

**coin**: A Computational Framework for Conditional Inference

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1 Introduction

The **coin** package provides a unified approach to conditional inference procedures commonly known as *permutation tests*. The theoretical basis for the design and implementation is the general framework for permutation tests given by Strasser and Weber (1999). For a very flexible formulation of multivariate linear statistics, Strasser and Weber (1999) derived the conditional expectation and covariance of the conditional (permutation) distribution as well as the multivariate limiting distribution. Test procedures for nominal, ordinal and continuous data with or without censoring are all part of this framework. For a more detailed overview see Hothorn *et al.* (2006).

The conceptual Strasser-Weber framework of permutation tests for arbitrary independence and symmetry problems are available via the generic functions `independence_test` and `symmetry_test` respectively. In addition to these very flexible procedures, a large set of convenience functions including well-known as well as lesser-known classical and non-classical procedures for tests of independence between two continuous variables, two- and K-sample tests for location and scale alternatives, tests of independence for contingency tables as well as tests of marginal homogeneity and symmetry have been implemented within the framework. Currently, the following conditional test procedures are available:
These convenience functions essentially perform a certain transformation of the data, e.g., a rank transformation, and then call \texttt{independence.test} or \texttt{symmetry.test} for the computation of the (multivariate) linear statistic and its conditional expectation and covariance as well as the scalar test statistic and its null distribution. The exact null distribution can be approximated by the asymptotic distribution or via conditional Monte Carlo resampling for all test procedures, whereas the exact null distribution is available for special cases only. Moreover, all test procedures allow for the specification of blocks pertaining to, e.g., stratification or repeated measurements.

2 Permutation Tests

In the following we assume that we are provided with $n$ observations

$$(Y_i, X_i, w_i, b_i), \quad i = 1, \ldots, n.$$  

The variables $Y$ and $X$ from sample spaces $\mathcal{Y}$ and $\mathcal{X}$ may be measured at arbitrary scales and may be multivariate as well. In addition to those measurements, case weights $w$ and a factor $b$ coding blocks may be available. For the sake of simplicity, we assume $w_i = 1$ and $b_i = 0$ for all observations $i = 1, \ldots, n$ for the moment.

We are interested in testing the null hypothesis of independence of $Y$ and $X$

$$H_0 : D(Y|X) = D(Y)$$
against arbitrary alternatives. Strasser and Weber (1999) suggest to derive scalar test statistics for testing $H_0$ from multivariate linear statistics of the form

$$\mathbf{T} = \text{vec}\left(\sum_{i=1}^{n} w_i g(X_i) h(Y_i, (Y_1, \ldots, Y_n))\right) \in \mathbb{R}^{pq}. \quad (1)$$

Here, $g : \mathcal{X} \to \mathbb{R}^p$ is a transformation of $X$ known as the regression function and $h : Y \times Y^n \to \mathbb{R}^q$ is a transformation of $Y$ known as the influence function, where the latter may depend on $(Y_1, \ldots, Y_n)$ in a permutation symmetric way. We will give specific examples on how to choose $g$ and $h$ later on.

The distribution of $\mathbf{T}$ depends on the joint distribution of $Y$ and $X$, which is unknown under almost all practical circumstances. At least under the null hypothesis one can dispose of this dependency by fixing $X_1, \ldots, X_n$ and conditioning on all possible permutations $S$ of the responses $Y_1, \ldots, Y_n$. This principle leads to test procedures known as permutation tests.

The conditional expectation $\mu \in \mathbb{R}^{pq}$ and covariance $\Sigma \in \mathbb{R}^{pq \times pq}$ of $\mathbf{T}$ under $H_0$ given all permutations $\sigma \in S$ of the responses are derived by Strasser and Weber (1999):

$$\mu = \mathbb{E}(\mathbf{T}|S) = \text{vec}\left(\sum_{i=1}^{n} w_i g(X_i) \mathbb{E}(h|S)\right),$$

$$\Sigma = \mathbb{V}(\mathbf{T}|S) = \frac{w}{w - 1} \mathbb{V}(h|S) \otimes \left(\sum_{i} w_i g(X_i) \otimes w_i g(X_i)^\top\right) - \frac{1}{w - 1} \mathbb{V}(h|S) \otimes \left(\sum_{i} w_i g(X_i)\right) \otimes \left(\sum_{i} w_i g(X_i)\right)^\top. \quad (2)$$

where $w = \sum_{i=1}^{n} w_i$ denotes the sum of the case weights, and $\otimes$ is the Kronecker product. The conditional expectation of the influence function is

$$\mathbb{E}(h|S) = w^{-1} \sum_{i} w_i h(Y_i, (Y_1, \ldots, Y_n)) \in \mathbb{R}^{q},$$

with corresponding $q \times q$ covariance matrix

$$\mathbb{V}(h|S) = w^{-1} \sum_{i} w_i \left(h(Y_i, (Y_1, \ldots, Y_n)) - \mathbb{E}(h|S)\right) \left(h(Y_i, (Y_1, \ldots, Y_n)) - \mathbb{E}(h|S)\right)^\top.$$

Having the conditional expectation and covariance at hand we are able to standardize a linear statistic $\mathbf{T} \in \mathbb{R}^{pq}$ of the form (1). Univariate test statistics $c$ mapping an observed linear statistic $\mathbf{t} \in \mathbb{R}^{pq}$ into the real line can be of arbitrary form. An obvious choice is the maximum of the absolute values of the standardized linear statistic

$$c_{\text{max}}(\mathbf{t}, \mu, \Sigma) = \max \left| \frac{\mathbf{t} - \mu}{\text{diag}(\Sigma)^{1/2}} \right|$$

utilizing the conditional expectation $\mu$ and covariance matrix $\Sigma$. The application of a quadratic form $c_{\text{quad}}(\mathbf{t}, \mu, \Sigma) = (\mathbf{t} - \mu)\Sigma^+(\mathbf{t} - \mu)^\top$ is one alternative, although computationally more expensive because the Moore-Penrose inverse $\Sigma^+$ of $\Sigma$ is involved.
The definition of one- and two-sided \( p \)-values used for the computations in the \texttt{coin} package is

\[
\begin{align*}
P(c(T, \mu, \Sigma) & \leq c(t, \mu, \Sigma)) \quad \text{(less)} \\
P(c(T, \mu, \Sigma) & \geq c(t, \mu, \Sigma)) \quad \text{(greater)} \\
P(|c(T, \mu, \Sigma)| & \geq |c(t, \mu, \Sigma)|) \quad \text{(two-sided)}.
\end{align*}
\]

Note that for quadratic forms only two-sided \( p \)-values are available and that in the one-sided case maximum type test statistics are replaced by

\[
\min \left( \frac{t - \mu}{\text{diag}(\Sigma)^{1/2}} \right) \quad \text{(less)} \quad \text{and} \quad \max \left( \frac{t - \mu}{\text{diag}(\Sigma)^{1/2}} \right) \quad \text{(greater)}.
\]

The conditional distribution and thus the \( p \)-value of the statistics \( c(t, \mu, \Sigma) \) can be computed in several different ways. For some special forms of the linear statistic, the exact distribution of the test statistic is tractable. For two-sample problems, the shift-algorithm by Streitberg and Röhmel (1986) and Streitberg and Röhmel (1987) and the split-up algorithm by van de Wiel (2001) are implemented as part of the package. Conditional Monte Carlo procedures can be used to approximate the exact distribution. Strasser and Weber (1999) proved (Theorem 2.3) that the conditional distribution of linear statistics \( T \) with conditional expectation \( \mu \) and covariance \( \Sigma \) tends to a multivariate normal distribution with parameters \( \mu \) and \( \Sigma \) as \( n, w \to \infty \). Thus, the asymptotic conditional distribution of test statistics of the form \( c_{\text{max}} \) is normal and can be computed directly in the univariate case (\( pq = 1 \)) or approximated by means of quasi-randomized Monte Carlo procedures in the multivariate setting (Genz, 1992). For quadratic forms \( c_{\text{quad}} \) which follow a \( \chi^2 \) distribution with degrees of freedom given by the rank of \( \Sigma \) (see Johnson and Kotz, 1970, Chapter 29), exact probabilities can be computed efficiently.

3 Illustrations and Applications

The main workhorse \texttt{independence.test} essentially allows for the specification of \( Y, X \) and \( b \) through a formula interface of the form \( y \sim x \mid b \), case weights can be defined by a formula with one variable on the right hand side only. Four additional arguments are available for the specification of the regression function \( g (x\text{trans}) \), the influence function \( h (y\text{trans}) \), the form of the test statistic \( c (\text{teststat}) \) and the null distribution (\text{distribution}).

**Independent \( K \)-Sample Problems.** When we want to compare the distribution of an univariate qualitative response \( Y \) in \( K \) groups given by a factor \( X \) at \( K \) levels, the transformation \( g \) is the dummy matrix coding the groups and \( h \) is either the identity transformation or a some form of rank transformation.

For example, the Kruskal-Wallis test may be computed as follows (example taken from Hollander and Wolfe, 1999, Table 6.3, page 200):

```r
R> library("coin")
R> YOY <- data.frame(
  length = c(46, 28, 46, 37, 32, 41, 42, 45, 38, 44, 42, 60, 32, 42, 45, 58, 27, 51, 42, 52, 38, 33, 26, 25, 28, 28, 26, 27, 27, 27, 31, 30, 27, 29, 30, 25, 25, 24, 27, 30),
  site = gl(4, 10, labels = as.roman(1:4))
R> independence.test(YOY["length"], YOY["site"], distribution = "asym", teststat = "sw", test.statistic = "max")
```


R> it <- independence_test(length ~ site, data = YOY, 
    ytrafo = function(data) 
      trafo(data, numeric_trafo = rank_trafo), 
      teststat = "quadratic")
R> it

Asymptotic General Independence Test

data: length by site (I, II, III, IV)
chi-squared = 22.852, df = 3, p-value = 4.335e-05

The linear statistic $T$ is the sum of the ranks in each group and can be extracted via

R> statistic(it, type = "linear")

<table>
<thead>
<tr>
<th></th>
<th>I</th>
<th>II</th>
<th>III</th>
<th>IV</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>278</td>
<td>307</td>
<td>119</td>
<td>116</td>
</tr>
</tbody>
</table>

Note that statistic(..., type = "linear") currently returns the linear statistic in matrix form, i.e.

$$
\sum_{i=1}^{n} w_{ig}(X_i) h(Y_{i, (Y_1, \ldots, Y_n)})^T \in \mathbb{R}^{p \times q}.
$$

The conditional expectation and covariance are available from

R> expectation(it)

<table>
<thead>
<tr>
<th></th>
<th>I</th>
<th>II</th>
<th>III</th>
<th>IV</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>205</td>
<td>205</td>
<td>205</td>
<td>205</td>
</tr>
</tbody>
</table>

R> covariance(it)

<table>
<thead>
<tr>
<th></th>
<th>I</th>
<th>II</th>
<th>III</th>
<th>IV</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>I</td>
<td>1019.0385</td>
<td>-339.6795</td>
<td>-339.6795</td>
</tr>
<tr>
<td></td>
<td>II</td>
<td>-339.6795</td>
<td>1019.0385</td>
<td>-339.6795</td>
</tr>
<tr>
<td></td>
<td>III</td>
<td>-339.6795</td>
<td>-339.6795</td>
<td>1019.0385</td>
</tr>
<tr>
<td></td>
<td>IV</td>
<td>-339.6795</td>
<td>-339.6795</td>
<td>-339.6795</td>
</tr>
</tbody>
</table>

and the standardized linear statistic $(T - \mu)\text{diag}(\Sigma)^{-1/2}$ is

R> statistic(it, type = "standardized")

<table>
<thead>
<tr>
<th></th>
<th>I</th>
<th>II</th>
<th>III</th>
<th>IV</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>I</td>
<td>2.286797</td>
<td>3.195250</td>
<td>-2.694035</td>
</tr>
</tbody>
</table>

5
Since a quadratic form of the test statistic was requested via `teststat = "quadratic"`, the test statistic is

```R
R> statistic(it)
[1] 22.85242
```

By default, the asymptotic distribution of the test statistic is computed, the p-value is

```R
R> pvalue(it)
[1] 4.334659e-05
```

Life is much simpler with convenience functions very similar to those available in package `stats` for a long time. Here, the exact null distribution of the Kruskal-Wallis test is approximated by Monte Carlo resampling using 10000 replicates via

```R
R> kt <- kruskal_test(length ~ site, data = YOY, 
                      distribution = approximate(nresample = 10000))
R> kt
```

```
Approximative Kruskal-Wallis Test
data: length by site (I, II, III, IV)
chi-squared = 22.852, p-value < 1e-04
```

with p-value (and 99 % confidence interval) of

```R
R> pvalue(kt)
[1] <1e-04
```

99 percent confidence interval:

```
0.0000000000 0.0005296914
```

Of course it is possible to choose a \(c_{\text{max}}\) type test statistic instead of a quadratic form.

**Independence in Contingency Tables.** Independence in general two- or three-dimensional contingency tables can be tested by the Cochran-Mantel-Haenszel test. Here, both \(g\) and \(h\) are dummy matrices (example data from Agresti, 2002, Table 7.8, page 288):

```R
R> data("jobsatisfaction", package = "coin")
R> ct <- cmh_test(jobsatisfaction)
R> ct
```

```
Asymptotic Generalized Cochran-Mantel-Haenszel Test
data: Job.Satisfaction by Income (<5000, 5000-15000, 15000-25000, >25000)
stratified by Gender
chi-squared = 10.2, df = 9, p-value = 0.3345
```

The standardized contingency table allowing for an inspection of the deviation from the null hypothesis of independence of income and jobsatisfaction (stratified by gender) is
Ordered Alternatives. Of course, both job satisfaction and income are ordered variables. When $Y$ is measured at $J$ levels and $X$ at $K$ levels, $Y$ and $X$ are associated with score vectors $\eta \in \mathbb{R}^J$ and $\gamma \in \mathbb{R}^K$, respectively. The linear statistic is now a linear combination of the linear statistic $T$ of the form

$$MT = \text{vec} \left( \sum_{i=1}^{n} w_i \gamma^T g(X_i) \left( \eta^T h(Y_i, (Y_1, \ldots, Y_n)) \right)^T \right) \in \mathbb{R}$$

with $M = \eta \otimes \gamma$.

By default, scores are $\eta = 1, \ldots, J$ and $\gamma = 1, \ldots, K$.

R> statistic(ct, type = "standardized")

<table>
<thead>
<tr>
<th></th>
<th>Very Dissatisfied</th>
<th>A Little Satisfied</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;5000</td>
<td>1.3112789</td>
<td>0.69201053</td>
</tr>
<tr>
<td>5000-15000</td>
<td>0.6481783</td>
<td>0.83462550</td>
</tr>
<tr>
<td>15000-25000</td>
<td>-1.0958361</td>
<td>-1.50130926</td>
</tr>
<tr>
<td>&gt;25000</td>
<td>-1.0377629</td>
<td>-0.08983052</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Moderately Satisfied</th>
<th>Very Satisfied</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;5000</td>
<td>-0.2478705</td>
<td>-0.9293458</td>
</tr>
<tr>
<td>5000-15000</td>
<td>0.5175755</td>
<td>-1.6257547</td>
</tr>
<tr>
<td>15000-25000</td>
<td>0.2361231</td>
<td>1.4614123</td>
</tr>
<tr>
<td>&gt;25000</td>
<td>-0.5946119</td>
<td>1.2031648</td>
</tr>
</tbody>
</table>

R> lbl_test(jobsatisfaction)

Asymptotic Linear-by-Linear Association Test

data: Job.Satisfaction (ordered) by
  Income (<5000 < 5000-15000 < 15000-25000 < >25000)
  stratified by Gender
Z = 2.5736, p-value = 0.01006
alternative hypothesis: two.sided

The scores $\eta$ and $\gamma$ can be specified to the linear-by-linear association test via a list whose names correspond to the variable names

R> lbl_test(jobsatisfaction, scores = list(Job.Satisfaction = c(1, 3, 4, 5), Income = c(3, 10, 20, 35)))

Asymptotic Linear-by-Linear Association Test

data: Job.Satisfaction (ordered) by
  Income (<5000 < 5000-15000 < 15000-25000 < >25000)
  stratified by Gender
Z = 2.4812, p-value = 0.01309
alternative hypothesis: two.sided

Alternatively, scores can be specified through of_trafo
Asymptotic Linear-by-Linear Association Test
data: Job.Satisfaction (ordered) by Income (<5000 < 5000-15000 < 15000-25000 < >25000) stratified by Gender
Z = 2.4812, p-value = 0.01309 alternative hypothesis: two.sided

Incomplete Randomised Blocks. Rayner and Best (2001), Chapter 7, discuss the application of Durbin’s test to data from sensory experiments, where incomplete block designs are common. As an example, data from taste-testing on ten dried eggs where mean scores for off-flavour from seven judges are given and one wants to assess whether there is any difference in the scores between the ten egg samples. The sittings are a block variable which can be added to the formula via ‘|’.

R> egg_data <- data.frame(  
  scores = c(9.7, 8.7, 5.4, 5.0, 9.6, 8.8, 5.6, 3.6, 9.0,  
    7.3, 3.8, 4.3, 9.3, 8.7, 6.8, 3.8, 10.0, 7.5,  
    4.2, 2.8, 9.6, 5.1, 4.6, 3.6, 9.8, 7.4, 4.4,  
    3.8, 9.4, 6.3, 5.1, 2.0, 9.4, 9.3, 8.2, 3.3,  
    8.7, 9.0, 6.0, 3.3, 9.7, 6.7, 6.6, 2.8, 9.3,  
    8.1, 3.7, 2.6, 9.8, 7.3, 5.4, 4.0, 9.0, 8.3,  
    4.8, 3.8, 9.3, 8.3, 6.3, 3.8),  
  sitting = factor(rep(c(1:15), rep(4, 15))),  
  product = factor(c(1, 2, 4, 5, 2, 3, 6, 10, 2, 4, 6, 7,  
    1, 3, 5, 7, 1, 4, 8, 10, 2, 7, 8, 9,  
    2, 5, 8, 10, 5, 7, 9, 10, 1, 2, 3, 9,  
    4, 5, 6, 9, 1, 6, 7, 10, 3, 4, 9, 10,  
    1, 6, 8, 9, 3, 4, 7, 8, 3, 5, 6, 8))
)

R> independence_test(scores ~ product | sitting,  
  data = egg_data, teststat = "quadratic",  
  ytrafo = function(data)  
    trafo(data, numeric_trafo = rank_trafo,  
      block = egg_data$sitting))

Asymptotic General Independence Test
data: scores by product (1, 2, 3, 4, 5, 6, 7, 8, 9, 10) stratified by sitting
chi-squared = 39.12, df = 9, p-value = 1.096e-05
and the Monte Carlo p-value can be computed via
If we assume that the products are ordered, the Page test is appropriate and can be computed as follows:

```r
R> independence_test(scores ~ product | sitting,
  data = egg_data,
  ytrafo = function(data)
    trafo(data, numeric_trafo = rank_trafo,
          block = egg_data$sitting),
  scores = list(product = 1:10))

Asymptotic General Independence Test

data: scores by product (1 < 2 < 3 < 4 < 5 < 6 < 7 < 8 < 9 < 10)
stratified by sitting
Z = -6.2166, p-value = 5.081e-10
alternative hypothesis: two.sided
```

### Multiple Tests.

One may be interested in testing multiple hypotheses simultaneously, either by using a linear combination of the linear statistic $K_T$, or by specifying multivariate variables $Y$ and/or $X$. For example, all pair comparisons may be implemented via:

```r
R> it <- independence_test(length ~ site, data = YOY,
                           xtrafo = mcp_trafo(site = "Tukey"),
                           teststat = "maximum",
                           distribution = "approximate")

R> pvalue(it)

[1] 1e-04
99 percent confidence interval:
 5.012541e-07 7.427741e-04
```

```r
R> pvalue(it, method = "single-step")

II - I  0.6618
III - I  0.0399
IV - I  0.0228
III - II  0.0001
IV - II  0.0001
IV - III  0.9989
```

9
When either $g$ or $h$ are multivariate, single-step adjusted $p$-values based on maximum-type statistics are computed as described in Westfall and Young (1993), algorithm 2.5 (page 47) and equation (2.8), page 50. Note that for the example shown above only the minimum $p$-value is adjusted appropriately because the subset pivotality condition is violated, i.e., the distribution of the test statistics under the complete null-hypothesis of no treatment effect of site is the basis of all adjustments instead of the corresponding partial null-hypothesis.

4 Quality Assurance

The test procedures implemented in package coin are continuously checked against results obtained by the corresponding implementations in package stats (where available). In addition, the test statistics and exact, approximative and asymptotic $p$-values for data examples given in the StatXact-6 user manual (Cytel Inc., 2003) are compared with the results reported in the StatXact-6 manual. Step-down multiple adjusted $p$-values have been checked against results reported by mt.maxT from package multtest (Pollard et al., 2008). For details on the test procedures we refer to the R transcript files in directory coin/tests.

5 Acknowledgements

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References


