

The Newsletter of the R Project

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Editorial

by Torsten Hothorn

Shortly before the end of 2007 it's a great pleasure for me to welcome you to the third and Christmas issue of R News. Also, it is the last issue for me as editorial board member and before John Fox takes over as editor-in-chief, I would like to thank Doug Bates, Paul Murrell, John Fox and Vince Carey whom I had the pleasure to work with during the last three years.

It is amazing to see how many new packages have been submitted to CRAN since October when Kurt Hornik previously provided us with the latest CRAN news. Kurt's new list starts at page 57. Most of us have already installed the first patch release in the 2.6.0 series. The most important facts about R 2.6.1 are given on page 56.

The contributed papers in the present issue may be divided into two groups. The first group focuses on applications and the second group reports on tools that may help to interact with R. Sanford Weisberg and Hadley Wickham give us some **hints** when our brain fails to remember the name of some important R function. Patrick Mair and Reinhold Hatzinger started a CRAN Psychometrics Task View and give us a snapshot of current developments. Robin Hankin deals with very large numbers in R using his **Brobdingnag** package. Two papers focus on graphical user interfaces. From a high-level point of view, John Fox shows how the functionality of his R Commander can be extended by plug-in packages. John Verzani gives an introduction to low-level GUI programming using the **gWidgets** package.

Applications presented here include a study on the performance of financial advices given in the Mad Money television show on CNBC, as investigated by Bill Alpert. Hee-Seok Oh and Donghoh Kim present a package for the analysis of scattered spherical data, such as certain environmental conditions measured over some area. Sebastián Luque follows aquatic animals into the depth of the sea and analyzes their diving behavior. Three packages concentrate on bringing modern statistical methodology to our computers: Parametric and semi-parametric Bayesian inference is implemented in the DPpackage by Alejandro Jara, Guido Schwarzer reports on the meta package for meta-analysis and, finally, a new version of the well-known multtest package is described by Sandra L. Taylor and her colleagues.

The editorial board wants to thank all authors and referees who worked with us in 2007 and wishes all of you a Merry Christmas and a Happy New Year 2008!

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SpherWave: An R Package for Analyzing Scattered Spherical Data by Spherical Wavelets

by Hee-Seok Oh and Donghoh Kim

Introduction

Given scattered surface air temperatures observed on the globe, we would like to estimate the temperature field for every location on the globe. Since the temperature data have inherent multiscale characteristics, spherical wavelets with localization properties are particularly effective in representing multiscale structures. Spherical wavelets have been introduced in Narcowich and Ward (1996) and Li (1999). A successful statistical application has been demonstrated in Oh and Li (2004).

SpherWave is an R package implementing the spherical wavelets (SWs) introduced by Li (1999) and the SW-based spatially adaptive methods proposed by Oh and Li (2004). This article provides a general description of SWs and their statistical applications, and it explains the use of the **SpherWave** package through an example using real data.

Before explaining the algorithm in detail, we first consider the average surface air temperatures (in degrees Celsius) during the period from December 1967 to February 1968 observed at 939 weather stations, as illustrated in Figure 1.



Figure 1: Average surface air temperatures observed at 939 weather stations during the years 1967-1968.

In the **SpherWave** package, the data are obtained by

```
> library("SpherWave")
> ### Temperature data from year 1961 to 1990
> ### list of year, grid, observation
> data("temperature")
> temp67 <- temperature$obs[temperature$year==1967]
> latlon <-
+ temperature$latlon[temperature$year==1967, ]</pre>
```

and Figure 1 is plotted by the following code.

> sw.plot(z=temp67, latlon=latlon, type="obs", + xlab="", ylab="")

Similarly, various signals such as meteorological or geophysical signal in nature can be measured at scattered and unevenly distributed locations. However, inferring the substantial effect of such signals at an arbitrary location on the globe is a crucial task. The first objective of using SWs is to estimate the signal at an arbitrary location on the globe by extrapolating the scattered observations. An example is the representation in Figure 2, which is obtained by extrapolating the observations in Figure 1. This result can be obtained by simply executing the function sbf (). The details of its arguments will be presented later.

- > netlab <- network.design(latlon=latlon,</pre>
- + method="ModifyGottlemann", type="regular", x=5)
- > eta <- eta.comp(netlab)\$eta
- > out.pls <- sbf(obs=temp67, latlon=latlon,</pre>
- + netlab=netlab, eta=eta, method="pls",
- + grid.size=c(100, 200), lambda=0.8)
- > sw.plot(out.pls, type="field", xlab="Longitude",
- ylab="Latitude")



Figure 2: An extrapolation for the observations in Figure 1.

Note that the representation in Figure 2 has inherent multiscale characteristics, which originate from the observations in Figure 1. For example, observe the global cold patterns near the north pole with local anomalies of the extreme cold in the central Canadian shield. Thus, classical methods such as spherical harmonics or smoothing splines are not very efficient in representing temperature data since they do not capture local properties. It is important to detect and explain local activities and variabilities as well as global trends. The second objective of using SWs is to decompose the signal properly according to spatial scales so as to capture the various activities of fields. Finally, SWs can be employed in developing a procedure to denoise the observations that are corrupted by noise. This article illustrates these procedures through an analysis of temperature data. In summary, the aim of this article is to explain how the **SpherWave** package is used in the following:

1) estimating the temperature field T(x) for an arbitrary location x on the globe, given the scattered observations $y_i, i = 1, ..., n$, from the model

$$y_i = T(x_i) + \epsilon_i, \quad i = 1, 2, ..., n,$$
 (1)

where x_i denote the locations of observations on the globe and e_i are the measurement errors;

- 2) decomposing the signal by the multiresolution analysis; and
- 3) obtaining a SW estimator using a thresholding approach.

As will be described in detail later, the multiresolution analysis and SW estimators of the temperature field can be derived from the procedure termed multiscale spherical basis function (SBF) representation.

Theory

In this section, we summarize the SWs proposed by Li (1999) and its statistical applications proposed by Oh and Li (2004) for an understanding of the methodology and promoting the usage of the **Spher-Wave** package.

Narcowich and Ward (1996) proposed a method to construct SWs for scattered data on a sphere. They proposed an SBF representation, which is a linear combination of localized SBFs centered at the locations of the observations. However, the Narcowich-Ward method suffers from a serious problem: the SWs have a constant spatial scale regardless of the intended multiscale decomposition. Li (1999) introduced a new multiscale SW method that overcomes the single-scale problem of the Narcowich-Ward method and truly represents spherical fields with multiscale structure.

When a network of *n* observation stations $\mathcal{N}_1 := \{x_i\}_{i=1}^n$ is given, we can construct nested networks $\mathcal{N}_1 \supset \mathcal{N}_2 \supset \cdots \supset \mathcal{N}_L$ for some *L*. We re-index the subscript of the location x_i so that x_{li} belongs to $\mathcal{N}_l \setminus \mathcal{N}_{l+1} = \{x_{li}\}_{i=1}^{M_l} \ (l = 1, \cdots, L; \mathcal{N}_{L+1} := \emptyset)$, and use the convention that the scale moves from the finest to the smoothest as the resolution level index *l* increases. The general principle of the multiscale SBF representation proposed by Li (1999) is to employ linear combinations of SBFs with various scale parameters to approximate the underlying field T(x) of the model in equation (1). That is, for some *L*

$$T_1(x) = \sum_{l=1}^{L} \sum_{i=1}^{M_l} \beta_{li} \phi_{\eta_l}(\theta(x, x_{li})),$$
(2)

where ϕ_{η_l} denotes SBFs with a scale parameter η_l and $\theta(x, x_i)$ is the cosine of the angle between two location x and x_i represented by the spherical coordinate system. Thus geodetic distance is used for spherical wavelets, which is desirable for the data on the globe. An SBF $\phi(\theta(x, x_i))$ for a given spherical location x_i is a spherical function of x that peaks at $x = x_i$ and decays in magnitude as x moves away from x_i . A typical example is the Poisson kernel used by Narcowich and Ward (1996) and Li (1999).

Now, let us describe a multiresolution analysis procedure that decomposes the SBF representation (2) into global and local components. As will be seen later, the networks N_l can be arranged in such a manner that the sparseness of stations in N_l increases as the index l increases, and the bandwidth of ϕ can also be chosen to increase with l to compensate for the sparseness of stations in N_l . By this construction, the index l becomes a true scale parameter. Suppose T_l , l = 1, ..., L, belongs to the linear subspace of all SBFs that have scales greater than or equal to l. Then T_l can be decomposed as

$$T_l(x) = T_{l+1}(x) + D_l(x),$$

where T_{l+1} is the projection of T_l onto the linear subspace of SBFs on the networks \mathcal{N}_{l+1} , and D_l is the orthogonal complement of T_l . Note that the field D_l can be interpreted as the field containing the local information. This local information cannot be explained by the field T_{l+1} which only contains the global trend extrapolated from the coarser network \mathcal{N}_{l+1} . Therefore, T_{l+1} is called the global component of scale l + 1and D_l is called the local component of scale l. Thus, the field T_1 in its SBF representation (equation (2)) can be successively decomposed as

$$T_1(x) = T_L(x) + \sum_{l=1}^{L-1} D_l(x).$$
 (3)

In general wavelet terminology, the coefficients of T_L and D_l of the SW representation in equation (3) can be considered as the smooth coefficients and detailed coefficients of scale l, respectively.

The extrapolated field may not be a stable estimator of the underlying field *T* because of the noise in the data. To overcome this problem, Oh and Li (2004) propose the use of thresholding approach pioneered by Donoho and Johnstone (1994). Typical thresholding types are hard and soft thresholding. By hard thresholding, small SW coefficients, considered as originating from the zero-mean noise, are set to zero while the other coefficients, considered as originating from the signal, are left unchanged. In soft thresholding, not only are the small coefficients set to zero but the large coefficients are also shrunk toward zero, based on the assumption that they are corrupted by additive noise. A reconstruction from these coefficients yields the SW estimators.

Network design and bandwidth selection

As mentioned previously, a judiciously designed network N_l and properly chosen bandwidths for the SBFs are required for a stable multiscale SBF representation.

In the **SpherWave** package, we design a network for the observations in Figure 1 as

```
> netlab <- network.design(latlon=latlon,
+ method="ModifyGottlemann", type="regular")</pre>
```

```
+ method="ModifyGottlemann", type="regular", x=5)
> sw.plot(z=netlab, latlon=latlon, type="network",
```

```
+ xlab="", ylab="", cex=0.6)
```

We then obtain the network in Figure 3, which consists of 6 subnetworks.

```
> table(netlab)
netlab
    1   2   3   4   5   6
686 104   72   44   25   8
```

Note that the number of stations at each level decreases as the resolution level increases. The most detailed subnetwork 1 consists of 686 stations while the coarsest subnetwork 6 consists of 8 stations.



Figure 3: Network Design

The network design in the **SpherWave** package depends only on the location of the data and the template grid, which is predetermined without considering geophysical information. To be specific, given a template grid and a radius for the spherical cap, we can design a network satisfying two conditions for stations: 1) choose the stations closest to the template grid so that the stations could be distributed as uniformly as possible over the sphere, and 2) select stations between consecutive resolution levels so that the resulting stations between two levels are not too close for the minimum radius of the spherical cap. This scheme ensures that the density of N_l decreases as the resolution level index l increases. The function network.design() is performed by the following parameters: latlon denotes the matrix of grid points (latitude, longitude) of the observation locations. The SpherWave package uses the following convention. Latitude is the angular distance in degrees of a point north or south of the equator and North and South are represented by "+" and "-" signs, respectively. Longitude is the angular distance in degrees of a point east or west of the prime (Greenwich) meridian, and East and West are represented by "+" and "-" signs, respectively. method has four options for making a template grid - "Gottlemann", "ModifyGottlemann", "Oh", and "cover". For details of the first three methods, see Oh and Kim (2007). "cover" is the option for utilizing the function cover.design() in the package fields. Only when using the method "cover", provide nlevel, which denotes a vector of the number of observations in each level, starting from the resolution level 1. type denotes the type of template grid; it is specified as either "regular" or "reduce". The option "reduce" is designed to overcome the problem of a regular grid, which produces a strong concentration of points near the poles. The parameter x is the minimum radius of the spherical cap.

Since the index l is a scale index in the resulting multiscale analysis, as l increases, the density of \mathcal{N}_l decreases and the bandwidth of ϕ_{η_l} increases. The bandwidths can be supplied by the user. Alternatively, the **SpherWave** package provides its own function for the automatic choosing of the bandwidths. For example, the bandwidths for the network design using "ModifyGottlemann" can be chosen by the following procedure.

> eta <- eta.comp(netlab)\$eta</pre>

Note that η can be considered as a spatial parameter of the SBF induced by the Poisson kernel: the SBF has a large bandwidth when η is small, while a large η produces an SBF with a small bandwidth. netlab denotes the index vector of the subnetwork level. Assuming that the stations are distributed equally over the sphere, we can easily find how many stations are required in order to cover the entire sphere with a fixed spatial parameter η and, conversely, how large a bandwidth for the SBFs is required to cover the entire sphere when the number of stations are given. The function eta.comp() utilizes this observation.

Multiscale SBF representation

Once the network and bandwidths are decided, the multiscale SBF representation of equation (2) can be implemented by the function sbf(). This function is controlled by the following arguments.

- obs : the vector of observations
- latlon : the matrix of the grid points of observation sites in degree
- netlab : the index vector of the subnetwork level
- eta: the vector of spatial parameters according to the resolution level

- method : the method for the calculation of coefficients of equation (2), "ls" or "pls"
- approx : approx = TRUE will use the approximation matrix
- grid.size: the size of the grid (latitude, longitude) of the extrapolation site
- lambda : smoothing parameter for method = "pls".

method has two options – "ls" and "pls". method = "ls" calculates the coefficients by the least squares method, and method = "pls" uses the penalized least squares method. Thus, the smoothing parameter lambda is required only when using method = "pls". approx = TRUE implies that we obtain the coefficients using m(< n) selected sites from among the n observation sites, while the interpolation method (approx = FALSE) uses all the observation sites. The function sbf() returns an object of class "sbf". See Oh and Kim (2006) for details. The following code performs the approximate multiscale SBF representation by the least squares method, and Figure 4 illustrates results.

- > out.ls <- sbf(obs=temp67, latlon=latlon,</pre>
- + netlab=netlab, eta=eta,
- + method="ls", approx=TRUE, grid.size=c(100, 200))
- > sw.plot(out.ls, type="field",
- + xlab="Longitude", ylab="Latitude")



Figure 4: An approximate multiscale SBF representation for the observations in Figure 1.

As can be observed, the result in Figure 4 is different from that in Figure 2, which is performed by the penalized least squares interpolation method. Note that the value of the smoothing parameter lambda used in Figure 2 is chosen by generalized crossvalidation. For the implementation, run the following procedure.

```
> lam <- seq(0.1, 0.9, length=9)
> gcv <- NULL
> for(i in 1:length(lam))
+ gcv <- c(gcv, gcv.lambda(obs=temp67,
+ latlon=latlon, netlab=netlab, eta=eta,
+ lambda=lam[i])$gcv)
> lam[gcv == min(gcv)]
[1] 0.8
```

Multiresolution analysis

Here, we explain how to decompose the multiscale SBF representation into the global field of scale l + 1, $T_{l+1}(x)$, and the local field of scale l, $D_l(x)$. Use the function swd() for this operation.

```
> out.dpls <- swd(out.pls)</pre>
```

The function swd() takes an object of class "sbf", performs decomposition with multiscale SWs, and returns an object of class "swd" (spherical wavelet decomposition). Refer to Oh and Kim (2006) for the detailed list of an object of class "swd". Among the components in the list are the smooth coefficients and detailed coefficients of the SW representation. The computed coefficients and decomposition results can be displayed by the function sw.plot() as shown in Figure 5 and Figure 6.

- > sw.plot(out.dpls, type="swcoeff", pch=19,
- + cex=1.1)
- > sw.plot(out.dpls, type="decom")



Figure 5: Plot of SW smooth coefficients and detailed coefficients at different levels l = 1, 2, 3, 4, 5.

Spherical wavelet estimators

We now discuss the statistical techniques of smoothing based on SWs. The theoretical background is based on the works of Donoho and Johnstone (1994) and Oh and Li (2004). The thresholding function swthresh() for SW estimators is

> swthresh(swd, policy, by.level, type, nthresh, + value=0.1, Q=0.05)

This function swthresh() thresholds or shrinks detailed coefficients stored in an swd object, and returns the thresholded detailed coefficients in a modified swd object. The thresh.info list of an swd object has the thresholding information. The available policies are "universal", "sure", "fdr", "probability", and "Lorentz". For the first three thresholding policies, see Donoho and Johnstone (1994, 1995) and Abramovich and Benjamini (1996).



Figure 6: Multiresolution analysis of the multiscale SBF representation $T_1(x)$ in Figure 2. Note that the field $T_1(x)$ is decomposed as $T_1(x) = T_6(x) + D_1(x) + D_2(x) + D_3(x) + D_4(x) + D_5(x)$.



Figure 7: Thresholding result obtained by using the FDR policy

Q specifies the false discovery rate (FDR) of the FDR policy. policy = "probability" performs thresholding using the user supplied threshold represented by a quantile value. In this case, the quantile value is supplied by value. The Lorentz policy takes the thresholding parameter λ as the mean sum of squares of the detailed coefficients.

by.level controls the methods estimating noise variance. In practice, we assume that the noise variances are globally the same or level-dependent. by.level = TRUE estimates the noise variance at each level *l*. Only for the universal, Lorentz, and FDR policies, a level-dependent thresholding is provided. The two approaches, hard and soft thresholding can be specified by type. In addition, the Lorentz type $q(t, \lambda) := \operatorname{sign}(t)\sqrt{t^2 - \lambda^2}I(|t| > \lambda)$ is supplied. Note that only soft type thresholding is appropriate for the SURE policy. By providing the number of resolution levels to be thresholded by nthresh, we can also specify the truncation parameter.

The following procedures perform thresholding using the FDR policy and the reconstruction. Comparing Figure 6 with Figure 7, we can observe that the local components of resolution level 1, 2, and 3 of Figure 7 are shrunk so that its reconstruction (Figure 8) illustrates a smoothed temperature field. For the reconstruction, the function swr() is used on an object of class "swd".

```
> ### Thresholding
```

```
> out.fdr <- swthresh(out.dpls, policy="fdr",</pre>
```

+ by.level=FALSE, type="soft", nthresh=3, Q=0.05)

```
> sw.plot(out.fdr, type = "decom")
```

```
> ### Reconstruction
```

- > out.reconfdr <- swr(out.fdr)
- > sw.plot(z=out.reconfdr, type="recon",
- + xlab="Longitude", ylab="Latitude")



Figure 8: Reconstruction

We repeatedly use sw.plot() for display. To summarize its usage, the function sw.plot() displays the observation, network design, SBF representation, SW coefficients, decomposition result or reconstruction result, as specified by type = "obs", "network", "field", "swcoeff", "decom" or "recon", respectively. Either argument sw or z specifies the object to be plotted. z is used for observations, subnetwork labels and reconstruction result and sw is used for an sbf or swd object.

Conclusion remarks

We introduce **SpherWave**, an R package implementing SWs. In this article, we analyze surface air temperature data using **SpherWave** and obtain meaningful and promising results; furthermore provide a step-by-step tutorial introduction for wide potential applicability of SWs. Our hope is that **SpherWave** makes SW methodology practical, and encourages interested readers to apply the SWs for real world applications.

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Bibliography

- F. Abramovich and Y. Benjamini. Adaptive thresholding of wavelet coefficients. *Computational Statistics & Data Analysis*, 22(4):351–361, 1996.
- D. L. Donoho and I. M. Johnstone. Ideal spatial adaptation by wavelet shrinkage. *Biometrika*, 81(3):425– 455, 1994.
- D. L. Donoho and I. M. Johnstone. Adapting to unknown smoothness via wavelet shrinkage *Journal of the American Statistical Association*, 90(432):1200– 1224, 1995.
- T-H. Li. Multiscale representation and analysis of spherical data by spherical wavelets. *SIAM Journal of Scientific Computing*, 21(3):924–953, 1999.
- F. J. Narcowich and J. D. Ward. Nonstationary wavelets on the *m*-sphere for scattered data. *Applied and Computational Harmonic Analysis*, 3(4): 324–336, 1996.
- H-S. Oh and D. Kim. **SpherWave**: Spherical wavelets and SW-based spatially adaptive methods, 2006. URL http://CRAN.R-project.org/src/contrib/Descriptions/SpherWave.html.
- H-S. Oh and D. Kim. Network design and preprocessing for multi-Scale spherical basis function representation. *Joournal of the Korean Statistical Society*, 36(2):209–228, 2007.
- H-S. Oh and T-H. Li. Estimation of global temperature fields from scattered observations by a spherical-wavelet-based spatially adaptive method. *Journal of the Royal Statistical Society B*, 66 (1):221–238, 2004.

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Diving Behaviour Analysis in R

An Introduction to the diveMove Package

by Sebastián P. Luque

Introduction

Remarkable developments in technology for electronic data collection and archival have increased researchers' ability to study the behaviour of aquatic animals while reducing the effort involved and impact on study animals. For example, interest in the study of diving behaviour led to the development of minute time-depth recorders (TDRs) that can collect more than 15 MB of data on depth, velocity, light levels, and other parameters as animals move through their habitat. Consequently, extracting useful information from TDRs has become a time-consuming and tedious task. Therefore, there is an increasing need for efficient software to automate these tasks, without compromising the freedom to control critical aspects of the procedure.

There are currently several programs available for analyzing TDR data to study diving behaviour. The large volume of peer-reviewed literature based on results from these programs attests to their usefulness. However, none of them are in the free software domain, to the best of my knowledge, with all the disadvantages it entails. Therefore, the main motivation for writing **diveMove** was to provide an R package for diving behaviour analysis allowing for more flexibility and access to intermediate calculations. The advantage of this approach is that researchers have all the elements they need at their disposal to take the analyses beyond the standard information returned by the program.

The purpose of this article is to outline the functionality of **diveMove**, demonstrating its most useful features through an example of a typical diving behaviour analysis session. Further information can be obtained by reading the vignette that is included in the package (vignette("diveMove")) which is currently under development, but already shows basic usage of its main functions. **diveMove** is available from CRAN, so it can easily be installed using install.packages().

The diveMove Package

diveMove offers functions to perform the following tasks:

• Identification of wet vs. dry periods, defined by consecutive readings with or without depth measurements, respectively, lasting more than a user-defined threshold. Depending on the sampling protocol programmed in the instrument, these correspond to wet vs. dry periods, respectively. Each period is individually identified for later retrieval.

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- Calibration of depth readings, which is needed to correct for shifts in the pressure transducer. This can be done using a **tcltk** graphical user interface (GUI) for chosen periods in the record, or by providing a value determined a priori for shifting all depth readings.
- Identification of individual dives, with their different phases (descent, bottom, and ascent), using various criteria provided by the user. Again, each individual dive and dive phase is uniquely identified for future retrieval.
- Calibration of speed readings using the method described by Blackwell et al. (1999), providing a unique calibration for each animal and deployment. Arguments are provided to control the calibration based on given criteria. Diagnostic plots can be produced to assess the quality of the calibration.
- Summary of time budgets for wet vs. dry periods.
- Dive statistics for each dive, including maximum depth, dive duration, bottom time, postdive duration, and summaries for each dive phases, among other standard dive statistics.
- tcltk plots to conveniently visualize the entire dive record, allowing for zooming and panning across the record. Methods are provided to include the information obtained in the points above, allowing the user to quickly identify what part of the record is being displayed (period, dive, dive phase).

Additional features are included to aid in analysis of movement and location data, which are often collected concurrently with TDR data. They include calculation of distance and speed between successive locations, and filtering of erroneous locations using various methods. However, **diveMove** is primarily a diving behaviour analysis package, and other packages are available which provide more extensive animal movement analysis features (e.g. **trip**).

The tasks described above are possible thanks to the implementation of three formal S4 classes to represent TDR data. Classes TDR and TDRspeed are used to represent data from TDRs with and without speed sensor readings, respectively. The latter class inherits from the former, and other concurrent data can be included with either of these objects. A third formal class (TDRcalibrate) is used to represent data obtained during the various intermediate steps described above. This structure greatly facilitates the retrieval of useful information during analyses.

Data Preparation

TDR data are essentially a time-series of depth readings, possibly with other concurrent parameters, typically taken regularly at a user-defined interval. Depending on the instrument and manufacturer, however, the files obtained may contain various errors, such as repeated lines, missing sampling intervals, and invalid data. These errors are better dealt with using tools other than R, such as awk and its variants, because such stream editors use much less memory than R for this type of problems, especially with the typically large files obtained from TDRs. Therefore, **diveMove** currently makes no attempt to fix these errors. Validity checks for the TDR classes, however, do test for time series being in increasing order.

Most TDR manufacturers provide tools for downloading the data from their TDRs, but often in a proprietary format. Fortunately, some of these manufacturers also offer software to convert the files from their proprietary format into a portable format, such as comma-separated-values (csv). At least one of these formats can easily be understood by R, using standard functions, such as read.table() or read.csv(). **diveMove** provides constructors for its two main formal classes to read data from files in one of these formats, or from simple data frames.

How to Represent TDR Data?

TDR is the simplest class of objects used to represent TDR data in **diveMove**. This class, and its TDRspeed subclass, stores information on the source file for the data, the sampling interval, the time and depth readings, and an optional data frame containing additional parameters measured concurrently. The only difference between TDR and TDRspeed objects is that the latter ensures the presence of a speed vector in the data frame with concurrent measurements. These classes have the following slots:

file: character,

dtime: numeric,

time: POSIXct,

depth: numeric,

concurrentData: data.frame

Once the TDR data files are free of errors and in a portable format, they can be read into a data frame, using e.g.:

```
R> ff <- system.file(file.path("data",
+ "dives.csv"), package = "diveMove")
R> tdrXcsv <- read.csv(ff)</pre>
```

and then put into one of the TDR classes using the function createTDR(). Note, however, that this approach requires knowledge of the sampling interval and making sure that the data for each slot are valid:

```
R> library("diveMove")
R> ddtt.str <- paste(tdrXcsv$date,
      tdrXcsv$time)
+
R> ddtt <- strptime(ddtt.str,
      format = "%d/%m/%Y %H:%M:%S")
+
R> time.posixct <- as.POSIXct(ddtt,</pre>
+
      tz = "GMT")
R> tdrX <- createTDR(time = time.posixct,</pre>
+
      depth = tdrXcsv$depth,
+
      concurrentData = tdrXcsv[,
+
          -c(1:3)], dtime = 5,
      file = ff
+
R> tdrX <- createTDR(time = time.posixct,
+
      depth = tdrXcsv$depth,
+
      concurrentData = tdrXcsv[,
          -c(1:3)], dtime = 5,
+
+
      file = ff, speed = TRUE)
```

If the files are in *.csv format, these steps can be automated using the readTDR() function to create an object of one of the formal classes representing TDR data (TDRspeed in this case), and immediately begin using the methods provided:

R> tdrX <- readTDR(ff, speed = TRUE) R> plotTDR(tdrX)



Figure 1: The plotTDR() method for TDR objects produces an interactive plot of the data, allowing for zooming and panning. Several arguments for readTDR() allow mapping of data from the source file to the different slots in diveMove's classes, the time format in the input and the time zone attribute to use for the time readings.

Various methods are available for displaying TDR objects, including show(), which provides an informative summary of the data in the object, extractors and replacement methods for all the slots. There is a plotTDR() method (Figure 1) for both TDR and TDRspeed objects. The interact argument allows for suppression of the tcltk interface. Information on these methods is available from methods?TDR.

TDR objects can easily be coerced to data frame (as.data.frame() method), without losing information from any of the slots. TDR objects can additionally be coerced to TDRspeed, whenever it makes sense to do so, using an as.TDRspeed() method.

Identification of Activities at Various Scales

One the first steps of dive analysis involves correcting depth for shifts in the pressure transducer, so that surface readings correspond to zero. Such shifts are usually constant for an entire deployment period, but there are cases where the shifts vary within a particular deployment, so shifts remain difficult to detect and dives are often missed. Therefore, a visual examination of the data is often the only way to detect the location and magnitude of the shifts. Visual adjustment for shifts in depth readings is tedious, but has many advantages which may save time during later stages of analysis. These advantages include increased understanding of the data, and early detection of obvious problems in the records, such as instrument malfunction during certain intervals, which should be excluded from analysis.

Zero-offset correction (ZOC) is done using the function zoc(). However, a more efficient method of doing this is with function calibrateDepth(), which takes a TDR object to perform three basic tasks. The first is to ZOC the data, optionally using the tcltk package to be able to do it interactively:

R> dcalib <- calibrateDepth(tdrX)</pre>

This command brings up a plot with **tcltk** controls allowing to zoom in and out, as well as pan across the data, and adjust the depth scale. Thus, an appropriate time window with a unique surface depth value can be displayed. This allows the user to select a depth scale that is small enough to resolve the surface value using the mouse. Clicking on the ZOC button waits for two clicks: i) the coordinates of the first click define the starting time for the window to be ZOC'ed, and the depth corresponding to the surface, ii) the second click defines the end time for the window (i.e. only the x coordinate has any meaning). This procedure can be repeated as many times as needed. If there is any overlap between time windows, then the last one prevails. However, if the offset is known a priori, there is no need to go through all this procedure, and the value can be provided as the argument offset to calibrateDepth(). For example, preliminary inspection of object tdrX would have revealed a 3 m offset, and we could have simply called (without plotting):

```
R> dcalib <- calibrateDepth(tdrX,
+ offset = 3)
```

Once depth has been ZOC'ed, the second step calibrateDepth() will perform is identify dry and wet periods in the record. Wet periods are those with depth readings, dry periods are those without them. However, records may have aberrant missing depth that should not define dry periods, as they are usually of very short duration¹. Likewise, there may be periods of wet activity that are too short to be compared with other wet periods, and need to be excluded from further analyses. These aspects can be controlled by setting the arguments dry.thr and wet.thr to appropriate values.

Finally, calibrateDepth() identifies all dives in the record, according to a minimum depth criterion given as its dive.thr argument. The value for this criterion is typically determined by the resolution of the instrument and the level of noise close to the surface. Thus, dives are defined as departures from the surface to maximal depths below dive.thr and the subsequent return to the surface. Each dive may subsequently be referred to by an integer number indicating its position in the time series.

Dive phases are also identified at this last stage. Detection of dive phases is controlled by three arguments: a critical quantile for rates of vertical descent (descent.crit.q), a critical quantile for rates of ascent (ascent.crit.q), and a proportion of maximum depth (wiggle.tol). The first two arguments are used to define the rate of descent below which the descent phase is deemed to have ended, and the rate of ascent above which the ascent phases is deemed to have started, respectively. The rates are obtained from all successive rates of vertical movement from the surface to the first (descent) and last (ascent) maximum dive depth. Only positive rates are considered for the descent, and only negative rates are considered for the ascent. The purpose of this restriction is to avoid having any reversals of direction or histeresis events resulting in phases determined exclusively by those events. The wiggle.tol argument determines the proportion of maximum dive depth above which wiggles are not allowed to terminate descent, or below which they should be considered as part of the bottom phase.

¹They may result from animals resting at the surface of the water long enough to dry the sensors.

A more refined call to calibrateDepth() for object tdrX may be:

```
R> dcalib <- calibrateDepth(tdrX,</pre>
```

```
+ offset = 3, wet.thr = 70,
```

+ dry.thr = 3610, dive.thr = 4,

```
+ descent.crit.q = 0.1,
```

+ ascent.crit.q = 0.1, wiggle.tol = 0.8)

The result (value) of this function is an object of class TDRcalibrate, where all the information obtained during the tasks described above are stored.

How to Represent Calibrated TDR Data?

Objects of class TDRcalibrate contain the following slots, which store information during the major procedures performed by calibrateDepth():

tdr: TDR. The object which was calibrated.

- **gross.activity:** list. This list contains four components with details on wet/dry activities detected, such as start and end times, durations, and identifiers and labels for each activity period. Five activity categories are used for labelling each reading, indicating dry (L), wet (W), underwater (U), diving (D), and brief wet (Z) periods. However, underwater and diving periods are collapsed into wet activity at this stage (see below).
- dive.activity: data.frame. This data frame contains three components with details on the diving activities detected, such as numeric vectors identifiying to which dive and post-dive interval each reading belongs to, and a factor labelling the activity each reading represents. Compared to the gross.activity slot, the underwater and diving periods are discerned here.
- dive.phases: factor. This identifies each reading with a particular dive phase. Thus, each reading belongs to one of descent, descent/bottom, bottom, bottom/ascent, and ascent phases. The descent/bottom and bottom/ascent levels are useful for readings which could not unambiguously be assigned to one of the other levels.

dry.thr: numeric.

wet.thr: numeric.

- dive.thr: numeric. These last three slots store information given as arguments to calibrateDepth(), documenting criteria used during calibration.
- **speed.calib.coefs:** numeric. If the object calibrated was of class TDRspeed, then this is a vector of length 2, with the intercept and the slope of the speed calibration line (see below).

All the information contained in each of these slots is easily accessible through extractor methods for objects of this class (see class?TDRcalibrate). An appropriate show() method is available to display a short summary of such objects, including the number of dry and wet periods identified, and the number of dives detected.

The TDRcalibrate plotTDR() method for these objects allows visualizing the major wet/dry activities throughout the record (Figure 2):

R> plotTDR(dcalib, concurVars = "light",

+ concurVarTitles = c("speed (m/s)",

+ "light"), surface = TRUE)



Figure 2: The plotTDR() method for TDRcalibrate objects displays information on the major activities identified throughout the record (wet/dry periods here).

The dcalib object contains a TDRspeed object in its tdr slot, and speed is plotted by default in this case. Additional measurements obtained concurrently can also be plotted using the concurVars argument. Titles for the depth axis and the concurrent parameters use separate arguments; the former uses ylab.depth, while the latter uses concurVarTitles. Convenient default values for these are provided. The surface argument controls whether post-dive readings should be plotted; it is FALSE by default, causing only dive readings to be plotted which saves time plotting and re-plotting the data. All plot methods use the underlying plotTD() function, which has other useful arguments that can be passed from these methods. A more detailed view of the record can be obtained by using a combination of the diveNo and the labels arguments to this plotTDR() method. This is useful if, for instance, closer inspection of certain dives is needed. The following call displays a plot of dives 2 through 8 (Figure 3):

R> plotTDR(dcalib, diveNo = 2:8, + labels = "dive.phase")



Figure 3: The plotTDR() method for TDRcalibrate objects can also display information on the different activities during each dive record (descent=D, descent/bottom=DB, bottom=B, bottom/ascent=BA, ascent=A, X=surface).

The labels argument allows the visualization of the identified dive phases for all dives selected. The same information can also be obtained with the extractDive() method for TDRcalibrate objects:

R> extractDive(dcalib, diveNo = 2:8)

Other useful extractors include: getGAct() and getDAct(). These methods extract the whole gross.activity and dive.activity, respectively, if given only the TDRcalibrate object, or a particular component of these slots, if supplied a string with the name of the component. For example: getGAct(dcalib, "trip.act") would retrieve the factor identifying each reading with a wet/dry activity and getDAct(dcalib, "dive.activity") would retrieve a more detailed factor with information on whether the reading belongs to a dive or a brief aquatic period.

With the information obtained during this calibration procedure, it is possible to calculate dive statistics for each dive in the record. A table providing summary statistics for each dive can be obtained with the function diveStats() (Figure 4).

diveStats() returns a data frame with the final summaries for each dive (Figure 4), providing the following information:

- The time of start of the dive, the end of descent, and the time when ascent began.
- The total duration of the dive, and that of the descent, bottom, and ascent phases.
- The vertical distance covered during the descent, the bottom (a measure of the level of "wiggling", i.e. up and down movement performed during the bottom phase), and the vertical distance covered during the ascent.
- The maximum depth attained.
- The duration of the post-dive interval.

A summary of time budgets of wet vs. dry periods can be obtained with timeBudget(), which returns a data frame with the beginning and ending times for each consecutive period (Figure 4). It takes a TDRcalibrate object and another argument (ignoreZ) controlling whether aquatic periods that were briefer than the user-specified threshold² should be collapsed within the enclosing period of dry activity.

These summaries are the primary goal of **dive-Move**, but they form the basis from which more elaborate and customized analyses are possible, depending on the particular research problem. These include investigation of descent/ascent rates based on the depth profiles, and bout structure analysis. Some of these will be implemented in the future.

In the particular case of TDRspeed objects, however, it may be necessary to calibrate the speed readings before calculating these statistics.

Calibrating Speed Sensor Readings

Calibration of speed sensor readings is performed using the procedure described by Blackwell et al. (1999). Briefly the method rests on the principle that for any given rate of depth change, the lowest measured speeds correspond to the steepest descent angles, i.e. vertical descent/ascent. In this case, measured speed and rate of depth change are expected to be equal. Therefore, a line drawn through the bottom edge of the distribution of observations in a plot of measured speed vs. rate of depth change would provide a calibration line. The calibrated speeds, therefore, can be calculated by reverse estimation of rate of depth change from the regression line.

Dive Summaries

²This corresponds to the value given as the wet.thr argument to calibrateDepth().

```
R> tdrXSumm1 <- diveStats(dcalib)</pre>
R> names(tdrXSumm1)
 [1] "begdesc"
                         "enddesc"
                                                  "begasc"
                                                                        "desctim"
[5] "botttim"
                         "asctim"
                                                  "descdist"
                                                                        "bottdist"
[9] "ascdist"
                          "desc.tdist"
                                                  "desc.mean.speed"
                                                                        "desc.angle"
[13] "bott.tdist"
                          "bott.mean.speed"
                                                  "asc.tdist"
                                                                        "asc.mean.speed"
[17] "asc.angle"
                           "divetim"
                                                  "maxdep"
                                                                        "postdive.dur"
[21] "postdive.tdist"
                          "postdive.mean.speed"
R> tbudget <- timeBudget(dcalib, ignoreZ = TRUE)
R> head(tbudget, 4)
 phaseno activity
                                   beg
                                                        end
       1 W 2002-01-05 11:32:00 2002-01-06 06:30:00
1
                L 2002-01-06 06:30:05 2002-01-06 17:01:10
2
       2
3
       3
                 W 2002-01-06 17:01:15 2002-01-07 05:00:30
4
        4
                L 2002-01-07 05:00:35 2002-01-07 07:34:00
R> trip.labs <- stampDive(dcalib, ignoreZ = TRUE)
R> tdrXSumm2 <- data.frame(trip.labs, tdrXSumm1)</pre>
R> names(tdrXSumm2)
 [1] "trip.no"
                           "trip.type"
                                                  "beg"
                                                                        "end"
 [5] "begdesc"
                           "enddesc"
                                                  "begasc"
                                                                        "desctim"
 [9] "botttim"
                           "asctim"
                                                  "descdist"
                                                                        "bottdist"
[13] "ascdist"
                           "desc.tdist"
                                                  "desc.mean.speed"
                                                                        "desc.angle"
[17] "bott.tdist"
                           "bott.mean.speed"
                                                  "asc.tdist"
                                                                        "asc.mean.speed"
[21] "asc.angle"
                           "divetim"
                                                  "maxdep"
                                                                        "postdive.dur"
[25] "postdive.tdist"
                           "postdive.mean.speed"
```

Figure 4: Per-dive summaries can be obtained with functions diveStats(), and a summary of time budgets with timeBudget(). diveStats() takes a TDRcalibrate object as a single argument (object dcalib above, see text for how it was created).

diveMove implements this procedure with function calibrateSpeed(). This function performs the following tasks:

- 1. Subset the necessary data from the record. By default only data corresponding to depth changes > 0 are included in the analysis, but higher constraints can be imposed using the z argument. A further argument limiting the data to be used for calibration is bad, which is a vector with the minimum **rate** of depth change and minimum speed readings to include in the calibration. By default, values > 0 for both parameters are used.
- 2. Calculate the binned bivariate kernel density and extract the desired contour. Once the proper data were obtained, a bivariate normal kernel density grid is calculated from the relationship between measured speed and rate of depth change (using the KernSmooth package). The choice of bandwidths for the binned kernel density is made using bw.nrd. The contour.level argument to calibrateSpeed() controls which particular contour should be extracted from the density grid. Since the interest is in defining a regression line passing through the lower densities of the grid, this value should be relatively low (it is set to 0.1 by default).
- 3. Define the regression line passing through the lower edge of the chosen contour. A quantile regression through a chosen quantile is used for this purpose. The quantile can be specified using the tau argument, which is passed to the rq() function in package **quantreg**. tau is set to 0.1 by default.
- 4. Finally, the speed readings in the TDR object are calibrated.

As recognized by Blackwell et al. (1999), the advantage of this method is that it calibrates the instrument based on the particular deployment conditions (i.e. controls for effects of position of the instrument on the animal, and size and shape of the instrument, relative to the animal's morphometry, among others). However, it is possible to supply the coefficients of this regression if they were estimated separately; for instance, from an experiment. The argument coefs can be used for this purpose, which is then assumed to contain the intercept and the slope of the line. calibrateSpeed() returns a TDRcalibrate object, with calibrated speed readings included in its tdr slot, and the coefficients used for calibration.

For instance, to calibrate speed readings using the 0.1 quantile regression of measured speed vs. rate of depth change, based on the 0.1 contour of the bivariate kernel densities, and including only changes in depth > 1, measured speeds and rates of depth

change > 0:

```
R> vcalib <- calibrateSpeed(dcalib,
+ tau = 0.1, contour.level = 0.1,
+ z = 1, bad = c(0, 0),
+ cex.pts = 0.2)
```



Figure 5: The relationship between measured speed and rate of depth change can be used to calibrate speed readings. The line defining the calibration for speed measurements passes through the bottom edge of a chosen contour, extracted from a bivariate kernel density grid.

This call produces the plot shown in Figure 5, which can be suppressed by the use of the logical argument plot. Calibrating speed readings allows for the meaningful interpretation of further parameters calculated by diveStats(), whenever a TDRspeed object was found in the TDRcalibrate object:

- The total distance travelled, mean speed, and diving angle during the descent and ascent phases of the dive.
- The total distance travelled and mean speed during the bottom phase of the dive, and the post-dive interval.

Summary

The **diveMove** package provides tools for analyzing diving behaviour, including convenient methods for the visualization of the typically large amounts of data collected by TDRs. The package's main strengths are its ability to:

- 1. identify wet vs. dry periods,
- 2. calibrate depth readings,
- 3. identify individual dives and their phases,
- 4. summarize time budgets,
- 5. calibrate speed sensor readings, and
- 6. provide basic summaries for each dive identified in TDR records.

Formal S4 classes are supplied to efficiently store TDR data and results from intermediate analysis, making the retrieval of intermediate results readily available for customized analysis. Development of the package is ongoing, and feedback, bug reports, or other comments from users are very welcome.

Acknowledgements

Many of the ideas implemented in this package developed over fruitful discussions with my mentors John P.Y. Arnould, Christophe Guinet, and Edward H. Miller. I would like to thank Laurent Dubroca who wrote draft code for some of **diveMove**'s functions. I am also greatly endebted to the regular contributors to the R-help newsgroup who helped me solve many problems during development.

Bibliography

S. Blackwell, C. Haverl, B. Le Boeuf, and D. Costa. A method for calibrating swim-speed recorders. *Marine Mammal Science*, 15(3):894–905, 1999.

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Very Large Numbers in R: Introducing Package Brobdingnag

Logarithmic representation for floating-point numbers

Robin K. S. Hankin

Introduction

The largest floating point number representable in standard double precision arithmetic is a little under 2^{1024} , or about 1.79×10^{308} . This is too small for some applications.

The R package **Brobdingnag** (Swift, 1726) overcomes this limit by representing a real number x using a double precision variable with value $\log |x|$, and a logical corresponding to $x \ge 0$; the S4 class of such objects is brob. Complex numbers with large absolute values (class glub) may be represented using a pair of brobs to represent the real and imaginary components.

The package allows user-transparent access to the large numbers allowed by Brobdingnagian arithmetic. The package also includes a vignette—brob which documents the S4 methods used and includes a step-by-step tutorial. The vignette also functions as a "Hello, World!" example of S4 methods as used in a simple package. It also includes a full description of the glub class.

Package Brobdingnag in use

Most readers will be aware of a googol which is equal to 10^{100} :

```
> require(Brobdingnag)
```

```
> googol <- as.brob(10)^100
```

[1] +exp(230.26)

Note the coercion of double value 10 to an object of class brob using function as.brob(): raising this to the power 100 (also double) results in another brob. The result is printed using exponential notation, which is convenient for very large numbers.

A googol is well within the capabilities of standard double precision arithmetic. Now, however, suppose we wish to compute its factorial. Taking the first term of Stirling's series gives

```
> stirling <- function(n) {
+     n^n * exp(-n) * sqrt(2 * pi * n)
+ }</pre>
```

which then yields

> stirling(googol)

[1] +exp(2.2926e+102)

Note the transparent coercion to brob form within function stirling().

It is also possible to represent numbers very close to 1. Thus

```
> 2^(1/googol)
```

[1] +exp(6.9315e-101)

It is worth noting that if *x* has an exact representation in double precision, then e^x is exactly representable using the system described here. Thus *e* and e^{1000} are represented exactly.

Accuracy

For small numbers (that is, representable using standard double precision floating point arithmetic), **Brobdingnag** suffers a slight loss of precision compared to normal representation. Consider the following function, whose return value for nonzero arguments is algebraically zero:

```
f <- function(x){
    as.numeric( (pi*x -3*x -(pi-3)*x)/x)
}</pre>
```

This function combines multiplication and addition; one might expect a logarithmic system such as described here to have difficulty with it.

```
> f(1/7)
[1] 1.700029e-16
> f(as.brob(1/7))
[1] -1.886393e-16
```

This typical example shows that Brobdingnagian numbers suffer a slight loss of precision for numbers of moderate magnitude. This degradation increases with the magnitude of the argument:

> f(1e+100)

[1] -2.185503e-16

- > f(as.brob(1e+100))
- [1] -3.219444e-14

Here, the brob's accuracy is about two orders of magnitude worse than double precision arithmetic: this would be expected, as the number of bits required to specify the exponent goes as $\log \log x$.

Compare

> f(as.brob(10)^1000)

[1] 1.931667e-13

showing a further degradation of precision. However, observe that conventional double precision arithmetic cannot deal with numbers this big, and the package returns about 12 correct significant figures.

A practical example

In the field of population dynamics, and especially the modelling of biodiversity (Hankin, 2007b; Hubbell, 2001), complicated combinatorial formulae often arise.

Etienne (2005), for example, considers a sample of *N* individual organisms taken from some natural population; the sample includes *S* distinct species, and each individual is assigned a label in the range 1 to *S*. The sample comprises n_i members of species *i*, with $1 \le i \le S$ and $\sum n_i = N$. For a given sample *D*, Etienne defines, amongst other terms, K(D, A) for $1 \le A \le N - S + 1$ as

$$\sum_{\left\{a_1,\dots,a_S\mid \sum_{i=1}^S a_i=A\right\}} \prod_{i=1}^S \frac{\overline{s}(n_i,a_i)\overline{s}(a_i,1)}{\overline{s}(n_i,1)}$$
(1)

where $\bar{s}(n, a)$ is the Stirling number of the second kind (Abramowitz and Stegun, 1965). The summation is over $a_i = 1, ..., n_i$ with the restriction that the a_i sum to A, as carried out by blockparts() of the **partitions** package (Hankin, 2006, 2007a).

Taking an intermediate-sized dataset due to Saunders¹ of only 5903 individuals—a relatively small dataset in this context—the maximal element of K(D, A) is about 1.435×10^{1165} . The accuracy of package **Brobdingnag** in this context may be assessed by comparing it with that computed by PARI/GP (Batut et al., 2000) with a working precision of 100 decimal places; the natural logs of the two values are 2682.8725605988689 and 2682.87256059887 respectively: identical to 14 significant figures.

Conclusions

The **Brobdingnag** package allows representation and manipulation of numbers larger than those cov-

ered by standard double precision arithmetic, although accuracy is eroded for very large numbers. This facility is useful in several contexts, including combinatorial computations such as encountered in theoretical modelling of biodiversity.

Acknowledgments

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Bibliography

- M. Abramowitz and I. A. Stegun. *Handbook of Mathematical Functions*. New York: Dover, 1965.
- C. Batut, K. Belabas, D. Bernardi, H. Cohen, and M. Olivier. User's guide to pari/gp. Technical Reference Manual, 2000. url: http://www.parigp-home.de/.
- R. S. Etienne. A new sampling formula for neutral biodiversity. *Ecology Letters*, 8:253–260, 2005. doi: 10.111/j.1461-0248.2004.00717.x.
- R. K. S. Hankin. Additive integer partitions in R. *Journal of Statistical Software*, 16(Code Snippet 1), May 2006.
- R. K. S. Hankin. Urn sampling without replacement: Enumerative combinatorics in R. *Journal of Statistical Software*, 17(Code Snippet 1), January 2007a.
- R. K. S. Hankin. Introducing **untb**, an R package for simulating ecological drift under the Unified Neutral Theory of Biodiversity, 2007b. Under review at the Journal of Statistical Software.
- S. P. Hubbell. *The Unified Neutral Theory of Biodiversity and Biogeography*. Princeton University Press, 2001.
- J. Swift. Gulliver's Travels. Benjamin Motte, 1726.
- W. N. Venables and B. D. Ripley. *Modern Applied Statistics with S-PLUS*. Springer, 1997.

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¹The dataset comprises species counts on kelp holdfasts; here saunders.exposed.tot of package untb (Hankin, 2007b), is used.

Applied Bayesian Non- and Semi-parametric Inference using DPpackage

by Alejandro Jara

Introduction

In many practical situations, a parametric model cannot be expected to describe in an appropriate manner the chance mechanism generating an observed dataset, and unrealistic features of some common models could lead to unsatisfactory inferences. In these cases, we would like to relax parametric assumptions to allow greater modeling flexibility and robustness against misspecification of a parametric statistical model. In the Bayesian context such flexible inference is typically achieved by models with infinitely many parameters. These models are usually referred to as Bayesian Nonparametric (BNP) or Semiparametric (BSP) models depending on whether all or at least one of the parameters is infinity dimensional (Müller & Quintana, 2004).

While BSP and BNP methods are extremely powerful and have a wide range of applicability within several prominent domains of statistics, they are not as widely used as one might guess. At least part of the reason for this is the gap between the type of software that many applied users would like to have for fitting models and the software that is currently available. The most popular programs for Bayesian analysis, such as **BUGS** (Gilks et al., 1992), are generally unable to cope with nonparametric models. The variety of different BSP and BNP models is huge; thus, building for all of them a general software package which is easy to use, flexible, and efficient may be close to impossible in the near future.

This article is intended to introduce an R package, DPpackage, designed to help bridge the previously mentioned gap. Although its name is motivated by the most widely used prior on the space of the probability distributions, the Dirichlet Process (DP) (Ferguson, 1973), the package considers and will consider in the future other priors on functional spaces. Currently, DPpackage (version 1.0-5) allows the user to perform Bayesian inference via simulation from the posterior distributions for models considering DP, Dirichlet Process Mixtures (DPM), Polya Trees (PT), Mixtures of Triangular distributions, and Random Bernstein Polynomials priors. The package also includes generalized additive models considering penalized B-Splines. The rest of the article is organized as follows. We first discuss the general syntax and design philosophy of the package. Next, the main features of the package and some illustrative examples are presented. Comments on future developments conclude the article.

Design philosophy and general syntax

The design philosophy behind **DPpackage** is quite different from that of a general purpose language. The most important design goal has been the implementation of model-specific MCMC algorithms. A direct benefit of this approach is that the sampling algorithms can be made dramatically more efficient.

Fitting a model in **DPpackage** begins with a call to an R function that can be called, for instance, DPmodel or PTmodel. Here "model" denotes a descriptive name for the model being fitted. Typically, the model function will take a number of arguments that govern the behavior of the MCMC sampling algorithm. In addition, the model(s) formula(s), data, and prior parameters are passed to the model function as arguments. The common elements in any model function are:

- i) prior: an object list which includes the values of the prior hyperparameters.
- ii) mcmc: an object list which must include the integers nburn giving the number of burnin scans, nskip giving the thinning interval, nsave giving the total number of scans to be saved, and ndisplay giving the number of saved scans to be displayed on screen: the function reports on the screen when every ndisplay scans have been carried out and returns the process's runtime in seconds. For some specific models, one or more tuning parameters for Metropolis steps may be needed and must be included in this list. The names of these tuning parameters are explained in each specific model description in the associated help files.
- iii) state: an object list giving the current values of the parameters, when the analysis is the continuation of a previous analysis, or giving the starting values for a new Markov chain, which is useful for running multiple chains starting from different points.
- iv) status: a logical variable indicating whether it is a new run (TRUE) or the continuation of a previous analysis (FALSE). In the latter case the

current values of the parameters must be specified in the object state.

Inside the R model function the inputs to the model function are organized in a more useable form, the MCMC sampling is performed by calling a shared library written in a compiled language, and the posterior sample is summarized, labeled, assigned into an output list, and returned. The output list includes:

- i) state: a list of objects containing the current values of the parameters.
- ii) save.state: a list of objects containing the MCMC samples for the parameters. This list contains two matrices randsave and thetasave which contain the MCMC samples of the variables with random distribution (errors, random effects, etc.) and the parametric part of the model, respectively.

In order to exemplify the extraction of the output elements, consider the abstract model fit:

The lists can be extracted using the following code:

```
fit$state
fit$save.state$randsave
fit$save.state$thetasave
```

Based on these output objects, it is possible to use, for instance, the **boa** (Smith, 2007) or the **coda** (Plummer et al., 2006) R packages to perform convergence diagnostics. For illustration, we consider the **coda** package here. It requires a matrix of posterior draws for relevant parameters to be saved as an mcmc object. As an illustration, let us assume that we have obtained fit1, fit2, and fit3, by independently running a model function three times, specifying different starting values each time. To compute the Gelman-Rubin convergence diagnostic statistic for the first parameter stored in the thetasave object, the following commands may be used,

where the fifth command saves the results as an object of class mcmc.list, and the sixth command computes the Gelman-Rubin statistic from these three chains.

Generic R functions such as print, plot, summary, and anova have methods to display the results of the **DPpackage** model fit. The function print displays the posterior means of the parameters in the model, and summary displays posterior summary statistics (mean, median, standard deviation, naive standard errors, and credibility intervals). By default, the function summary computes the 95% HPD intervals using the Monte Carlo method proposed by Chen & Shao (1999). Note that this approximation is valid when the true posterior distribution is symmetric. The user can display the order statistic estimator of the 95% credible interval by using the following code,

summary(fit, hpd=FALSE)

The plot function displays the trace plots and a kernel-based estimate of the posterior distribution for the model parameters. Similarly to summary, the plot function displays the 95% HPD regions in the density plot and the posterior mean. The same plot but considering the 95% credible region can be obtained by using,

plot(fit, hpd=FALSE)

The anova function computes simultaneous credible regions for a vector of parameters from the MCMC sample using the method described by Besag et al. (1995). The output of the anova function is an ANOVA-like table containing the pseudo-contour probabilities for each of the factors included in the linear part of the model.

Implemented Models

Currently **DPpackage** (version 1.0-5) contains functions to fit the following models:

- Density estimation: DPdensity, PTdensity, TDPdensity, and BDPdensity using DPM of normals, Mixtures of Polya Trees (MPT), Triangular-Dirichlet, and Bernstein-Dirichlet priors, respectively. The first two functions allow uni- and multi-variate analysis.
- ii) Nonparametric random effects distributions in mixed effects models: DP1mm and DPM1mm, using a DP/Mixtures of DP (MDP) and DPM of normals prior, respectively, for the linear mixed effects model. DPg1mm and DPMg1mm, using a DP/MDP and DPM of normals prior, respectively, for generalized linear mixed effects models. The families (links) implemented by these functions are binomial (logit, probit), poisson (log) and gamma (log). DPo1mm and DPMo1mm, using a DP/MDP and DPM of normals prior, respectively, for the ordinal-probit mixed effects model.
- iii) Semiparametric IRT-type models: DPrasch and FPTrasch, using a DP/MDP and finite PT (FPT)/MFPT prior for the Rasch

model with a binary distribution, respectively. DPraschpoisson and FPTraschpoisson, employing a Poisson distribution.

- iv) Semiparametric meta-analysis models: DPmeta and DPMmeta for the random (mixed) effects meta-analysis models, using a DP/MDP and DPM of normals prior, respectively.
- v) Binary regression with nonparametric link: CSDPbinary, using Newton et al. (1996)'s centrally standardized DP prior. DPbinary and FPTbinary, using a DP and a finite PT prior for the inverse of the link function, respectively.
- vi) AFT model for interval-censored data: DPsurvint, using a MDP prior for the error distribution.
- vii) ROC curve estimation: DProc, using DPM of normals.
- viii) Median regression model: PTlm, using a median-0 MPT prior for the error distribution.
- ix) Generalized additive models: PSgam, using penalized B-Splines.

Additional tools included in the package are DPelicit, to elicit the DP prior using the exact and approximated formulas for the mean and variance of the number of clusters given the total mass parameter and the number of subjects (see, Jara et al. 2007); and PsBF, to compute the Pseudo-Bayes factors for model comparison.

Examples

Bivariate Density Estimation

As an illustration of bivariate density estimation using DPM normals (DPdensity) and MPT models (PTdensity), part of the dataset in Chambers et al. (1983) is considered. Here, n = 111 bivariate observations $\mathbf{y}_i = (y_{i1}, y_{i2})^T$ on radiation y_{i1} and the cube root of ozone concentration y_{i2} are modeled. The original dataset has the additional variables wind speed and temperature. These were analyzed by Müller et al. (1996) and Hanson (2006).

The DPdensity function considers the multivariate extension of the univariate Dirichlet Process Mixture of Normals model discussed in Escobar & West (1995),

$$\boldsymbol{y}_{i} \mid \boldsymbol{G} \stackrel{iid}{\sim} \int N_{k} \left(\boldsymbol{\mu}, \boldsymbol{\Sigma}\right) \boldsymbol{G}(d\boldsymbol{\mu}, d\boldsymbol{\Sigma})$$
$$\boldsymbol{G} \mid \boldsymbol{M}, \boldsymbol{G}_{0} \sim \boldsymbol{D}\boldsymbol{P} \left(\boldsymbol{\alpha}\boldsymbol{G}_{0}\right)$$
$$\boldsymbol{G}_{0} \equiv N_{k}(\boldsymbol{\mu} \mid \boldsymbol{m}_{1}, \boldsymbol{\kappa}_{0}^{-1}\boldsymbol{\Sigma}) \boldsymbol{I} \boldsymbol{W}_{k} \left(\boldsymbol{\Sigma} \mid \boldsymbol{\nu}_{1}, \boldsymbol{\Psi}_{1}\right)$$

 $\alpha \sim \Gamma(a_0, b_0)$

$$m_{1} \mid m_{2}, S_{2} \sim N_{k} (m_{2}, S_{2})$$

$$\kappa_{0} \mid \tau_{1}, \tau_{2} \sim \Gamma (\tau_{1}/2, \tau_{2}/2)$$

$$\Psi_{1} \mid \nu_{2}, \Psi_{2} \sim IW_{k} (\nu_{2}, \Psi_{2})$$

where $N_k(\mu, \Sigma)$ refers to a *k*-variate normal distribution with mean and covariance matrix μ and Σ , respectively, $IW_k(\nu, \Psi)$ refers to an inverted-Wishart distribution with shape and scale parameter ν and Ψ , respectively, and $\Gamma(a, b)$ refers to a gamma distribution with shape and rate parameter, *a* and *b*, respectively. Note that the inverted-Wishart prior is parameterized such that its mean is given by $\frac{1}{\nu-k-1}\Psi^{-1}$.

The PTdensity function considers a Mixture of multivariate Polya Trees model discussed in Hanson (2006),

$$\boldsymbol{y}_i | \boldsymbol{G} \stackrel{iid}{\sim} \boldsymbol{G}, \tag{1}$$

$$G \mid \boldsymbol{\alpha}, \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{M} \sim \boldsymbol{P} T^{\boldsymbol{M}}(\Pi^{\boldsymbol{\mu}, \boldsymbol{\Sigma}}, \mathcal{A}^{\boldsymbol{\alpha}}),$$
(2)

$$p(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \propto |\boldsymbol{\Sigma}|^{-(d+1)/2},$$
 (3)

$$x|a_0, b_0 \sim \Gamma(a_0, b_0),$$
 (4)

where the PT prior is centered around a $N_k(\mu, \Sigma)$ distribution. To fit these models we used the following commands:

Data
 data("airquality")
 attach(airquality)
 ozone <- Ozone**(1/3)
 radiation <- Solar.R</pre>

```
# Prior information
priorDPM <- list(a0 = 1, b0 = 1/5,
    nu1 = 4, nu2 = 4,
    s2 = matrix(c(10000,0,0,1),ncol = 2),
    m2 = c(180,3),
    psiinv2 = matrix(c(1/10000,0,0,1),ncol = 2),
    tau1 = 0.01, tau2 = 0.01)</pre>
```

```
priorMPT <- list(a0 = 5, b0 = 1, M = 4)
```

tune3 = 2.1)

fitMPT <- PTdensity(
 y = cbind(radiation,ozone),
 prior = priorMPT,mcmc = mcmcMPT,
 state = NULL,status = TRUE,
 na.action = na.omit)</pre>

We illustrate the results from these analyses in Figure 1. This figure shows the contour plots of the posterior predictive density for each model.



Figure 1: Density estimate for the New York Air Quality Measurements dataset, using (a) DPdensity and (b) PTdensity, respectively.

Figure 1 clearly shows a departure from the normality assumption for these data. The results indicate the existence of at least two clusters of data. We refer to Hanson (2006) for more details and comparisons between these models.

Interval-Censored Data

The DPsurvint function implements the algorithm described by Hanson & Johnson (2004) for semiparametric accelerated failure time (AFT) models. We illustrate the function on a dataset involving time to cosmetic deterioration of the breast for women with stage 1 breast cancer who have undergone a lumpectomy, for two treatments, these being radiation, and radiation coupled with chemotherapy. Radiation is known to cause retraction of the breast, and there is some evidence that chemotherapy worsens this effect. There is interest in the cosmetic impact of the treatments because both are considered very effective in preventing recurrence of this early stage cancer.

The data come from a retrospective study of 46 patients who received radiation only and 48 who received radiation plus chemotherapy. Patients were observed typically every four to six months and at each observation a clinician recorded the level of breast retraction that had taken place since the last visit: none, moderate, or severe. The time-to-event considered was the time until moderate or severe breast retraction, and this time is interval censored between patient visits or right censored if no breast retraction was detected over the study period of 48 months. As the observed intervals were the result of pre-scheduled visits, an independent noninformative censoring process can be assumed. The data were analyzed by Hanson & Johnson (2004) and also given in Klein & Moeschberger (1997).

In the analysis of survival data with covariates, the semiparametric proportional hazards (PH) model is the most popular choice. It is flexible and easily fitted using standard software, at least for right-censored data. However, the assumption of proportional hazard functions may be violated and we may seek a proper alternative semiparametric model. One such model is the AFT model. Whereas the PH model assumes the covariates act multiplicatively on a baseline hazard function, the AFT model assumes that the covariates act multiplicatively on the argument of the baseline survival distribution, *G*, $P(T > t | \mathbf{x}) = G((t \exp{\{\mathbf{x}_i^T \boldsymbol{\beta}\}, +\infty)})$, thus providing a model with a simple interpretation of the regression coefficients for practitioners.

Classical treatments of the semiparametric AFT model with interval-censored data were presented, for instance, in Lin & Zhang (1998). Note, however, that for semiparametric AFT models there is nothing comparable to a partial likelihood function. Therefore, the vector of regression coefficients and the baseline survival distribution must be estimated simultaneously, complicating matters enormously in the interval-censored case. The more recent classical approaches only provide inferences about the regression coefficients and not for the survival function.

In the Bayesian semiparametric context, Christensen & Johnson (1998) assigned a simple DP prior, centered in a single distribution, to baseline survival for nested interval-censored data. A marginal likelihood for the vector of regression coefficients β is maximized to provide a point estimate and resulting survival curves. However, this approach does not allow the computation of credible intervals for the parameters. Moreover, it may be difficult in practice to specify a single centering distribution for the DP prior and, once specified, a single centering distribution may affect inferences. To overcome these difficulties, a MDP prior can be considered. Under this approach, it is not very difficult to demonstrated that the computations involved for a full Bayesian solution are horrendous at best, even for the noncensored data problem. The analytic intractability of the Bayesian semiparametric AFT model has been overcome using MCMC methods by Hanson & Johnson (2004).

To test whether chemotherapy in addition to radiotherapy has an effect on time to breast retraction, an AFT model $T_i = \exp(-x_i^T \beta) V_i$, i = 1, ..., n, was considered. We model the baseline distribution in the AFT model using a MDP prior centered in a standard parametric family, the lognormal distribution,

iid

$$V_1, \dots, V_n | G \stackrel{\text{nu}}{\sim} G,$$

$$G | \alpha, \mu, \sigma^2 \sim DP(\alpha G_0), \quad G_0 \equiv LN(\mu, \sigma^2),$$

$$\mu | m_0, s_0 \sim N(m_0, s_0),$$

$$\sigma^{-2} | \tau_1, \tau_2 \sim \Gamma(\tau_1/2, \tau_2/2),$$

$$\beta | \beta_0, S_{\beta_0} \sim N_p(\beta_0, S_{\beta_0}),$$

where $LN(m, s^2)$ and $N(m, s^2)$ refer to a log-normal and normal distribution, respectively, with location m and scale parameter s^2 . The precision parameter of the MDP prior was chosen to be $\alpha = 10$, allowing for moderate deviations from the log-normal family. We allow the parametric family to hold only approximately, and the resulting model is robust against mis-specification of the baseline survival distribution. The covariate of interest is $trt_i = 0$ if the ith patient had radiotherapy only and $trt_i = 1$ if the ith patient had radiotherapy and chemotherapy. The following commands were used to fit the model,

prior <- list(alpha = 10, beta0 = rep(0,1),
 Sbeta0 = diag(100,1), m0 = 0,
 s0 = 1, tau1 = 0.01, tau2 = 0.01)</pre>

In our analysis, the posterior mean and 95% HPD associated with trt was 0.50 (0.12, 0.82), indicating that including chemotherapy significantly reduces the time to deterioration. Figure 2 (page 22) displays posterior summary statistics for the parameters of interest. In this case, the output includes the log of the Conditional Predictive Ordinate (CPO) (see, Geisser & Eddy 1979) for each data point, the AFT regression

tribution, and the number of clusters. Inferences about the survival curves can be obtained from the MCMC output. Indeed, given a sample of the parameters of size J, a sample of the survival curve for a given x can be drawn as follows: for the MCMC scan j of the posterior distribution, with j = 1, ..., J, we sample from $S^{(j)}(t|\mathbf{x}, data) \sim Beta(a^{(j)}(t), b^{(j)}(t))$ where $a^{(j)}(t) = \alpha^{(j)}G_0^{(j)}\left((t\exp(\mathbf{x}^T\boldsymbol{\beta}^{(j)}), +\infty)\right)$ + $\sum_{i=1}^{n} \delta_{V_{i}^{(j)}} \left((t \exp(\mathbf{x}^{T} \boldsymbol{\beta}^{(j)}), +\infty) \right)$, and $b^{(j)}(t) =$ $\alpha^{(j)} + N - a^{(j)}(t)$. This approach is implemented in the function predict.DPsurvint. For user-specified values of the covariates, xnew, and the grid where the survival function is evaluated, grid, posterior information for the survival curves can be obtained using the following commands,

coefficients, the parameters of the DP centering dis-

```
xnew <- matrix(c(0,1), nrow=2, ncol=1)
grid <- seq(0.01,70,1)
pred <- predict(fit, xnew=xnew, grid=grid)
plot(pred, all=FALSE, band=TRUE)</pre>
```

The resulting survival curves and point-wise 95% HPD intervals are given in Figure 3 (page 23).

Semiparametric Generalized Linear Mixed Model

Lesaffre & Spiessens (2001) analyzed data from a multicentre randomized comparison of two oral treatments for toe-nail infection (dermatophyte onychomycosis) involving two groups of 189 patients evaluated at seven visits; on week 0, 4, 8, 12, 24, 36, and 48. Onychomycosis, known popularly as toenail fungus, is a fairly common condition that not only can disfigure and sometimes destroy the nail but that also can lead to social and self-image issues for sufferers. Onychomycosis can be caused by several types of fungi known as dermatophytes, as well as by non-dermatophytic yeasts or molds. Dermatophyte onychomycosis corresponds to the type caused by dermatophytes. Here we are interested in the degree of onycholysis which expresses the degree of separation of the nail plate from the nail-bed and which was scored in four categories (0, absent; 1, mild; 2, moderate; 3, severe). These data were analyzed by Lesaffre & Spiessens (2001) using generalized estimating equations (GEE) and generalized linear mixed models (GLMM).

```
> summary(fit)
Bayesian Semiparametric AFT Regression Model
Call:
DPsurvint.default(formula = y ~ trt, prior = prior, mcmc = mcmc,
   state = state, status = TRUE)
Posterior Predictive Distributions (log):
  Min. 1st Qu. Median Mean 3rd Qu.
                                            Max.
-4.5920 -2.3570 -1.4600 -1.6240 -0.7121 -0.1991
Regression coefficients:
             Median Std. Dev. Naive Std.Error 95%HPD-Low 95%HPD-Upp
    Mean
trt 0.502282 0.513219 0.195521 0.001955
                                                  0.120880
                                                             0.820614
Baseline distribution:
                          Std. Dev. Naive Std.Error 95%HPD-Low 95%HPD-Upp
       Mean
             Median
       3.255374 3.255518 0.173132 0.001731 2.917770
                                                               3.589759
mu
sigma2 1.021945 0.921764 0.469061 0.004691
                                                               1.908676
                                                   0.366900
Precision parameter:
         Mean
               Median
                            Std. Dev. Naive Std.Error 95%HPD-Low 95%HPD-Upp
ncluster 27.58880 28.00000 3.39630
                                       0.03396
                                                      20.00000
                                                                 33.00000
Acceptance Rate for Metropolis Step = 0.2637435
Number of Observations: 94
```

Figure 2: Posterior summary for the Breast Cancer Data fit using DPsurvint.

GLMM provide a popular framework for the analysis of longitudinal measures and clustered data. The models account for correlation among clustered observations by including random effects in the linear predictor component of the model. Although GLMM fitting is typically complex, standard random intercept and random intercept/slope models with normally distributed random effects can now be routinely fitted in standard software. Such models are quite flexible in accommodating heterogenous behavior, but they suffer from the same lack of robustness against departures from distributional assumptions as other statistical models based on Gaussian distributions.

A common strategy for guarding against such mis-specification is to build more flexible distributional assumptions for the random effects into the model. Following Lesaffre & Spiessens (2001), we consider a logistic mixed effects model to examine the probability of moderate or severe toenail separation Y = 1 versus the probability of absent or mild Y = 0, including as covariates treatment (trt) (0 or 1), time (t) (continuous), and time×treatment interaction,

 $logit \left\{ P\left(Y_{ij} = 1 \mid \boldsymbol{\beta}, \theta_i\right) \right\} = \theta_i + \beta_1 \operatorname{Trt}_i + \beta_2 \operatorname{Time}_{ij} + \beta_3 \operatorname{Trt}_i \times \operatorname{Time}_{ij}.$

However, we replace the normality assumption of the random intercepts by using a DPM of normals

prior (see, e.g., Müller et al. 2007), $\theta_i \mid G \stackrel{iid}{\sim} G,$ $G \mid P, \Sigma_k \sim \int N(m, \Sigma_k) P(dm),$ $P \mid \alpha, \mu, \Sigma \sim DP(\alpha N(\mu, \Sigma)),$ $\beta \sim N_p(\beta_0, S_{\beta_0}),$ $\Sigma_k \mid \nu_0, T \sim IW_k(\nu_0, T),$ $\mu \mid m_b, S_b \sim N_q(m_b, S_b),$ $\Sigma \mid \nu_0, T_b \sim IW_k(\nu_b, T_b),$ $\alpha \mid a_0, b_0 \sim \Gamma(a_0, b_0).$

The semiparametric GLMM using DPM of normals model can be fitted using function DPMglmm and the following code,

Sbeta0 = diag(100,3))

- # Fitting the model
- fitDPM <- DPMglmm(fixed = infect^{*}trt+ time*trt, random = ~ 1|idnr, family = binomial(logit), prior = prior, mcmc = mcmc, state = NULL, status = TRUE)



Figure 3: Breast cancer data: Posterior probability of no evidence of breast retraction for (a) radiotherapy only and (b) radiotherapy plus chemotherapy, respectively.

Figure 4 shows the posterior estimate of the random effects distribution. The predictive density is overlaid on a plot of the posterior means of the random effects. The results clearly indicate departure from the normality assumption, suggesting the existence of groups of patients with respect to the resistance against the infection.



Figure 4: Toe-nail data: Random effects distribution and posterior means estimated using DPMglmm.

Figure 5 (page 24) reports summary statistics for the posterior distribution of the parameters of interest. It includes posterior means and 95% HPD intervals for the parameters along with two model performance measures: DIC and LPML. DIC is the deviance information criterion of Spiegelhalter et al. (2002). LPML is the log pseudo marginal likelihood of Geisser & Eddy (1979), which is a leave-one-out cross validatory measure based on predictive densities. A parametric analysis of these data (not shown), considering equivalent prior distributions, gave a DIC and LPML of 964.2 and -484.0, respectively. The results, therefore, indicate that the DPM version of the model outperforms the normal model using either the LPML or DIC statistic, suggesting that the semiparametric model is better both for explaining the observed data and from a predictive point of view.

Figure 5 (page 24) and the Pseudo Contour probabilities of the covariates in the model (see below) suggest a significant effect of time on the degree of toe-nail infection. As expected because of randomization of the patients to the treatment groups, no significant difference between the two treatment groups at baseline was observed. The results also suggest a non-significant difference in the evolution in time between the treatment groups, contradicting the results under the parametric normal model. The posterior mean (95% HPD interval) for β_3 (Trt × Time) under the normal assumption for the random effects was -0.138 (-0.271; -0.005). These results illustrate the consequences of the incorrect use of traditional model assumptions in the GLMM context.

```
> anova(fitDPM)
Table of Pseudo Contour Probabilities
```

Response: infect				
\mathtt{Df}	PsCP			
1	0.512			
1	<0.01	***		
	Df 1	infect Df PsCP 1 0.512 1 <0.01		

```
> summary(fitDPM)
Bayesian semiparametric generalized linear mixed effect model
Call:
DPMglmm.default(fixed = infect ~ trt + time * trt, random = ~1 |
   idnr, family = binomial(logit), prior = prior, mcmc = mcmc,
   state = state, status = TRUE)
Posterior Predictive Distributions (log):
             1st Qu. Median
     Min.
                                           Mean
                                                    3rd Qu.
                                                                    Max.
-9.644e+00 -2.335e-01 -4.190e-02 -2.442e-01 -8.629e-03 -4.249e-05
Model's performance:
                 pD
          Dhat
                          DIC
                                   LPML
  Dbar
   753.0
          603.6
                   149.4 902.5 -466.0
Regression coefficients:
            Mean Median Std. Dev. Naive Std.Error 95%HPD-Low 95%HPD-Upp
(Intercept) -2.508419 -2.440589 0.762218 0.005390 -4.122867 -1.091684

        0.300309
        0.304453
        0.478100
        0.003381

        -0.392343
        -0.390384
        0.046101
        0.000326

        -0.128891
        -0.128570
        0.072272
        0.000511

trt
                                                               -0.669604
                                                                            1.242553
time
                                                              -0.482329 -0.302442
trt:time
                                                                -0.265813 0.018636
Kernel variance:
                   Mean
                              Median
                                          Std. Dev. Naive Std.Error 95%HPD-Low 95%HPD-Upp
sigma-(Intercept) 0.0318682 0.0130737 0.0966504 0.0006834
                                                                       0.0009878
                                                                                   0.1069456
Baseline distribution:
                              Median Std. Dev. Naive Std.Error 95%HPD-Low 95%HPD-Upp
                   Mean
                    -2.624227 -2.558427 1.405269 0.009937 -5.621183
mub-(Intercept)
                                                                                   0.008855
sigmab-(Intercept) 26.579978 23.579114 13.640300 0.096451
                                                                         7.714973 52.754246
Precision parameter:
          Mean
                 Median
                              Std. Dev. Naive Std.Error 95%HPD-Low 95%HPD-Upp
ncluster
           70.6021 64.0000 36.7421
                                          0.2598 11.0000
                                                                        143.0000
           38.4925 25.7503
                              44.1123
alpha
                                            0.3119
                                                             1.1589
                                                                        112.1120
Acceptance Rate for Metropolis Steps = 0.8893615 0.9995698
Number of Observations: 1908
Number of Groups: 294
```

Figure 5: Posterior summary for the Toe-nail Data fit using DPMglmm.

```
trt:time 1 0.075 .
                                                        prior = prior, mcmc = mcmc,
                                                        state = state, status = TRUE)
Signif. codes: 0 '***' 0.001 '**' 0.01
'*' 0.05 '.' 0.1 ' ' 1
                                                   Posterior mean of subject-specific components:
Finally, information about the posterior distribution
                                                         (Intercept)
of the subject-specific effects can be obtained by us-
                                                          1.6239
                                                    1
ing the DPMrandom function as follows,
                                                           .
> DPMrandom(fitDPM)
                                                    383
                                                          2.0178
Random effect information for the DP object:
Call:
DPMglmm.default(fixed = infect ~ trt +
    time * trt, random = ~1 |idnr,
    family = binomial(logit),
```

Summary and Future Developments

As the main obstacle for the practical use of BSP and BNP methods has been the lack of estimation tools, we presented an R package for fitting some frequently used models. Until the release of **DPpackage**, the two options for researchers who wished to fit a BSP or BNP model were to write their own code or to rely heavily on particular parametric approximations to some specific processes using the **BUGS** code given in Peter Congdon's books (see, e.g., Congdon 2001). **DPpackage** is geared primarily towards users who are not willing to bear the costs associated with both of these options.

Many improvements to the current status of the package can be made. For example, all **DPpackage** modeling functions compute CPOs for model comparison. However, only some of them compute the effective number of parameters pD and the deviance information criterion (DIC), as presented by Spiegelhalter et al. (2002). These and other model comparison criteria will be included for all the functions in future versions of **DPpackage**.

The implementation of more models, the development of general-purpose sampling functions, and the ability to run several Markov chains at once and to handle large dataset problems through the use of sparse matrix techniques, are areas of further improvement.

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Bibliography

- J. Besag, P. Green, D. Higdon, and K. Mengersen. Bayesian computation and stochastic systems (with Discussion). *Statistical Science*, 10:3–66, 1995.
- J. M. Chambers, S. Cleveland, and A. P. Tukey. Graphical Methods for Data Analysis. *Boston*, *USA: Duxbury*, 1983.

- M. H. Chen and Q. M. Shao. Monte Carlo estimation of Bayesian credible and HPD intervals. *Journal of Computational and Graphical Statistics*, 8(1):69–92, 1999.
- R. Christensen and W. O. Johnson. Modeling Accelerated Failure Time With a Dirichlet Process. *Biometrika*, 75:693–704, 1998.
- P. Congdon. *Bayesian Statistical Modelling*. New York, USA: John Wiley and Sons, 2001.
- M. D. Escobar and M. West. Bayesian density estimation and inference using mixtures. *Journal of the American Statistical Association*, 90:577–588, 1995.
- T. S. Ferguson. A Bayesian analysis of some nonparametric problems. *The Annals of Statistics*, 1:209–230, 1973.
- S. Geisser and W. Eddy. A predictive approach to model selection. *Journal of the American Statistical Association*, 74:153–160, 1979.
- W. R. Gilks, A. Thomas, and D. J. Spiegelhalter. Software for Gibbs sampler *Computing Science and Statistics* 24:439–448, 1992.
- T. Hanson. Inference for Mixtures of Finite Polya Tree Models. *Journal of the American Statistical Association*, 101:1548–1565, 2006.
- T. Hanson and W. O. Johnson. A Bayesian Semiparametric AFT Model for Interval-Censored Data. *Journal of Computational and Graphical Statistics* 13(2):341–361, 2004.
- A. Jara, M. J. Garcia-Zattera, and E. Lesaffre. A Dirichlet Process Mixture model for the analysis of correlated binary responses. *Computational Statistics and Data Analysis*, 51:5402–5415, 2007.
- J. Klein and M. Moeschberger. *Survival Analysis*. New York, USA: Springer-Verlag, 1997.
- E. Lesaffre and B. Spiessens. On the effect of the number of quadrature points in a logistic random-effects model: an example. *Applied Statistics* 50: 325–335, 2001.
- G. Lin and C. Zhang. Linear Regression With Interval Censored Data. *The Annals of Statistics* 26:1306– 1327, 1998.
- P. Müller and F.A. Quintana. Nonparametric Bayesian Data Analysis. *Statistical Science* 19(1):95– 110, 2004.
- P. Müller, A. Erkanli, and M. West. Bayesian Curve Fitting Using Multivariate Normal Mixtures. *Biometrika*, 83:67–79, 1996.
- P. Müller, F. A. Quintana, and G. Rosner. Semiparametric Bayesian Inference for Multilevel Repeated Measurement Data. *Biometrics*, 63(1):280– 289, 2007.

- M. A. Newton, C. Czado, and R. Chappell. Bayesian inference for semiparametric binary regression. *Journal of the American Statistical Association* 91:142– 153, 1996.
- M. Plummer, N. Best, K. Cowles, and K. Vines. CODA: Output analysis and diagnostics for MCMC. *R package version* 0.12-1, 2007.
- B. J. Smith. boa: Bayesian Output Analysis Program (BOA) for MCMC. *R package version* 1.1.6-1, 2007.

An Introduction to gWidgets

by John Verzani

Introduction

CRAN has several different packages that interface R with toolkits for making graphical user interfaces (GUIs). For example, among others, there are RGtk2 (Lawrence and Temple Lang, 2006), rJava, and tcltk (Dalgaard, 2001). These primarily provide a mapping between library calls for the toolkits and similarly named R functions. To use them effectively to create a GUI, one needs to learn quite a bit about the underlying toolkit. Not only does this add complication for many R users, it can also be tedious, as there are often several steps required to set up a basic widget. The gWidgets package adds another layer between the R user and these packages providing an abstract, simplified interface that tries to be as familiar to the R user as possible. By abstracting the toolkit it is possible to use the gWidgets interface with many different toolkits. Although, open to the criticism that such an approach can only provide a least-common-denominator user experience, we'll see that gWidgets, despite not being as feature-rich as any underlying toolkit, can be used to produce fairly complicated GUIs without having as steep a learning curve as the toolkits themselves.

As of this writing there are implementations for three toolkits, **RGtk2**, **tcltk**, and **rJava** (with progress on a port to **RwxWidgets**). The **gWidgetsRGtk2** package was the first and is the most complete. Whereas **gWidgetstcltk** package is not as complete, due to limitations of the base libraries, but it has many useful widgets implemented. Installation of these packages requires the base toolkit libraries be installed. For **gWidgetstcltk** these are bundled with the windows distribution, for others they may require a separate download. S. D. Spiegelhalter, N. G.Best, B. P. Carlin, and A. Van der Linde. Bayesian measures of model complexity and fit. *Journal of the Royal Statistical Society: Series B* 64:583–639, 2002.

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Dialogs

We begin by loading the package. Both the package and at least one toolkit implementation must be installed prior to this. If more than one toolkit implementation has been installed, you will be queried as to which one to use.

library("gWidgets")

The easiest GUI elements to create are the basic dialogs (Figure 1). These are useful for sending out quick messages, such as: 1

```
gconfirm("Are we having fun?")
```



Figure 1: Simple dialog created by gconfirm using the **RGtk2** toolkit.

A basic dialog could be used to show error messages

```
options(error = function() {
  err = geterrmessage()
  gmessage(err, icon="error")
})
```

or, be an alternative to file.choose

```
source(gfile())
```

In **gWidgets**, these basic dialogs are modal, meaning the user must take some action before control of R is returned. The return value is a logical or string, as appropriate, and can be used as input to a further command. Modal dialogs can be confusing

¹The code for these examples is available from http://www.math.csi.cuny.edu/pmg/gWidgets/rnews.R

if the dialog gets hidden by another window. Additionally, modal dialogs disrupt a user's flow. A more typical GUI will allow the R session to continue and will only act when a user initiates some action with the GUI by mouse click, text entry, etc. The GUI designer adds handlers to respond to these events. The **gWidgets** programming interface is based around facilitating the following basic tasks in building a GUI: constructing widgets that a user can control to affect the state of the GUI, using generic functions to programmatically manipulate these widgets, simplifying the layout of widgets within containers, and facilitating the assigning of handlers to events initiated by the user of the GUI.

Selecting	а	CRAN	site
-----------	---	------	------

X	Se	ect a	CF	RAN mirro)r		23
Filter b	y Cou	ntry =	:=	USA	•		
Name			Co	untry	City	7	\Box
USA	(CA	1)	U۵	A	Berł	celey	
USA	(CA	2)	U۵	A	Los	Angeles	
USA	(CA	3)	U۵	A	Dav:	is	
USA	(IA)		U۵	A	Ames	5	
USA	(IL)		U۵	A	Chio	cago	
USA	(MI)		U۵	A	Houg	ghton	
USA	(MO)		U۵	A	St.	Louis	
USA	(NC)		U۵	A	Chap	pel Hill	
USA	(PA	1)	U۵	A	Pitt	sburgh	
USA	(PA	2)	U۵	A	Pitt	sburgh	
USA	(TX)		UΒ	5A	Dall	las	
USA	(WA)		U۵	A	Seat	tle	
							7
						\geq	

Figure 2: GUI to select a CRAN mirror shown using **gWidgetstcltk**. The filter feature of gtable has been used to narrow the selection to USA sites. Double clicking a row causes the CRAN repository to be set.

Selecting an item from a list of items or a table of items is a very common task in GUIs. Our next example presents a GUI that allows a user to select with the mouse a CRAN repository from a table. The idea comes from a **tcltk** GUI created by the chooseCRANmirror function. This example shows how the widget constructors allow specification of both containers and event handlers.

We will use this function to set the CRAN repository from a URL.

```
setCRAN <- function(URL) {
  repos = getOption("repos")
  repos["CRAN"] <- gsub("/$", "", URL)
  options(repos=repos)
}</pre>
```

To begin our GUI we first create a top-level window to contain our table widget.

win <- gwindow("Select a CRAN mirror")</pre>

A call to gwindow will pop-up a new window on the screen and return an object which can be manipulated later. The argument sets the window title.

The widget we create will show the possible CRAN values in a tabular format for easy selection by a mouse. Selection occurs when a row is clicked. We will assign this function to respond to a double click event:

```
handler = function(h,...) {
    URL <- svalue(tbl) # get value of widget
    setCRAN(URL) # set URL
    dispose(win) # close window
}</pre>
```

The svalue function is a new generic function which retrieves the selected value for a widget, in this case one called tbl constructed below. The dispose function is a new generic which for windows causes them to be destroyed. So this handler will set the chosen URL and then destroy the top-level window.

The gtable function constructs a widget allowing the user to select a value from a data frame and returns an object for which generic functions are defined. The row of the value is selected with a mouse click, whereas, the selected column is specified at the time the widget is constructed using the chosencol argument. Additionally, this function allows the specification of a column whose unique values can be used to filter the display of possible values to select from.

```
tbl <- gtable(
    items=utils:::getCRANmirrors(),
    chosencol=4,
    filter.column=2,
    container=win,
    handler=handler
)</pre>
```

Figure 2 shows the final widget using the **tcltk** toolkit.

Using gWidgets

We now go through the basic steps of building a GUI using **gWidgets** a little more systematically.

Containers

As illustrated previously a top-level window is created using gwindow. The **gWidgets** package only allows one widget to be packed into a top-level window. As such, typically a container that can hold more than one object is packed into the top-level window. There are several types of containers available. The ggroup function produces a container that may be visualized as a box that allows new widgets to be packed in from left to right (the default) or from top to bottom (horizontal=FALSE). Nesting such containers gives a wide range of flexibility.

Widgets are added to containers through the container argument at the time of construction (which hereafter we shorten to cont) or using the add method for containers. However, **gWidgetstcltk** requires one to use the container argument when a widget is constructed. That is, except with **gWidgetstcltk**

```
win <- gwindow("test")
b <- gbutton("click me", cont=win)</pre>
```

is equivalent to

```
win <- gwindow("test")
add(win, gbutton("click me"))</pre>
```

The latter is a bit more convenient as it allows one to keep separate the widget's construction and its layout, but the former allows more portability of code.



Figure 3: Expanding group example after resizing window. The button, label and text widgets use nested ggroup containers for their layout.

To illustrate nested ggroup containers and the add and delete generics for containers, the following example shows how to create a widget that can hide or show its contents when a button is clicked. This is more fully implemented in the gexpandgroup container.

We begin by defining a top-level window and immediately add a ggroup instance which packs in its widgets from top to bottom.

```
win <- gwindow("Expanding group")
g <- ggroup(horizontal=FALSE, cont=win)</pre>
```

Inside of g we add a nested group which will contain a button and a label.

Finally, we add a ggroup instance to the g container to hold the widgets that we wish to hide and put a widget into the new container.

```
g2 <- ggroup(cont=g, expand=TRUE)
e <- gedit("Hide this with button",
    cont=g2)</pre>
```

That finishes the layout. Figure 3 shows the GUI in the expanded state. To make this example do something interesting, we define functions to respond to clicking on the button or the label. These functions toggle whether or not the g2 container is packed into the g container using the add and delete generics for containers.

```
expandGroup = function()
  add(g,g2, expand=TRUE)
hideGroup = function() delete(g,g2)
```

The add generic is used to add a widget (or container) to a container. In this case, the argument expand=TRUE is given to force the added widget to take up as much space as possible. The delete generic removes a widget from a container. The widget is not destroyed, as with dispose, just removed from its container.

Next, we define a handler to be called when the button or label is clicked. This involves arranging a means to toggle between states and to adjust the button text accordingly.

```
state <- TRUE # a global
changeState <- function(h,...) {
    if(state) {
        hideGroup()
        svalue(button) <- ">"
    } else {
        expandGroup()
        svalue(button) <- "V"
    }
    state <<- !state
}</pre>
```

We used the <<- operator so that the value of state is updated in the global environment, rather than the environment of the handler.

Finally, we bind this handler to both the button and the label, so that it is called when they are clicked.

- ID <- addHandlerClicked(button, handler=changeState)
- ID <- addHandlerClicked(label, handler=changeState)

There are just a few options for the layout of widgets within a ggroup container, compared to those available in the various toolkits. We illustrated the expand argument. With rJava and tcltk there is also an anchor argument which takes a value of the form c(x,y) where x or y are -1, 0, or 1. These are used to specify which corner of the space allocated by the container the widget should add itself in.

Additionally, the ggroup instances have methods addSpace to add a fixed amount of blank space and addSpring to add a "spring" which forces the remaining widgets to be pushed to the right (or the bottom) of the containers. This simple example shows how these can be used to put buttons on the right side of a dialog. First we pack a ggroup instance into a top-level container.

X	Mock up			
	>	Cancel	∨ <u>о</u> к	

Figure 4: Illustration of addSpace and addSpring methods of ggroup using the **gWidgetsRGTk2** package after resizing main window. The buttons are pushed to the right side by addSpring.

```
win <- gwindow("Mock up")
bg <- ggroup(cont=win, expand=TRUE)
addSpring(bg)  # push to right</pre>
```

Now we add two buttons and a bit of space, 10 pixels, between them. By default, packing is done from left to right, starting on the left. The use of addSpring pushes the packed in containers and widgets to the right side of the container.

```
b1 <- gbutton("cancel", cont=bg)
addSpace(bg,10) # add some space
b2 <- gbutton("ok", cont=bg)</pre>
```

The expand=TRUE value for bg ensures that that container expands to fill the space it can, otherwise the button widgets would push to the boundary of the button group and not the outside container win. Figure 4 shows the widget.

Other containers are illustrated in the examples below. These include glayout for laying out widgets in a grid, gnotebook for holding multiple widgets at once with tabs used to select between the widgets, and gpanedgroup which uses a movable pane to allocate space between widgets. Additionally, gframe is similar to ggroup, but with an external frame and area for a label.

Basic widgets

A GUI is composed of widgets packed into containers. In **gWidgets** there are a number of familiar widgets. We've illustrated labels and buttons (glabel and gbutton). Additionally there are widgets to select from a list of items (gradio, gdroplist, and gcheckboxgroup); widgets to select from a table of values (gtable); widgets to select files or dates (gfile, gcalendar); widgets to edit text (gedit, gtext); a widget to edit a data frame (gdf); a widget to display graphic files (gimage); and others. Not all are available for each toolkit.

The following example, modified from a recent R News article on the **rpanel** package (Bowman et al., 2006), illustrates how many of these widgets can be combined to create a GUI to demonstrate confidence intervals. This example uses the glayout container to lay out its widgets in a grid.

First we pack the container into a top level window.

win <- gwindow("CI example")
tbl <- glayout(cont=win)</pre>

The glayout container uses matrix-like notation to specify where the widgets are placed. When the assigned value is a string, a glabel is used.

X	CI example	
mu	0	
sigma	1.0 -	
n		
	5 28 51 74 97	
conf. level		0.95
No. intervals	10	
	○ 25	
	○ 50	
	○ 100	
	resample	

Figure 5: GUI for a confidence interval demonstration, using **gWidgetsrJava**, illustrating several different widgets: gedit for single-line editing; and gdroplist, gslider, gspinbox, and gradio for selection from a fixed set of items.

```
tbl[1,1] <- "mu"
tbl[1,2] <-
  (mu <- gedit("0", cont=tbl,</pre>
    coerce.with=as.numeric))
tbl[2,1] <- "sigma"
tb1[2,2] <-
  (sigma <- gdroplist(c(1,5,10),</pre>
    cont=tbl))
tbl[3,1] <- "n"
tbl[3,2] <- (
  n <- gslider(from=5,to=100, by=1,</pre>
    value = 10, cont=tbl))
tbl[4,1] <- "conf. level"
tb1[4,2, expand=TRUE] <-
  (confLevel <- gspinbutton(</pre>
    from=0.5, to=0.99, by=0.01,
    value=0.95, cont=tbl))
tbl[5,1] <- "No. intervals"</pre>
tb1[5,2] <-
  (noIntervals <- gradio(c(10,25,</pre>
    50,100), cont=tbl))
tb1[6,2] <-
  (resample <- gbutton("resample",</pre>
    cont=tbl))
visible(tbl) <- TRUE
```

The last line with visible is necessary for **gWidgetsRGtk2** to produce the layout.

The matrix-notation refers to where the widget is placed. An assignment like

```
tbl[1:2,2:3] <- "testing"
```

would place a label within the area for the first and second rows and second and third columns. Unlike matrices, the notation is not used to vectorize the placement of several widgets, extract widgets, or replace a widget. The above code completes the widget construction and layout. Figure 5 shows a realization using **rJava**.

The widgets have various arguments to specify their values that depend on what the widget does. For example, the slider and spinbutton select a value from a sequence, so the arguments mirror those of seq. Some widgets have a coerce.with argument which allows a text-based widget, like gedit, to return numeric values through svalue. The gdroplist widget is used above to pop up its possible values for selection. Additionally, if the editable=TRUE argument is given, it becomes a combo-box allowing a user to input a different value.

In Figure 5 we see in the slider widget one of the limitations of the **gWidgets** approach – it is not as feature rich as any individual toolkit. Although the underlying JSlider widget has some means to adjust the labels on the slider, **gWidgets** provides none in its API, which in this case is slightly annoying, as Java's chosen values of 5, 28, 51, 74, and 97 just don't seem right.

The values specified by these widgets are to be fed into the function makeCIs, which is not shown here, but uses matplot to construct a graphic displaying simulated confidence intervals. To make this GUI interactive, the following handler will be used to respond to changes in the GUI. We need to call svalue on each of the widgets and then pass these results to the makeCIs function. This task is streamlined by using lapply and do.call:

```
allWidgets <- list(mu,sigma,noIntervals,
    n, confLevel, resample)
plotCI <- function(h, ...) {
    lst <- lapply(allWidgets,svalue)
    do.call(makeCIs,lst)
}
```

Again we use lapply to add the handler to respond to the different widget default events all at once.

```
invisible(sapply(allWidgets,function(i)
    addHandlerChanged(i,handler=plotCI))
)
```

Interacting with widgets programmatically

In **gWidgets**, the widget and container constructors return S4 objects of various classes. These objects are accessed programmatically with generic functions. As was sensible, generic methods familiar to R users were used, and when not possible, new generics were added. For example, for widgets which store values to select from, the generics [and [<- are used to refer to the possible values. For other widgets, as appropriate, the generics dim, names, length, etc., are defined. To get and set a widget's "selected" value, the new generic functions svalue and svalue<- were defined. The term "selected" is loosely defined, e.g., applying to a button's text when clicked.

This simple example shows how selecting values in a checkbox group can be used to set the possible values in a drop list. First we create a container to hold the two widgets.

```
win <- gwindow("methods example")
g <- ggroup(cont=win)</pre>
```

The construction of the two widgets is straightforward: simply specify the available values using items.

```
cb <- gcheckboxgroup(items=letters[1:5],
    cont=g)
dl <- gdroplist(items="", cont=g)</pre>
```

To finish, the following adds a handler to cb which will update the possible values of dl when the user changes the value of the checkbox group.

ID <- addHandlerChanged(cb, function(h,...) { dl[] <- svalue(cb) })

A few other new generics are defined in **gWidgets** for the basic widgets such as font<- for setting font properties, size<- to adjust the size in pixels for a widget, enabled<- to adjust if the widget can accept input, and the pair tag and tag<-, which is like attr only its values are stored with the widget. This latter function is useful as its values can be updated within a function call, such as a handler, as this next example shows. The expanding group example with the state variable would have been a good place to use this feature.

```
> x = gbutton("test", cont=gwindow())
> tag(x,"ex") <- attr(x,"ex") <- "a"
> f = function(y)
+ tag(y,"ex") <- attr(y,"ex") <- "b"
> c(tag(x,"ex"),attr(x,"ex"))
[1] "a" "a"
> f(x)
> c(tag(x,"ex"),attr(x,"ex"))
[1] "b" "a"
```

Handlers

A GUI user initiates an event to happen when a button is clicked, or a key is pressed, or a drag and drop is initiated, etc. The **gWidgets** package allows one to specify a handler, or callback, to be called when an event occurs. These handlers may be specified when a widget is constructed using the handler argument, or added at a later time. To add the default handler, use the addHandlerChanged generic. Most, but not all, widgets have just one type of event for which a handler may be given. For instance, the gedit widget has the default handler respond to the event of a user pressing the ENTER key. Whereas, the addHandlerKeystroke method can be used to add a handler that responds to any keystroke. Officially, only one handler can be assigned per event, although some toolkits allow more.

Handlers return an ID which can be used with removeHandler to remove the response to the event.

The signature of a handler function has a first argument, h, to which is passed a list containing components obj, action and perhaps others. The obj component refers to the underlying widget. In the examples above we found this widget after storing it to a variable name, this provides an alternative. The action component may be used to passed along an arbitrary value to the handler. The other components depend on the widget. For the ggraphics widget (currently just **gWidgetsRGtk2**), the components x and y report the coordinates of a mouse click for addHandlerClicked. Whereas, for addDropTarget the dropdata component contains a string specifying the value being dragged.

To illustrate the drag-and-drop handlers the following creates two buttons. The drop source needs a handler which returns the value passed along to the dropdata component of the drop target handler. In this example, clicking on the first button and dragging its value onto the label will change the text displayed on the label.

```
g = ggroup(cont=gwindow("DnD example"))
11 <- gbutton("drag me", cont=g)
12 <- glabel("drop here", cont=g)
ID <- addDropSource(11, handler=
   function(h,...) svalue(h$obj))
ID <- addDropTarget(12, handler =
   function(h,...)</pre>
```

svalue(h\$obj) <- h\$dropdata)

Drag and drop works with all the toolkits except **gWidgetsrJava** where only what is provided natively through the Java libraries is working.

An application

This last example shows how to make a more ambitious GUI for a task; in this case, an interface to download and visualize stock prices. New widgets and containers shown are the toolbar widget; the notebook container, which is used to present different simultaneous summaries of a stock; the variable selector widget, for selecting variables from the workspace; and the generic widget constructor, which creates a simple GUI based on a function's arguments, as found by formal. Although more involved than the examples above, it is meant to show how specialized GUIs can be formed relatively easily by gluing together the pieces available through **gWidgets**. Figure 6 shows the result of running the following code, then downloading data for Google into the session.



Figure 6: Stock browser widget using **gWidgetsRGtk2**. This illustrates a toolbar, the variable selector, and a notebook container.

We begin by loading the **tseries** package which contains the get.hist.quote() function for retrieving stock data from www.yahoo.com and calls in the handy **zoo** package by Achim Zeileis and Gabor Grothendieck or use for later use.

invisible(require("tseries"))

In previous examples we used the global environment to store our variables. This works well for a single GUI, but can quickly lead to problems with colliding variable names with multiple GUIs. Setting up a separate environment for each GUI is one way around this potential conflict. Similarly, the **proto** package can be used effectively to provide an environment and more. Other possible methods are to use namespaces or the environment within a function body. In this example, we create a new environment to store our global variables.

e <- new.env()

The environment e is accessed using list-like syntax.

To download stock information we use get.hist.quote. We define this function to reduce the number of arguments so that ggenericwidget produces a simpler GUI (Figure 7).

```
getQuotes = function(
    inst = "GODG",
    quote = c("Open","High","Low","Close"),
    start, end)
get.hist.quote(inst, start=start,
    end=end, quote=quote)
```



Figure 7: The GUI for getQuotes created by ggenericwidget using the **RGtk2** toolkit.

We define two functions to display graphical summaries of the stock, using the **zoo** package to produce the plots. Rather than use a plot device (as only **gWidgetsRGtk2** implements an embeddable one through ggraphics), we choose instead to make a file containing the plot as a graphic and display this using the gimage widget. In **gWidgetstcltk** the number of graphic formats that can be displayed is limited, so we use an external program, convert, to create a gif file. This is not needed if using **RGtk2** or **rJava**.

```
showTrend <- function(stock) {</pre>
  trendPlotFile <- e$trendPlotFile</pre>
  png(trendPlotFile)
 plot(stock, main="Trend plot")
  lines(rollmean(stock, k = 30), lwd=2,
    lty=2, col=gray(.7))
  lines(rollmean(stock, k = 90), lwd=2,
    lty=3, col=gray(.7))
  legend(index(stock)[length(stock)],
   min(stock),
   legend=c("30 day MA","90 day MA"),
   lty=2:3,xjust=1, yjust=0)
  dev.off()
  ## create a gif file
  system(paste("convert ",
    trendPlotFile," ",
    trendPlotFile,".gif",sep=""))
  svalue(e$trendPlot) = paste(
    trendPlotFile,".gif",sep="")
}
```

The function showDiscount is similarly defined but not shown.

The main function below is used to update the notebook pages when a new stock is selected, or the graphing parameters are changed. This function refers to widgets defined in a subsequent code chunk.

```
updateNB <- function(h,...) {
    ## update data set
    ifelse(e$curDSName != "",
        e$curDS <- get(e$curDSName),
        return())
    ## get data within specified range</pre>
```

```
start <- svalue(e$startD)
if(start == "") start=NULL
end <- svalue(e$endD)
if(end == "") end = NULL
dataSet = window(e$curDS,
   start=start,end=end)
## update summaries
svalue(e$noSum) =
   capture.output(summary(dataSet))
showDiscount(dataSet,
   svalue(e$discRate))
showTrend(dataSet)
}</pre>
```

Now the main application is defined. First some variables.

```
e$curDSName <- ""
e$curDS <- NA
e$tsPlotFile <- tempfile()
e$trendPlotFile <- tempfile()
```

Next we define the main window and a container to hold the subsequent widgets.

The first widget will be a toolbar. This basic one has two actions, one to open a dialog allowing a user to download stock information from the internet, the other a quit button. To be more friendly to R users, The gtoolbar() constructor uses a list to specify the toolbar structure, rather than, say, XML. Basically, each named component of this list should be a list with a handler component and optionally an icon component. Menubars are similarly defined, only nesting is allowed.

```
## Set up simple toolbar
tb <- list()
tb$"Get quotes"$handler <- function(...)
ggenericwidget("getQuotes",
    container=gwindow("Get quotes"))
tb$"Get quotes"$icon <- "ts"
tb$Quit$handler <- function(...)
dispose(e$win)
tb$Quit$icon <- "cancel"
theTB <- gtoolbar(tb, cont=e$gp)</pre>
```

This application has widgets to adjust the interest rate (used as a discounting factor), and the start and end dates. The date widgets use the gcalendar() constructor for easier date selection.

```
## Now add parameters
e$pg <- ggroup(horizontal=TRUE,
    cont = e$gp)
## the widgets
1 <- glabel("Discount rate (%):",
    cont=e$pg)
e$discRate <- gedit(0, cont=e$pg,</pre>
```

```
coerce.with=as.numeric,
handler=updateNB)
e$pg <- ggroup(horizontal=TRUE,
cont = e$gp)
1 <- glabel("Range of dates:",
cont=e$pg)
curDate <- Sys.Date()
1 <- glabel("from=", cont=e$pg)
e$startD <-
gcalendar(as.character(curDate-365),
handler=updateNB, cont=e$pg)
1 <- glabel("to=", cont=e$pg)
e$endD <-
gcalendar(as.character(curDate),
handler=updateNB, cont=e$pg)
```

A paned group is used for the final layout, alllowing the user to adjust the amount of room for each major part of the GUI. One part is a variable selection widget provided by gvarbrowser(). Double clicking a row calls the updateNB handler to update the notebook pages.

```
e$gpg <- gpanedgroup(cont=e$gp,
expand=TRUE)
e$varSel <- gvarbrowser(
cont= e$gpg,
handler = function(h,...) {
    e$curDSName <- svalue(e$varSel)
    updateNB()
})
```

The other major part of the GUI is a notebook container to hold the three different summaries of the stock.

```
e$nb <- gnotebook(cont=e$gpg)
```

Finally, we add pages to the notebook container below. The additional label argument sets the text for the tab. (These can be adjusted later using names<-.)

```
## A numeric summary of the data set
e$noSum <- gtext("Numeric summary",
    cont=e$nb, label="Summary")
## First graphic summary
e$tsPlot <- gimage(e$tsPlotFile,</pre>
```

```
cont=e$nb, label="Time series plot")
size(e$tsPlot) <- c(480,480)
## secondGraphicSummary
e$trendPlot <- gimage(e$trendPlotFile,
    cont=e$nb, label="Trend plot")</pre>
```

Acknowledgments

The **gWidgets** package was designed as an extension of the **iWidgets** package (Urbanek, 2007) of Simon Urbanek for Michael Lawrence's **RGtk2** package (an extension of Duncan Temple Lang's **RGtk** package). Michael had done an initial port. Philippe Grosjean suggested to the author to abstract the code to make it independent of toolkit and Simon Urbanek contributed several key ideas for this. The author would like to thank all of the above for helpful comments, and the thoughtful and thorough report of an anonymous referee of an initial version of this article.

Bibliography

- A. Bowman, E. Crawford, and R. Bowman. rpanel: Making graphs move with tcltk. *R News*, 6(5):12– 17, October 2006.
- P. Dalgaard. The R-Tcl/Tk interface. In F. Leisch and K. Hornik, editors, *Proceedings of the 2nd International Workshop on Distributed Statistical Computing* (*DSC 2001*), March 2001. ISSN: 1609-395X.
- M. Lawrence and D. Temple Lang. RGTK2-A GUI Toolkit for R. *Statistical Computing and Graphics*, 17(1), 2006. Pusblished at http://www.amstat-online.org/sections/ graphics/newsletter/newsletter.html.
- S. Urbanek. iWidgets. http://www.rforge.net/ iWidgets/.

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Financial Journalism with R

Bill Alpert

R proved itself a sharp tool in testing the stock picks of Jim Cramer, a popular US financial journalist. We examined Cramer's advice for a recent cover story in *Barron's*, the Dow Jones & Co. stock market weekly, where I am a reporter and floundering R user (Alpert, 2007). The August 20, 2007 story should be accessible without subscription at the *Barron's* website (http://www.barrons.com).

The 52-year-old Cramer once ran a hedge fund which racked up 24% annualized returns over about a dozen years. His current celebrity comes from the *Mad Money* television show on the cable network CNBC, in which he makes Buy and Sell recommendations to the accompaniment of wacky sound effects and clownish antics. A few have attempted to measure the performance of modest samples of Cramer's picks (Engelberg et al., 2007; Nayda, 2006). Yet Cramer makes almost 7,000 recommendations a year, according to the count of a database at his *Mad Money* website (http://madmoney.thestreet. com/). He has never reported the performance of all those stock picks. I figured I'd try.

As in most projects, data collection was the hard part. I called Cramer and asked for any records of his Mad Money picks. After ripping into me and all journalists who've reviewed his show, he stopped taking my calls. Meanwhile, I found a website maintained by a retired stock analyst, who had tallied about 1,300 of Cramer's Mad Money recommendations over two years. I also found the abovementioned database at Cramer's official website, which recorded over 3,400 recommendations from the preceding six months. This Cramer site classified his picks in ways useful for subsetting in R, but conspicuously lacked any performance summaries. I turned these Web records of his stock picks into Excel spreadsheets. Then I downloaded stock price histories from Edgar Online's I-Metrix service (http: //I-Metrix.Edgar-Online.com), using some Excel macros. None of this was trivial work, because I wanted a year's worth of stock prices around each recommendation and the date ranges varied over the thousands of stocks. Financial data suppliers can deliver a wealth of information for a single, common date range, but an "event study" like mine involved hundreds of date ranges for thousands of stocks. Most finance researchers deal with this hassle by using SAS and a third-party add-on called Eventus that eases data collection. But I wanted to use R.

I reached out to quantitative finance programmer Pat Burns and Pat wrote some R code for our event study style analysis. Pat has posted his own working paper on our study at his website (http: //www.burns-stat.com). R's flexibility was useful because we needed a novel data structure for the Cramer analysis. In most analyses, the data for prices (or for returns) are in a matrix where each column is a different stock and each row is a specific date. In our case, each stock recommendation had the same number of data points, so a matrix was a logical choice. However, instead of each row being a specific date, it was a specific offset from the recommendation date. We still needed the actual date, though, in order to get the difference in return between the stocks and the S&P 500 on each day – to see if Cramer's picks "beat the market." Pat's solution was to have a matrix of dates as a companion to the matrix of prices. It was then a trivial subscripting exercise to get a matrix of S&P returns that matched the matrix of returns for the recommendations. Many stocks were recommended multiple times, so the column names of the matrices were not unique.

Once the data were in R, it was fairly easy to test various investment strategies, such as buying the day after Cramer's 6 pm show or, instead, waiting two days before buying. Any investment strategy that actively picks stocks should at least beat the returns you'd get from a passive marketmimicking portfolio with comparable risk (that is, similar return variance) - and it should beat the market by enough to cover trading costs. Otherwise you ought to keep your money in an index fund. You can see the importance of marketadjusting Cramer's returns by comparing the red and blue lines in Figure 1. The Nasdaq Composite Index is arguably a better match to the riskiness of Cramer's widely-varying returns. We made his performance look better when we used the S&P.



Figure 1: Average cumulative percentage log return from the day of broadcast for approx. 1,100 Mad Money recommendations recorded at http://www. yourmoneywatch.com. Blue line shows return relative to S&P 500 Index.

The red line shows his average pick's unadjusted log return, while the blue shows the log return relative to the Standard & Poors 500 Index. The data were roughly 1,100 Buy recommendations over the period from July 2005 to July 2007. The lines' lefthand peaks mark the trading day after each evening broadcast, when enthusiastic fans have bid up Cramer's pick. We ultimately tested several dozen investment strategies.

The results were disappointing for someone who wants to follow Cramer's advice. You could not beat the market by a statistically significant amount if you followed his recommendations in any way readily available to a viewer. But we did find that you might make an interesting return if you went against Cramer's recommendations – shorting his Buys the morning after his shows, while putting on offsetting S&P 500 positions. This shorting opportunity appears in Figure 1, as the widening difference between the red and blue lines. If a viewer shorted only Cramer's recommendations that jumped 2% or more on the day after his broadcasts, that difference could earn the viewer an annualized 12% on average (less trading costs). The bootstrapped 95% confidence intervals of this difference ranged from 3% to 21%. (For background on bootstrap techniques, see Efron and Tibshirani, 1993)



Figure 2: Cumulative log return relative to S&P 500 on about 480 of Cramer's off-the-cuff Lightning Round Sell recommendations, as recorded at madmoney.thestreet.com. The yellow band is a bootstrapped 95% confidence interval, showing that the negative return – desirable for Sell recommendations – is clearly different from zero

One reason we tested so many different strategies is that when I finally started getting responses from Cramer and CNBC, they kept changing their story. They argued about selection. Neither of my databases were reliable records of Cramer's picks, CNBC said, not even the database endorsed by

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Cramer at his website. Instead of giving me a record of his two-years' of stock picks, they suggested that I watch tapes of all his shows, which they'd gladly provide me. It reminded me of the endless tasks assigned in fairy tales – separating peas from the ash pile.

They also argued that certain subsets of Cramer's recommendations were the only proper ones to count ... as if viewers would somehow know which of his screaming "Buys" he meant them to ignore. As it happened, the segment of his show that Cramer argued most shrilly for us to deselect (the "Lightning Round" with his impromptu responses to phoned-in questions) was the only segment with any statistically-significant marketbeating returns – in this case, on the Sell recommendations (see Figure 2). Embarrassingly, the Sell recommendations that Cramer prepared in advance went up (see Figure 3).

Negative featured or discussed



Figure 3: Cumulative log return relative to S&P 500 on about 160 of Cramer's Prepared Sell recommendations as recorded at madmoney.thestreet.com

CNBC and Cramer also kept shifting their claim about when Cramer advises his audience to act on his picks. After I told Cramer that viewers got market-lagging returns if they bought the day after his recommendations (when most viewers clearly do their buying), he angrily said that he "always" advises waiting until the second day. When I came back with evidence that a second-day purchase also lagged the market (as is clear in Figure 1), CNBC said that Cramer's advice had "always" been to wait a week or two after each show. Later still, they said that a good test should wait exactly five days.

Such data dredging and methodological debates are probably not unfamiliar to readers of this newsletter who use R for high stakes evaluations of pharmaceuticals or government interventions, but journalism may be extreme in its extensive interaction with the subjects of its analyses. Academics rarely contact authors they critique – indeed, postpublication data repositories aim to make it easy to replicate a study without questioning the authors. Good journalists do the opposite: we contact the subjects of our investigations early and often.

And of course, R let us flexibly change our analysis every time CNBC and Cramer changed their story. When they argued for a different selection, R made it easy to create a new data subset. When they argued for a different holding strategy, R's indexing facility let us start and stop our analysis on different dates. In fact, when I begged CNBC for their own analysis of Cramer's performance, they said something that should warm the hearts of all you folks who've made R the powerful environment it is. CNBC told me not to expect a timely response from them because it was obvious that Pat and I had spent *months* on our analysis. In truth, Pat put in less than a week's work.

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Need A Hint?

Sanford Weisberg and Hadley Wickham

Suppose you have created an object in R, for example from a regression fit using lm or loess. You know that auxiliary functions exist that do useful computations on the object, but you can't remember their names. You need a hint on what to do next.

The hints function in the hints package does just this, finding a list of appropriate functions to jog your memory. For example, Figure 1 shows a list of hints for a lm object.

The output lists methods for generic functions like print specific to the class you specify, as well as searching the documentation to find all mentions of the class. You can then use the usual help mechanism to learn more about each of these methods and functions.

The hints function has three arguments:

hints(x, class=class(x), all.packages=FALSE)

If specified, the argument x can be any R object. For example, x might have been created by $x \le lm(y z)$. hints determines the S3 class of the object, and then looks for functions that operate on that class. The S3 class of an object is a character vector, and may consist of multiple strings, as, for example, a generalized linear model which has class c("glm",

macros by Edgar Online analyst Elias-John Kies and from Tufts University undergraduate Madison Mcgaffin; wise statistical pointers from Tim Hesterberg, of Insightful Corp. in Seattle ... none of whom bear responsibility for any woebegone errors.

Bibliography

- B. Alpert. Shorting Cramer. Barron's, 2007.
- B. Efron and R. Tibshirani. *Introduction to the Bootstrap*. Chapman and Hall, 1993.
- J. Engelberg, C. Sasseville, and J. Williams. Attention and Asset Prices: the Case of Mad Money. Technical report, Kellogg School of Management, 2007. http://papers.ssrn.com.
- N. Nayda. You! Me! Let's Get Ready to Make Mad Money!!! Technical report, Elmont Virginia Elementary School, 2006. Science fair project.

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"lm"). If x is not given, then you can specify the class you want hints about as character vector.

The hints function will look for methods and functions in all currently loaded packages. For example, the hints for 1m would be different if either the **car** or the **alr3** packages have been loaded, since both of these add methods and functions for 1m objects. Similarly, hints(class="lda") would return methods only if the package **MASS** were loaded, since all the relevant methods and functions are in that package. You can get hints for all your packages by setting all.packages=TRUE, but note that this works by require'ing all available packages so may be time consuming.

The **hints** package also includes an xtable method so, for example, xtable(hints(m1)) would have produced a version of Figure 1, but in LATEX format.

The function isn't foolproof, as it depends on the quality of documentation written by others. It may find irrelevant functions if the name of the class appears in the documentation for the irrelevant function. It can miss functions, too. For example, the function coeftest in the **Imtest** package can be used with Im objects by applying the function coeftest.default.
```
> hints(class = "lm")
```

Functions for lm in package 'base' Estimate the Condition Number kappa base-defunct Defunct Functions in Base Package Functions for 1m in package 'methods' Specify Names for Old-Style Classes setOldClass Functions for lm in package 'stats' add1 Add or Drop All Possible Single Terms to a Model alias Find Aliases (Dependencies) in a Model ANOVA for Linear Model Fits anova.lm Case and Variable Names of Fitted Models case.names.lm cooks.distance.lm Regression Deletion Diagnostics dfbeta.lm Regression Deletion Diagnostics dfbetas.lm Regression Deletion Diagnostics Add or Drop All Possible Single Terms to a Model drop1.lm Extract Coefficients in Original Coding dummy.coef.lm effects Effects from Fitted Model family.lm Accessing Linear Model Fits formula.lm Accessing Linear Model Fits hatvalues.lm Regression Deletion Diagnostics influence.lm Regression Diagnostics labels.lm Accessing Linear Model Fits logLik Extract Log-Likelihood Extracting the "Environment" of a Model Formula model.frame.lm Construct Design Matrices model.matrix.lm plot.lm Plot Diagnostics for an lm Object predict.lm Predict method for Linear Model Fits print.lm Fitting Linear Models Projections of Models proj residuals.lm Accessing Linear Model Fits rstandard.lm Regression Deletion Diagnostics rstudent.lm Regression Deletion Diagnostics summary.lm Summarizing Linear Model Fits variable.names.lm Case and Variable Names of Fitted Models Calculate Variance-Covariance Matrix for a Fitted Model vcov Object case.names Case and Variable Names of Fitted Models dummy.coef Extract Coefficients in Original Coding influence.measures Regression Deletion Diagnostics Fitting Linear Models lm lm.influence Regression Diagnostics lm.fit Fitter Functions for Linear Models model.frame Extracting the "Environment" of a Model Formula model.matrix Construct Design Matrices stats-defunct Defunct Functions in Package stats Functions for 1m in package 'unknown' confint.lm NΑ deviance.lm ΝA extractAIC.lm NA simulate.lm NA

Figure 1: Hints for the lm class.

Hints can't figure this out because there is no explicit mention of 1m in the function or the documentation, and so it misses the function. If the regression had been done using glm rather than 1m, hints would have found coeftest.glm.

The explanations of what the methods and functions do may be more generic than one might want, if the title of the help page is too generic. In some cases, no explanation is found. For example, simulate.lm is shown in Figure 1, but its description is missing. The help page for simulate mentions the lm class, but no page is available for simulate.lm, and so the hints function doesn't know where to get documentation. Finally, the hints function can only find hints for S3 objects, not for S4. Nevertheless, this simple function can be a useful tool, if you are willing to take a hint.

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Psychometrics Task View

Patrick Mair, Reinhold Hatzinger

Psychometrics is concerned with the design and analysis of research and the measurement of human characteristics. Psychometricians have also worked collaboratively with those in the field of statistics and quantitative methods to develop improved ways to organize and analyze data. In our task view we subdivide "Psychometrics" into the following methodological areas: Item Response Theory (IRT), Correspondence Analysis (CA), Structural Equation Models (SEM) and related methods such as Factor Analysis (FA) and Principal Component Analysis (PCA), Multidimensional Scaling (MDS), Classical Test Theory (CTT), and other approaches related to psychometrics.

Since much functionality is already contained in base R and there is considerable overlap between tools for psychometry and tools described in other views, particularly in SocialSciences, we only give a brief overview of packages that are closely related to psychometric methodology. Recently, Journal of Statistical Software (JSS) published a special volume on Psychometrics in R in which some new R packages were published. For an overview see de Leeuw and Mair (2007).

Item Response Theory (IRT)

The **eRm** package fits extended Rasch models, i.e. the ordinary Rasch model for dichotomous data (RM), the linear logistic test model (LLTM), the rating scale model (RSM) and its linear extension (LRSM), the partial credit model (PCM) and its linear extension (LPCM) using conditional ML estimation.

The package **ltm** also fits the simple RM. Additionally, functions for estimating Birnbaum's 2- and 3-parameter models based on a marginal ML approach are implemented as well as the graded response model for polytomous data, and the linear multidimensional logistic model.

Item and ability parameters can be calibrated using the package **plink**. It provides various functions for conducting separate calibration of IRT singleformat or mixed-format item parameters for multiple groups using the Mean/Mean, Mean/Sigma, Haebara, and Stocking-Lord methods. It includes symmetric and non-symmetric optimization and chainlinked rescaling of item and ability parameters.

The package **plRasch** computes maximum likelihood estimates and pseudo-likelihood estimates of parameters of Rasch models for polytomous (or dichotomous) items and multiple (or single) latent traits. Robust standard errors for the pseudolikelihood estimates are also computed.

A multilevel Rasch model can be estimated using the package **lme4** with functions for mixed-effects models with crossed or partially crossed random effects.

Other packages of interest are: **mokken** in the JSS special issue as a package to compute nonparametric item analysis, the **RaschSampler** allowing for the construction of exact Rasch model tests by generating random zero-one matrices with given marginals, **mprobit** fitting the multivariate binary probit model, and **irtoys** providing a simple interface to the estimation and plotting of IRT models. Simple Rasch computations such a simulating data and joint maximum likelihood are included in the **MiscPsycho** package.

Gaussian ordination, related to logistic IRT and also approximated as maximum likelihood estimation through canonical correspondence analysis is implemented in various forms in the package VGAM.

Two additional IRT packages (for Microsoft Windows only) are available and documented on the JSS site. The package **mlirt** computes multilevel IRT models, and **cirt** uses a joint hierarchically built up likelihood for estimating a two-parameter normal ogive model for responses and a log-normal model for response times. Bayesian approaches for estimating item and person parameters by means of Gibbs-Sampling are included in **MCMCpack**.

Correspondence Analysis (CA)

Simple and multiple correspondence analysis can be performed using corresp() and mca() in package MASS (and in the corresponding bundle VR). The package ca comprises two parts, one for simple correspondence analysis and one for multiple and joint correspondence analysis. Within each part, functions for computation, summaries and visualization in two and three dimensions are provided, including options to display supplementary points and perform subset analyses. Other features are visualization functions that offer features such as different scaling options for biplots and three-dimensional maps using the rgl package. Graphical options include shading and sizing plot symbols for the points according to their contributions to the map and masses respectively.

The package **ade4** contains an extensive set of functions covering, e.g., principal components, simple and multiple, fuzzy, non symmetric, and decentered correspondence analysis. Additional functionality is provided at Bioconductor in the package **made4**.

The **PTAk** package provides a multiway method to decompose a tensor (array) of any order, as a generalisation of SVD also supporting non-identity metrics and penalisations. 2-way SVD with these extensions is also available. Additionally, the package includes some other multiway methods: PCAn (Tucker-n) and PARAFAC/CANDECOMP with extensions.

The package **cocorresp** fits predictive and symmetric co-correspondence analysis (CoCA) models to relate one data matrix to another data matrix.

Apart from several factor analytic methods **FactoMineR** performs CA including supplementary row and/or column points and multiple correspondence analysis (MCA) with supplementary individuals, supplementary quantitative variables and supplementary qualitative variables.

Package **vegan** supports all basic ordination methods, including non-metric multidimensional scaling. The constrained ordination methods include constrained analysis of proximities, redundancy analysis, and constrained (canonical) and partially constrained correspondence analysis.

Other extensions of CA and MCA which also generalize many common IRT models can be found on the PsychoR page.

Structural Equation Models (SEM) and related methods

Ordinary factor analysis (FA) and principal component analysis (PCA) are in the package stats as functions factanal() and princomp(). Additional rotation methods for FA based on gradient projection algorithms can be found in the package **GPArotation**. The package **nFactors** produces a non-graphical solution to the Cattell scree test. Some graphical PCA representations can be found in the **psy** package.

The **sem** package fits general (i.e., latentvariable) SEMs by FIML, and structural equations in observed-variable models by 2SLS. Categorical variables in SEMs can be accommodated via the **polycor** package. The **systemfit** package implements a wider variety of estimators for observed-variables models, including nonlinear simultaneous-equations models. See also the **pls** package, for partial least-squares estimation, the gR task view for graphical models and the SocialSciences task view for other related packages.

FA and PCA with supplementary individuals and supplementary quantitative/qualitative variables can be performed using the **FactoMineR** package. The **homals** package can do various forms of mixed data PCA whereas **MCMCpack** has some options for sampling from the posterior for ordinal and mixed factor models.

Independent component analysis (ICA) can be computed using the packages **mlica** and **fastICA**. Independent factor analysis (IFA) with independent non-Gaussian factors can be performed with the **ifa** package. A desired number of robust principal components can be computed with the **pcaPP** package.

The package **psych** includes functions such as fa.parallel() and VSS() for estimating the appropriate number of factors/components as well as ICLUST() for item clustering.

Multidimensional Scaling (MDS)

MASS (and the corresponding bundle VR) as well as stats provide functionalities for computing classical MDS using the cmdscale() function. Sammon mapping sammon() and non-metric MDS isoMDS() are other relevant functions. Non-metric MDS can additionally be performed with metaMDS() in vegan. Furthermore, labdsv and ecodist provide the function nmds() and other relevant routines can be found in xgobi.

Principal coordinate analysis can be computed with capscale() in **vegan**; in **labdsv** and **ecodist** using pco() and with dudi.pco() in **ade4**.

Individual differences in multidimensional scaling can be computed with indscal() in the **SensoMineR** package. The package **MLDS** allows for the computation of maximum likelihood difference scaling (MLDS).

Classical Test Theory (CTT)

The package **psychometric** contains functions useful for correlation theory, meta-analysis (validitygeneralization), reliability, item analysis, inter-rater reliability, and classical utility. Cronbach alpha, kappa coefficients, and intra-class correlation coefficients (ICC) can be found in the **psy** package.

A number of routines for scale construction and reliability analysis useful for personality and experimental psychology are contained in the packages **psych** and **MiscPsycho**. Additional measures for reliability and concordance can be computed with the **concord** package.

Other related packages

Latent class analysis can be performed using the function lca() from package **e1071**. Further packages are **mmlcr** and **poLCA**. They compute mixed-mode latent class regression and polytomous variable latent class analysis, respectively.

The **cfa** package allows for the computation of simple, more-sample, and stepwise configural frequency analysis (CFA).

Coefficients for interrater reliability and agreements can be computed with the **irr** package. Psychophysical data can be analyzed with the **psyphy** package. Bradley-Terry models for paired comparisons are implemented in the package **BradleyTerry** and in **eba**. The latter allowes also for the computation of elimination-by-aspects models. Confidence intervals for standardized effect sizes can be found in **MBESS**.

Bibliography

J. de Leeuw and P. Mair. An Introduction to the Special Volume on Psychometrics in R *Journal* of Statistical Software, 20(1):1-5, 2007. URL http: //www.jstatsoft.org/v20/i01/

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meta: An R Package for Meta-Analysis

by G. Schwarzer

Introduction

The statistical method of meta-analysis can be used to combine two or more individual study results. More specificly, an overall effect is estimated by calculating a weighted average of estimates in individual studies. Various methods of meta-analysis exist that differ mainly in the weighting scheme utilised. Meta-analysis provides a statistical method to evaluate the direction and size of the effect as well as the question whether the effect is consistent across different studies.

The package **meta** is a comprehensive set of functions for meta-analysis. Initially, the package was intended to provide statistical methods for metaanalysis available in Review Manager, Version 4 (RevMan 4), the Cochrane Collaboration's program for preparing and maintaining Cochrane reviews (see http://www.cc-ims.net/RevMan/). The statistical capabilities of RevMan 4 have been extended over time.

The package provides methods for meta-analysis of studies comparing two groups with either binary or continuous outcome (function metabin() and metacont(), respectively). Furthermore, the package can be used in a more general way by using the function metagen(), e.g., to combine hazard ratios for survival outcomes.

Statistical methods for fixed effect and random effects models (Fleiss, 1993) are available as well as functions to draw the most commonly used graphical displays (forest plots, funnel plots, and radial plots). Various statistical tests for funnel plot asymmetry, which is often taken as an indication of publication bias, are implemented. Some additional functions are available which will not be described in detail in this article, e.g. the function trimfill() for the trim-and-fill method, which can be used to correct for funnel plot asymmetry (Duval and Tweedie, 2000), and the function read.mtv() to read data analysis files exported from RevMan 4.

Another package for meta-analysis exists, called **rmeta**, which also provides functions for fixed effect and random effects models. As compared to the package **meta**, functions implementing statistical methods for funnel plot asymmetry, specific methods for continuous outcomes, the Peto method for pooling as well as the additional functions mentioned in the last paragraph are not available in the package **rmeta**.

Meta-analysis of binary outcomes

The function metabin() provides methods for the meta-analysis of studies comparing two groups with binary outcomes. Output from metabin() is an object with classes "metabin" and "meta".

The summary measure to compare the two groups (parameter sm) can be

• the relative risk (RR, default): $\frac{p_E}{p_C}$

• the odds ratio (OR):
$$\frac{p_E/(1-p_E)}{p_C/(1-p_C)}$$

- the risk difference (RD): $p_E p_C$
- the arcsine difference (AS): $\arcsin(\sqrt{p_E}) - \arcsin(\sqrt{p_C})$

with p_E and p_C denoting the event probabilities for experimental and control group, respectively.

At a minimum, the number of events (event.e, event.c) and the sample size in both groups (n.e, n.c) are needed as input to metabin(). Further parameters could be set, e.g., the type of fixed effect method to be utilised (parameter method):

- Inverse variance method, available for all effect measures (Fleiss, 1993),
- Mantel-Haenszel method, available for RR, OR, and RD (Greenland and Robins, 1985; Robins et al., 1986),
- Peto method, only available for OR (Yusuf et al., 1985).

In any case, results of a random effects meta-analysis based on the inverse variance method and a method of moments estimator for the between-study variance are also calculated (DerSimonian and Laird, 1986).

Zero cell frequencies

Several parameters of metabin() are concerned with the handling of studies with zero cell frequencies.

The estimated event probability \hat{p}_E or \hat{p}_C is zero if either the number of events in the experimental or control group is zero; accordingly, the estimated odds ratio and risk ratio are either 0 or infinite. If both event numbers are zero, odds ratio and relative risk are undefined (see below). Furthermore, variance estimates of log odds ratio and log relative risk are infinite due to division by zero. For the risk difference, the estimated effect is always finite, but the variance estimate can be zero. Thus, an adjustment for zero cell frequencies is necessary for odds ratio, relative risk, and risk difference. On the other hand, no adjustment for zero cell frequencies is necessary for the arcsine difference as summary measure. It is common practice to add a small constant, typically 0.5, to each cell count in the case of zero cell frequencies (Gart and Zweifel, 1967; Pettigrew et al., 1986); a different value for this increment can be chosen (parameter incr). This modification can be used in general, but it is typically only applied if any of the cell counts is zero.

Three meta-analytic strategies are implemented in metabin() to adjust for zero cell frequencies:

- add 0.5 only to cell counts of two-by-two tables with zero cell counts (default),
- add 0.5 to all two-by-two tables in the case of zero cell counts in one or more studies (parameter allincr=TRUE),
- add 0.5 to all two-by-two tables (parameter addincr=TRUE).

To calculate the Mantel-Haenszel and the Peto estimate, there is no need to adjust for zero cell frequencies. However, an adjustment is utilised for the Mantel-Haenszel method in commonly used software for meta-analysis like RevMan 4 or the Stata procedure metan (http://www.stata.com/). Accordingly, an adjustment is also used by default for the Mantel-Haenszel method in metabin(); the exact Mantel-Haenszel estimate without adjustment can be calculated by setting the parameter MH.exact=TRUE.

For odds ratio and relative risk, studies with zero events in both groups are typically excluded from the meta-analysis, which is the default behaviour in metabin(). However, it is possible to include these studies in the meta-analysis by setting the parameter allstudies=TRUE.

Example: aspirin in myocardial infarction

A dataset of seven randomised controlled trials of the effectiveness of aspirin versus placebo in preventing death after myocardial infarction (Fleiss, 1993) is included in the package **meta**.

The result of conducting a meta-analysis of these trials using the odds ratio as measure of treatment effect is given in Figure 1. The assignment

```
> m1 <- metabin(...)
```

results in an object of classes "metabin" and "meta". Accordingly, the command

> m1

utilises the generic function print.meta() to print individual results of the seven trials as well as summaries for the fixed effect and random effects model. The columns %W(fixed) and %W(random) give the percentage weights of individual trials in the fixed effect and random effects model, respectively.

```
> data("Fleiss93")
> m1 <- metabin(event.e, n.e, event.c, n.c,
+
               data=Fleiss93, studlab=paste(study, year),
               sm="OR")
+
> m1
               OR.
                              95%-CI %W(fixed) %W(random)
MRC-1 1974 0.7197 [0.4890; 1.0593]
                                          3.18
                                                     8.21
CDP 1976
           0.6808 [0.4574; 1.0132]
                                          3.10
                                                     7.85
MRC-2 1979 0.8029 [0.6065; 1.0629]
                                         5.68
                                                    13.23
                                         1.80
GASP 1979 0.8007 [0.4863; 1.3186]
                                                    5.36
PARIS 1980 0.7981 [0.5526; 1.1529]
                                         3.22
                                                     8.89
AMIS 1980 1.1327
                   [0.9347; 1.3728]
                                         10.15
                                                    20.70
ISIS-2 1988 0.8950 [0.8294; 0.9657]
                                         72.88
                                                    35.77
Number of trials combined: 7
                         ΠR
                                       95%-CI
                                                    z p.value
Fixed effects model 0.8969
                             [0.8405; 0.9570] -3.2876
                                                        0.001
Random effects model 0.8763 [0.7743; 0.9917] -2.0918
                                                        0.0365
Quantifying heterogeneity:
tau<sup>2</sup> = 0.0096; H = 1.29 [1; 1.99]; I<sup>2</sup> = 39.7% [0%; 74.6%]
Test of heterogeneity:
    Q d.f. p.value
9.95
        6 0.1269
Method: Mantel-Haenszel method
```

Figure 1: Meta-analysis with binary outcome – myocardial infarction trials (Fleiss, 1993); output of function metabin().

Summary and forest plot

The command

> summary(m1)

results in the same output as given in Figure 1 but omitting results for individual studies; actually, the function summary.meta() is called inside print.meta(). The function summary.meta() results in an object of class "summary.meta" with corresponding function print.summary.meta().

An object of class "summary.meta" contains information on several summary statistics. For example, the command

```
> summary(m1)$fixed
```

gives a list of elements with results for the fixed effect meta-analysis.

The function summary.meta() can also be used to conduct a sub-group analysis. For example, the following command results in a sub-group analysis of the myocardial infarction trials based on the year of publication:

> summary(m1, byvar=Fleiss93\$year<1980, + bylab="year<1980")</pre>

The result of a meta-analysis can be shown graphically by using the function plot.meta(). Figure 2 was generated by the command



> plot(m1, comb.f=TRUE, comb.r=TRUE)

Figure 2: Forest plot of the myocardial infarction trials (Fleiss, 1993); output of function plot.meta().

This type of figure is usually called a forest plot. For individual trials, the estimated odds ratio with 95% confidence interval is plotted. Fixed effect and random effects estimate and 95% confidence interval are depicted by the diamonds.

Meta-analysis of continuous outcomes

The function metacont() provides methods for the meta-analysis of continuous outcomes; an object of classes "metacont" and "meta" is generated. The following summary measures (parameter sm) are available:

- weighted mean difference (WMD, default): $\bar{x}_E \bar{x}_C$
- standardised mean difference (SMD): $\frac{\bar{x}_E \bar{x}_C}{SD}$

with \bar{x}_E and \bar{x}_C denoting the mean values in the two groups and SD denoting the average standard deviation. Hedges' adjusted g (Cooper and Hedges, 1994) is utilised for the standardised mean difference.

At a minimum, sample sizes (n.e, n.c), mean values (mean.e, mean.c), and standard deviations (sd.e, sd.c) are needed as input to metacont(). Both fixed effect and random effects summary estimates are calculated based on the inverse variance method (Fleiss, 1993).

The generic functions print(), summary(), and plot() described in the last section are also available for meta-analyses with continuous outcomes.

Meta-analysis based on generic inverse variance method

The function metagen() provides methods for the meta-analysis of any outcome. At a minimum, the estimated effect (TE) and its standard error (seTE) are needed as input to metagen(). Both fixed effect and random effects summary estimates are calculated based on the inverse variance method (Fleiss, 1993).

For example, the function metagen() can be utilised to summarise

- adjusted estimates (e.g. from logistic regression),
- log hazard ratios for survival outcomes (Parmar et al., 1998),
- estimates from cross-over trials (Curtin et al., 2002),
- estimates from both direct and indirect comparisons (Bucher et al., 1997).

The generic functions print(), summary(), and plot() described in the section on meta-analyses of binary outcomes can be utilised for objects generated by metagen().

Statistical methods to detect smallstudy effects

In meta-analyses it sometimes happens that smaller studies show different, often larger, treatment effects. One possible reason for such "small study effects" is publication bias. This is said to occur when the chance of a smaller study being published is increased if it shows a stronger effect. If this occurs, it in turn biases the result of the meta-analysis. A comprehensive review of these issues is given in Rothstein et al. (2005).

Funnel plot

A natural way of visualising the evidence for possible small study effects/publication bias is the funnel plot (Light and Pillemer, 1984), which plots each study's treatment effect (x-axis) against a measure of its variability (y-axis); usually this is the standard error, although other options are preferable in different situations (Sterne and Egger, 2001). The funnel plot gives an idea of whether there is any dependence of treatment effect on precision.

In principal, at least two sources of asymmetry in funnel plots exist. Publication bias, the first of them, is well known. The second reason is heterogeneity, for example, smaller studies may select patients who are more likely to benefit from the intervention. Effects like these have been referred to as "small study effects" (Sterne et al., 2000).

A funnel plot of the myocardial infarction trials generated by the command

> funnel(m1, level=0.95)

is plotted in Figure 3. In this figure, a gap in the lower right part is somewhat suggestive of asymmetry in the funnel plot.



Figure 3: Funnel plot of the myocardial infarction trials (Fleiss, 1993); output of function funnel().

Tests for funnel plot asymmetry

A number of tests for small study effects/publication bias have been developed and are available in the function metabias(). Output of this command is an object of class "htest" which utilises the default print() function available with basic R.

Tests for small study effects/publication bias fall into two classes:

- non-parametric tests using rank-correlation methods, going back to Begg and Mazumdar (1994),
- regression tests, represented by the so-called Egger test (Egger et al., 1997).

The tests assume that under the null hypothesis of no "publication bias" among studies included in a meta-analysis, there is no association between treatment effect and precision.

While this assumption is plausible when the outcome is quantitative, as assuming normality the sample mean is statistically independent of the sample variance, it is not generally true for binary data. Specifically, suppose the outcome is binary and the effect is summarised by the log relative risk (logRR) or log odds ratio (logOR). The variance estimators of both the logRR and logOR are statistically dependent on the estimated logRR and logOR. Even in the absence of small study effects, this dependence induces asymmetry in the funnel plot (Macaskill et al., 2001; Schwarzer et al., 2002).

This observation has motivated recent proposals to modify existing tests for binary outcomes (Harbord et al., 2006; Peters et al., 2006; Schwarzer et al., 2007; Rücker et al., 2007). These tests are available in the function metabias() (parameter method).

In Figure 4, results for two different tests on funnel plot asymmetry (Begg and Mazumdar, 1994; Harbord et al., 2006) are given for the meta-analysis of the myocardial infarction trials. Both tests are non-significant (p-value ≥ 0.1); thus, there is no clear indication of funnel plot asymmetry.

Summary

The package **meta** is a comprehensive set of functions for meta-analysis and provides functions for the most commonly used outcomes, i.e., metabin() for binary and metacont() for continuous outcomes. Furthermore, the package can be used in a more general way by using the function metagen(). Generic functions to print and plot the results of a metaanalysis and to conduct sub-group analyses are available. Various statistical tests for funnel plot asymmetry which is often taken as an indication of publication bias are implemented.

Acknowledgments

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Bibliography

- C. B. Begg and M. Mazumdar. Operating characteristics of a rank correlation test for publication bias. *Biometrics*, 50:1088–1101, 1994.
- H. C. Bucher, G. H. Guyatt, L. E. Griffith, and S. D. Walter. The results of direct and indirect treatment comparisons in meta-analysis of randomized controlled trials. *Journal of Clinical Epidemiology*, 50: 683–91, 1997.
- H. Cooper and L. V. Hedges, editors. *The Handbook of Research Synthesis*. Russell Sage Foundation, Newbury Park, CA, 1994.
- F. Curtin, D. G. Altman, and D. Elbourne. Metaanalysis combining parallel and cross-over clinical trials. I: Continuous outcomes. *Statistics in Medicine*, 21:2131–2144, 2002.
- R. DerSimonian and N. Laird. Meta-analysis in clinical trials. *Controlled Clinical Trials*, 7:177–188, 1986.
- S. Duval and R. Tweedie. A nonparametric "Trim and Fill" method of accounting for publication bias in meta-analysis. *Journal of the American Statistical Association*, 95:89–98, 2000.
- M. Egger, G. D. Smith, M. Schneider, and C. Minder. Bias in meta-analysis detected by a simple, graphical test. *British Medical Journal*, 315:629–634, 1997.
- J. L. Fleiss. The statistical basis of meta-analysis. *Statistical Methods in Medical Research*, 2:121–145, 1993.
- J. J. Gart and J. R. Zweifel. On the bias of various estimators of the logit and its variance with application to quantal bioassay. *Biometrika*, 54:181–187, 1967.
- S. Greenland and J. M. Robins. Estimation of a common effect parameter from sparse follow-up data. *Biometrics*, 41:55–68, 1985. (C/R: V45 p1323–1324).
- R. M. Harbord, M. Egger, and J. A. Sterne. A modified test for small-study effects in meta-analyses of controlled trials with binary endpoints. *Statistics in Medicine*, 25(20):3443–3457, 2006.
- R. J. Light and D. B. Pillemer. *Summing up. The science of reviewing research*. Harvard University Press, Cambridge, Massachusetts, 1984.
- P. Macaskill, S. D. Walter, and L. Irwig. A comparison of methods to detect publication bias in metaanalysis. *Statistics in Medicine*, 20:641–654, 2001.

```
> metabias(m1, meth="rank")
Rank correlation test of funnel plot asymmetry
data: m1
z = -1.3517, p-value = 0.1765
alternative hypothesis: true is 0
sample estimates:
      ks
              se.ks
-9.000000 6.658328
> metabias(m1, meth="score")
Linear regression test of funnel plot asymmetry (efficient score)
data: m1
t = -0.9214, df = 5, p-value = 0.3991
alternative hypothesis: true is 0
sample estimates:
      bias
               se.bias
                              slope
-0.72587833 0.78775820 -0.05932016
```

Figure 4: Statistical tests for funnel plot asymmetry – myocardial infarction trials (Fleiss, 1993); output of function metabias().

- M. K. B. Parmar, V. Torri, and L. Stewart. Extracting summary statistics to perform meta-analyses of the published literature for survival endpoints. *Statistics in Medicine*, 17:2815–2834, 1998.
- J. L. Peters, A. J. Sutton, D. R. Jones, K. R. Abrams, and L. Rushton. Comparison of two methods to detect publication bias in meta-analysis. *Journal of the American Medical Association*, 295:676–680, 2006.
- H. M. Pettigrew, J. J. Gart, and D. G. Thomas. The bias and higher cumulants of the logarithm of a binomial variate. *Biometrika*, 73:425–435, 1986.
- J. Robins, N. E. Breslow, and S. Greenland. Estimators of the Mantel-Haenszel variance consistent in both sparse data and large-strata limiting models. *Biometrics*, 42:311–323, 1986.
- H. R. Rothstein, A. J. Sutton, and M. Borenstein. *Publication bias in meta analysis: prevention, assessment and adjustments.* Wiley, Chichester, 2005.
- G. Rücker, G. Schwarzer, and J. R. Carpenter. Arcsine test for publication bias in meta-analyses with binary outcomes. *Statistics in Medicine*, 2007. Accepted.
- G. Schwarzer, G. Antes, and M. Schumacher. Inflation of type I error rate in two statistical tests for

the detection of publication bias in meta-analyses with binary outcomes. *Statistics in Medicine*, 21: 2465–2477, 2002.

- G. Schwarzer, G. Antes, and M. Schumacher. A test for publication bias in meta-analysis with sparse binary data. *Statistics in Medicine*, 26(4):721–733, 2007.
- J. A. C. Sterne and M. Egger. Funnel plots for detecting bias in meta-analysis: Guideline on choice of axis. *Journal of Clinical Epidemiology*, 54:1046–1055, 2001.
- J. A. C. Sterne, D. Gavaghan, and M. Egger. Publication and related bias in meta-analysis: Power of statistical tests and prevalence in the literature. *Journal of Clinical Epidemiology*, 53:1119–1129, 2000.
- S. Yusuf, R. Peto, J. Lewis, R. Collins, and P. Sleight. Beta blockade during and after myocardial infarction: An overview of the randomized trials. *Progress in Cardiovascular Diseases*, 27:335–371, 1985.

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Extending the R Commander by "Plug-In" Packages

by John Fox

This article describes how the **Rcmdr** package can be extended by suitably designed "plug-in" packages. Embodied in the **Rcmdr** package, the **R Commander** was originally conceived as a basic-statistics graphical user interface ("GUI") to **R**. The **R Commander**'s capabilities have since been extended substantially beyond this original purpose, although it still accesses only a small fraction of the statistical and data-management capabilities of the standard **R** distribution, not to mention those of the more than 1000 contributed packages now on CRAN.

In addition to enhancing the usefulness of the **R Commander** as a teaching tool, the plug-in package mechanism allows interested package developers to add graphical interfaces to their **R** software, with the **R Commander** providing most of the necessary intrastructure, and without — as was previously the case — requiring the developer to maintain an independent version of the **Rcmdr** package [e.g., **Dusa** (2007)].

The **Rcmdr** package is based on the **tcltk** package (Dalgaard, 2001, 2002), which provides an **R** interface to the **Tcl/Tk** GUI builder. Because **Tcl/Tk** and the **tcltk** package are available for all of the computing platforms on which **R** is commonly run, the **R Commander** GUI runs on all of these platforms as well.

The main **R** Commander window is shown in Figure 1. Along the top are the **R** Commander menus: *File, Edit, Data, Statistics,* and so on. Below the menus is a tool bar, containing buttons for selecting, editing, and viewing the "active" data set, and for selecting the "active" statistical model. Below the toolbar are script, output, and messages windows: Commands generated by the **R** Commander appear in the script window; these commands can be edited and re-executed. Printed output is displayed in the output window, while error messages, warnings, and notes appear in the messages window. A more detailed description of the **R** Commander interface may be found in Fox (2005).

Workflow in the **R Commander** is straightforward, and is based on a single rectangular (i.e., caseby-variable) data set being "active" at any given time. Users can import, select, or modify the active data set via the **R Commander**'s *Data* menu. Various statistical methods are provided by the *Statistics* and *Graphs* menus. The **R Commander** recognizes certain classes of objects as statistical models. There can be an active statistical model that is manipulated via the *Models* menu. As long as a package conforms to this simple design (and does not, for example, require access to several data frames simultaneously), it should be possible to integrate it with the **R Commander**.

From a very early stage in its development, the **R** Commander was designed to be extensible: The menus for the R Commander interface are not hardcoded in the package sources, but rather are defined in a plain-text configuration file that installs into the Rcmdr package's etc subdirectory. Similarly, when it starts up, the **R Commander** will automatically source files with .R extensions that reside in the Rcmdr etc subdirectory; such files can contain **R** code to build **R** Commander dialog boxes, for example. Nevertheless, extending the R Commander has been relatively inconvenient, requiring either that users modify the installed package (e.g., by editing the **R** Commander menu-configuration file), or that they modify and recompile the **Rcmdr** source package.¹

Starting with version 1.3-0, the Rcmdr makes alternative provision for extension by "plug-in" packages — standard R packages that are developed, maintained, distributed, and installed independently of the Rcmdr package. Plug-in packages can augment the **R** Commander menus, and can provide additional dialog boxes and statistical functionality. Once installed on the user's system, plugin packages are automatically detected when the **R** Commander starts up and can be loaded from the R Commander's Tools menu. Plug-in packages can alternatively be loaded independently via R's library command; in this event, the Rcmdr package will also be loaded with the plug-in's menus installed in the **R** Commander menu bar. Finally, plug-in packages can be loaded automatically along with the Rcmdr package by setting the **Rcmdr** plugins option; for example, the command

```
options(Rcmdr=list(plugins=
    "RcmdrPlugin.TeachingDemos"))
```

causes the **RcmdrPlugin.TeachingDemos** plug-in package (described below) to load when the **R Commander** starts up.

The remainder of this article explains in some detail how to design **R Commander** plug-in packages. I begin with a description of the **R Commander** menu-definition file, because the format of this file is shared by **R Commander** plug-in packages. I then very briefly explain how to write functions for constructing **R Commander** dialog boxes. Finally, I

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¹In at least one instance, this inconvenience led to the distribution of a complete, alternative version of the **Rcmdr** package, Richard Heiberger and Burt Holland's **Rcmdr.HH** package. Exploiting the new facilities for extending the **Rcmdr** described in this article, Professor Heiberger has redesigned **Rcmdr.HH** as an **R Commander** plug-in package (Heiberger with Holland, 2007).

74 R Commander	
File Edit Data Statistics Graphs Models Distributions Tools Help	
Rata set: Summaries Script Window Contingency tables data (Prest Proportions Variances Nonparametric tests Dimensional analysis Linear regression Fit models Linear model Ordinal regression model Ordinal regression model	
	>
Output Window	
> data(Prestige)	
	>
Messages	
NOTE: The dataset Prestige has 102 rows and 6 columns.	
3	

Figure 1: The **R Commander** interface (under **Windows XP**), showing menus, script, output, and messages windows.

describe the structure of plug-in packages.

The Menu-Definition File

The standard **R Commander** menus are defined in the file Rcmdr-menus.txt, which resides in the installed **Rcmdr** package's etc subdirectory. Each line in the file comprises seven text fields, separated by white space. Fields with embedded blanks must be enclosed in single or double-quotes; unused fields are specified by an empty character string, "".

The Rcmdr-menus.txt file is quite large, and so I will not reproduce it here (though you may want to look at it in a text editor as you read the following description). Let us instead examine some representative lines in the file. The first line in Rcmdr-menus.txt defines the top-level *File* menu:

menu fileMenu topMenu "" "" ""

- The first, or "operation type", field menu indicates that we are defining a menu; it is also possible to define a menu item, in which case the operation type is item (see below).
- The second field fileMenu gives an arbitrary name to the new menu; any valid **R** name can be employed.
- The third field topMenu specifies the "parent" of the menu, in this case signifying that fileMenu is a top-level menu, to be installed directly in the **R Commander** menu bar. It is also possible to define a submenu of another menu (see below).
- The remaining four fields are empty.

The second line in Rcmdr-menus.txt defines a menu item under fileMenu:²

item fileMenu command "Open script file..."
 loadLog "" ""

- As explained previously, the first field indicates the definition of a menu item.
- The second field indicates that the menu item belongs to fileMenu.
- The third field specifies that the menu item invokes a command.
- The fourth field gives the text corresponding to the menu item that will be displayed when a user opens the *File* menu; the ellipses (...) are a conventional indication that selecting this menu item leads to a dialog box (see Figure 2).

- The fifth field specifies the name of the function (loadLog) to be called when the menu item is selected. This function is defined in the **Rcmdr** package, but any **R** function that has no required arguments can serve as a menu-item call-back function.
- In this case, the sixth and seventh fields are empty; I will explain their purpose presently.

Open			? 🗙
Look in:	🚞 R-2.5.0	R G 🕫 📂 🖽-	
My Recent Documents Desktop My Documents	Din doc include include ibrary modules share src Td		
My Computer			
	File name:	· · · · · · · · · · · · · · · · · · ·	Open
My Network	Files of type:	Script Files (*.R)	Cancel

Figure 2: The dialog box produced by the **R Com-mander** loadLog function.

A little later in Rcmdr-menus.txt, the following line appears:

menu exitMenu fileMenu "" "" ""

This line defines a submenu, named exitMenu, under fileMenu. Subsequent lines (not shown here) define menu items belonging to exitMenu.

Still later, we encounter the lines

item fileMenu cascade "Exit" exitMenu "" ""
item topMenu cascade "File" fileMenu "" ""

Each of these lines installs a menu and the items that belong to it, "cascading" the menu under its parent: exitMenu is cascaded under fileMenu, and will appear with the label *Exit*, while fileMenu is installed as a top-level menu with the label *File*. Again, the last two fields are not used.

Fields six and seven control, respectively, the conditional activation and conditional installation of the corresponding item. Each of these fields contains an \mathbf{R} expression enclosed in quotes that evaluates either to TRUE or FALSE. Here is an example from Rcmdr-menus.txt:

```
item tablesMenu command "Multi-way table..."
multiWayTable
"factorsP(3)" "packageAvailable('abind')"
```

²I have broken this — and other — menu lines for purposes of display because they are too long to show on a single line.

This line defines an item under tablesMenu (which is a submenu of the *Statistics* menu); the item leads to a dialog box, produced by the call-back function multiWayTable, for constructing multi-way contingency tables.

The activation field, "factorsP(3)", returns TRUE if the active dataset contains at least three factors — it is, of course, not possible to construct a multiway table from fewer than three factors. When factorsP(3) is TRUE, the menu item is activated; otherwise, it is inactive and "grayed out."

The function that constructs multi-way contingency tables requires the abind package, both in the sense that it needs this package to operate and in the literal sense that it executes the command require(abind). If the abind package is available on the user's system, the command packageAvailable('abind') returns TRUE. Under these circumstances, the menu item will be installed when the **R Commander** starts up; otherwise, it will not be installed.

Through judicious use of the activation and installation fields, a menu designer, therefore, is able to prevent the user from trying to do some things that are inappropriate in the current context, and even from seeing menu items that cannot work.

R Commander Dialogs

Most **R** Commander menu items lead to dialog boxes. A call-back function producing a dialog can make use of any appropriate tcltk commands, and indeed in writing such functions it helps to know something about Tcl/Tk. The articles by Dalgaard (2001, 2002) mentioned previously include basic orienting information, and there is a helpful web site of **R** tcltk examples compiled by James Wettenhall, at http://bioinf.wehi.edu.au/~wettenhall/RTclTkExamples/. Welch et al. (2003) provide a thorough introduction to Tcl/Tk.

In addition, however, the **Rcmdr** package exports a number of functions meant to facilitate the construction of **R Commander** dialogs, and to help insure that these dialogs have a uniform appearance. For example, the **Rcmdr** radioButtons function constructs a related set of radio buttons (for selecting one of several choices) in a single simple command (see below). One relatively painless way to proceed, if it is applicable, is to find an existing **R Commander** dialog box that is similar to what you intend to construct and to adapt it.

A reasonably typical, if simple, **Rcmdr** dialog box, for computing a paired *t*-test, is shown in Figure 3. This dialog box is produced by the call-back function pairedTTest shown in Figure 4, which illustrates the use of a number of functions exported by the **Rcmdr** package, such as initializeDialog, variableListBox, and radioButtons, as well as some **tlctk** functions that are called directly, such as tclvalue, tkentry, and tkgrid. Additional information about the functions provided by the **Rcmdr** package may be found in Fox (2005) and via ?Rcmdr.Utilities.

74 Paired t-Test	
First variable (pick one)	Second variable (pick one)
scent	scent
subj unscent 🗸	subj <u>unspent</u>
Alternative Hypothesis	Confidence Level
Two-sided 💿	.95
Difference < 0 🔿	
Difference > 0 C	
OK Car	ncel Help

Figure 3: **R Commander** dialog produced by the function pairedTTest.

Writing Plug-In Packages

I have contributed an illustrative plug-in package to CRAN, **RcmdrPlugin.TeachingDemos**. The name was selected so that this package will sort alphabetically after the **Rcmdr** package on CRAN; I suggest that other writers of **Rcmdr** plug-ins adopt this naming convention. The **RcmdrPlugin.TeachingDemos** package adds menus to the **R Commander** for some of the demonstrations in Greg Snow's intriguing **TeachingDemos** package (Snow, 2005). In particular, a *Visualize distributions* sub-menu with several items is cascaded under the standard **R Commander** toplevel *Distributions* menu, and a new *Demos* top-level menu, also with several menu items, is installed in the **R Commander** menu bar.

An **R** Commander plug-in package is, in the first instance, an ordinary **R** package. Detailed instructions for creating packages are available in the manual *Writing R Extensions* (**R** Development Core Team, 2007), which ships with **R**.

The DESCRIPTION file for the **RcmdrPlugin.**-**TeachingDemos** package is given in Figure 5. All of the fields in this DESCRIPTION file are entirely standard, with the exception of the last, Models:. Certain classes of objects are recognized by the **R Commander** as statistical models, including objects of class lm, glm, multinom, and polr. You can add to this list here, separating the entries by commas, if there are more than one. The **RcmdrPlugin.TeachingDemos** package specifies no additional models; it is, therefore, not necessary to include the Models: field in the DESCRIPTION file — I have done so simply to indicate its format.

Figure 6 shows the .First.lib function for the **RcmdrPlugin.TeachingDemos** package. As is stan-

```
pairedTTest <- function(){</pre>
    initializeDialog(title=gettextRcmdr("Paired t-Test"))
    .numeric <- Numeric()</pre>
    xBox <- variableListBox(top, .numeric,</pre>
        title=gettextRcmdr("First variable (pick one)"))
    yBox <- variableListBox(top, .numeric,</pre>
        title=gettextRcmdr("Second variable (pick one)"))
    onOK <- function(){</pre>
        x <- getSelection(xBox)</pre>
        y <- getSelection(yBox)</pre>
        if (length(x) == 0 | length(y) == 0){
            errorCondition(recall=pairedTTest,
                message=gettextRcmdr("You must select two variables."))
            return()
            }
        if (x == y){
            errorCondition(recall=pairedTTest,
                message=gettextRcmdr("Variables must be different."))
            return()
            }
        alternative <- as.character(tclvalue(alternativeVariable))</pre>
        level <- tclvalue(confidenceLevel)</pre>
        closeDialog()
        .activeDataSet <- ActiveDataSet()</pre>
        doItAndPrint(paste("t.test(", .activeDataSet, "$", x, ", ",
             .activeDataSet, "$", y,
             ", alternative='", alternative, "', conf.level=", level,
            ", paired=TRUE)", sep=""))
        tkfocus(CommanderWindow())
        }
    OKCancelHelp(helpSubject="t.test")
    radioButtons(top, name="alternative",
        buttons=c("twosided", "less", "greater"),
        values=c("two.sided", "less", "greater"),
        labels=gettextRcmdr(c("Two-sided", "Difference < 0",</pre>
            "Difference > 0")),
        title=gettextRcmdr("Alternative Hypothesis"))
    confidenceFrame <- tkframe(top)</pre>
    confidenceLevel <- tclVar(".95")</pre>
    confidenceField <- tkentry(confidenceFrame, width="6",</pre>
        textvariable=confidenceLevel)
    tkgrid(getFrame(xBox), getFrame(yBox), sticky="nw")
    tkgrid(tklabel(confidenceFrame,
        text=gettextRcmdr("Confidence Level"), fg="blue"))
    tkgrid(confidenceField, sticky="w")
    tkgrid(alternativeFrame, confidenceFrame, sticky="nw")
    tkgrid(buttonsFrame, columnspan=2, sticky="w")
    dialogSuffix(rows=3, columns=2)
    }
```

Figure 4: The pairedTTest function.

```
Package: RcmdrPlugin.TeachingDemos
Type: Package
Title: Rcmdr Teaching Demos Plug-In
Version: 1.0-3
Date: 2007-11-02
Author: John Fox <jfox@mcmaster.ca>
Maintainer: John Fox <jfox@mcmaster.ca>
Depends: Rcmdr (>= 1.3-0), rgl, TeachingDemos
Description: This package provides an Rcmdr "plug-in" based on the
TeachingDemos package, and is primarily for illustrative purposes.
License: GPL (>= 2)
Models:
```

Figure 5: The DESCRIPTION file from the RcmdrPlugin.TeachingDemos package.

dard in **R**, this function executes when the package is loaded, and serves to load the **Rcmdr** package, with the plug-in activated, if the **Rcmdr** is not already loaded. .First.lib is written so that it can (and should) be included in every **R Commander** plug-in package.³

Every **R** Commander plug-in package must include a file named menus.txt, residing in the installed package's etc subdirectory. This file, therefore, should be located in the source package's inst/etc subdirectory. A plug-in package's menus.txt file has the same structure as Rcmdr-menus.txt, described previously. For example, the line

```
menu demosMenu topMenu "" "" ""
```

in the menus.txt file for the **RcmdrPlugin.**-**TeachingDemos** package creates a new top-level menu, demosMenu;

```
item demosMenu command
  "Central limit theorem..."
  centralLimitTheorem
  "" "packageAvailable('TeachingDemos')"
```

creates an item under this menu; and

item topMenu cascade "Demos" demosMenu
 "" "packageAvailable('TeachingDemos')"

installs the new menu, and its items, in the menu bar (see Figure 7).



Figure 7: The *Demos* menu provided by the **RcmdrPlugin.TeachingDemos** package.

The **R** Commander takes care of reconciling the menus.txt files for plug-in packages with the master Rcmdr-menus.txt file: New top-level menus appear to the left of the standard *Tools* and *Help* menus; when new sub-menus or items are inserted into existing menus, they appear at the end. The **RcmdrPlug**in.TeachingDemos package also includes **R** code, for example for the centralLimitTheorem call-back function, which creates a dialog box.

Concluding Remarks

It is my hope that the ability to define plug-in packages will extend the utility of the **R Commander** interface. The availability of a variety of specialized plug-ins, and the possibility of writing one's own plug-in package, should allow instructors to tailor the **R Commander** more closely to the specific needs of their classes. Similarly **R** developers wishing to add a GUI to their packages have a convenient means of doing so. An added benefit of having a variety of optionally loaded plug-ins is that unnecessary menus and menu items need not be installed: After all, one of the *disadvantages* of an extensive GUI is that users can easily become lost in a maze of menus and dialogs.

Bibliography

- P. Dalgaard. A primer on the R-Tcl/Tk package. R News, 1(3):27-31, September 2001. URL http: //CRAN.R-project.org/doc/Rnews/.
- P. Dalgaard. Changes to the R-Tcl/Tk package. R News, 2(3):25-27, December 2002. URL http:// CRAN.R-project.org/doc/Rnews/.
- A. Dusa. *QCAGUI: QCA Graphical User Interface,* 2007. R package version 1.3-0.

³I am grateful to Richard Heiberger for help in writing this function, and, more generally, for his suggestions for the design of the **Rcmdr** plug-in facility.

```
.First.lib <- function(libname, pkgname){
    if (!interactive()) return()
    Rcmdr <- options()$Rcmdr
    plugins <- Rcmdr$plugins
    if ((!pkgname %in% plugins) && !getRcmdr("autoRestart")) {
        Rcmdr$plugins <- c(plugins, pkgname)
        options(Rcmdr=Rcmdr)
        closeCommander(ask=FALSE, ask.save=TRUE)
        Commander()
      }
}</pre>
```

Figure 6: The .First.lib function from the RcmdrPlugin.TeachingDemos package.

- J. Fox. The R Commander: A basic-statistics graphical user interface to R. Journal of Statistical Software, 14(9):1–42, Aug. 2005. ISSN 1548-7660. URL http://www.jstatsoft.org/counter. php?id=134&url=v14/i09/v14i09.pdf&ct=1.
- R. M. Heiberger and with contributions from Burt Holland. *RcmdrPlugin.HH: Rcmdr support for the HH package*, 2007. R package version 1.1-4.
- R Development Core Team. *Writing R Extensions*. 2007.

- G. Snow. *TeachingDemos: Demonstrations for teaching and learning*, 2005. R package version 1.5.
- B. B. Welch, K. Jones, and J. Hobbs. *Practical Programming in Tcl/Tk, Fourth Edition*. Prentice Hall, Upper Saddle River NJ, 2003.

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Improvements to the Multiple Testing Package multtest

by Sandra L. Taylor, Duncan Temple Lang, and Katherine S. Pollard

Introduction

The R package multtest (Dudoit and Ge, 2005) contains multiple testing procedures for analyses of high-dimensional data, such as microarray studies of gene expression. These methods include various marginal p-value adjustment procedures (the mt.rawp2adjp function) as well as joint testing procedures. A key component of the joint testing methods is estimation of a null distribution for the vector of test statistics, which is accomplished via permutations (Westfall and Young, 1993; Ge et al., 2003) or the non-parametric bootstrap (Pollard and van der Laan, 2003; Dudoit et al., 2004). Statistical analyses of high-dimensional data often are computationally intensive. Application of resampling-based statistical methods such as bootstrap or permutation methods to these large data sets further increases computational demands. Here we report on improvements incorporated into multtest version 1.16.1 available via both Bioconductor and CRAN. These updates have significantly increased the computational speed of using the bootstrap procedures.

The **multtest** package implements multiple testing procedures with a bootstrap null distribution through the main user function MTP. Eight test statistic functions (meanX, diffmeanX, FX, blockFX, twowayFX, lmX, lmY, coxY) are used to conduct one and two sample *t*-tests, one and two-way ANOVAS, simple linear regressions and survival analyses, respectively. To generate a bootstrap null distribution, the MTP function calls the function boot.null. This function then calls boot.resample to generate bootstrap samples. Thus, the call stack for the bootstrap is MTP -> boot.null -> boot.resample. Finally, the test statistic function is applied to each sample, and boot.null returns a matrix of centered and scaled bootstrap test statistics.

We increased the computational speed of generating this bootstrap null distribution through three main modifications:

- 1. optimizing the R code of the test statistics;
- 2. implementing two frequently used tests (two sample *t*-test and *F*-test) in C; and

3. integrating an option to run the bootstrap in parallel on a computer cluster.

Changes to Test Statistic Functions

Since the test statistic functions are applied to each bootstrap sample, even small increases in the speed of these functions yielded noticeable improvements to the overall bootstrap procedure. Through profiling the R code of the test statistic functions, we identified several ways to increase the speed of these First, the function ifelse was comfunctions. monly used in the test statistic functions. Changing ifelse to an if...else construct yielded the largest speed improvements. The ifelse function is designed to evaluate vectors quickly but is less efficient at evaluating single values. Small gains were achieved with changing unique to unique.default, mean to mean.default, and sort to sort.init. These changes eliminated the need to assess the object class before selecting the appropriate method when each function was called. The functions 1mX and 1mY benefitted from using rowSums (i.e., rowSums(is.na(covar))) rather than using apply (i.e., apply(is.na(covar),1,sum)).

The greatest improvements were achieved for the one-sample *t*-test (meanX) and the regression tests (1mX and 1mY). We conducted a simulation to evaluate the speed improvements. For the one-sample t-test, we randomly generated 100 and 1,000 Normal(0,1) variables for sample sizes of 50 and 100. We tested the null hypotheses that the means for each of the 100 or 1,000 variables were 0. For the twosample *t*-test, we randomly generated 100 and 1,000 Normal(0,1) variables for two groups consisting of 50 and 100 samples each. For the F-test, we used three groups of 50 and 100 samples each. We tested the null hypotheses of equal group means for each of the variables. We evaluated the speed of 1,000 and 10,000 iterations when computing the bootstrap null distributions.

We reduced computational times for the onesample *t*-test by nearly 60% when the sample size was 50 and from 40% to 46% when the sample size was 100. The number of variables tested and the number of bootstrap iterations did not influence the relative improvement of the revised functions. Changes in R code yielded more modest improvements for the two-sample *t*-test and *F*-test. Computational times were reduced by 25% to 28%, and by about 10%, respectively. As with the one-sample *t*test, the speed improvements were not affected by the number of variables tested or the number of bootstrap iterations. Sample size had a very small effect for the two-sample test, but did not influence computation speed for the *F*-test.

Because two-sample *t*-tests and *F*-tests are some of the most commonly used tests in **multtest** and

only modest improvements were achieved through changes in the R code, we implemented these statistics in C to further increase speed. These modifications took advantage of C code for calculating test statistics in permutation tests that was already in the package. While moving computations into C increases the complexity of the code, the availability of a reference implementation in R allowed us to easily test the new code, easing the transition.

We evaluated the speed improvements of our C implementation with the same approach used to evaluate the R code modifications. By executing the two-sample *t*-test in C, computational time was reduced by about one-half ranging from 46% when the sample size was 100 to 52% for a sample size of 50. The results were more dramatic for the *F*-test; time was reduced by 79% to 82% with the C code implementation. Relative improvements did not vary with the number of bootstrap iterations or variables evaluated. Some further optimization could be done by profiling the C code.

Integration of Parallel Processing

Although we increased the computational speed of generating bootstrap null distributions considerably through improvements to the test statistics code, some analyses still require a long time to complete using a single CPU. Many institutions have computer clusters that can greatly increase computational speed through parallel processing. Bootstrapping is a straightforward technique to conduct in parallel, since each resampled data set is independently generated with no communication needed between individual iterations (Tierney et al., 2007). Thus, synchronizing cluster nodes only entails dispatching tasks to each node and combining the results.

Running the bootstrap on a cluster requires the R package snow (Tierney et al., 2007). Through functions in this package, the user can create a cluster object using makeCluster and then dispatch jobs to nodes of the cluster through several apply functions designed for use with a cluster. We integrated use of a cluster for generating a bootstrap null distribution by adding an argument to the main user interface function (MTP) called cluster. When this argument is 1 (the default value), the bootstrap is executed on a single CPU. To implement the bootstrap in parallel, the user either supplies a cluster object created using the function makeCluster in **snow** or identifies the number of nodes to use in a cluster which MTP then uses to create a cluster. In this case, the type of interface system to use must be specified in the type argument. MPI and PVM interfaces require Rmpi and rpvm packages, respectively. MTP will check if these packages are installed and load them if necessary.

To use a cluster, multtest and Biobase (required

by **multtest**) must be loaded on each node in the cluster. MTP checks if these packages are installed and loads them on each node. However, if these packages are not installed in a directory in R's library search path, the user will need to create a cluster, load the packages on each node and supply the cluster object as the argument to cluster as shown in the following example code. This code loads the **snow** package, makes a cluster consisting of two nodes and loads **Biobase** and **multtest** onto each node of the cluster using clusterEvalQ.

```
library("snow")
cl <- makeCluster(2, "MPI")
clusterEvalQ(cl, {library("Biobase");
    library("multtest")})</pre>
```

Use of the cluster for the bootstrap is then accomplished by specifying the cluster object as the argument to cluster in the MTP function.

```
diffMeanData <- matrix(rnorm(100*100),100)
group <- gl(2, 100)
MTP(X=diffMeanData, Y=group,
   test="t.twosamp.unequalvar",
   alternative="two.sided", B=1000,
   method="sd.minP", cluster=cl)</pre>
```

In **multtest**, we use the **snow** package function clusterApplyLB to dispatch bootstrap iterations to cluster nodes. This function automatically balances tasks among available nodes. The user can specify the number or percentage of bootstrap samples to dispatch at a time to each node via the dispatch argument. We set the default value for the dispatch argument to 5% based on simulation results. We considered bootstraps with 100, 1,000 and 10,000 iterations and evaluated dispatching between 1 and 2,500 samples at a time with cluster sizes ranging from 2 to 4 nodes. Dispatching small numbers of iterations to each node took the longest (Figure 1); in these cases the I/O time became substantial. Processing times initially declined as the number of iterations transmitted at one time increased but then leveled off at 10 to 25 iterations for 100 iterations, 25 to 50 for 1,000 iterations and 250 to 500 for 10,000 iterations. Based on these results, we chose to dispatch 5% of the bootstrap iterations at a time as the default value.

Overall Speed Improvements

To assess the overall speed improvements achieved, we compared the speed of the original user interface function MTP and supporting test statistic functions with the new interface function and supporting functions. We compared the speed of 10,000, 25,000 and 50,000 bootstrap iterations for one-sample *t*-tests, two-sample *t*-tests and *F*-tests with 100 and 1,000 variables and group sample sizes of 50 and 100. To assess the effect of a cluster, we used a Linux cluster consisting of 3 nodes. Each node was a Dual Core AMD Opteron 2411.127 MHz Processor with 4 GB of memory.



Figure 1: Time to execute 100, 1, 000, and 10, 000 bootstrap iterations for 2, 3, and 4 nodes and varying numbers of samples dispatched at a time.

Computational speed increased substantially with the new methods. For the one-sample *t*-test, computation times were reduced by about 75% for a sample size of 50 and 49% to 69% for a sample size of 100 (Figure 2). Evaluating 1,000 variables in a sample of 50 based on 10,000 bootstrap iterations required 26 minutes with the original functions but only 6.5 minutes with the new functions. The two-sample *t*-test showed the greatest improvement for 50,000 bootstrap iterations, with speed increasing by up to 96%. At 10,000 bootstrap iterations, the new methods were 64% to 90% faster. For 1,000 variables, two groups of 50 and 10,000 bootstrap iterations, computation time was reduced from over an hour to 20 minutes. Speed increases for the *F*-test were more consistent ranging

from 78% to 98%. The new methods reduced computation time for 1,000 variables in 3 groups of 50 and based on 10,000 bootstrap iterations from over 3 hours to about 20 minutes. The non-monotone pattern of improvement versus number of bootstrap iterations for the one-sample *t*-test with 100 variables and a sample size of 100 and the F-test for 1,000 variables and a sample size of 50 reflects sampling variability of a single observation for each combination.

Summary

Substantial increases in computational speed for implementing the bootstrap null distribution were achieved through optimizing the R code, executing calculations of test statistics in C code, and using a cluster. Through these changes, computational times typically were reduced by more than 75% and up to 96%. Computations that previously required several hours to complete can now be accomplished in half an hour.

Bibliography

- S. Dudoit and Y. Ge. Multiple testing procedures, R package, 2005.
- S. Dudoit, M. van der Laan, and K. Pollard. Multiple testing. Part I. Single-step procedures for control of general type I error rates. Statistical Applications in Genetics and Molecular Biology, 3(1):1– 69, 2004. URL http://www.bepress.com/sagmb/ vol3/iss1/art13.
- Y. Ge, S. Dudoit, and T. Speed. Resamplingbased multiple testing for microarray data analysis. TEST, 12(1):1-44, 2003. URL http://www.stat.berkeley.edu/users/ sandrine/Docs/Papers/Test_spe.pdf.
- K. Pollard and M. van der Laan. Resampling-based multiple testing: Asymptotic control of type I error and applications to gene expression data. Technical Report 121, Division of Biostatistics, University of California, Berkeley, pages 1–37, 2003. URL http: //www.bepress.com/ucbbiostat/paper121.
- L. Tierney, A. Rossini, N. Li, and H. Sevcikova. Simple network of workstations, R package, 2007.
- P. Westfall and S. Young. Resampling-based Multiple Testing: Examples and Methods for p-value Adjustment. John Wiley and Sons, 1993.



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Figure 2: Percent improvement in time to generate bootstrap null distributions based on 10,000, 25,000, and 50,000 iterations for one-sample t-tests, twosample *t*-tests, and F-tests. For the simulations, sample sizes within groups for each test were 50 (dotted lines) or 100 (solid lines). Mean differences were tested for 100 (blue lines) and 1,000 variables (red lines) at each sample size.

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Changes in R 2.6.1

by the R Core Team

New features

- The data.frame and factor methods for [[now support the exact argument introduced in 2.6.0.
- plot.lm() gains a new argument cex.caption to allow the size of the captions to be controlled.
- A series of changes make the CHARSXP cache introduced in 2.6.0 faster (and in some cases many times faster) in sessions with a large number (e.g., a million) of unique character strings, and also if there are many empty strings.
- embedFonts(), bitmap() and dev2bitmap() explicitly turn off auto-rotation in Ghostscript when generating PDF.
- The canonical architecture is no longer checked when loading packages using a non-empty sub-architecture, since it is possible to (e.g.) build packages for i386-pc-linux-gnu on both that architecture and on x86_64-unknownlinux-gnu.
- Deparsing will (if option warnIncomplete is set) warn on strings longer than the parser limit (8192 bytes).
- url() now uses the UserAgent header in http transactions in the same way as download.file() (making use of option "HTTPUserAgent").

Bug fixes

- iconv() is again able to translate character strings with embedded nuls (such as those in UCS-2).
- new.packages() and update.packages() failed when called on an empty library, since old.packages() threw an error. old.packages() now returns NULL (as documented) in that case.
- Builds on Mac OS X 10.4 or higher now allocate enough space in the binary headers to relocate dependent libraries into the framework.
- R CMD build now computes the exclusion list on the copy it makes: this avoids problems if the original sources contain symbolic links

(which are resolved in the copy). Thanks to Michael Lawrence for diagnosis and patch.

- object.size() had slightly too low a size for objects of type "S4".
- symbol() in plotmath expressions was only accepting valid character strings, which made it impossible to specify symbols such as aleph (obtained by symbol("300")) in a UTF-8 locale.
- An event handling issue caused autorepeat functions to misbehave with **tcltk** (notably scrollbars).
- plot(sin, -5, 5) gives ylab "sin(x)" again, where it resulted in "x(x)" in 2.6.0. Further, plot(sin) again plots from [0,1] also in cases where a previously used coordinate system differs.
- curve() with unspecified from, to and xlim now reuses the previous *x* limits, and not slightly larger ones.
- It was intended that R code filenames in packages should start with an ASCII letter or digits (and R CMD INSTALL uses that), but the test used in R CMD build ([A-Za-z0-9]) was locale-specific (and excluded t to y in Estonian, for example). (PR#10351)
- R CMD build could misbehave when faced with files with CRLF line endings *and* no line ending on the final line of the file, removing the last byte of the file.
- DF[i, j] failed in 2.6.0 if j was a logical vector selecting a single column.
- Unix x11() would fail if a valid display was specified but DISPLAY was unset. (PR#10379)
- postscript() was not always ignoring .Postscript.Options in the workspace (where it should not have occurred).
- help.search() would give an error if it found a badly installed package, even if package was not specified.
- tclServiceMode() (package tcltk) now works under Unix-alikes. (Although documented, it used only to work under Windows.)
- As Mac OS X 10.5.0 comes with incompatible /bin/sh shell, we force SHELL=/bin/bash (which is ok) in that case. [Only for 2.6.x: another solution is used in 2.7.0.]
- Deliberately using malformed source attributes no longer causes deparsing/printing of functions to crash R. (PR#10437)

- R CMD check and R CMD INSTALL now work with (some) directory names containing spaces.
- choose(n, k) gave incorrect values for negative n and small k.
- plot.ts(x,y) could use wrong default labels; fixed thanks to Antonio Fabio di Narzo.

Changes on CRAN

by Kurt Hornik

New contributed packages

- **BARD** Better Automated ReDistricting and heuristic exploration of redistricter revealed preference. By Micah Altman.
- **CellularAutomaton** An object-oriented implementation of one-dimensional cellular automata. Supports many of the features offered by Mathematica, including elementary rules, userdefined rules, radii, user-defined seeding, and plotting. By John Hughes.
- **ComPairWise** Compare phylogenetic or population genetic data alignments. By Trina E. Roberts.
- **EDR** Estimation of the effective dimension reduction (EDR) space in multi-index regression models. By Joerg Polzehl.
- **FGN** Fractional Gaussian Noise (FGN) model fitting, including MLEs for the *H* parameter and regression with FGN errors, and simulation of FGN. By A. I. McLeod.
- **FKBL** Fuzzy Knowledge Base Learning, an R/C implementation of a fuzzy inference engine supporting several inference methods. By Alvaro Gonzalez Alvarez.
- **FieldSim** Routines to simulate random fields. By Alexandre Brouste and Sophie Lambert-Lacroix.
- **GLDEX** Fitting single and mixture of Generalized Lambda Distributions (RS and FMKL) using Discretized and Maximum Likelihood methods. The fitting algorithms considered have two major objectives. One is to provide a smoothing device to fit distributions to data using the weight and unweighted discretized approach based on the bin width of the histogram. The other is to provide a definitive fit

- reshape() got column names out of sync with contents in some cases; found by Antonio Fabio Di Narzo.
- ar(x) for short x (i.e., length ≤ 10) could fail because the default order.max was ≥ length(x) which is non-sensical.
- Keyboard events in getGraphicsEvent() could cause stack imbalance errors (PR#10453)

to the data set using the maximum likelihood estimation. Diagnostics on goodness of fit can be done via QQ-plots, KS-resample tests and comparing mean, variance, skewness and kurtosis of the data with the fitted distribution. By Steve Su.

- GillespieSSA Gillespie's Stochastic Simulation Algorithm (SSA). Provides a simple to use, intuitive, and extensible interface to several stochastic simulation algorithms for generating simulated trajectories of finite population continuous-time models. Currently it implements Gillespie's exact stochastic simulation algorithm (Direct method) and several approximate methods (Explicit tau-leap, Binomial tau-leap, and Optimized tau-leap). Also contains a library of template models that can be run as demo models and can easily be customized and extended. Currently the following models are included: decayingdimerization reaction set, linear chain system, logistic growth model, Lotka predatorprey model, Rosenzweig-MacArthur predatorprey model, Kermack-McKendrick SIR model, and a meta-population SIRS model. By Mario Pineda-Krch.
- HardyWeinberg Exploration of bi-allelic marker data. Focuses on the graphical representation of the results of tests for Hardy-Weinberg equilibrium in a ternary plot. Routines for several tests for Hardy-Weinberg equilibrium are included. By Jan Graffelman.
- HiddenMarkov Hidden Markov Models. Contains functions for the analysis of Discrete Time Hidden Markov Models, Markov Modulated GLMs and the Markov Modulated Poisson Process. Includes functions for simulation, parameter estimation, and the Viterbi algorithm. The algorithms are based of those of Walter Zucchini. By David Harte.

JADE JADE and ICA performance criteria. The

package ports J.-F. Cardoso's JADE algorithm as well as his function for joint diagonalization. There are also several criteria for performance evaluation of ICA algorithms. By Klaus Nordhausen, Jean-Francois Cardoso, Hannu Oja, and Esa Ollila.

- JudgeIt Calculates bias, responsiveness, and other characteristics of two-party electoral systems, with district-level electoral and other data. By Andrew Gelman, Gary King, and Andrew C. Thomas.
- **NestedCohort** Estimate hazard ratios, standardized survival and attributable risks for cohorts with missing covariates, for Cox models or Kaplan-Meier. By Hormuzd A. Katki.
- **ProfessR** Grades setting and exam maker. Programs to determine student grades and create examinations from question banks. Programs will create numerous multiple choice exams, randomly shuffled, for different versions of same question list. By Jonathan M. Lees.
- **RFOC** Graphics for statistics on a sphere, as applied to geological fault data, crystallography, earthquake focal mechanisms, radiation patterns, ternary plots and geographical/geological maps. By Jonathan M. Lees.
- **RHmm** Discrete, univariate or multivariate Gaussian, mixture of univariate or multivariate Gaussian HMM functions for simulation and estimation. By Ollivier Taramasco.
- **RPMG** R Poor Man's Gui: create interactive R analysis sessions. By Jonathan M. Lees.
- **RPyGeo** ArcGIS Geoprocessing in R via Python. Provides access to (virtually any) ArcGIS Geoprocessing tool from within R by running Python geoprocessing scripts without writing Python code or touching ArcGIS. Requires ArcGIS \geq 9.2, a suitable version of Python (currently 2.4), and Windows. By Alexander Brenning.
- **RSAGA** SAGA Geoprocessing and Terrain Analysis in R. Provides access to geocomputing and terrain analysis functions of SAGA (http://www. saga-gis.org/) from within R by running the command line version of SAGA. In addition, several R functions for handling and manipulating ASCII grids are provided, including a flexible framework for applying local or focal functions to grids. By Alexander Brenning.
- **RcmdrPlugin.FactoMineR** Rcmdr plugin for package **FactoMineR**. By Francois Husson, Julie Josse, and Sebastien Le.

- **Rsundials** SUite of Nonlinear DIfferential ALgebraic equations Solvers in R. Provides an interface for the package of nonlinear differential algebraic equation solvers that comprise SUNDIALS. ODEs are expressed as R functions or as compiled code. By Selwyn-Lloyd McPherson.
- **Rvelslant** Code for interactively analyzing downhole seismic data and interpreting layered velocity models of constant velocity layers accounting for refractions across layer boundaries. Original method by Dave Boore, R port and some additions by Eric M. Thompson.
- **SASxport** Functions for reading, listing the contents of, and writing SAS XPORT format files. The functions support reading and writing of either individual data frames or sets of data frames. Further, a mechanism has been provided for customizing how variables of different data types are stored. By Gregory R. Warnes.
- **SoDA** Utilities and examples from the book "Software for Data Analysis: Programming with R". By John M Chambers.
- **StatDA** Offers different possibilities to make statistical analysis for environmental data. By Peter Filzmoser and Barbara Steiger.
- **TSMySQL** Time Series Database Interface extensions for MySQL. By Paul Gilbert.
- **TSSQLite** Time Series Database Interface extensions for SQLite. By Paul Gilbert.
- **TSdbi** Time Series Database Interface. By Paul Gilbert.
- **TSpadi** TSdbi Interface to PADI Time Series Server (for e.g. Fame). Provides methods for generics in the **TSdbi** package to connect through a protocol for application database interface (PADI) to a time series database (e.g., Fame). By Paul Gilbert.
- **TTR** Functions and data to construct Technical Trading Rules. By Josh Ulrich.
- **animation** Various functions for animations in statistics, covering many areas such as probability theory, mathematical statistics, multivariate statistics, nonparamatric statistics, sampling survey, linear models, time series, computational statistics, data mining and machine learning. These functions might be of help in teaching statistics and data analysis. By Yihui Xie.
- **bnlearn** Bayesian network structure learning via constraint-based (also known as "conditional independence") algorithms. This package implements the Grow-Shrink (GS) algorithm, the

Incremental Association (IAMB) algorithm, the Interleaved-IAMB (Inter-IAMB) algorithm and the Fast-IAMB (Fast-IAMB) algorithm for both discrete and Gaussian networks. Simulation and some score functions are implemented for discrete networks. By Marco Scutari.

- **bs** A collection of utilities for the Birnbaum-Saunders distribution (BSD). By Víctor Leiva, Hugo Hernández, and Marco Riquelme.
- **cacher** Tools for caching statistical analyses in keyvalue databases which can subsequently be distributed over the web. By Roger D. Peng.
- **calib** Statistical tool for calibration of plate based bioassays. By Dan Samarov and Perry Haaland.
- **caret** Classification And REgression Training: functions for training and plotting classification and regression models. By Max Kuhn, Jed Wing, Steve Weston, and Andre Williams.
- caretLSF Classification And REgression Training LSF style. By Max Kuhn.
- caretNWS Classification And REgression Training in parallel Using NetworkSpaces. By Max Kuhn and Steve Weston.
- **cggd** Continuous Generalized Gradient Descent. Efficient procedures for fitting an entire regression sequences with different model types. By Cun-Hui Zhang and Ofer Melnik.
- **demogR** Construction and analysis of matrix population models in R. By James Holland Jones.
- dice Calculate probabilities of various dice-rolling events. By Dylan Arena.
- **dtw** Implementation of Dynamic Time Warp (DTW) and its generalizations. DTW finds the optimal mapping (local time stretch) between a given query into a given template time series. Implements symmetric, asymmetric, and custom step patterns with weights. Supports windowing (none, Itakura, Sakoe-Chiba, custom). Outputs minimum cumulative distance, warping paths, etc. By Toni Giorgino, with contributions from Paolo Tormene.
- ecespa Some wrappers, functions and data sets for for spatial point pattern analysis, used in the book "Introduccion al Analisis Espacial de Datos en Ecologia y Ciencias Ambientales: Metodos y Aplicaciones". By Marcelino de la Cruz Rot, with contributions of Philip M. Dixon.
- **fAsianOptions** Rmetrics: EBM and Asian option valuation. By Diethelm Wuertz and many others.

- **fAssets** Rmetrics: Assets selection and modeling. By Diethelm Wuertz and many others.
- **fBonds** Rmetrics: Bonds and interest rate models. By Diethelm Wuertz and many others.
- **fExoticOptions** Rmetrics: Exotic option valuation. By Diethelm Wuertz and many others.
- **fGarch** Rmetrics: Autoregressive conditional heteroskedastic modeling. By Diethelm Wuertz and many others.
- **fImport** Rmetrics: Economic and financial data import. By Diethelm Wuertz and many others.
- **fNonlinear** Rmetrics: Nonlinear and chaotic time series modeling. By Diethelm Wuertz and many others.
- **fRegression** Rmetrics: Regression based decision and prediction. By Diethelm Wuertz and many others.
- **fTrading** Rmetrics: Technical trading analysis. By Diethelm Wuertz and many others.
- **fUnitRoots** Rmetrics: Trends and unit roots. By Diethelm Wuertz and many others.
- **fUtilities** Rmetrics utilities. By Diethelm Wuertz and many others.
- ff Flat file database designed for large vectors and multi-dimensional arrays. By Daniel Adler, Oleg Nenadic, Walter Zucchini, and Christian Glaeser.
- **fuzzyFDR** Exact calculation of fuzzy decision rules for multiple testing. Choose to control FDR (false discovery rate) using the Benjamini and Hochberg method, or FWER (family wise error rate) using the Bonferroni method. By Alex Lewin.
- gamlss.cens An add on package to GAMLSS for fitting interval response variables using gamlss.family distributions. By Mikis Stasinopoulos, Bob Rigby, and Nicoleta Mortan.
- **glasso** Graphical lasso. By Jerome Friedman and R. Tibshirani.
- **hbim** Hill/Bliss Independence Model for combination vaccines. Calculate expected relative risk and proportion protected assuming normally distributed log10 transformed antibody dose for several component vaccine. Uses Hill models for each component which are combined under Bliss independence. By M. P. Fay.
- **hints** Gives hints on what functions you might want to apply to an object you have created. By Hadley Wickham and Sanford Weisberg.

- ig A collection of utilities for robust and classical versions of the inverse Gaussian distribution known as inverse Gaussian type distribution (IGTD). By Víctor Leiva, Hugo Hernández, and Antonio Sanhueza.
- **lga** Tools for linear grouping analysis (LGA). By Justin Harrington.
- **logilasso** Analysis of sparse contingency tables with penalization approaches. By Corinne Dahinden.
- **Itsa** Linear time series analysis. Methods are given for loglikelihood computation, forecasting and simulation. By A. I. McLeod, Hao Yu, and Zinovi Krougly.
- **matrixcalc** A collection of functions to support matrix differential calculus as presented in Magnus and Neudecker (1999) "Matrix Differential Calculus with Applications in Statistics and Econometrics", Second Edition, John Wiley, New York. Some of the functions are comparable to APL and J functions which are useful for actuarial models and calculations. By Frederick Novomestky.
- **mefa** Faunistic count data handling and reporting. The name "mefa" stands for the term "metafaunistics" indicating that handling of basic data is only the first, but the most critical and sometimes most time consuming part of data analysis. It contains functions to create and manage objects combining basic faunistic (sample/species/count or crosstabulated) count data and sample/species attribute tables. Segments within the count data and samples with zero count can be indicated and used in subsequent operations. Reports can be generated in plain text or LATEX format. By Peter Solymos.
- **mlegp** Maximum Likelihood Estimates of Gaussian Processes for univariate and multi-dimensional outputs with diagnostic plots and sensitivity analysis. By Garrett M. Dancik.
- **mra** Analysis of mark-recapture (capture-recapture) data using individual, time, and individualtime varying covariates. Contains functions to estimate live-capture Cormack-Jolly-Seber open population models. By Trent McDonald.
- **nnls** An R interface to the Lawson-Hanson NNLS algorithm for non-negative least squares that solves the least squares problem Ax = b with the constraint $x \ge 0$. By Katharine M. Mullen.
- **nonbinROC** ROC-type analysis for non-binary gold standards. Estimate and compare the accuracies of diagnostic tests in situations where the

gold standard is continuous, ordinal or nominal. By Paul Nguyen.

- **paleoTSalt** Modeling evolution in paleontological time-series (alternate parametrization). Facilitates the analysis of paleontological sequences of trait values from an evolving lineage. Functions are provided to fit, using maximum likelihood, evolutionary models including unbiased random walks, directional evolution, stasis and Ornstein-Uhlenbeck (OU) models. Performs many of the same functions as package **paleoTS**, but does so using a different parametrization of the evolutionary models. By Gene Hunt.
- **playwith** A GUI for interactive plots using GTK+. Tries to work out the structure of a plot, in order to interact with it. The built-in features include: navigating the data space, identifying data points, editing and annotating the plot, and saving to a file. New tools can be defined. Note: the interaction features do not work with multiple-plot layouts. Based on **RGtk2**, and so requires the GTK+ libraries, and still very much under development.
- **ppls** Linear and nonlinear regression methods based on Partial Least Squares and Penalization Techniques. By Nicole Kraemer and Anne-Laure Boulesteix.
- **predbayescor** Classification rule based on naive Bayes models with feature selection bias corrected. By Longhai Li.
- **predmixcor** Classification rule based on Bayesian mixture models with feature selection bias corrected. By Longhai Li.
- **pseudo** Various functions for computing pseudoobservations for censored data regression. By Mette Gerster and Maja Pohar Perme.
- ramps Bayesian geostatistical modeling of Gaussian processes using a reparametrized and marginalized posterior sampling (RAMPS) algorithm designed to lower autocorrelation in MCMC samples. Package performance is tuned for large spatial datasets. By Brian J. Smith, Jun Yan, and Mary Kathryn Cowles.
- realized Realized Variance Toolkit. By Scott Payseur.
- **regsubseq** Detect and test regular sequences and subsequences. For a sequence of event occurrence times, we are interested in finding subsequences in it that are too "regular" (in the sense of being significantly different from a homogeneous Poisson process). By Yanming Di.
- **sendplot** A tool for sending interactive plots. By Daniel P Gaile, Lori A. Shepherd, Lara Sucheston, Andrew Bruno, and Kenneth F. Manly.

- sets Data structures and basic operations for ordinary sets, and generalizations such as fuzzy sets, multisets, and fuzzy multisets. By David Meyer and Kurt Hornik.
- **surv2sample** Two-sample tests for survival analysis. Provides tests for comparing two survival distributions, testing equality of two cumulative incidence functions under competing risks and checking goodness of fit of proportional rate models (proportional hazards, proportional odds) for two samples. By David Kraus.
- **zoeppritz** Zoeppritz equations: calculate and plot scattering matrix coefficients for plane waves

at interface. By Jonathan M. Lees.

Other changes

- Packages FLCore, FLEDA, FortranCallsR, GammaTest, InfNet, RcppTemplate, edci, limma, rcompletion, and roblm were moved to the Archive.
- Packages **StoppingRules** and **pwt** were removed from CRAN.

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