, optional (default='linear')*) – probability conversion method. It must be one of 'linear' or 'unify'.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

set_params(***params*)

Set the parameters of this estimator. The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Returns **self**

Return type object

pyod.models.xgbod module

XGBOD: Improving Supervised Outlier Detection with Unsupervised Representation Learning. A semi-supervised outlier detection framework.

class pyod.models.xgbod.**XGBOD**(*estimator_list=None*, *standardization_flag_list=None*, *max_depth=3*, *learning_rate=0.1*, *n_estimators=100*, *silent=True*, *objective='binary:logistic'*, *booster='gbtree'*, *n_jobs=1*, *nthread=None*, *gamma=0*, *min_child_weight=1*, *max_delta_step=0*, *subsample=1*, *colsample_bytree=1*, *colsample_bylevel=1*, *reg_alpha=0*, *reg_lambda=1*, *scale_pos_weight=1*, *base_score=0.5*, *random_state=0*, *missing=None*, ***kwargs*)

Bases: *pyod.models.base.BaseDetector*

XGBOD class for outlier detection. It first use the passed in unsupervised outlier detectors to extract richer representation of the data and then concatenate the newly generated features to the original feature for constructing the augmented feature space. An XGBoost classifier is then applied on this augmented feature space. Read more in the [BZH18].

Parameters

- **estimator_list** (*list, optional (default=None)*) – The list of pyod detectors passed in for unsupervised learning
- **standardization_flag_list** (*list, optional (default=None)*) – The list of boolean flags for indicating whether to take standardization for each detector.
- **max_depth** (*int*) – Maximum tree depth for base learners.
- **learning_rate** (*float*) – Boosting learning rate (xgb's "eta")
- **n_estimators** (*int*) – Number of boosted trees to fit.
- **silent** (*boolean*) – Whether to print messages while running boosting.
- **objective** (*string or callable*) – Specify the learning task and the corresponding learning objective or a custom objective function to be used (see note below).
- **booster** (*string*) – Specify which booster to use: gbtree, gblinear or dart.
- **n_jobs** (*int*) – Number of parallel threads used to run xgboost. (replaces `nthread`)
- **gamma** (*float*) – Minimum loss reduction required to make a further partition on a leaf node of the tree.
- **min_child_weight** (*int*) – Minimum sum of instance weight(hessian) needed in a child.
- **max_delta_step** (*int*) – Maximum delta step we allow each tree's weight estimation to be.
- **subsample** (*float*) – Subsample ratio of the training instance.
- **colsample_bytree** (*float*) – Subsample ratio of columns when constructing each tree.
- **colsample_bylevel** (*float*) – Subsample ratio of columns for each split, in each level.
- **reg_alpha** (*float (xgb's alpha)*) – L1 regularization term on weights.
- **reg_lambda** (*float (xgb's lambda)*) – L2 regularization term on weights.
- **scale_pos_weight** (*float*) – Balancing of positive and negative weights.

- **base_score** – The initial prediction score of all instances, global bias.
- **random_state** (*int*) – Random number seed. (replaces seed)
- **missing** (*float, optional*) – Value in the data which needs to be present as a missing value. If None, defaults to np.nan.
- **importance_type** (*string, default "gain"*) – The feature importance type for the feature_importances_ property: either "gain", "weight", "cover", "total_gain" or "total_cover".
- ****kwargs** (*dict, optional*) – Keyword arguments for XGBoost Booster object. Full documentation of parameters can be found here: https://github.com/dmlc/xgboost/blob/master/doc/parameter.rst. Attempting to set a parameter via the constructor args and **kwargs dict simultaneously will result in a TypeError.

  Note: **kwargs is unsupported by scikit-learn. We do not guarantee that parameters passed via this argument will interact properly with scikit-learn.

n_detector_
The number of unsupervised of detectors used.

Type int

clf_
The XGBoost classifier.

Type object

decision_scores_
The outlier scores of the training data. The higher, the more abnormal. Outliers tend to have higher scores. This value is available once the detector is fitted.

Type numpy array of shape (n_samples,)

labels_
The binary labels of the training data. 0 stands for inliers and 1 for outliers/anomalies. It is generated by applying threshold_ on decision_scores_.

Type int, either 0 or 1

decision_function(*X*)
Predict raw anomaly scores of X using the fitted detector.

The anomaly score of an input sample is computed based on the fitted detector. For consistency, outliers are assigned with higher anomaly scores.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples. Sparse matrices are accepted only if they are supported by the base estimator.

Returns **anomaly_scores** – The anomaly score of the input samples.

Return type numpy array of shape (n_samples,)

fit(*X*, *y*)
Fit the model using X and y as training data.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – Training data.
- **y** (*numpy array of shape (n_samples,)*) – The ground truth (binary label)
  - 0 : inliers
  - 1 : outliers

Returns self

Return type object

fit_predict(*X*, *y*)
DEPRECATED

Fit detector first and then predict whether a particular sample is an outlier or not.

X [numpy array of shape (n_samples, n_features)] The input samples.

y [numpy array of shape (n_samples,), optional (default=None)] The ground truth of the input samples (labels).

outlier_labels [numpy array of shape (n_samples,)] For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Deprecated since version 0.6.9: *fit_predict* will be removed in pyod 0.8.0.; it will be replaced by calling *fit* function first and then accessing *labels_* attribute for consistency.

fit_predict_score(*X*, *y*, *scoring='roc_auc_score'*)
Fit the detector, predict on samples, and evaluate the model by predefined metrics, e.g., ROC.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.
- **y** (*numpy array of shape (n_samples,), optional (default=None)*) – The ground truth of the input samples (labels).
- **scoring** (*str, optional (default='roc_auc_score')*) – Evaluation metric:
  - 'roc_auc_score': ROC score
  - 'prc_n_score': Precision @ rank n score

Returns score

Return type float

get_params(*deep=True*)
Get parameters for this estimator.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Parameters **deep** (*boolean, optional*) – If True, will return the parameters for this estimator and contained subobjects that are estimators.

Returns **params** – Parameter names mapped to their values.

Return type mapping of string to any

predict(*X*)
Predict if a particular sample is an outlier or not. Calling xgboost *predict* function.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. 0 stands for inliers and 1 for outliers.

Return type numpy array of shape (n_samples,)

predict_proba(*X*)
Predict the probability of a sample being outlier. Calling xgboost *predict_proba* function.

Parameters **X** (*numpy array of shape (n_samples, n_features)*) – The input samples.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

set_params(***params*)
Set the parameters of this estimator. The method works on simple estimators as well as on nested objects (such as pipelines). The latter have parameters of the form `<component>__<parameter>` so that it's possible to update each component of a nested object.

See http://scikit-learn.org/stable/modules/generated/sklearn.base.BaseEstimator.html and sklearn/base.py for more information.

Returns **self**

Return type object

Module contents

References

2.5.2 Utility Functions

pyod.utils.data module

Utility functions for manipulating data

pyod.utils.data.**check_consistent_shape**(*X_train*, *y_train*, *X_test*, *y_test*, *y_train_pred*, *y_test_pred*)
Internal shape to check input data shapes are consistent.

Parameters

- **X_train** (*numpy array of shape (n_samples, n_features)*) – The training samples.
- **y_train** (*list or array of shape (n_samples,)*) – The ground truth of training samples.
- **X_test** (*numpy array of shape (n_samples, n_features)*) – The test samples.
- **y_test** (*list or array of shape (n_samples,)*) – The ground truth of test samples.
- **y_train_pred** (*numpy array of shape (n_samples, n_features)*) – The predicted binary labels of the training samples.
- **y_test_pred** (*numpy array of shape (n_samples, n_features)*) – The predicted binary labels of the test samples.

Returns

- **X_train** (*numpy array of shape (n_samples, n_features)*) – The training samples.

- **y_train** (*list or array of shape (n_samples,)*) – The ground truth of training samples.
- **X_test** (*numpy array of shape (n_samples, n_features)*) – The test samples.
- **y_test** (*list or array of shape (n_samples,)*) – The ground truth of test samples.
- **y_train_pred** (*numpy array of shape (n_samples, n_features)*) – The predicted binary labels of the training samples.
- **y_test_pred** (*numpy array of shape (n_samples, n_features)*) – The predicted binary labels of the test samples.

pyod.utils.data.**evaluate_print**(*clf_name*, *y*, *y_pred*)

Utility function for evaluating and printing the results for examples. Default metrics include ROC and Precision @ n

Parameters

- **clf_name** (*str*) – The name of the detector.
- **y** (*list or numpy array of shape (n_samples,)*) – The ground truth. Binary (0: inliers, 1: outliers).
- **y_pred** (*list or numpy array of shape (n_samples,)*) – The raw outlier scores as returned by a fitted model.

pyod.utils.data.**generate_data**(*n_train=1000*, *n_test=500*, *n_features=2*, *contamination=0.1*, *train_only=False*, *offset=10*, *behaviour='old'*, *random_state=None*)

Utility function to generate synthesized data. Normal data is generated by a multivariate Gaussian distribution and outliers are generated by a uniform distribution.

Parameters

- **n_train** (*int, (default=1000)*) – The number of training points to generate.
- **n_test** (*int, (default=500)*) – The number of test points to generate.
- **n_features** (*int, optional (default=2)*) – The number of features (dimensions).
- **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set. Used when fitting to define the threshold on the decision function.
- **train_only** (*bool, optional (default=False)*) – If true, generate train data only.
- **offset** (*int, optional (default=10)*) – Adjust the value range of Gaussian and Uniform.
- **behaviour** (*str, default='old'*) – Behaviour of the returned datasets which can be either 'old' or 'new'. Passing `behaviour='new'` returns "X_train, y_train, X_test, y_test", while passing `behaviour='old'` returns "X_train, X_test, y_train, y_test".

  New in version 0.7.0: `behaviour` is added in 0.7.0 for back-compatibility purpose.

  Deprecated since version 0.7.0: `behaviour='old'` is deprecated in 0.20 and will not be possible in 0.7.2.

  Deprecated since version 0.7.2.: `behaviour` parameter will be deprecated in 0.7.2 and removed in 0.8.0.

- **random_state** (*int, RandomState instance or None, optional (default=None)*) – If int, random_state is the seed used by the random number

generator; If RandomState instance, random_state is the random number generator; If None, the random number generator is the RandomState instance used by *np.random*.

Returns

- **X_train** (*numpy array of shape (n_train, n_features)*) – Training data.
- **y_train** (*numpy array of shape (n_train,)*) – Training ground truth.
- **X_test** (*numpy array of shape (n_test, n_features)*) – Test data.
- **y_test** (*numpy array of shape (n_test,)*) – Test ground truth.

pyod.utils.data.**generate_data_clusters**(*n_train=1000*, *n_test=500*, *n_clusters=2*, *n_features=2*, *contamination=0.1*, *size='same'*, *density='same'*, *dist=0.25*, *random_state=None*, *return_in_clusters=False*)

Utility function to generate synthesized data in clusters. Generated data can involve the low density pattern problem and global outliers which are considered as difficult tasks for outliers detection algorithms.

Parameters

- **n_train** (*int, (default=1000)*) – The number of training points to generate.
- **n_test** (*int, (default=500)*) – The number of test points to generate.
- **n_clusters** (*int, optional (default=2)*) – The number of centers (i.e. clusters) to generate.
- **n_features** (*int, optional (default=2)*) – The number of features for each sample.
- **contamination** (*float in (0., 0.5), optional (default=0.1)*) – The amount of contamination of the data set, i.e. the proportion of outliers in the data set.
- **size** (*str, optional (default='same')*) – Size of each cluster: 'same' generates clusters with same size, 'different' generate clusters with different sizes.
- **density** (*str, optional (default='same')*) – Density of each cluster: 'same' generates clusters with same density, 'different' generate clusters with different densities.
- **dist** (*float, optional (default=0.25)*) – Distance between clusters. Should be between 0. and 1.0 It is used to avoid clusters overlapping as much as possible. However, if number of samples and number of clusters are too high, it is unlikely to separate them fully even if `dist` set to 1.0
- **random_state** (*int, RandomState instance or None, optional (default=None)*) – If int, random_state is the seed used by the random number generator; If RandomState instance, random_state is the random number generator; If None, the random number generator is the RandomState instance used by *np.random*.
- **return_in_clusters** (*bool, optional (default=False)*) – If True, the function returns x_train, y_train, x_test, y_test each as a list of numpy arrays where each index represents a cluster. If False, it returns x_train, y_train, x_test, y_test each as numpy array after joining the sequence of clusters arrays,

Returns

- **X_train** (*numpy array of shape (n_train, n_features)*) – Training data.
- **y_train** (*numpy array of shape (n_train,)*) – Training ground truth.
- **X_test** (*numpy array of shape (n_test, n_features)*) – Test data.

- **y_test** (*numpy array of shape (n_test,)*) – Test ground truth.

pyod.utils.data.**get_color_codes**(*y*)
Internal function to generate color codes for inliers and outliers. Inliers (0): blue; Outlier (1): red.

Parameters **y** (*list or numpy array of shape (n_samples,)*) – The ground truth. Binary (0: inliers, 1: outliers).

Returns **c** – Color codes.

Return type numpy array of shape (n_samples,)

pyod.utils.data.**get_outliers_inliers**(*X*, *y*)
Internal method to separate inliers from outliers.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The input samples
- **y** (*list or array of shape (n_samples,)*) – The ground truth of input samples.

Returns

- **X_outliers** (*numpy array of shape (n_samples, n_features)*) – Outliers.
- **X_inliers** (*numpy array of shape (n_samples, n_features)*) – Inliers.

pyod.utils.example module

Utility functions for running examples

pyod.utils.example.**data_visualize**(*X_train*, *y_train*, *show_figure=True*, *save_figure=False*)
Utility function for visualizing the synthetic samples generated by generate_data_cluster function.

Parameters

- **X_train** (*numpy array of shape (n_samples, n_features)*) – The training samples.
- **y_train** (*list or array of shape (n_samples,)*) – The ground truth of training samples.
- **show_figure** (*bool, optional (default=True)*) – If set to True, show the figure.
- **save_figure** (*bool, optional (default=False)*) – If set to True, save the figure to the local.

pyod.utils.example.**visualize**(*clf_name*, *X_train*, *y_train*, *X_test*, *y_test*, *y_train_pred*, *y_test_pred*, *show_figure=True*, *save_figure=False*)
Utility function for visualizing the results in examples. Internal use only.

Parameters

- **clf_name** (*str*) – The name of the detector.
- **X_train** (*numpy array of shape (n_samples, n_features)*) – The training samples.
- **y_train** (*list or array of shape (n_samples,)*) – The ground truth of training samples.

- **X_test** (*numpy array of shape (n_samples, n_features)*) – The test samples.
- **y_test** (*list or array of shape (n_samples,)*) – The ground truth of test samples.
- **y_train_pred** (*numpy array of shape (n_samples, n_features)*) – The predicted binary labels of the training samples.
- **y_test_pred** (*numpy array of shape (n_samples, n_features)*) – The predicted binary labels of the test samples.
- **show_figure** (*bool, optional (default=True)*) – If set to True, show the figure.
- **save_figure** (*bool, optional (default=False)*) – If set to True, save the figure to the local.

pyod.utils.stat_models module

A collection of statistical models

pyod.utils.stat_models.**pairwise_distances_no_broadcast**(*X*, *Y*)

Utility function to calculate row-wise euclidean distance of two matrix. Different from pair-wise calculation, this function would not broadcast.

For instance, X and Y are both (4,3) matrices, the function would return a distance vector with shape (4,), instead of (4,4).

Parameters

- **X** (*array of shape (n_samples, n_features)*) – First input samples
- **Y** (*array of shape (n_samples, n_features)*) – Second input samples

Returns **distance** – Row-wise euclidean distance of X and Y

Return type array of shape (n_samples,)

pyod.utils.stat_models.**pearsonr_mat**(*mat*, *w=None*)

Utility function to calculate pearson matrix (row-wise).

Parameters

- **mat** (*numpy array of shape (n_samples, n_features)*) – Input matrix.
- **w** (*numpy array of shape (n_features,)*) – Weights.

Returns **pear_mat** – Row-wise pearson score matrix.

Return type numpy array of shape (n_samples, n_samples)

pyod.utils.stat_models.**wpearsonr**(*x*, *y*, *w=None*)

Utility function to calculate the weighted Pearson correlation of two samples.

See https://stats.stackexchange.com/questions/221246/such-thing-as-a-weighted-correlation for more information

Parameters

- **x** (*array, shape (n,)*) – Input x.
- **y** (*array, shape (n,)*) – Input y.
- **w** (*array, shape (n,)*) – Weights w.

Returns **scores** – Weighted Pearson Correlation between x and y.

Return type float in range of [-1,1]

pyod.utils.utility module

A set of utility functions to support outlier detection.

pyod.utils.utility.**argmaxn**(*value_list*, *n*, *order='desc'*)

Return the index of top n elements in the list if order is set to 'desc', otherwise return the index of n smallest ones.

Parameters

- **value_list** (*list, array, numpy array of shape (n_samples,)*) – A list containing all values.
- **n** (*int*) – The number of elements to select.
- **order** (*str, optional (default='desc')*) – The order to sort {'desc', 'asc'}:
  - 'desc': descending
  - 'asc': ascending

Returns **index_list** – The index of the top n elements.

Return type numpy array of shape (n,)

pyod.utils.utility.**check_detector**(*detector*)

Checks if fit and decision_function methods exist for given detector

Parameters **detector** (*pyod.models*) – Detector instance for which the check is performed.

pyod.utils.utility.**check_parameter**(*param*, *low=-2147483647*, *high=2147483647*, *param_name=''*, *include_left=False*, *include_right=False*)

Check if an input is within the defined range.

Parameters

- **param** (*int, float*) – The input parameter to check.
- **low** (*int, float*) – The lower bound of the range.
- **high** (*int, float*) – The higher bound of the range.
- **param_name** (*str, optional (default='')*) – The name of the parameter.
- **include_left** (*bool, optional (default=False)*) – Whether includes the lower bound (lower bound <=).
- **include_right** (*bool, optional (default=False)*) – Whether includes the higher bound (<= higher bound).

Returns **within_range** – Whether the parameter is within the range of (low, high)

Return type bool or raise errors

pyod.utils.utility.**generate_bagging_indices**(*random_state*, *bootstrap_features*, *n_features*, *min_features*, *max_features*)

Randomly draw feature indices. Internal use only.

Modified from sklearn/ensemble/bagging.py

Parameters

- **random_state** (*RandomState*) – A random number generator instance to define the state of the random permutations generator.
- **bootstrap_features** (*bool*) – Specifies whether to bootstrap indice generation
- **n_features** (*int*) – Specifies the population size when generating indices
- **min_features** (*int*) – Lower limit for number of features to randomly sample
- **max_features** (*int*) – Upper limit for number of features to randomly sample

Returns **feature_indices** – Indices for features to bag

Return type numpy array, shape (n_samples,)

pyod.utils.utility.**generate_indices**(*random_state*, *bootstrap*, *n_population*, *n_samples*)
Draw randomly sampled indices. Internal use only.

See sklearn/ensemble/bagging.py

Parameters

- **random_state** (*RandomState*) – A random number generator instance to define the state of the random permutations generator.
- **bootstrap** (*bool*) – Specifies whether to bootstrap indice generation
- **n_population** (*int*) – Specifies the population size when generating indices
- **n_samples** (*int*) – Specifies number of samples to draw

Returns **indices** – randomly drawn indices

Return type numpy array, shape (n_samples,)

pyod.utils.utility.**get_label_n**(*y*, *y_pred*, *n=None*)
Function to turn raw outlier scores into binary labels by assign 1 to top n outlier scores.

Parameters

- **y** (*list or numpy array of shape (n_samples,)*) – The ground truth. Binary (0: inliers, 1: outliers).
- **y_pred** (*list or numpy array of shape (n_samples,)*) – The raw outlier scores as returned by a fitted model.
- **n** (*int, optional (default=None)*) – The number of outliers. if not defined, infer using ground truth.

Returns **labels** – binary labels 0: normal points and 1: outliers

Return type numpy array of shape (n_samples,)

Examples

```
>>> from pyod.utils.utility import get_label_n
>>> y = [0, 1, 1, 0, 0]
>>> y_pred = [0.1, 0.5, 0.3, 0.2, 0.7]
>>> get_label_n(y, y_pred)
array([0, 1, 0, 0, 1])
```

pyod.utils.utility.**invert_order**(*scores*, *method='multiplication'*)
Invert the order of a list of values. The smallest value becomes the largest in the inverted list. This is useful while combining multiple detectors since their score order could be different.

Parameters

- **scores** (*list, array or numpy array with shape (n_samples,)*) – The list of values to be inverted
- **method** (*str, optional (default='multiplication')*) – Methods used for order inversion. Valid methods are:
  - 'multiplication': multiply by -1
  - 'subtraction': max(scores) - scores

Returns **inverted_scores** – The inverted list

Return type numpy array of shape (n_samples,)

Examples

```
>>> scores1 = [0.1, 0.3, 0.5, 0.7, 0.2, 0.1]
>>> invert_order(scores1)
array([-0.1, -0.3, -0.5, -0.7, -0.2, -0.1])
>>> invert_order(scores1, method='subtraction')
array([0.6, 0.4, 0.2, 0. , 0.5, 0.6])
```

pyod.utils.utility.**precision_n_scores**(*y*, *y_pred*, *n=None*)
Utility function to calculate precision @ rank n.

Parameters

- **y** (*list or numpy array of shape (n_samples,)*) – The ground truth. Binary (0: inliers, 1: outliers).
- **y_pred** (*list or numpy array of shape (n_samples,)*) – The raw outlier scores as returned by a fitted model.
- **n** (*int, optional (default=None)*) – The number of outliers. if not defined, infer using ground truth.

Returns **precision_at_rank_n** – Precision at rank n score.

Return type float

pyod.utils.utility.**score_to_label**(*pred_scores*, *outliers_fraction=0.1*)
Turn raw outlier outlier scores to binary labels (0 or 1).

Parameters

- **pred_scores** (*list or numpy array of shape (n_samples,)*) – Raw outlier scores. Outliers are assumed have larger values.
- **outliers_fraction** (*float in (0,1)*) – Percentage of outliers.

Returns **outlier_labels** – For each observation, tells whether or not it should be considered as an outlier according to the fitted model. Return the outlier probability, ranging in [0,1].

Return type numpy array of shape (n_samples,)

pyod.utils.utility.**standardizer**(*X*, *X_t=None*, *keep_scalar=False*)
Conduct Z-normalization on data to turn input samples become zero-mean and unit variance.

Parameters

- **X** (*numpy array of shape (n_samples, n_features)*) – The training samples

- **X_t** (*numpy array of shape (n_samples_new, n_features), optional (default=None)*) – The data to be converted
- **keep_scalar** (*bool, optional (default=False)*) – The flag to indicate whether to return the scalar

Returns

- **X_norm** (*numpy array of shape (n_samples, n_features)*) – X after the Z-score normalization
- **X_t_norm** (*numpy array of shape (n_samples, n_features)*) – X_t after the Z-score normalization
- **scalar** (*sklearn scalar object*) – The scalar used in conversion

2.5.3 Module contents

2.6 Known Issues & Warnings

This is the central place to track known issues.

2.6.1 Installation

There are some known dependency issues/notes. Refer installation for more information.

2.6.2 Neural Networks

SO_GAAL and MO_GAAL may only work under Python 3.5+.

2.6.3 Differences between PyOD and scikit-learn

Although PyOD is built on top of scikit-learn and inspired by its API design, some differences should be noted:

- All models in PyOD follow the tradition that the outlying objects come with higher scores while the normal objects have lower scores. scikit-learn has an inverted design–lower scores stand for outlying objects.
- PyOD uses "0" to represent inliers and "1" to represent outliers. Differently, scikit-learn returns "-1" for anomalies/outliers and "1" for inliers.
- Although Isolation Forests, One-class SVM, and Local Outlier Factor are implemented in both PyOD and scikit-learn, users are not advised to mix the use of them, e.g., calling one model from PyOD and another model from scikit-learn. It is recommended to only use one library for consistency (for three models, the PyOD implementation is indeed a set of wrapper functions of scikit-learn).
- PyOD models may not work with scikit-learn's check_estimator function. Similarly, scikit-learn models would not work with PyOD's check_estimator function.

2.7 Outlier Detection 101

Outlier detection broadly refers to the task of identifying observations which may be considered anomalous given the distribution of a sample. Any observation belonging to the distribution is referred to as an inlier and any outlying point is referred to as an outlier.

In the context of machine learning, there are three common approaches for this task:

1. **Unsupervised Outlier Detection**
    - Training data (unlabelled) contains both normal and anomalous observations.
    - The model identifies outliers during the fitting process.
    - This approach is taken when outliers are defined as points that exist in low-density regions in the data.
    - Any new observations that do not belong to high-density regions are considered outliers.
2. **Semi-supervised Novelty Detection**
    - Training data consists only of observations describing normal behavior.
    - The model is fit on training data and then used to evaluate new observations.
    - This approach is taken when outliers are defined as points differing from the distribution of the training data.
    - Any new observations differing from the training data within a threshold, even if they form a high-density region, are considered outliers.
3. **Supervised Outlier Classification**
    - The ground truth label (inlier vs outlier) for every observation is known.
    - The model is fit on imbalanced training data and then used to classify new observations.
    - This approach is taken when ground truth is available and it is assumed that outliers will follow the same distribution as in the training set.
    - Any new observations are classified using the model.

The algorithms found in *PyOD* focus on the first two approaches which differ in terms of how the training data is defined and how the model's outputs are interpreted. If interested in learning more, please refer to our Anomaly Detection Resources page for relevant related books, papers, videos, and toolboxes.

2.8 Citations & Achievements

2.8.1 Citing PyOD

PyOD paper is published in JMLR (machine learning open-source software track). If you use PyOD in a scientific publication, we would appreciate citations to the following paper:

```
@article{zhao2019pyod,
  author  = {Zhao, Yue and Nasrullah, Zain and Li, Zheng},
  title   = {PyOD: A Python Toolbox for Scalable Outlier Detection},
  journal = {Journal of Machine Learning Research},
  year    = {2019},
  volume  = {20},
  number  = {96},
  pages   = {1-7},
  url     = {http://jmlr.org/papers/v20/19-011.html}
}
```

or:

```
Zhao, Y., Nasrullah, Z. and Li, Z., 2019. PyOD: A Python Toolbox for Scalable Outlier␣
↪Detection. Journal of machine learning research (JMLR), 20(96), pp.1-7.
```

2.8.2 Scientific Work Using or Referencing PyOD

We are appreciated that PyOD has been increasingly referred and cited in scientific works. An incomplete list is provided below:

2019

Ishii, Y. and Takanashi, M., 2019. Low-cost Unsupervised Outlier Detection by Autoencoders with Robust Estimation. *Journal of Information Processing*, 27, pp.335-339.

Klaeger, T., Schult, A. and Oehm, L., 2019. Using anomaly detection to support classification of fast running (packaging) processes. arXiv preprint arXiv:1906.02473.

Krishnan, S. and Wu, E., 2019. AlphaClean: Automatic Generation of Data Cleaning Pipelines. arXiv preprint arXiv:1904.11827.

Kumar Das, S., Kumar Mishra, A. and Roy, P., 2019. Automatic Diabetes Prediction Using Tree Based Ensemble Learners. *International Journal of Computational Intelligence & IoT*, 2(2).

Ramakrishnan, J., Shaabani, E., Li, C. and Sustik, M.A., 2019. Anomaly Detection for an E-commerce Pricing System. arXiv preprint arXiv:1902.09566.

Trinh, H.D., Giupponi, L. and Dini, P., 2019. Urban Anomaly Detection by processing Mobile Traffic Traces with LSTM Neural Networks. *IEEE International Conference on Sensing, Communication and Networking (IEEE SECON)*.

Wan, C., Li, Z. and Zhao, Y., 2019. SynC: A Unified Framework for Generating Synthetic Population with Gaussian Copula. arXiv preprint arXiv:1904.07998.

Weng, Y., Zhang, N. and Xia, C., 2019. Multi-Agent-Based Unsupervised Detection of Energy Consumption Anomalies on Smart Campus. *IEEE Access*, 7, pp.2169-2178.

Zhao, Y., Hryniewicki, M.K., Nasrullah, Z., and Li, Z., 2019. LSCP: Locally Selective Combination in Parallel Outlier Ensembles. *SIAM International Conference on Data Mining (SDM)*, SIAM.

2018

Kalaycı, İ. and Ercan, T., 2018, October. Anomaly Detection in Wireless Sensor Networks Data by Using Histogram Based Outlier Score Method. In *2018 2nd International Symposium on Multidisciplinary Studies and Innovative Technologies (ISMSIT)* (pp. 1-6). IEEE.

Zhao, Y. and Hryniewicki, M.K., 2018. DCSO: Dynamic Combination of Detector Scores for Outlier Ensembles. *ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD), Workshop on Outlier Detection De-constructed*, 2018, London, UK.

Zhao, Y. and Hryniewicki, M.K., 2018, July. XGBOD: improving supervised outlier detection with unsupervised representation learning. In *2018 International Joint Conference on Neural Networks (IJCNN) (pp. 1-8)*. IEEE.

2.8.3 Featured Posts & Achievements

PyOD has been well acknowledged by the machine learning community with a few featured posts and tutorials.

Analytics Vidhya: An Awesome Tutorial to Learn Outlier Detection in Python using PyOD Library

KDnuggets: Intuitive Visualization of Outlier Detection Methods

KDnuggets: An Overview of Outlier Detection Methods from PyOD

Towards Data Science: Anomaly Detection for Dummies

Computer Vision News (March 2019): Python Open Source Toolbox for Outlier Detection

FLOYDHUB: Introduction to Anomaly Detection in Python

awesome-machine-learning: General-Purpose Machine Learning

Workshop/Showcase using PyOD:

- Detecting the Unexpected: An Introduction to Anomaly Detection Methods, *KISS Technosignatures Workshop* by Dr. Kiri Wagstaff @ Jet Propulsion Laboratory, California Institute of Technology. [Workshop Video] [PDF]

GitHub Python Trending:

- 2019: Jul 8th-9th, Apr 5th-6th, Feb 10th-11th, Jan 23th-24th, Jan 10th-14th
- 2018: Jun 15, Dec 8th-9th

Miscellaneous:

- PythonAwesome
- awesome-python
- PapersWithCode

2.9 Frequently Asked Questions

2.9.1 What is the Next?

This is the central place to track important things to be fixed/added:

- GPU support
- Installation efficiency improvement, such as using docker
- Add contact channel with Gitter
- Support additional languages, see Manage Translations
- Fix the bug that numba enabled function may be excluded from code coverage
- Decide which Python interpreter should readthedocs use. 3.X invokes Python 3.7 which has no TF supported for now.

Feel free to open on issue report if needed. See Issues.

2.9.2 How to Contribute

You are welcome to contribute to this exciting project:

- Please first check Issue lists for "help wanted" tag and comment the one you are interested. We will assign the issue to you.
- Fork the master branch and add your improvement/modification/fix.
- Create a pull request to **development branch** and follow the pull request template PR template
- Automatic tests will be triggered. Make sure all tests are passed. Please make sure all added modules are accompanied with proper test functions.

To make sure the code has the same style and standard, please refer to abod.py, hbos.py, or feature_bagging.py for example.

You are also welcome to share your ideas by opening an issue or dropping me an email at zhaoy@cmu.edu :)

2.9.3 Inclusion Criteria

Similarly to scikit-learn, We mainly consider well-established algorithms for inclusion. A rule of thumb is at least two years since publication, 50+ citations, and usefulness.

However, we encourage the author(s) of newly proposed models to share and add your implementation into PyOD for boosting ML accessibility and reproducibility. This exception only applies if you could commit to the maintenance of your model for at least two year period.

2.10 About us

2.10.1 Core Development Team

Yue Zhao (initialized the project in 2017): Homepage

Zain Nasrullah (joined in 2018): LinkedIn (Zain Nasrullah)

Winston (Zheng) Li (joined in 2018): LinkedIn (Winston Li)

Yahya Almardeny (joined in 2019): LinkedIn (Yahya Almardeny)

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