coin: A Computational Framework for Conditional Inference

Torsten Hothorn¹, Kurt Hornik², Mark van de Wiel³ and Achim Zeileis²

¹Institut für Medizininformatik, Biometrie und Epidemiologie Friedrich-Alexander-Universität Erlangen-Nürnberg Waldstraße 6, D-91054 Erlangen, Germany Torsten.Hothorn@R-project.org

²Department für Statistik und Mathematik, Wirtschaftsuniversität Wien Augasse 2-6, A-1090 Wien, Austria Kurt.Hornik@R-project.org
Achim.Zeileis@R-project.org

³Department of Mathematics, Vrije Universiteit De Boelelaan 1081a, 1081 HV Amsterdam, The Netherlands mark.vdwiel@vumc.nl

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-Nemec test koziol_test Two- and K-sample Fisher-Pitman permutation test oneway_test wilcox_test Wilcoxon-Mann-Whitney test kruskal_test Kruskal-Wallis test Two- and K-sample van der Waerden test normal_test median_test Two- and K-sample Brown-Mood median test Two- and K-sample Savage test savage_test Two- and K-sample Taha test taha_test klotz_test Two- and K-sample Klotz test Two- and K-sample Mood test mood_test ansari_test Two- and K-sample Ansari-Bradley test Two- and K-sample Fligner-Killeen test fligner_test conover_test Two- and K-sample Conover-Iman test Two- and K-sample weighted logrank tests logrank_test (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

Pearson χ^2 test chisq_test

Generalized Cochran-Mantel-Haenszel test cmh_test

lbl_test Linear-by-linear association test Marginal homogeneity tests mh_test

(McNemar test, Cochran Q test, Stuart-Maxwell test, . . .)

Generalized maximally selected statistics maxstat_test

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 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 bcoding blocks may be available. For the sake of simplicity, we assume $w_i = 1$ and $b_i = 0$ for all observations i = 1, ..., n for the moment.

We are interested in testing the null hypothesis of independence of Y and 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 $(\mathbf{Y}_1, \dots, \mathbf{Y}_n)$ 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):

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

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

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

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

$$(2)$$

where $\mathbf{w} = \sum_{i=1}^{n} w_i$ 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

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

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

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

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

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

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 $\mathbf{y} \sim \mathbf{x} \mid \mathbf{b}$, 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 h (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):

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")

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)

I 205

II 205

III 205

IV 205

R> covariance(it)

I II III IV

I 1019.0385 -339.6795 -339.6795 -339.6795

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 $(\mathbf{T} - \mu) \operatorname{diag}(\Sigma)^{-1/2}$ is

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

I 2.286797

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)
```

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

```
R> pvalue(it)
```

[1] 22.85242

```
[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

```
data: length by site (I, II, III, IV)
chi-squared = 22.852, p-value < 1e-04</pre>
```

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

```
R> pvalue(kt)
```

```
[1] <1e-04
99 percent confidence interval:
0.0000000000 0.0005296914</pre>
```

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 I	ittle 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	Moderately Satisfied -0.2478705	Very Satisfied -0.9293458
<5000 5000-15000	•	•
	-0.2478705	-0.9293458

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 $\eta = 1, ..., J$ and $\gamma = 1, ..., K$.

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

Asymptotic Linear-by-Linear Association Test

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(
       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
```

```
R> pvalue(independence_test(scores ~ product | sitting,
              data = egg_data, teststat = "quadratic",
              ytrafo = function(data)
                   trafo(data, numeric_trafo = rank_trafo,
                         block = egg_data$sitting),
              distribution = approximate(nresample = 19999)))
[1] <5.00025e-05
99 percent confidence interval:
0.00000000 0.000264894
If we assume that the products are ordered, the Page test is appropriate and can be computed
as follows
R> independence_test(scores ~ product | sitting,
       data = egg_data,
       ytrafo = function(data)
           trafo(data, numeric_trafo = rank_trafo,
                  block = egg_data$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 KT, or by specifying multivariate variables Y
and/or 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**.

5 Acknowledgements

We would like to thank Helmut Strasser for discussions on the theoretical framework. Henric Winell provided clarification and examples for the Stuart-Maxwell test.

References

- Agresti A (2002). Categorical Data Analysis. 2nd edition. John Wiley & Sons, Hoboken, New Jersey.
- Cytel Inc (2003). StatXact 6: Statistical Software for Exact Nonparametric Inference. Cytel Software Corporation, Cambridge, MA. URL http://www.cytel.com/.
- Genz A (1992). "Numerical Computation of Multivariate Normal Probabilities." *Journal of Computational and Graphical Statistics*, **1**, 141–149.
- Hollander M, Wolfe DA (1999). *Nonparametric Statistical Inference*. 2nd edition. John Wiley & Sons, New York.
- Hothorn T, Hornik K, van de Wiel MA, Zeileis A (2006). "A Lego System for Conditional Inference." The American Statistician, 60(3), 257–263. doi:10.1198/000313006X118430.
- Johnson NL, Kotz S (1970). Distributions in Statistics: Continuous Univariate Distributions 2. John Wiley & Sons, New York.
- Pollard KS, Ge Y, Dudoit S (2008). multtest: Resampling-Based Multiple Hypothesis Testing. R package version 1.21.1, URL http://CRAN.R-project.org/package=multtest.
- Rayner JCW, Best DJ (2001). A Contingency Table Approach to Nonparametric Testing. Chapman & Hall, New York.
- Strasser H, Weber C (1999). "On the Asymptotic Theory of Permutation Statistics." *Mathematical Methods of Statistics*, **8**(2), 220–250. Preprint available from http://epub.wu-wien.ac.at/dyn/openURL?id=oai:epub.wu-wien.ac.at:epub-wu-01_94c.

- Streitberg B, Röhmel J (1986). "Exact Distributions for Permutation and Rank Tests: An Introduction to Some Recently Published Algorithms." *Statistical Software Newsletter*, **12**(1), 10–17. ISSN 1609-3631.
- Streitberg B, Röhmel J (1987). "Exakte Verteilungen für Rang- und Randomisierungstests im allgemeinen c-Stichprobenfall." EDV in Medizin und Biologie, $\mathbf{18}(1)$, 12-19.
- van de Wiel MA (2001). "The Split-Up Algorithm: A Fast Symbolic Method for Computing p-Values of Distribution-Free Statistics." Computational Statistics, 16, 519–538.
- Westfall PH, Young SS (1993). Resampling-Based Multiple Testing. John Wiley & Sons, New York.