Package ‘dsos’

January 18, 2022

Title Dataset Shift with Outlier Scores

Version 0.1.0

Description Test for no adverse shift in two-sample comparison when we have a training set, the reference distribution, and a test set. The approach is flexible and relies on a robust and powerful test statistic, the weighted AUC. Technical details are in Kamulete, V. M. (2021) <arXiv:1908.04000>. Modern notions of outlyingness such as trust scores and prediction uncertainty can be used as the underlying scores for example.

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URL https://github.com/vathymut/dsos

BugReports https://github.com/vathymut/dsos/issues

Imports data.table (>= 1.14.0), ggplot2 (>= 3.3.3), isotree (>= 0.2.7), ranger (>= 0.12.1), scales (>= 1.1.1), simctest (>= 2.6), stats (>= 3.6.1), WeightedROC (>= 2020.1.31)

Suggests fdrtool (>= 1.2.16), knitr (>= 1.33), rmarkdown (>= 2.7), testthat (>= 3.0.2)

VignetteBuilder knitr

Encoding UTF-8

Language en-US

RoxygenNote 7.1.2

NeedsCompilation no

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Repository CRAN

Date/Publication 2022-01-18 08:32:51 UTC
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**cp_at**  
*Dataset Shift via Class Probabilities*

**Description**

Test for no adverse shift via class probabilities for two-sample comparison. The scores are out-of-bag predictions from random forests with the package `ranger`. The prefix `cp` stands for class probability, whether the instance belongs to the training or test set. The probability of belonging to the test set is the relevant notion of outlyingness.

**Usage**

```r
cp_at(x_train, x_test, R = 1000, num_trees = 500, sub_ratio = 1/2)
```

**Arguments**

- `x_train` Training sample.
- `x_test` Test sample.
- `R` The number of permutations. May be ignored.
- `num_trees` The number of trees in random forests.
- `sub_ratio` Subsampling ratio for sample splitting. May be ignored.

**Details**

The suffix `at` refers to the asymptotic test statistic. This variant uses the asymptotic null distribution for the weighted AUC (WAUC), the test statistic. Li & Fine (2010) derives its null distribution. This approximation is reliable in large sample; otherwise, prefer permutations for inference. The example below uses datasets with small samples, which is generally not advisable, is for illustration only.
Value

A named list or object of class outlier.test containing:

- **statistic**: observed WAUC statistic
- **seq_mct**: sequential Monte Carlo test, if applicable
- **p_value**: p-value
- **outlier_scores**: outlier scores from training and test set

Notes

Please see references for the classifier two-sample test, the inspiration behind this approach. Note that Ciemcon et al. (2009) uses both sample splitting for inference and the AUC, rather than the WAUC. Most supervised method for binary classification can replace random forests, the default in this implementation.

References


See Also

- [cp_ss()] for asymptotic p-value via sample splitting.
- [cp_pt()] for p-value approximation via permutations.

Other classifiers: cp_pt(), cp_ss()

Examples

```r
library(dsos)
set.seed(12345)
data(iris)
x_train <- iris[1:50, 1:4]  # Training sample: Species == 'setosa'
x_test <- iris[51:100, 1:4]  # Test sample: Species == 'versicolor'
iris_test <- cp_at(x_train, x_test)  # Can also use: cp_ss and cp_pt
str(iris_test)
```
Description

Test for no adverse shift via class probabilities for two-sample comparison. The scores are out-of-bag predictions from random forests with the package \texttt{ranger}. The prefix \textit{cp} stands for class probability, whether the instance belongs to the training or test set. The probability of belonging to the test set is the relevant notion of outlyingness.

Usage

\begin{verbatim}
cp_pt(x_train, x_test, R = 1000, num_trees = 500, sub_ratio = 1/2)
\end{verbatim}

Arguments

\begin{itemize}
  \item \texttt{x_train} \hspace{1cm} Training sample.
  \item \texttt{x_test} \hspace{1cm} Test sample.
  \item \texttt{R} \hspace{1cm} The number of permutations. May be ignored.
  \item \texttt{num_trees} \hspace{1cm} The number of trees in random forests.
  \item \texttt{sub_ratio} \hspace{1cm} Subsampling ratio for sample splitting. May be ignored.
\end{itemize}

Details

The empirical null distribution uses \texttt{R} permutations to estimate the p-value. For speed, this is implemented as a sequential Monte Carlo test with the \texttt{simctest} package. See Gandy (2009) for details. The suffix \texttt{pt} refers to permutation test. It does not use the asymptotic (theoretical) null distribution for the weighted AUC (WAUC), the test statistic. This is the recommended approach for small samples.

Value

A named list or object of class \texttt{outlier.test} containing:

- \texttt{statistic}: observed WAUC statistic
- \texttt{seq_mct}: sequential Monte Carlo test, if applicable
- \texttt{p_value}: p-value
- \texttt{outlier_scores}: outlier scores from training and test set

Notes

Please see references for the classifier two-sample test, the inspiration behind this approach. Note that Ciemencon et al. (2009) uses both sample splitting for inference and the AUC, rather than the WAUC. Most supervised method for binary classification can replace random forests, the default in this implementation.
References


See Also

Other classifiers: cp_at(), cp_ss()

Examples

library(dsos)
set.seed(12345)
data(iris)
x_train <- iris[1:50, 1:4] # Training sample: Species == ‘setosa’
x_test <- iris[51:100, 1:4] # Test sample: Species == ‘versicolor’
iris_test <- cp_at(x_train, x_test) # Can also use: cp_ss and cp_pt
str(iris_test)

---

**cp_ss** Dataset Shift via Class Probabilities

**Description**

Test for no adverse shift via class probabilities for two-sample comparison. The scores are out-of-bag predictions from random forests with the package ranger. The prefix *cp* stands for class probability, whether the instance belongs to the training or test set. The probability of belonging to the test set is the relevant notion of outlyingness.

**Usage**

cp_ss(x_train, x_test, sub_ratio = 1/2, R = 1000, num_trees = 500)
Arguments

\begin{itemize}
\item \texttt{x_train} \hspace{1cm} Training sample.
\item \texttt{x_test} \hspace{1cm} Test sample.
\item \texttt{sub_ratio} \hspace{1cm} Subsampling ratio for sample splitting. May be ignored.
\item \texttt{R} \hspace{1cm} The number of permutations. May be ignored.
\item \texttt{num_trees} \hspace{1cm} The number of trees in random forests.
\end{itemize}

Details

This approach uses sample splitting to compute the p-value for inference. \texttt{sub_ratio} splits each sample into two parts: one half for estimation (calibration) and the half for inference, if \texttt{sub_ratio} is 1/2. In other words, it sacrifices some predictive accuracy for inferential robustness as in Rinaldo et al. (2019). The suffix \texttt{ss} refers to sample splitting. Sample splitting relies on the asymptotic null distribution for the weighted AUC (WAUC), the test statistic. Li & Fine (2010) derives its null distribution.

Value

A named list or object of class \texttt{outlier.test} containing:

\begin{itemize}
\item \texttt{statistic} \hspace{1cm} observed WAUC statistic
\item \texttt{seq_mct} \hspace{1cm} sequential Monte Carlo test, if applicable
\item \texttt{p_value} \hspace{1cm} p-value
\item \texttt{outlier_scores} \hspace{1cm} outlier scores from training and test set
\end{itemize}

Notes

Please see references for the classifier two-sample test, the inspiration behind this approach. Note that Cienmencon et al. (2009) uses both sample splitting for inference and the AUC, rather than the WAUC. Most supervised method for binary classification can replace random forests, the default in this implementation.

References

See Also

Other classifiers: `cp_at()`, `cp_pt()`

Examples

```r
library(dsos)
set.seed(12345)
data(iris)
x_train <- iris[1:50, 1:4] # Training sample: Species == 'setosa'
x_test <- iris[51:100, 1:4] # Test sample: Species == 'versicolor'
iris_test <- cp_at(x_train, x_test) # Can also use: cp_ss and cp_pt
str(iris_test)
```

---

**od_pt**  
*Dataset Shift via Isolation Scores*

**Description**

Test for no adverse shift via isolation scores for two-sample comparison. The scores are predictions from extended isolation forest with the package *isotree*. The prefix *od* stands for outlier detection, the relevant notion of outlyingness.

**Usage**

```r
od_pt(x_train, x_test, R = 1000, num_trees = 500, sub_ratio = 1/2)
```

**Arguments**

- `x_train`: Training sample.
- `x_test`: Test sample.
- `R`: The number of permutations. May be ignored.
- `num_trees`: The number of trees in random forests.
- `sub_ratio`: Subsampling ratio for sample splitting. May be ignored.

**Details**

The empirical null distribution uses `R` permutations to estimate the p-value. For speed, this is implemented as a sequential Monte Carlo test with the *simctest* package. See Gandy (2009) for details. The suffix *pt* refers to permutation test. It does not use the asymptotic (theoretical) null distribution for the weighted AUC (WAUC), the test statistic. This is the recommended approach for small samples.
Value

A named list or object of class `outlier.test` containing:

- **statistic**: observed WAUC statistic
- **seq_mct**: sequential Monte Carlo test, if applicable
- **p_value**: p-value
- **outlier_scores**: outlier scores from training and test set

Notes

Isolation forest detects *isolated* points, instances that are typically out-of-distribution relative to the high-density regions of the data distribution. Any performant method for density-based out-of-distribution detection can replace isolation forest, the default in this implementation.

References


Examples

```r
library(dsos)
set.seed(12345)
data(iris)
x_train <- iris[1:50, 1:4] # Training sample: Species == 'setosa'
x_test <- iris[51:100, 1:4] # Test sample: Species == 'versicolor'
iris_test <- od_pt(x_train, x_test) # Can also use: od_ss
str(iris_test)
```

plot.outlier.test

Plot the result of the D-SOS test.

Description

Plot the result of the D-SOS test.
### rd_pt

**Usage**

```r
## S3 method for class 'outlier.test'
plot(x, ...)
```

**Arguments**

- `x`: A `outlier.test` object from a D-SOS test.
- `...`: Placeholder to be compatible with S3 `plot` generic.

**Value**

A `ggplot2` plot with outlier scores and p-value.

**Examples**

```r
set.seed(12345)
data(iris)
x_train <- iris[1:50, 1:4]  # Training sample: Species == 'setosa'
x_test <- iris[51:100, 1:4]  # Test sample: Species == 'versicolor'
iris_test <- od_pt(x_train, x_test)
plot(iris_test)
```

---

**Description**

Test for no adverse shift via residuals for multivariate two-sample comparison. The scores are obtained using out-of-bag predictions from random forest with the package `ranger` to get the residuals. The prefix `rd` stands for residual diagnostics, the relevant notion of outlier. This test assumes that both training and test sets are labeled.

**Usage**

```r
dr_pt(
  x_train,
  x_test,
  R = 1000,
  num_trees = 500L,
  sub_ratio = 1/2,
  response_name = "label"
)
```
Arguments

- `x_train` Training sample.
- `x_test` Test sample.
- `R` The number of permutations. May be ignored.
- `num_trees` The number of trees in random forests.
- `sub_ratio` Subsampling ratio for sample splitting. May be ignored.
- `response_name` The column name of the categorical outcome to predict.

Details

The empirical null distribution uses $R$ permutations to estimate the p-value. For speed, this is implemented as a sequential Monte Carlo test with the `simctest` package. See Gandy (2009) for details. The suffix `pt` refers to permutation test. It does not use the asymptotic (theoretical) null distribution for the weighted AUC (WAUC), the test statistic. This is the recommended approach for small samples.

Value

A named list or object of class `outlier.test` containing:

- `statistic`: observed WAUC statistic
- `seq_mct`: sequential Monte Carlo test, if applicable
- `p_value`: p-value
- `outlier_scores`: outlier scores from training and test set

Notes

Residuals traditionally underpin diagnostics (misspecification) tests in supervised learning. For a contemporaneous example of this approach also using machine learning, see Janková et al. (2020) and references therein.

References


Examples

```r
library(dsos)
set.seed(12345)
data(iris)
idx <- sample(nrow(iris), 2 / 3 * nrow(iris))
xy_train <- iris[idx, ]
xy_test <- iris[-idx, ]
iris_test <- rd_pt(xy_train, xy_test, response_name = "Species")
str(iris_test)
```

---

**rue_pt**  
*Dataset Shift via Resampling (Prediction) Uncertainty*

Description

Test for no adverse shift via prediction uncertainty for two-sample comparison. The scores are out-of-bag predictions from random forests with the package *ranger*. The prefix *rue* stands for resampling uncertainty, the relevant notion of outlier. This uncertainty is the standard error of the mean predictions. This assumes that both training and test sets are labeled.

Usage

```r
rue_pt(
  x_train,
  x_test,
  R = 1000,
  sub_ratio = 1/2,
  num_trees = 500L,
  response_name = "label"
)
```

Arguments

- **x_train**: Training sample.
- **x_test**: Test sample.
- **R**: The number of permutations. May be ignored.
- **sub_ratio**: Subsampling ratio for sample splitting. May be ignored.
- **num_trees**: The number of trees in random forests.
- **response_name**: The column name of the categorical outcome to predict.
Details
The empirical null distribution uses R permutations to estimate the p-value. For speed, this is implemented as a sequential Monte Carlo test with the simctest package. See Gandy (2009) for details. The suffix pt refers to permutation test. It does not use the asymptotic (theoretical) null distribution for the weighted AUC (WAUC), the test statistic. This is the recommended approach for small samples.

Value
A named list or object of class outlier.test containing:

- statistic: observed WAUC statistic
- seq_mct: sequential Monte Carlo test, if applicable
- p_value: p-value
- outlier_scores: outlier scores from training and test set

Notes
For resampling uncertainty, we essentially implement the approach in Schulam & Saria (2019) with random forests. The standard errors of the mean predictions are the underlying scores. Any performant method for confidence-based out-of-distribution detection can replace random forests, the default in this implementation.

References

Examples
library(dsos)
set.seed(12345)
data(iris)
idx <- sample(nrow(iris), 2 / 3 * nrow(iris))
xy_train <- iris[idx, ]
xy_test <- iris[-idx, ]
iris_test <- rue_pt(xy_train, xy_test, response_name = "Species")
str(iris_test)
Description

Computes the weighted AUC with the weighting scheme described in Kamulete, V. M. (2021). This assumes that the training set is the reference distribution and specifies a particular functional form to derive weights from threshold scores.

Usage

```r
wauc_from_os(os_train, os_test)
```

Arguments

- `os_train` Outlier scores in training set.
- `os_test` Outlier scores in test set.

Value

The value (scalar) of the weighted AUC given the weighting scheme.

References


Examples

```r
library(dsos)
set.seed(12345)
os_train <- runif(n = 100)
os_test <- runif(n = 100)
test_stat <- wauc_from_os(os_train, os_test)
```
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