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:

spearman_test	Spearman correlation test		
_ fisyat_test	Fisher-Yates correlation test		
quadrant_test	Quadrant test		
- koziol_test	Koziol-Nemec test		
oneway_test	Two- and K-sample Fisher-Pitman permutation test		
wilcox_test	Wilcoxon-Mann-Whitney test		
kruskal_test	Kruskal-Wallis test		
normal_test	Two- and K -sample van der Waerden test		
median_test	Two- and K-sample Brown-Mood median test		
savage_test	Two- and K-sample Savage test		
taha_test	Two- and K -sample Taha test		
klotz_test	Two- and K -sample Klotz test		
mood_test	Two- and K-sample Mood test		
ansari_test	Two- and K-sample Ansari-Bradley test		
fligner_test	Two- and K-sample Fligner-Killeen test		
conover_test	Two- and K-sample Conover-Iman test		
logrank_test	Two- and K -sample weighted logrank tests		
	(Logrank test, Gehan-Breslow test, Tarone-Ware test,)		
sign_test	Sign test		
wilcoxsign_test	Wilcoxon signed-rank test		
friedman_test	Friedman test and Page test		
quade_test	Quade test		
chisq_test	Pearson χ^2 test		
cmh_test	Generalized Cochran-Mantel-Haenszel test		
lbl_test	Linear-by-linear association test		
mh_test	Marginal homogeneity tests		
	(McNemar test, Cochran Q test, Stuart-Maxwell test,)		
maxstat_test	Generalized maximally selected statistics		

These convenience functions essentially perform a certain transformation of the data, e.g., a rank transformation, and then call independence_test or 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

$$(\mathbf{Y}_i, \mathbf{X}_i, w_i, b_i), \quad i = 1, \dots, n$$

The variables \mathbf{Y} and \mathbf{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 ${f Y}$ and ${f X}$

$$H_0: D(\mathbf{Y}|\mathbf{X}) = D(\mathbf{Y})$$

against arbitrary alternatives. Strasser and Weber (1999) suggest to derive scalar test statistics for testing H_0 from multivariate linear statistics of the form

$$\mathbf{T} = \operatorname{vec}\left(\sum_{i=1}^{n} w_i g(\mathbf{X}_i) h(\mathbf{Y}_i, (\mathbf{Y}_1, \dots, \mathbf{Y}_n))^{\top}\right) \in \mathbb{R}^{pq}.$$
(1)

Here, $g: \mathcal{X} \to \mathbb{R}^p$ is a transformation of **X** known as the *regression function* and $h: \mathcal{Y} \times \mathcal{Y}^n \to \mathbb{R}^q$ is a transformation of **Y** known as the *influence function*, where the latter may depend on $(\mathbf{Y}_1, \ldots, \mathbf{Y}_n)$ 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 \mathbf{Y} and \mathbf{X} , which is unknown under almost all practical circumstances. At least under the null hypothesis one can dispose of this dependency by fixing $\mathbf{X}_1, \ldots, \mathbf{X}_n$ and conditioning on all possible permutations S of the responses $\mathbf{Y}_1, \ldots, \mathbf{Y}_n$. 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 **T** under H_0 given all permutations $\sigma \in S$ of the responses are derived by Strasser and Weber (1999):

$$\mu = \mathbb{E}(\mathbf{T}|S) = \operatorname{vec}\left(\left(\sum_{i=1}^{n} w_{i}g(\mathbf{X}_{i})\right)\mathbb{E}(h|S)^{\top}\right),$$

$$\Sigma = \mathbb{V}(\mathbf{T}|S)$$

$$= \frac{\mathbf{w}}{\mathbf{w}} \mathbb{V}(h|S) \otimes \left(\sum_{i} w_{i}g(\mathbf{X}_{i}) \otimes w_{i}g(\mathbf{X}_{i})^{\top}\right)$$

$$- \frac{1}{\mathbf{w}} \mathbb{V}(h|S) \otimes \left(\sum_{i} w_{i}g(\mathbf{X}_{i})\right) \otimes \left(\sum_{i} w_{i}g(\mathbf{X}_{i})\right)^{\top}$$
(2)

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

$$\mathbb{E}(h|S) = \mathbf{w}_{\cdot}^{-1} \sum_{i} w_{i}h(\mathbf{Y}_{i}, (\mathbf{Y}_{1}, \dots, \mathbf{Y}_{n})) \in \mathbb{R}^{q}$$

with corresponding $q \times q$ covariance matrix

$$\mathbb{V}(h|S) = \mathbf{w}_{\cdot}^{-1} \sum_{i} w_{i} \left(h(\mathbf{Y}_{i}, (\mathbf{Y}_{1}, \dots, \mathbf{Y}_{n})) - \mathbb{E}(h|S) \right)$$
$$\left(h(\mathbf{Y}_{i}, (\mathbf{Y}_{1}, \dots, \mathbf{Y}_{n})) - \mathbb{E}(h|S) \right)^{\top}.$$

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

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

utilizing the conditional expectation μ and covariance matrix Σ . 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 Σ^+ of Σ is involved.

The definition of one- and two-sided p-values used for the computations in the **coin** package is

$$\begin{array}{lll} P(c(\mathbf{T}, \mu, \Sigma) &\leq c(\mathbf{t}, \mu, \Sigma)) & (\text{less}) \\ P(c(\mathbf{T}, \mu, \Sigma) &\geq c(\mathbf{t}, \mu, \Sigma)) & (\text{greater}) \\ P(|c(\mathbf{T}, \mu, \Sigma)| &\geq |c(\mathbf{t}, \mu, \Sigma)|) & (\text{two-sided}). \end{array}$$

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

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

The conditional distribution and thus the *p*-value of the statistics $c(\mathbf{t}, \mu, \Sigma)$ 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 \mathbf{T} with conditional expectation μ and covariance Σ tends to a multivariate normal distribution with parameters μ and Σ as $n, \mathbf{w}. \to \infty$. Thus, the asymptotic conditional distribution of test statistics of the form c_{\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_{quad} which follow a χ^2 distribution with degrees of freedom given by the rank of Σ (see Johnson and Kotz, 1970, Chapter 29), exact probabilities can be computed efficiently.

3 Illustrations and Applications

The main workhorse independence_test essentially allows for the specification of \mathbf{Y}, \mathbf{X} and b through a formula interface of the form $\mathbf{y} ~ \mathbf{x} | \mathbf{b}$, 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 (xtrans), the influence function h (ytrans), the form of the test statistic c (teststat) and the null distribution (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> 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 \mathbf{T} is the sum of the ranks in each group and can be extracted via

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

I 278 II 307 III 119 IV 116

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

$$\sum_{i=1}^{n} w_i g(\mathbf{X}_i) h(\mathbf{Y}_i, (\mathbf{Y}_1, \dots, \mathbf{Y}_n))^\top \in \mathbb{R}^{p \times q}.$$

The conditional expectation and covariance are available from

R> expectation(it) Ι 205 II 205 III 205 IV 205 R> covariance(it) ΙI III ΙV Ι 1019.0385 -339.6795 -339.6795 -339.6795 I II -339.6795 1019.0385 -339.6795 -339.6795 III -339.6795 -339.6795 1019.0385 -339.6795 IV -339.6795 -339.6795 -339.6795 1019.0385 and the standardized linear statistic $(\mathbf{T}-\mu)\mathrm{diag}(\Sigma)^{-1/2}$ is R> statistic(it, type = "standardized") 2.286797 Ι II 3.195250 III -2.694035 IV -2.788013

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

R> statistic(it)

[1] 22.85242

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

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

0.000000000 0.0005296914

Of course it is possible to choose a c_{\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> data("jobsatisfaction", package = "coin")
R> ct <- cmh_test(jobsatisfaction)
R> ct
```

Asymptotic Generalized Cochran-Mantel-Haenszel Test

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

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

	Very Dissatisfied A	Little Satisfied
<5000	1.3112789	0.69201053
5000-15000	0.6481783	0.83462550
15000-25000	-1.0958361	-1.50130926
>25000	-1.0377629	-0.08983052
	Moderately Satisfied	Very Satisfied
<5000	-0.2478705	-0.9293458
5000-15000	0.5175755	-1.6257547
15000-25000	0.2361231	1.4614123
>25000	-0.5946119	1.2031648

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

$$\mathbf{MT} = \operatorname{vec}\left(\sum_{i=1}^{n} w_i \gamma^{\top} g(\mathbf{X}_i) \left(\eta^{\top} h(\mathbf{Y}_i, (\mathbf{Y}_1, \dots, \mathbf{Y}_n))^{\top}\right) \in \mathbb{R} \text{ with } \mathbf{M} = \eta \otimes \gamma.$$

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

R> lbl_test(jobsatisfaction)

Asymptotic Linear-by-Linear Association Test

The scores η and γ can be specified to the linear-by-linear association test via a list whose names correspond to the variable names

Alternatively, scores can be specified through of_trafo

```
R> lbl_test(jobsatisfaction,
    ytrafo = function(data)
        trafo(data, ordered_trafo = function(y)
            of_trafo(y, scores = c(1, 3, 4, 5))),
    xtrafo = function(data)
        trafo(data, ordered_trafo = function(x)
            of_trafo(x, scores = 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
```

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(</pre>
       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

```
99 percent confidence interval:
0.00000000 0.000264894
```

If we assume that the products are ordered, the Page test is appropriate and can be computed as follows

Multiple Tests. One may be interested in testing multiple hypotheses simultaneously, either by using a linear combination of the linear statistic \mathbf{KT} , or by specifying multivariate variables \mathbf{Y} and/or \mathbf{X} . For example, all pair comparisons may be implemented via

```
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> 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
```

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**.

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