News

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Editorial

by Torsten Hothorn

Welcome to the first issue of R News for 2007, which follows the release of R version 2.5.0. This major revision, in addition to many other features, brings better support of JAVA and Objective C to our desks. Moreover, there is a new recommended package, **codetools**, which includes functions that automagically check R code for possible problems.

Just before the release of R 2.5.0 the fifth developer conference on "Directions in Statistical Computing" was held in Auckland, NZ, the birthplace of R. Hadley Wickham reports on the highlights of this meeting. The R user community is not only active in conferences. Volume 7, like the preceding volumes of R News since 2001, wouldn't be what it is without the outstanding support of our referees. The editorial board would like to say "Thank you!" to all who contributed criticism and encouragement during the last year—the complete list of referees in 2006 is given at the end of this issue.

The scientific part of Volume 7 starts with an article by Paul Murrell, our former editor-in-chief, on handling binary files with tools provided by the **hexView** package. Andrew Robinson teaches how R users can make use of standard Unix tools, for example `mail` for auto-generating large amounts of email (not spam!). Many of us are regularly confronted with data lacking a unique definition of missing values–the **gdata** package can help in this situation, as Gregor Gorjanc explains.

Bettina Grün and Fritz Leisch give an introduction to the **flexmix** package for finite mixture modeling, analyzing a dataset on 21 different whiskey brands. The analysis of field agricultural experiments by means of additive main effect multiplicative interactions is discussed by Andrea Onofri and Egidio Ciriciofolo. Tests and confidence intervals for ratios of means, such as ratios of regression coefficients, implemented in package **mratio** are described by Gemechis Dilba and colleagues. The **npmlreg** package for fitting random effect models is introduced by Jochen Einbeck and his co-workers. Mathieu Ribatet models peaks over a threshold by **POT**, and financial instruments like stocks or options are (back-)tested by Kyle Campbell and colleagues.

Finally, I would like to remind everyone that the next "useR!" conference is taking place in Ames, Iowa, August 8–10. I hope to see you there!

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Viewing Binary Files with the hexView Package

by Paul Murrell

I really like plain text files.

I like them because I can see exactly what is in them. I can even easily modify the file if I'm feeling dangerous. This makes me feel like I understand the file.

I am not so fond of binary files. I always have to use specific software to access the contents and that software only shows me an interpretation of the basic content of the file. The raw content is hidden from me.

Sometimes I want to know more about a real binary file, for example when I need to read data in a binary format that no existing R function will read. When things go wrong, like when an R workspace file becomes "corrupt", I may have a strong *need* to know more.

Hex editors are wonderful tools that provide a view of the raw contents of a binary (or text) file, whether just to aid in understanding the file or to inspect or recover a file. The **hexView** package is an attempt to bring this sort of facility to R.

Viewing raw text files

The `viewRaw()` function reads and displays the raw content of a file. The content is displayed in three columns: the left column provides a byte offset within the file, the middle column shows the raw bytes, and the right column displays each byte as an ASCII character. If the byte does not correspond to a printable ASCII character then a full stop is displayed.

As a simple example, we will look at a plain text file, `"rawTest.txt"`, that contains a single line of text. This file was created using the following code (on a Linux system).

```
> writeLines("test pattern", "rawTest.txt")
```

A number of small example files are included as part of the **hexView** package and the `hexViewFile()` function is provided to make it convenient to refer to these files. The `readLines()` function from the **base** package reads in the lines of a plain text file as a vector of strings, so the plain text content of the file `"rawTest.txt"` can be retrieved as follows.

```
> readLines(hexViewFile("rawTest.txt"))

[1] "test pattern"
```

The following code uses the `viewRaw()` function from **hexView** to display the *raw* contents of this file.

```
> viewRaw(hexViewFile("rawTest.txt"))

0  :  74 65 73 74 20 70 61 74  |  test pat
8  :  74 65 72 6e 0a           |  tern.
```

As this example shows, by default, the raw bytes are printed in hexadecimal format. The first byte in this file is `74`, which is $7 * 16 + 4 = 116$ in decimal notation—the ASCII code for the character `t`. This byte pattern can be seen several times in the file, wherever there is a `t` character.

The `machine` argument to the `viewRaw()` function controls how the raw bytes are displayed. It defaults to `"hex"` for hexadecimal output, but also accepts the value `"binary"`, which means that the raw bytes are printed in binary format, as shown below.

```
> viewRaw(hexViewFile("rawTest.txt"),
          machine="binary")

 0  :  01110100 01100101 01110011  |  tes
 3  :  01110100 00100000 01110000  |  t p
 6  :  01100001 01110100 01110100  |  att
 9  :  01100101 01110010 01101110  |  ern
12  :  00001010                    |  .
```

One noteworthy feature of this simple file is the last byte, which has the hexadecimal value `0a` (or `00001010` in binary; the decimal value `10`) and no printable ASCII interpretation. This is the ASCII code for the *newline* or *line feed* (LF) special character that indicates the end of a line in text files. This is a simple demonstration that even plain text files have details that are hidden from the user by standard viewing software; viewers will show text on separate lines, but do not usually show the "character" representing the start of a new line.

The next example provides a more dramatic demonstration of hidden details in text files. The file we will look at contains the same text as the previous example, but was created on a Windows XP system with Notepad using "Save As..." and selecting "Unicode" as the "Encoding". The `readLines()` function just needs the file to be opened with the appropriate encoding, then it produces the same result as before.

```
> readLines(
      file(hexViewFile("rawTest.unicode"),
           encoding="UCS-2LE"))

[1] "test pattern"
```

However, the raw content of the file is now very different.

```
> viewRaw(hexViewFile("rawTest.unicode"))
```

```
 0  :  ff fe 74 00 65 00 73 00  |  ..t.e.s.
 8  :  74 00 20 00 70 00 61 00  |  t. .p.a.
16  :  74 00 74 00 65 00 72 00  |  t.t.e.r.
24  :  6e 00 0d 00 0a 00        |  n.....
```

It is fairly straightforward to identify some parts of this file. The ASCII codes from the previous example are there again, but there is an extra 00 byte after each one. This reflects the fact that, on Windows, Unicode text is stored using two bytes per character[1].

Instead of the 13 bytes in the original file, we might expect 26 bytes in this file, but there are actually 30 bytes. Where did the extra bytes come from?

The first two bytes at the start of the file are a *byte order mark* (BOM). With two bytes to store for each character, there are two possible orderings of the bytes; for example, the two bytes for the character t could be stored as 74 00 (called *little endian*) or as 00 74 (*big endian*). The BOM tells software which order has been used. Another difference occurs at the end of the file. The newline character is there again (with an extra 00), but just before it there is a 0d character (with an extra 00). This is the *carriage return* (CR) character. On Windows, a new line in a text file is signalled by the combination CR+LF, but on UNIX a new line is just indicated by a single LF.

As this example makes clear, software sometimes does a lot of work behind the scenes in order to display even "plain text".

Viewing raw binary files

An example of a binary file is the native binary format used by R to store information via the `save()` function. The following code was used to create the file `"rawTest.bin"`.

```
> save(rnorm(50), file="rawTest.bin")
```

We can view this file with the following code; the `nbytes` argument is used to show the raw data for only the first 80 bytes.

```
> viewRaw(hexViewFile("rawTest.bin"),
          nbytes=80)

 0  :  1f 8b 08 00 00 00 00 00  |  ........
 8  :  00 03 01 c0 01 3f fe 52  |  .....?.R
16  :  44 58 32 0a 58 0a 00 00  |  DX2.X...
24  :  00 02 00 02 05 00 00 02  |  ........
32  :  03 00 00 00 04 02 00 00  |  ........
40  :  00 01 00 00 10 09 00 00  |  ........
48  :  00 01 7a 00 00 00 0e 00  |  ..z.....
56  :  00 00 32 3f e7 60 e6 49  |  ..2?.`.I
64  :  c6 fe 0d 3f e1 3b c5 2f  |  ...?.;./
72  :  bb 4e 18 bf c4 9e 0f 1a  |  .N......
```

This is a good example of a binary file that is intriguing to view, but there is little hope of retrieving any useful information because the data has been compressed (encoded). In other cases, things are a not so hopeless, and it is not only possible to view the raw bytes, but also to see useful patterns and structures.

The next example looks at a binary file with a much simpler structure. The file `"rawTest.int"` only contains (uncompressed) integer values and was created by the following code.

```
> writeBin(1:50, "rawTest.int", size=4)
```

This file only contains the integers from 1 to 50, with four bytes used for each integer. The raw contents are shown below; this time the `nbytes` argument has been used to show only the raw data for the first 10 integers (the first 40 bytes).

```
> viewRaw(hexViewFile("rawTest.int"),
          nbytes=40)

 0  :  01 00 00 00 02 00 00 00  |  ........
 8  :  03 00 00 00 04 00 00 00  |  ........
16  :  05 00 00 00 06 00 00 00  |  ........
24  :  07 00 00 00 08 00 00 00  |  ........
32  :  09 00 00 00 0a 00 00 00  |  ........
```

None of the bytes correspond to printable ASCII characters in this case, so the right column of output is not terribly interesting. The `viewRaw()` function has two arguments, `human` and `size`, which control the way that the raw bytes are interpreted and displayed. In this case, rather than interpreting each byte as an ASCII character, it makes sense to interpret each block of four bytes as an integer. This is done in the following code using `human="int"` and `size=4`.

```
> viewRaw(hexViewFile("rawTest.int"),
          nbytes=40, human="int", size=4)

 0  :  01 00 00 00 02 00 00 00  |   1   2
 8  :  03 00 00 00 04 00 00 00  |   3   4
16  :  05 00 00 00 06 00 00 00  |   5   6
24  :  07 00 00 00 08 00 00 00  |   7   8
32  :  09 00 00 00 0a 00 00 00  |   9  10
```

With this simple binary format, we can see how the individual integers are being stored. The integer 1 is stored as the four bytes 01 00 00 00, the integer 2 as 02 00 00 00, and so on. This clearly demonstrates the idea of little endian byte order; the least-significant byte, the value 1, is stored first. In big endian byte order, the integer 1 would be 00 00 00 01 (as we shall see later).

The other option for interpreting bytes is `"real"` which means that each block of `size` bytes is interpreted as a floating-point value. A simple example

[1] Over-simplification alert! Windows *used to* use the UCS-2 encoding, which has two bytes per character, but now it uses UTF-16, which has two or four bytes per character. There are only two bytes per character in this case because these are common english characters.

is provided by the file "rawTest.real", which was generated by the following code. I have deliberately used big endian byte order because it will make it easier to see the structure in the resulting bytes.

```
> writeBin(1:50/50, "rawTest.real", size=8,
          endian="big")
```

Here is an example of reading this file and interpreting each block of 8 bytes as a floating-point number. This also demonstrates the use of the width argument to explicitly control how many bytes are displayed per line of output.

```
> viewRaw(hexViewFile("rawTest.real"),
          nbytes=40, human="real", width=8,
          endian="big")

 0  :  3f 94 7a e1 47 ae 14 7b  |  0.02
 8  :  3f a4 7a e1 47 ae 14 7b  |  0.04
16  :  3f ae b8 51 eb 85 1e b8  |  0.06
24  :  3f b4 7a e1 47 ae 14 7b  |  0.08
32  :  3f b9 99 99 99 99 99 9a  |  0.10
```

Again, we are able to see how individual floating-point values are stored. The following code takes this a little further and allows us to inspect the bit representation of the floating point numbers. The output is shown in Figure 1.

```
> viewRaw(hexViewFile("rawTest.real"),
          nbytes=40, human="real",
          machine="binary", width=8,
          endian="big")
```

The bit representation adheres to the IEEE Standard for Binary Floating-Point Arithmetic (IEEE, 1985; Wikipedia, 2006). Each value is stored in the form $sign \times mantissa \times 2^{exponent}$. The first (left-most) bit indicates the sign of the number, the next 11 bits describe the *exponent* and the remaining 52 bits describe the *mantissa*. The mantissa is a binary fraction, with bit i corresponding to 2^{-i}.

For the first value in "rawTest.real", the first bit has value 0 indicating a positive number, the exponent bits are 0111111 1001 = 1017, from which we subtract 1023 to get -6, and the mantissa is an implicit 1 plus $0 \times 2^{-1} + 1 \times 2^{-2} + 0 \times 2^{-3} + 0 \times 2^{-4} + 0 \times 2^{-5} + 1 \times 2^{-6} ... = 1.28$.[2] So we have the value $1.28 \times 2^{-6} = 0.02$.

Viewing a Binary File in Blocks

As the examples so far have hopefully demonstrated, being able to see the raw contents of a file can be a very good way to teach concepts such as endianness, character encodings, and floating-point representations of real numbers. Plus, it is just good fun to poke around in a file and see what is going on.

In this section, we will look at some more advanced functions from the **hexView** package, which will allow us to take a more detailed look at more complex binary formats and will allow us to perform some more practical tasks.

We will start by looking again at R's native binary format. The file "rawTest.XDRint" contains the integers 1 to 50 saved as a binary R object and was produced using the following code. The compress=FALSE is important to allow us to see the structure of the file.

```
> save(1:50, file="rawTest.XDRint",
       compress=FALSE)
```

We can view (the first 80 bytes of) the raw file using viewRaw() as before and this does show us some interesting features. For example, we can see the text RDX2 at the start of the file (it is common for files to have identifying markers at the start of the file). If we look a little harder, we can also see the first few integers (1 to 9); the data is stored in an XDR format (Wikipedia, 2006a), which uses big endian byte order, so the integers are in consecutive blocks of four bytes that look like this: 00 00 00 01, then 00 00 00 02, and so on.

```
> viewRaw(hexViewFile("rawTest.XDRint"),
          width=8, nbytes=80)

 0  :  52 44 58 32 0a 58 0a 00  |  RDX2.X..
 8  :  00 00 02 00 02 04 00 00  |  ........
16  :  02 03 00 00 00 04 02 00  |  ........
24  :  00 00 01 00 00 10 09 00  |  ........
32  :  00 00 01 78 00 00 00 0d  |  ...x....
40  :  00 00 00 32 00 00 00 01  |  ...2....
48  :  00 00 00 02 00 00 00 03  |  ........
56  :  00 00 00 04 00 00 00 05  |  ........
64  :  00 00 00 06 00 00 00 07  |  ........
72  :  00 00 00 08 00 00 00 09  |  ........
```

It is clear that there is some text in the file and that there are some integers in the file, so neither viewing the whole file as characters nor viewing the whole file as integers is satisfactory. What we need to be able to do is view the text sections as characters and the integer sections as integers. This is what the functions memFormat(), memBlock(), and friends are for.

The memBlock() function creates a description of a block of memory, specifying how many bytes are in the block; the block is interpreted as ASCII characters. The atomicBlock() function creates a description of a memory block that contains a single value of a specified type (e.g., a four-byte integer), and the vectorBlock() function creates a description of a memory block consisting of 1 or more memory blocks.

A number of standard memory blocks are predefined: integer4 (a four-byte integer) and integer1,

[2] At least, as close as it is possible to get to 1.28 with a finite number of bits. Another useful thing about viewing raw values is that it makes explicit the fact that most decimal values do not have an exact floating-point representation.

```
 0  :  00111111 10010100 01111010 11100001 01000111 10101110 00010100 01111011  |  0.02
 8  :  00111111 10100100 01111010 11100001 01000111 10101110 00010100 01111011  |  0.04
16  :  00111111 10101110 10111000 01010001 11101011 10000101 00011110 10111000  |  0.06
24  :  00111111 10110100 01111010 11100001 01000111 10101110 00010100 01111011  |  0.08
32  :  00111111 10111001 10011001 10011001 10011001 10011001 10011001 10011010  |  0.10
```

Figure 1: The floating point representation of the numbers 0.02 to 0.10 following IEEE 754 in big endian byte order.

`integer2`, and `integer8`; `real8` (an eight-byte floating-point number, or *double*) and `real4`; and `ASCIIchar` (a single-byte character). There is also a special `ASCIIline` memory block for a series of single-byte characters terminated by a newline.

The `memFormat()` function collects a number of memory block descriptions together and `viewFormat()` reads the memory blocks and displays them.

As an example, the following code reads in the `"RDX2"` header line of the file `"rawTest.XDRint"`, treats the next 39 bytes as just raw binary, ignoring any structure, then reads the first nine integers (as integers). A new memory block description is needed for the integers because the XDR format is big endian (the predefined `integer4` is little endian). The names of the memory blocks within the format are used to separate the blocks of output.

```
> XDRint <- atomicBlock("int", endian="big")
> viewFormat(hexViewFile("rawTest.XDRint"),
      memFormat(saveFormat=ASCIIline,
                rawBlock=memBlock(39),
                integers=vectorBlock(XDRint,
                                     9)))

========saveFormat
  0  :  52 44 58 32 0a           |  RDX2.
========rawBlock
  5  :  58 0a 00 00 00 02 00     |  X......
 12  :  02 04 00 00 02 03 00     |  .......
 19  :  00 00 04 02 00 00 00     |  .......
 26  :  01 00 00 10 09 00 00     |  .......
 33  :  00 01 78 00 00 00 0d     |  ..x....
 40  :  00 00 00 32              |  ...2
========integers
 44  :  00 00 00 01 00 00 00 02  |  1 2
 52  :  00 00 00 03 00 00 00 04  |  3 4
 60  :  00 00 00 05 00 00 00 06  |  5 6
 68  :  00 00 00 07 00 00 00 08  |  7 8
 76  :  00 00 00 09              |  9
```

The raw 39 bytes can be further broken down—see the description of R's native binary format on pages 11 and 12 of the "R Internals" manual (R Development Core Team, 2006) that is distributed with R—but that is beyond the scope of this article.

[3]There is a `readRaw()` function too.

Extracting Blocks from a Binary File

As well as viewing different blocks of a binary file, we may want to extract the values from each block. For this purpose, the `readFormat()` function is provided to read a binary format, as produced by `memFormat()`, and generate a `"rawFormat"` object (but not explicitly print it[3]). A `"rawFormat"` object is a list with a component `"blocks"` that is itself a list of `"rawBlock"` objects, one for each memory block defined in the memory format. A `"rawBlock"` object contains the raw bytes read from a file.

The `blockValue()` function extracts the interpreted value from a `"rawBlock"` object. The `blockString()` function is provided specifically for extracting a null-terminated string from a `"rawBlock"` object.

The following code reads in the file `"rawTest.XDRint"` and just extracts the 50 integer values.

```
> XDRfile <-
    readFormat(hexViewFile("rawTest.XDRint"),
      memFormat(saveFormat=ASCIIline,
                rawBlock=memBlock(39),
                integers=vectorBlock(XDRint,
                                     50)))
> blockValue(XDRfile$blocks$integers)

 [1]  1  2  3  4  5  6  7  8  9 10 11 12 13
[14] 14 15 16 17 18 19 20 21 22 23 24 25 26
[27] 27 28 29 30 31 32 33 34 35 36 37 38 39
[40] 40 41 42 43 44 45 46 47 48 49 50
```

A Caution

On a typical 32-bit platform, R uses 4 bytes for representing integer values in memory and 8 bytes for floating-point values. This means that there may be limits on what sort of values can be *interpreted* correctly by **hexView**.

For example, if a file contains 8-byte integers, it is possible to view each set of 8 bytes as an integer, but on my system R can only represent an integer using 4 bytes, so 4 of the bytes are (silently) dropped. The following code demonstrates this effect by reading

the file "testRaw.int" and interpreting its contents as 8-byte integers.

```
> viewRaw(hexViewFile("rawTest.int"),
          nbytes=40, human="int", size=8)

 0  :  01 00 00 00 02 00 00 00  |  1
 8  :  03 00 00 00 04 00 00 00  |  3
16  :  05 00 00 00 06 00 00 00  |  5
24  :  07 00 00 00 08 00 00 00  |  7
32  :  09 00 00 00 0a 00 00 00  |  9
```

An extended example: Reading EViews Files

On November 18 2006, Dietrich Trenkler sent a message to the R-help mailing list asking for a function to read files in the native binary format used by Eviews, an econometrics software package (http://www.eviews.com/). No such function exists, but John C Frain helpfully pointed out that an unofficial description of the basic structure of Eviews files had been made available by Allin Cottrell (creator of gretl, the Gnu Regression, Econometrics and Time-series Library). The details of Allin Cottrell's reverse-engineering efforts are available on the web (http://www.ecn.wfu.edu/~cottrell/eviews_format/).

In this section, we will use the **hexView** package to explore an Eviews file and produce a new function for reading files in this format. The example data file we will use is from Ramu Ramanathan's Introductory Econometrics text (Ramanathan, 2002). The data consists of four variables measured on single family homes in University City, San Diego, in 1990:

price: sale price in thousands of dollars.

sqft: square feet of living area.

bedrms: number of bedrooms.

baths: number of bath rooms.

The data are included in both plain text format, as "data4-1.txt", and Eviews format, as "data4-1.wf1", as part of the **hexViews** package.[4] For later comparison, the data from the plain text format are shown below, having been read in with the read.table() function.

```
> read.table(hexViewFile("data4-1.txt"),
             col.names=c("price", "sqft",
               "bedrms", "baths"))

   price sqft bedrms baths
1  199.9 1065      3  1.75
2  228.0 1254      3  2.00
3  235.0 1300      3  2.00
4  285.0 1577      4  2.50
5  239.0 1600      3  2.00
6  293.0 1750      4  2.00
7  285.0 1800      4  2.75
8  365.0 1870      4  2.00
9  295.0 1935      4  2.50
10 290.0 1948      4  2.00
11 385.0 2254      4  3.00
12 505.0 2600      3  2.50
13 425.0 2800      4  3.00
14 415.0 3000      4  3.00
```

An Eviews file begins with a header, starting with the text "New MicroTSP Workfile" and including important information about the size of the header and the number of variables and the number of observations in the file. The following code defines an appropriate "memFormat" object for this header information.

```
> EViewsHeader <-
    memFormat(firstline=memBlock(80),
              headersize=integer8,
              unknown=memBlock(26),
              numvblesplusone=integer4,
              date=vectorBlock(ASCIIchar, 4),
              unkown=memBlock(2),
              datafreq=integer2,
              startperiod=integer2,
              startobs=integer4,
              unkown=memBlock(8),
              numobs=integer4)
```

We can use readFormat() to read this header from the file as follows. The number of variables reported is one greater than the actual number of variables and also includes two "boiler plate" variables that are always included in Eviews files (hence 7 instead of the expected 4).

```
> data4.1.header <-
      readFormat(hexViewFile("data4-1.wf1"),
                 EViewsHeader)
> data4.1.header

=========firstline
   0  :  4e 65 77 20 4d 69                  |  New Mi
   6  :  63 72 6f 54 53 50                  |  croTSP
  12  :  20 57 6f 72 6b 66                  |   Workf
  18  :  69 6c 65 00 00 00                  |  ile...
  24  :  d8 5e 0e 01 00 00                  |  .^....
  30  :  00 00 00 00 08 00                  |  ......
  36  :  15 00 00 00 00 00                  |  ......
  42  :  ff ff ff ff 21 00                  |  ....!.
  48  :  00 00 00 00 00 00                  |  ......
  54  :  00 00 06 00 00 00                  |  ......
  60  :  0f 00 00 00 06 00                  |  ......
  66  :  00 00 01 00 01 00                  |  ......
  72  :  66 03 00 00 00 00                  |  f.....
  78  :  00 00                              |  ..
=========headersize
  80  :  90 00 00 00 00 00 00 00            |  144
=========unknown
  88  :  01 00 00 00 01 00                  |  ......
```

[4] The original source of the files was: http://ricardo.ecn.wfu.edu/pub/gretl_cdrom/data/

```
  94  :  00 00 01 00 00 00                    |  ......
 100  :  00 00 00 00 00 00                    |  ......
 106  :  00 00 00 00 00 00                    |  ......
 112  :  00 00                                |  ..
=========numvblesplusone
 114  :  07 00 00 00                          |  7
=========date
 118  :  d5 b7 0d 3a                          |  ...:
=========unkown
 122  :  06 00                                |  ..
=========datafreq
 124  :  01 00                                |  1
=========startperiod
 126  :  00 00                                |  0
=========startobs
 128  :  01 00 00 00                          |  1
=========unkown
 132  :  00 5d 67 0e 01 59                    |  .]g..Y
 138  :  8b 41                                |  .A
=========numobs
 140  :  0e 00 00 00                          |  14
```

We can extract some pieces of information from this header and use them to look at later parts of the file.

```
> headerSize <-
      blockValue(
          data4.1.header$blocks$headersize)
> numObs <-
      blockValue(
          data4.1.header$blocks$numobs)
```

At a location 26 bytes beyond the header size, there are several blocks describing each variable in the Eviews file. Each of these blocks is 70 bytes long and contains information on the variable name and the location within the file where the data values reside for that variable. The following code creates a description of a block containing variable information, then uses `readFormat()` to read the information for the first variable (the number of bath rooms); the `offset` argument is used to start reading the block at the appropriate location within the file. We also extract the location of the data for this variable.

```
> EViewsVbleInfo <-
    memFormat(unknown=memBlock(6),
              recsize=integer4,
              memsize=integer4,
              ptrtodata=integer8,
              vblename=vectorBlock(ASCIIchar,
                32),
              ptrtohistory=integer8,
              vbletype=integer2,
              unknown=memBlock(6))
> data4.1.vinfo <-
      readFormat(hexViewFile("data4-1.wf1"),
                 EViewsVbleInfo,
                 offset=headerSize + 26)
> data4.1.vinfo
```

```
=========unknown
 170  :  00 00 00 00 0b 00                    |  ......
=========recsize
 176  :  86 00 00 00                          |  134
=========memsize
 180  :  70 00 00 00                          |  112
=========ptrtodata
 184  :  f6 03 00 00 00 00 00 00              |  1014
=========vblename
 192  :  42 41 54 48 53 00 00 00 00 00  |  BATHS.....
 202  :  00 00 00 00 00 00 00 00 00 00  |  ..........
 212  :  00 00 00 00 00 00 00 00 00 00  |  ..........
 222  :  00 00                          |  ..
=========ptrtohistory
 224  :  00 00 00 00 d5 b7 0d 3a        |  0
=========vbletype
 232  :  2c 00                          |  44
=========unknown
 234  :  60 02 10 00 01 00              |  `.....
```

```
> firstVbleLoc <-
    blockValue(data4.1.vinfo$blocks$ptrtodata)
```

The data for each variable is stored in a block containing some preliminary information followed by the data values stored as eight-byte floating-point numbers. The code below creates a description of a block of variable data and then reads the data block for the first variable.

```
> EViewsVbleData <- function(numObs) {
      memFormat(numobs=integer4,
                startobs=integer4,
                unknown=memBlock(8),
                endobs=integer4,
                unknown=memBlock(2),
                values=vectorBlock(real8,
                  numObs))
  }
> viewFormat(hexViewFile("data4-1.wf1"),
             EViewsVbleData(numObs),
             offset=firstVbleLoc)
```

```
=========numobs
1014  :  0e 00 00 00                          |  14
=========startobs
1018  :  01 00 00 00                          |  1
=========unknown
1022  :  00 00 00 00 00 00                    |  ......
1028  :  00 00                                |  ..
=========endobs
1030  :  0e 00 00 00                          |  14
=========unknown
1034  :  00 00                                |  ..
=========values
1036  :  00 00 00 00 00 00 fc 3f              |  1.75
1044  :  00 00 00 00 00 00 00 40              |  2.00
1052  :  00 00 00 00 00 00 00 40              |  2.00
1060  :  00 00 00 00 00 00 04 40              |  2.50
1068  :  00 00 00 00 00 00 00 40              |  2.00
1076  :  00 00 00 00 00 00 00 40              |  2.00
1084  :  00 00 00 00 00 00 06 40              |  2.75
1092  :  00 00 00 00 00 00 00 40              |  2.00
1100  :  00 00 00 00 00 00 04 40              |  2.50
1108  :  00 00 00 00 00 00 00 40              |  2.00
1116  :  00 00 00 00 00 00 08 40              |  3.00
1124  :  00 00 00 00 00 00 04 40              |  2.50
1132  :  00 00 00 00 00 00 08 40              |  3.00
1140  :  00 00 00 00 00 00 08 40              |  3.00
```

This manual process of exploring the file structure can easily be automated within a function. The **hexView** package includes such a function under the

name `readEViews()`. With this function, we can read in the data set from the Eviews file as follows.

```
> readEViews(hexViewFile("data4-1.wf1"))

Skipping boilerplate variable
Skipping boilerplate variable
   BATHS BEDRMS PRICE SQFT
1   1.75      3 199.9 1065
2   2.00      3 228.0 1254
3   2.00      3 235.0 1300
4   2.50      4 285.0 1577
5   2.00      3 239.0 1600
6   2.00      4 293.0 1750
7   2.75      4 285.0 1800
8   2.00      4 365.0 1870
9   2.50      4 295.0 1935
10  2.00      4 290.0 1948
11  3.00      4 385.0 2254
12  2.50      3 505.0 2600
13  3.00      4 425.0 2800
14  3.00      4 415.0 3000
```

This solution is not the most efficient way to read Eviews files, but the **hexView** package does make it easy to gradually build up a solution, it makes it easy to view the results, and it does provide a way to solve the problem without having to resort to C code.

Summary

The **hexView** package provides functions for viewing the raw byte contents of files. This is useful for exploring a file structure and for demonstrating how information is stored on a computer. More advanced functions make it possible to read quite complex binary formats using only R code.

Acknowledgements

At the heart of the **hexView** package is the `readBin()` function and the core facilities for working with `"raw"` binary objects in R code (e.g., `rawToChar()`); thanks to the R-core member(s) who were responsible for developing those features.

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FlexMix: An R Package for Finite Mixture Modelling

by Bettina Grün and Friedrich Leisch

Introduction

Finite mixture models are a popular method for modelling unobserved heterogeneity or for approximating general distribution functions. They are applied in a lot of different areas such as astronomy, biology, medicine or marketing. An overview on these models with many examples for applications is given in the recent monographs McLachlan and Peel (2000) and Frühwirth-Schnatter (2006).

Due to this popularity there exist many (standalone) software packages for finite mixture modelling (see McLachlan and Peel, 2000; Wedel and Kamakura, 2001). Furthermore, there are several different R packages for fitting finite mixture models available on CRAN. Packages which use the EM algo-

rithm for model estimation are **flexmix**, **fpc**, **mclust**, **mixreg**, **mixtools**, and **mmlcr**. Packages with other model estimation methods are **bayesmix**, **depmix**, **moc**, **vabayelMix** and **wle**. A short description of these packages can be found in the CRAN task view on clustering (`http://cran.at.r-project.org/src/contrib/Views/Cluster.html`).

Finite mixture models

A finite mixture model is given by a convex combination of K different components, i.e. the weights of the components are non-negative and sum to one. For each component it is assumed that it follows a parametric distribution or is given by a more complex model, such as a generalized linear model (GLM).

In the following we consider finite mixture densities $h(\cdot|\cdot)$ with K components, dependent variables $\boldsymbol{y}$ and (optional) independent variables $\boldsymbol{x}$:

$$h(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{w}, \Theta) = \sum_{k=1}^{K} \pi_k(\boldsymbol{w}, \boldsymbol{\alpha}) f(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\vartheta}_k)$$

where $\forall \boldsymbol{w}, \boldsymbol{\alpha}$:

$$\pi_k(\boldsymbol{w}, \boldsymbol{\alpha}) \geq 0 \, \forall k \quad \wedge \quad \sum_{k=1}^{K} \pi_k(\boldsymbol{w}, \boldsymbol{\alpha}) = 1$$

and

$$\boldsymbol{\vartheta}_k \neq \boldsymbol{\vartheta}_l \quad \forall k \neq l.$$

We assume that the component distributions $f(\cdot|\cdot)$ are from the same distributional family with component specific parameters $\boldsymbol{\vartheta}_k$. The component weights or prior class probabilities π_k optionally depend on the concomitant variables $\boldsymbol{w}$ and the parameters $\boldsymbol{\alpha}$ and are modelled through multinomial logit models as suggested for example in Dayton and Macready (1988). A similar model class is also described in McLachlan and Peel (2000, p. 145). The model can be estimated using the EM algorithm (see Dempster et al., 1977; McLachlan and Peel, 2000) for ML estimation or using MCMC methods for Bayesian analysis (see for example Frühwirth-Schnatter, 2006).

A possible extension of this model class is to either have mixtures with components where the parameters of one component are fixed a-priori (e.g. zero-inflated models; Grün and Leisch, 2007b) or to even allow different component specific models (e.g. for modelling noise in the data; Dasgupta and Raftery, 1998).

Design principles of FlexMix

The main reason for the implementation of the package was to allow easy extensibility and to have the possibility for rapid prototyping in order to be able to try out new mixture models. The package was implemented using S4 classes and methods.

The EM algorithm provides a common basis for estimation of a general class of finite mixture models and the package **flexmix** tries to enable the user to exploit this commonness. **flexmix** provides the E-step and takes care of all data handling while the user is supposed to supply the M-step via model drivers for the component-specific model and the concomitant variable model. For the M-step available functions for weighted maximum likelihood estimation can be used as for example `glm()` for fitting GLMs or `multinom()` in **MASS** for multinomial logit models.

Currently model drivers are available for model-based clustering of multivariate Gaussian distributions with diagonal or unrestricted variance-covariance matrices (`FLXMCmvnorm()`) and multivariate Bernoulli and Poisson distributions (`FLXMCmvbinary()` and `FLXMCmvpois()`) where the dimensions are mutually independent. **flexmix** does not provide functionality for estimating mixtures of Gaussian distributions with special variance-covariance structures, as this functionality has already been implemented in the R package **mclust** (Fraley and Raftery, 2006).

For mixtures of regressions the Gaussian, binomial, Poisson and gamma distribution can be specified (`FLXMRglm()`). If some parameters are restricted to be equal over the components the model driver `FLXMRglmfix()` can be used. Zero-inflated Poisson and binomial regression models can be fitted using `FLXMRziglm()`. For an example of zero-inflated models see `example("FLXMRziglm")`. For the concomitant variable models either constant component weights (default) can be used or multinomial logit models (`FLXPmultinom()`) can be fitted.

Estimation problems can occur if the components become too small during the EM algorithm. In order to avoid these problems a minimum size can be specified for each component. This is especially important for finite mixtures of multivariate Gaussian distributions where full variance-covariance matrices are estimated for each component.

Further details on the implementation and the design principles as well as exemplary applications of the package can be found in the accompanying vignettes `"flexmix-intro"` which is an updated version of Leisch (2004) and `"regression-examples"` and in Grün and Leisch (2007a). Note that this article uses the new version 2.0 of the package, where the names of some driver functions have changed compared with older versions of **flexmix**.

Exemplary applications

In the following we present two examples for using the package. The first example demonstrates model-based clustering, i.e., mixtures without independent variables, and the second example gives an application for fitting mixtures of generalized linear regres-

sion models.

Model-based clustering

The following dataset is taken from Edwards and Allenby (2003) who refer to the Simmons Study of Media and Markets. It contains all households which used any whiskey brand during the last year and provides a binary incidence matrix on their brand use for 21 whiskey brands during this year. This means only the information on the different brands used in a household is available.

We first load the package and the dataset. The `whiskey` dataset contains observations from 2218 households. The relative frequency of usage for each brand is given in Figure 1. Additional information is available for the brands indicating the type of whiskey: blend or single malt.

```
R> library("flexmix")
R> data("whiskey")
R> set.seed(1802)
```

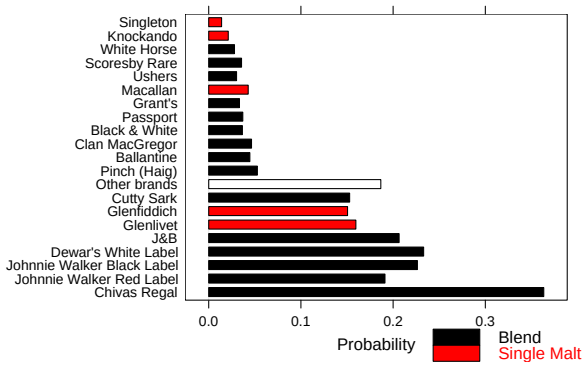

Figure 1: Relative frequency of the whiskey brands.

We fit a mixture of binomial distributions to the dataset where the variables in each component specific models are assumed to be independent. The EM algorithm is repeated `nrep = 3` times using random initialization, i.e. each observation is assigned to one component with an a-posteriori probability of 0.9 and 0.1 otherwise and the component is selected with equal probability.

```
R> wh_mix <- stepFlexmix(Incidence ~ 1,
+   weights = ~ Freq, data = whiskey,
+   model = FLXMCmvbinary(truncated = TRUE),
+   control = list(minprior = 0.005),
+   k = 1:7, nrep = 3)
```

Model-based clustering uses no explanatory variables, hence the right hand side of the formula `Incidence ~ 1` is constant. The model driver is `FLXMCmvbinary()` with argument `truncated = TRUE`, as the number of non-users is not available and a truncated likelihood is maximized in each M-step again using the EM-algorithm. We vary the number of components for `k = 1:7`. The best solution with respect to the log-likelihood for each of the different numbers of components is returned in an object of class `"stepFlexmix"`. The control argument can be used to control the fitting with the EM algorithm. With `minprior` the minimum relative size of the components is specified, components falling below this threshold are removed during the EM algorithm.

The dataset contains only the unique binary patterns observed with the corresponding frequency. We use these frequencies for the weights argument instead of transforming the dataset to have one row for each observation. The use of a weights argument allows to use only the number of unique observations for fitting, which can substantially reduce the size of the model matrix and hence speed up the estimation process. For this dataset this means that the model matrix has 484 instead of 2218 rows.

Model selection can be made using information criteria, as for example the BIC (see Fraley and Raftery, 1998). For this example the BIC suggests a mixture with 5 components:

```
R> BIC(wh_mix)

      1       2       3       4
27705.1 26327.6 25987.7 25683.2
      5       6       7
25647.0 25670.3 25718.6

R> wh_best <- getModel(wh_mix, "BIC")
R> wh_best

Call:
stepFlexmix(Incidence ~ 1,
    weights = ~Freq, data = whiskey,
    model = FLXMCmvbinary(truncated = TRUE),
    control = list(minprior = 0.005),
    k = 5, nrep = 3)

Cluster sizes:
  1   2   3   4   5
283 791 953  25 166

convergence after 180 iterations
```

The estimated parameters can be inspected using accessor functions such as `prior()` or `parameters()`.

```
R> prior(wh_best)

[1] 0.1421343 0.3303822
[3] 0.4311072 0.0112559
[5] 0.0851203

R> parameters(wh_best, component=4:5)[1:2,]

                    Comp.4
center.Singleton 0.643431
center.Knockando 0.601124
                       Comp.5
center.Singleton 2.75013e-02
center.Knockando 1.13519e-32
```

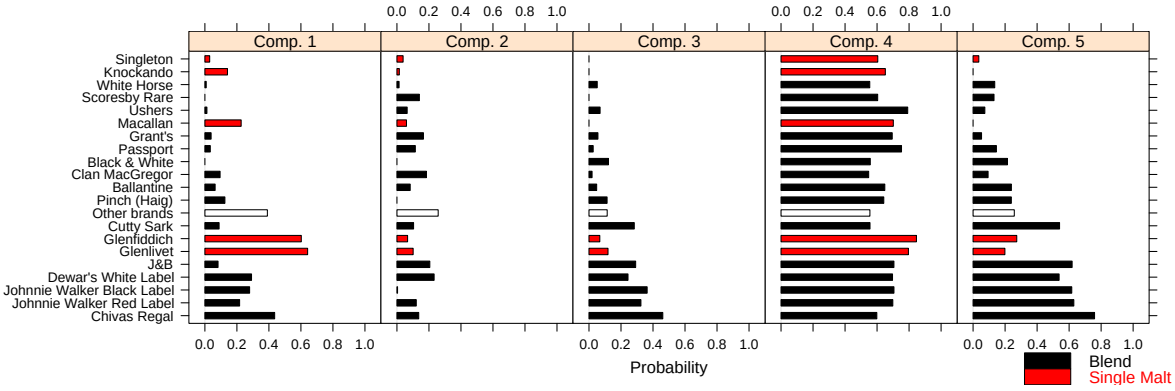

Figure 2: Estimated probability of usage for the whiskey brands for each component.

The fitted parameters of the mixture for each component are given in Figure 2. It can be seen that component 4 (1.1% of the households) contains the households which bought the greatest number of different brands and all brands to a similar extent. Households from component 5 (8.5%) also buy a wide range of whiskey brands, but tend to avoid single malts. Component 3 (43.1%) has a similar usage pattern as component 5 but buys less brands in general. Component 1 (14.2%) seems to favour single malt whiskeys and component 2 (33%) is especially fond of other brands and tends to avoid Johnnie Walker Black Label.

Mixtures of regressions

The patent data given in Wang et al. (1998) includes 70 observations on patent applications, R&D spending and sales in millions of dollar from pharmaceutical and biomedical companies in 1976 taken from the National Bureau of Economic Research R&D Masterfile. The data is given in Figure 3.

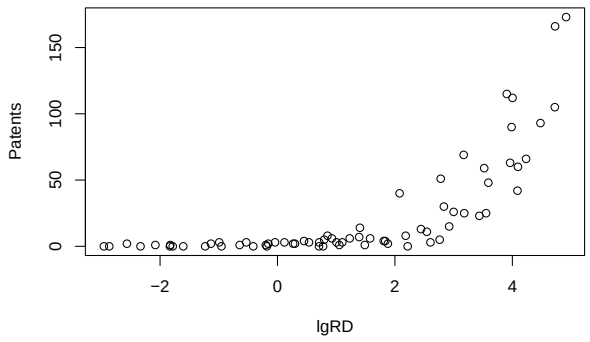

Figure 3: Patent dataset.

The model which is chosen as the best in Wang et al. (1998) is a finite mixture of three Poisson regression models with `Patents` as dependent variable, the logarithmized R&D spending `lgRD` as independent variable and the R&D spending per sales `RDS` as concomitant variable. This model can be fitted in R with the component-specific model driver `FLXMRglm()` which allows fitting of finite mixtures of GLMs. As concomitant variable model driver `FLXPmultinom()` is used for a multinomial logit model where the posterior probabilities are the dependent variables.

```
R> data("patent")
R> pat_mix <- flexmix(Patents ~ lgRD,
+   k = 3, data = patent,
+   model = FLXMRglm(family = "poisson"),
+   concomitant = FLXPmultinom(~RDS))
```

The observed values together with the fitted values for each component are given in Figure 4. The coloring and characters used for plotting the observations are according to the component assignment using the maximum a-posteriori probabilities, which are obtained using `cluster(pat_mix)`.

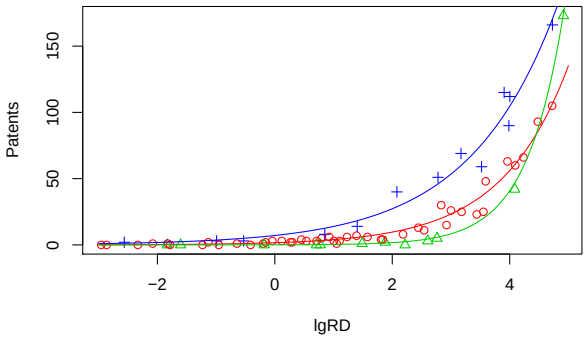

Figure 4: Patent data with fitted values for each component.

In Figure 5 a rootogram of the posterior probabilities of the observations is given. This is the default plot of the `"flexmix"` objects returned by the fitting function. It can be used for arbitrary mixture models and indicates how well the observations are clustered by the mixture. For ease of interpretation the observations with a-posteriori probability less than `eps`$=10^{-4}$ are omitted as otherwise the peak at zero would dominate the plot. The observations where the a-posteriori probability is largest for the third component are colored differently. The plot is generated using the following command.

```
R> plot(pat_mix, mark = 3)
```

The posteriors of all three components have modes at 0 and 1, indicating well-separated clusters (Leisch, 2004). Note that the object returned by the plot function is of class "trellis", and that the plot itself is produced by the corresponding show() method (Sarkar, 2002).

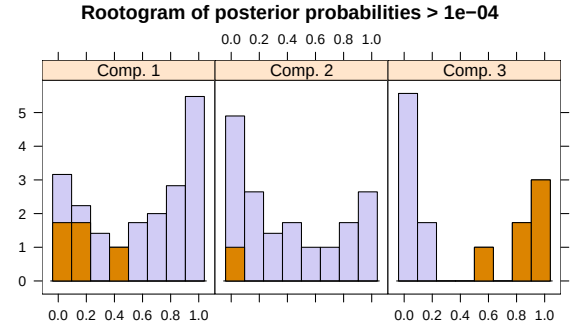

Figure 5: Rootogram of the posterior probabilities.

Further details of the fitted mixture can be obtained with refit() which returns the fitted values together with approximate standard deviations and significance tests, see Figure 6. The standard deviations are only approximative because they are determined separately for each component and it is not taken into account that the components have been estimated simultaneously. In the future functionality to determine the standard deviations using either the full Hesse matrix or the parametric bootstrap shall be provided.

The estimated coefficients are given in Figure 7. The black lines indicate the (approximative) 95% confidence intervals. This is the default plot for the objects returned by refit() and is obtained with the following command.

```
R> plot(refit(pat_mix), bycluster = FALSE)
```

The argument bycluster indicates if the clusters/components or the different variables are used as conditioning variables for the panels.

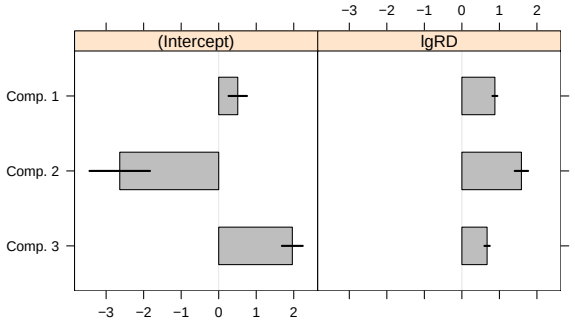

Figure 7: Estimated coefficients of the component specific models with corresponding 95% confidence intervals.

The plot indicates that the estimated coefficients vary between all components even though the coefficients for lgRD are similar for the first and third component. A smaller model where these coefficients are restricted to be equal can be fitted using the model driver FLXMRglmfix(). The EM algorithm can be initialized in the original solution using the estimated posterior probabilities for the cluster argument. As in this case the first and third component are restricted to have the same coefficient for lgRD, the posteriors of the fitted mixture are used for initialization after reordering the components to have these two components next to each other. The modified model is compared to the original model using the BIC.

```
R> Model_2 <- FLXMRglmfix(family = "poisson",
+   nested = list(k = c(1,2),
+     formula = ~lgRD))
R> Post_1 <- posterior(pat_mix)[,c(2,1,3)]
R> pat_mix2 <- flexmix(Patents ~ 1,
+   concomitant = FLXPmultinom(~RDS),
+   data = patent, cluster = Post_1,
+   model = Model_2)
R> c(M_1 = BIC(pat_mix), M_2 = BIC(pat_mix2))

    M_1     M_2
437.836 445.243
```

In this example, the original model is preferred by the BIC.

Summary

flexmix provides infrastructure for fitting finite mixture models with the EM algorithm and tools for model selection and model diagnostics. We have shown the application of the package for model-based clustering as well as for fitting finite mixtures of regressions.

In the future we want to implement new model drivers, e.g., for generalized additive models with smooth terms, as well as to extend the tools for model selection, diagnostics and model validation. Additional functionality will be added which allows to fit mixture models with different component specific models. The implementation of zero-inflated models has been a first step in this direction.

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```
R> refit(pat_mix)

Call:
refit(pat_mix)

Number of components: 3

$Comp.1
             Estimate Std. Error z value Pr(>|z|)
(Intercept)  0.50819    0.12366    4.11 3.96e-05 ***
lgRD         0.87976    0.03328   26.43  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

$Comp.2
             Estimate Std. Error z value Pr(>|z|)
(Intercept)  -2.6368     0.4043  -6.522 6.95e-11 ***
lgRD          1.5866     0.0899  17.648  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

$Comp.3
             Estimate Std. Error z value Pr(>|z|)
(Intercept)  1.96217    0.13968   14.05   <2e-16 ***
lgRD         0.67190    0.03572   18.81   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Figure 6: Details of the fitted mixture model for the patent data.

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Using R to Perform the AMMI Analysis on Agriculture Variety Trials

by Andrea Onofri & Egidio Ciriciofolo

Introduction

Field agricultural experiments are generally planned to evaluate the actual effect produced by man-made chemical substances or human activities on crop yield and quality, environmental health, farmers' income and so on. Field experiments include the testing of new and traditional varieties (genotypes), fertilizers (types and doses), pesticides (types and doses) and cultural practices. With respect to greenhouse or laboratory experiments, field trials are much more strongly subjected to environmental variability that forces researchers into repeating experiments across seasons and/or locations. A significant 'treatment x environment' interaction may introduce some difficulties in exploring the dataset, summarizing results and determining which treatment (genotype, herbicide, pesticide...) was the best.

In such conditions, the AMMI (Additive Main effect Multiplicative Interaction) analysis has been proposed as an aid to visualize the dataset and explore graphically its pattern and structure (Gollob, 1968; Zobel et al., 1988); this technique has received a particular attention from plant breeders (see for example Abamu and Alluri, 1998; Annichiarico et al., 1995; Annichiarico, 1997; Ariyo, 1998) and recently it has been stated as superior to other similar techniques, such as the GGE (Gauch, 2006). Unfortunately, such technique is not yet very well exploited by agricultural scientists, who often prefer a more traditional approach to data analysis, based on ANOVA and multiple comparison testing. Without disregarding the importance of such an approach, one cannot deny that sometimes this does not help unveil the underlying structure of experimental data, which may be more important than hypothesis testing, especially at the beginning of data analyses (Exploratory Data Analysis; NIST/SEMATECH, 2004) or at the very end, when graphs have to be drawn for publication purposes.

To make more widespread the acceptance and the use of such powerful tool within agronomists, it is necessary to increase the availability of both practical information on how to perform and interpret an AMMI analysis and simple software tools that give an easily understandable output, aimed at people with no specific and deep statistical training, such as students and field technicians.

The aim of this paper was to show how R can be easily used to perform an AMMI analysis and produce 'biplots', as well as to show how these tools can be very useful within variety trials in agriculture.

Some basic statistical aspects

The AMMI analysis combines the ANalysis OF VAriance (ANOVA) and the Singular Value Decomposition (SVD) and it has been explained in detail by Gollob (1968). If we specifically refer to a variety trial, aimed at comparing the yield of several genotypes in several environments (years and/or locations), the ANOVA partitions the total sum of squares into two main effects (genotypes and environments) plus the interaction effect (genotypes x environments). This latter effect may be obtained by taking the observed averages for each 'genotype x environment' combination and doubly-centering them (i.e., subtracting to each data the appropriate genotype and environment means and adding back the grand mean). The interaction effect is arranged on a two-way matrix γ (one row for each genotype and one column for each environment) and submitted to SVD, as follows:

$$\gamma = \sum_{i=1}^{r} \lambda_i \cdot g_{ik} \cdot e_{ij} \qquad (1)$$

where r is the rank of γ, λ_i is the singular value for principal component i, g_{ik} is the eigenvector score for genotype k and Principal Component (PC) i (left singular vector), while e_{ij} is the eigenvector score for environment j and PC i (right singular vector). If PC scores are multiplied by the square root of the singular value, equation 1 is transformed into:

$$\gamma = \sum_{i=1}^{r} \left(\lambda_i^{0.5} \cdot g_{ik}\right)\left(\lambda_i^{0.5} \cdot e_{ij}\right) = \sum_{i=1}^{r} G_{ik} \cdot E_{ij} \qquad (2)$$

In this way the additive interaction in the ANOVA model is obtained by multiplication of genotype PC scores by environment PC scores, appropriately scaled. If a reduced number of PCs is used ($r = 1$ or 2, typically) a dimensionality reduction is achieved with just a small loss in the descriptive ability of the model. This makes it possible to plot the interaction effect, via the PC scores for genotypes and environments. Such graphs are called biplots, as they contain two kinds of data; typically, a AMMI1 and a AMMI2 biplots are used: the AMMI1 biplot has main effects (average yields for genotypes and environments) on the x-axis and PC1 scores on the y-axis, while the AMMI2 biplot has PC1 scores on the x-axis and PC2 scores on the y-axis.

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Table 1: Field averages (three replicates) for six genotypes compared in seven years.

Genotype	1996	1997	1998	1999	2000	2001	2002	Average
COLOSSEO	6.35	6.46	6.70	6.98	6.44	7.07	4.90	6.41
CRESO	5.60	6.09	6.13	7.13	6.08	6.45	4.33	5.97
DUILIO	5.64	8.06	7.15	7.99	5.18	7.88	4.24	6.59
GRAZIA	6.26	6.74	6.35	6.84	4.75	7.30	4.34	6.08
IRIDE	6.04	7.72	6.39	7.99	6.05	7.71	4.96	6.70
SANCARLO	5.70	6.77	6.81	7.41	5.66	6.67	4.50	6.22
SIMETO	5.08	7.19	6.44	7.07	4.82	7.55	3.34	5.93
SOLEX	6.14	6.39	6.44	6.87	5.45	7.52	4.79	6.23
Average	5.85	6.93	6.55	7.29	5.55	7.27	4.42	6.27

The dataset

To show how the AMMI analysis can be easily performed with R, we will use a dataset obtained from a seven-years field trial on durum wheat, carried out from 1996 to 2003 in central Italy, on a randomised block design with three replicates. For the present analysis, eight genotypes were chosen, as they were constantly present throughout the years (Colosseo, Creso, Duilio, Grazia, Iride, Sancarlo, Simeto, Solex). Yield data referred to the standard humidity content of 13% (Tab. 1) have been previously published in Belocchi et al. (2003), Ciriciofolo et al. (2002); Ciriciofolo et al. (2001); Desiderio et al. (2000), Desiderio et al. (1999), Desiderio et al. (1998), Desiderio et al. (1997). The interaction matrix (which is submitted to SVD) is given in table 2.

The AMMI with R

To perform the AMMI analysis, an R function was defined, as shown on page 17.

The `AMMI()` function requires as inputs a vector of genotype codes (factor), a vector of environment codes (factor), a vector of block codes (factor) and a vector of yields (numerical). PC is the number of PCs to be considered (set to 2 by default) and biplot is the type of biplot to be drown (1 for AMM1 and 2 for AMMI2). It should be noted that the script is very elementary and that it does not use any difficult function or programming construct. It was simply coded by translating the algebraic procedure proposed by Gollob (1968) into R statements, which is a very easy task, even without a specific programming training. Wherever possible, built-in R functions were used, to simplify the coding process and to facilitate the adaptation of the script to other kinds of AMMI models.

The first part uses the function `tapply()` to calculate some descriptive statistics, such as genotype means, environment means and 'genotype x environment' means, which are all included in the final output.

The second part uses the function `aov()` to perform the ANOVA by using a randomised block design repeated in different environments with a different randomisation in each environment (LeClerg et al., 1962). The interaction matrix γ is calculated by using the function `model.tables()` applied to the output of the function `aov()`; the way the R script is coded, the interaction matrix is actually the transpose of the matrix shown in table 2, but this does not change much in terms of the results. The interaction matrix is then submitted to SVD, by using the built-in R function `svd()`.

The significant PCs are assessed by a series of F tests as shown by Zobel et al. (1988) and PC scores, genotype means and environment means are used to produce biplots, by way of the functions `plot()` and `points()`.

Table 2: Interaction effects for the dataset in table 1.

Genotype	1996	1997	1998	1999	2000	2001	2002
COLOSSEO	0.35	-0.62	0.00	-0.45	0.74	-0.34	0.33
CRESO	0.04	-0.54	-0.13	0.14	0.82	-0.52	0.20
DUILIO	-0.54	0.80	0.28	0.38	-0.70	0.29	-0.51
GRAZIA	0.60	-0.01	-0.02	-0.27	-0.62	0.21	0.10
IRIDE	-0.24	0.37	-0.59	0.28	0.07	0.01	0.11
SANCARLO	-0.10	-0.11	0.31	0.17	0.16	-0.55	0.12
SIMETO	-0.43	0.60	0.23	0.13	-0.40	0.62	-0.75
SOLEX	0.33	-0.50	-0.07	-0.38	-0.07	0.29	0.40

```
$Additive_ANOVA
                         Df  Sum Sq Mean Sq  F value    Pr(>F)
Environments              6 159.279  26.547 178.3996 < 2.2e-16 ***
Genotypes                 7  11.544   1.649  11.0824 2.978e-10 ***
Blocks(Environments)     14   3.922   0.280   1.8826   0.03738 *
Environments x Genotypes 42  27.713   0.660   4.4342 6.779e-10 ***
Residuals                98  14.583   0.149
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

$Mult_Interaction
     Effect        SS DF        MS         F        Prob.
1       PC1 18.398624 12 1.5332187 10.303612 7.958058e-13
2       PC2  5.475627 10 0.5475627  3.679758 3.339881e-04
3       PC3  1.961049  8 0.2451311  1.647342 1.212529e-01
4 Residuals  1.877427 12 0.1564522  1.051398 4.094193e-01

$Environment_scores
            PC1         PC2         PC3
1996  0.4685599 -0.62599974  0.01665148
1997 -0.8859669  0.21085535 -0.19553672
1998 -0.1572887 -0.00567589  0.80162642
1999 -0.3139136  0.51881710 -0.13286326
2000  0.8229290  0.59868592 -0.03330554
2001 -0.5456613 -0.49726356 -0.18138908
2002  0.6113417 -0.19941917 -0.27518331

$Genotype_scores
                PC1         PC2           PC3
COLOSSEO  0.74335025 -0.02451524  0.1651197989
CRESO     0.63115567  0.47768803 -0.0001969871
DUILIO   -0.87632103  0.17923645  0.1445152042
GRAZIA   -0.07625519 -0.74659598 -0.0108977060
IRIDE    -0.12683903  0.28634343 -0.7627600696
SANCARLO  0.18186612  0.35076556  0.3753706117
SIMETO   -0.78109997  0.04751457  0.1740113396
SOLEX     0.30414317 -0.57043681 -0.0851621918
```

Figure 1: Results from ANOVA and AMMI analyses.

Results

Results (Fig. 1) show a highly significant 'genotypes x environments' interaction (GE) on the ANOVA, that does not permit to define an overall ranking of varieties across environments.

The SVD decomposition of the interaction matrix was performed by extracting three PCs, though only the first two are significant. It is possible to observe that the first PC accounts for 66% of the interaction sum of squares, while the second one accounts for an additional 20%.

The AMMI1 biplot shows contemporarily main effects (genotypes and environments average yields) and interaction, as PC1 scores (Fig. 2). This graph is relevant as it accounts for 87% of total data variability.

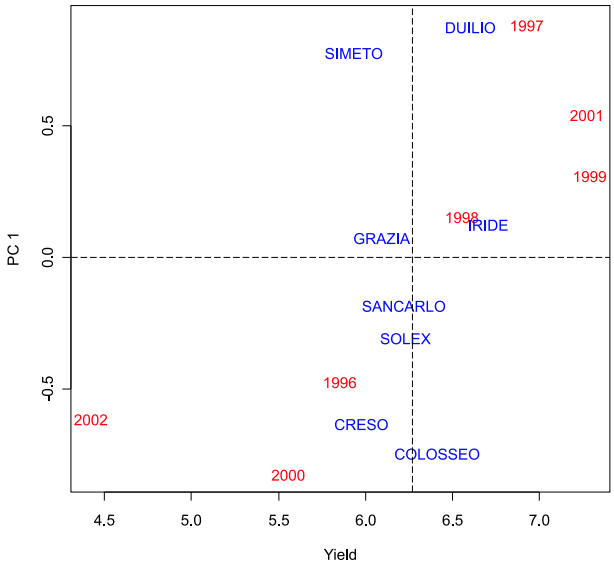

Figure 2: AMMI1 biplot.

```
AMMI <- function(variety, envir, block, yield, PC = 2, biplot = 1) {
## 1 - Descriptive statistics
  overall.mean <- mean(yield)
  envir.mean <- tapply(yield, envir, mean)
  var.mean <- tapply(yield, variety, mean)
  int.mean <- tapply(yield, list(variety,envir), mean)
  envir.num <- length(envir.mean)
  var.num <- length(var.mean)
## 2 - ANOVA (additive model)
  variety <- factor(variety)
  envir <- factor(envir)
  block <- factor(block)
  add.anova <- aov(yield ~ envir + block %in% envir + variety + envir:variety)
  modelTables <- model.tables(add.anova, type = "effects", cterms = "envir:variety")
  int.eff <- modelTables$tables$"envir:variety"
  add.anova.residual.SS <- deviance(add.anova)
  add.anova.residual.DF <- add.anova$df.residual
  add.anova.residual.MS <- add.anova.residual.SS/add.anova.residual.DF
  anova.table <- summary(add.anova)
  row.names(anova.table[[1]]) <- c("Environments", "Genotypes", "Blocks(Environments)",
                                   "Environments x Genotypes", "Residuals")
## 3 - SVD
  dec <- svd(int.eff, nu = PC, nv = PC)
  if (PC > 1) {
    D <- diag(dec$d[1:PC])
  } else {
    D <- dec$d[1:PC]
  }
  E <- dec$u %*% sqrt(D)
  G <- dec$v %*% sqrt(D)
  Ecolnumb <- c(1:PC)
  Ecolnames <- paste("PC", Ecolnumb, sep = "")
  dimnames(E) <- list(levels(envir), Ecolnames)
  dimnames(G) <- list(levels(variety), Ecolnames)
## 4 - Significance of PCs
  numblock <- length(levels(block))
  int.SS <- (t(as.vector(int.eff)) %*% as.vector(int.eff))*numblock
  PC.SS <- (dec$d[1:PC]^2)*numblock
  PC.DF <- var.num + envir.num - 1 - 2*Ecolnumb
  residual.SS <- int.SS - sum(PC.SS)
  residual.DF <- ((var.num - 1)*(envir.num - 1)) - sum(PC.DF)
  PC.SS[PC + 1] <- residual.SS
  PC.DF[PC + 1] <- residual.DF
  MS <- PC.SS/PC.DF
  F <- MS/add.anova.residual.MS
  probab <- pf(F, PC.DF, add.anova.residual.DF, lower.tail = FALSE)
  percSS <- PC.SS/int.SS
  rowlab <- c(Ecolnames, "Residuals")
  mult.anova <- data.frame(Effect = rowlab, SS = PC.SS, DF = PC.DF, MS = MS, F = F, Prob. = probab)
## 5 - Biplots
  if (biplot == 1) {
    plot(1, type = 'n', xlim = range(c(envir.mean, var.mean)), ylim = range(c(E[,1], G[,1])), xlab = "Yield",
     ylab = "PC 1")
    points(envir.mean, E[,1], col = "red", lwd = 5)
    plot(1, type = 'n', xlim = range(c(envir.mean, var.mean)), ylim = range(c(E[,1], G[,1])), xlab = "Yield",
      ylab = "PC 1")
    points(envir.mean, E[,1], "n", col = "red", lwd = 5)
    text(envir.mean, E[,1], labels = row.names(envir.mean), adj = c(0.5, 0.5), col = "red")
    points(var.mean, G[,1], "n", col = "blue", lwd = 5)
    text(var.mean, G[,1], labels = row.names(var.mean), adj = c(0.5, 0.5), col = "blue")
    abline(h = 0, v = overall.mean, lty = 5)
  } else {
    plot(1, type = 'n', xlim = range(c(E[,1], G[,1])), ylim = range(c(E[,2], G[,2])), xlab = "PC 1",
     ylab = "PC 2")
    points(E[,1], E[,2], "n",col = "red", lwd = 5)
    text(E[,1], E[,2], labels = row.names(E),adj = c(0.5,0.5),col = "red")
    points(G[,1],G[,2], "n", col = "blue", lwd = 5)
    text(G[,1], G[,2], labels = row.names(G),adj = c(0.5, 0.5), col = "blue")
  }
## 6 - Other results
  list(Genotype_means = var.mean, Environment_means = envir.mean,  Interaction_means = int.mean,
       Additive_ANOVA = anova.table, Mult_Interaction = mult.anova, Environment_scores = E,
       Genotype_scores = G)
}
```

To read this biplot, it is necessary to remember that genotypes and environments on the right side of the graph shows yield levels above the average. Besides, genotypes and environments laying close to the x-axis (PC 1 score close to 0) did not interact with each other, while data with positive/negative score on y-axis interacted positively with environments characterised by a score of same sign.

Indeed, environmental variability was much higher than genotype variability (Fig. 2, see also the ANOVA in Fig. 1). Iride showed the highest average yield and did not interact much with the environment (PC1 score close to 0). Duilo ranked overall second, but showed a high interaction with the environment, i.e., its yield was above the average in 1997 (first ranking), 2001 (first ranking) and 1999 (second ranking), while it was below the average in 1996, 2000 and 2002. Colosseo gave also a good average yield, but its performances were very positive in 1996, 2000 and 2002, while they were below the average in 1997, 2000 and 2002.

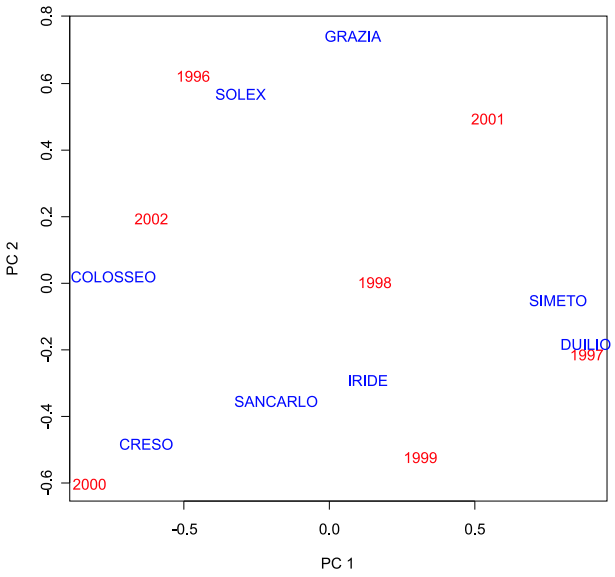

Figure 3: AMMI2 biplot.

The AMMI2 biplot (Fig. 3) is more informative on the GE interaction as it accounts for 86% of the sum of squares of this latter effect. Remember that genotypes and environments in the center of the graph did not show a relevant interaction, while genotypes and environment lying close on the external parts of the graph interacted positively. Duilio and Simeto were particularly brilliant in 1997 (compared to their average performances; notice in tab. 1 that Simeto was the third in this year, which is very good compared to its seventh position on the ranking based on average yield). Solex and Grazia were brilliant in 1997 (they were third and second respectively, in spite of the eighth and fifth ranking based on average yield). Likewise, Creso and Colosseo were the best in 2000 and 2002, while Iride and Sancarlo interacted positively with 1999.

Discussion and conclusions

The above example should be discussed with reference to two main aspects: the AMMI analysis and the use of R. Concerning the first aspect, the example confirms the graphical power of the biplots; indeed, all the above comments are just an excerpt of what can be easily grasped at first sight from the AMMI1 and AMMI2 biplots. It is worth to notice that obtaining such information from table 1 is not as immediate and quick. Of course, the AMMI analysis should be followed by other procedures to explore the relationship between the behaviour of each variety and the environmental conditions of each year.

It is also necessary to mention that in the present example the analyses were aimed only at graphically exploring the underlying structure of the dataset. In other cases, whenever hypothesis testing is more important, the F procedure employed on the script may be too liberal and other techniques may be better suited to evaluate the significance of PCs (Cornelius, 1993).

Concerning R, the above example confirms that this environment can be easily used to perform statistical analyses in the agricultural field. Thanks to its ability to deal with linear models and to the facilities for matrix manipulation, it is very easy to accomplish also rather complex statistical tasks, such as the AMMI analysis. Indeed, calculations can be performed having in mind the usual algebraic notation, as one can find in statistical literature, without a deep knowledge of programming constructs. Indeed, this script has been coded in an elementary fashion, following the calculation pattern proposed by Gollob (1968) and including some built-in R functions when possible.

Of course, it is necessary to mention that this elementary coding style may be useful for simple scripts, but should not be regarded as optimal, especially for more advanced applications. Indeed, in such cases an object-oriented approach is much more advisable to exploit the statistical power of R. In any case, elementary scripts such this one may be always used as the starting point to perform other types of statistical analyses. In particular, with slight modifications, this script (available on: `www.unipg.it/~onofri/software.htm`) could be used to draw the GGE biplot, that has received a certain attention in the last years (Yan and Tinker, 2005).

However, when re-using this script, one should bear in mind some limitations. Indeed, it is important to notice that this script has been aimed at a specific experimental design (completely randomised block experiment repeated across years or environments), as commonly found in field variety trials. Other designs will require some adaptations into the code and unbalanced designs (especially those with missing combinations of genotypes and environments) should not be analysed with this script.

Furthermore, the 'environment' effect has been considered as 'fixed' and changes to the code should be made in case it should be considered as 'random'.

In spite of the the above limitations, it is clear that also users with a limited background in computer programming (which is often the case in agriculture) can benefit from the use of R: an elementary knowledge of R statements and functions is already enough to perform also the 'less traditional' statistical analysis, with a very slight effort.

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Inferences for Ratios of Normal Means

by Gemechis Dilba, Frank Schaarschmidt, Ludwig A. Hothorn

Introduction

Inferences concerning ratios of means of normally distributed random variables or ratios of regression coefficients arise in a variety of problems in biomedical research. For example, in tests for non-inferiority of one or more experimental treatments against a positive control, it is often easier to define and also to interpret the non-inferiority margin as percentage changes (or fraction retained compared to the mean of the control group). In bioassay problems, one is also interested in ratios of regression coefficients, for instance in parallel line or slope ratio assays. Our aim here is to introduce an R extension package called **mratios** which can perform inferences about one or more such ratio parameters in the general linear model. For two-sample problems, the package is capable of constructing Fieller confidence intervals and performing the related tests when the group variances are assumed homogeneous or heterogeneous. In simultaneous inferences for multiple ratios, the package can (i) perform multiple tests, (ii) construct simultaneous confidence intervals using a variety of techniques, and (iii) calculate the sample sizes required for many-to-one comparisons in simultaneous tests for non-inferiority (or superiority) based on relative margins. We demonstrate the functionality of the package by using several data examples.

Two-sample Problem

The two-sample problem is one of the standard methods routinely used in practice. Here the interest is in comparing the means of two independent normally distributed random variables in terms of the ratio of their means. This can be accomplished by using the `t.test.ratio` function. If the variances are homogeneous, this function performs a ratio formatted t-test (also known as Sasabuchi test) and computes Fieller's confidence interval. If variance homogeneity is not tenable (the default), the test proposed by Tamhane and Logan (2004) is performed using Satterthwaite adjusted degrees of freedom. For confidence interval estimation under variance heterogeneity, Satterthwaite degrees of freedom depends on the unknown ratio. To circumvent this problem, we plug in the maximum likelihood estimate of the ratio (i.e., ratio of sample means) in the approximate expression for the number of degrees of freedom.

Example 1. Consider the mutagenicity assay data described in the **mratios** package. A first step in the analysis of the data could be to test whether the active control (cyclophosphamide at dose 25mg/kg) results in a significantly higher number of mutations than the vehicle control. The data appear to be heteroscedastic, and therefore we use the unequal variances option (the default) to compare the two treatments.

```
> library("mratios")
> data("Mutagenicity")
> muta2 <- subset(Mutagenicity, Treatment ==
+     "Vehicle" | Treatment == "Cyclo25")
> t.test.ratio(MN ~ Treatment, data = muta2,
+     alternative = "greater")

    Ratio t-test for unequal variances

data:  Cyclo25 and Vehicle
t = 5.0071, df = 3.07, p-value = 0.0073
 alternative hypothesis: true ratio of means
    is greater than 1
95 percent confidence interval:
 5.110079      Inf
sample estimates:
   mean Cyclo25    mean Vehicle
      25.000000        2.571429
Cyclo25/Vehicle
       9.722222
```

Note that when testing a ratio of means against 1, the p-value computed by the `t.test.ratio` function is exactly the same as that computed by `t.test` when testing the difference of means against 0.

Simultaneous Inferences

In this section we consider inferential problems involving one or more ratio parameters. The basic distribution underlying the analyses is the multivariate t-distribution. Under the assumption of normality and homogeneous variance for the error terms, the joint distribution of the test statistics associated with the various contrasts of interest follows a multivariate t-distribution. For the computation of the related multivariate t probabilities and equi-coordinate critical points, we refer to Hothorn et al. (2001).

Multiple Tests

Assume a normal one-way ANOVA model with homogeneous variances. The interest is in simultaneous tests for several ratios of linear combinations of the treatment means. Such tests for ratio hypotheses (ratios of normal means) appear, for example, in tests for non-inferiority (or superiority) of several experimental treatments compared to a control

(placebo). These are so called many-to-one comparisons. In the R-function `simtest.ratio`, most of the routinely used multiple comparison procedures [e.g., many-to-one (Dunnett type), all pairs (Tukey type), sequence (successive comparisons of ordered treatment effects)] are implemented in the context of ratio hypotheses. In general, the function also allows for any user-defined contrast matrices.

Let $\gamma_j = \boldsymbol{c}_j'\boldsymbol{\mu}/\boldsymbol{d}_j'\boldsymbol{\mu},\ j = 1,\ldots,r$ denote the ratios of interest, where $\boldsymbol{\mu} = (\mu_1,\ldots,\mu_k)'$ is a vector of the treatment means, $\boldsymbol{c}_j$ and $\boldsymbol{d}_j$ are known vectors of real constants each of dimension $k \times 1$, and r is the number of ratios. To specify the ratios, we define two contrast matrices, namely, numerator and denominator contrast matrices. The numerator contrast matrix is a matrix whose row vectors are $\boldsymbol{c}_1',\ldots,\boldsymbol{c}_r'$, and the denominator contrast matrix is a matrix whose row vectors are $\boldsymbol{d}_1',\ldots,\boldsymbol{d}_r'$. Therefore, the dimensions of both the numerator and denominator contrast matrices are each $r \times k$. Further, let $(\psi_1,\ldots,\psi_r)'$ denote the set of margins against which we test the r ratios. Then, for example, for one-sided upper-tailed alternative hypotheses, the hypotheses of interest are $H_{0j} : \gamma_j \leq \psi_j$ versus $H_{1j} : \gamma_j > \psi_j$, $j = 1,\ldots,r$.

Given a data frame containing the observations, the contrast matrices, the vector of margins, and the family-wise type I error rate, the function `simtest.ratio` calculates the point estimates of the ratios, the test statistics, the raw p-values and the multiplicity adjusted p-values. The adjusted p-values are computed by adapting the results of Westfall et al. (1999) for ratio hypotheses and general contrasts.

In general, note that the function `simtest.ratio` allows for varying margins for the set of comparisons. This can be quite appealing, for example, in test problems involving a mixture of non-inferiority and superiority hypotheses.

Example 2. Bauer et al. (1998) analyzed data from a multi-dose experiment including a positive control and placebo. In the experiment, patients with chronic stable angina pectoris were randomized to five treatment arms (placebo, three doses of a new compound, and an active control). The response variable is the difference in the duration of an exercise test before and after treatment. Now, due to the unavailability of the original data values, we randomly generated independent samples (from a normal distribution) that satisfy the summary statistics given in Table II of Bauer et al. (1998). This data set is available in the **mratios** package. The interest is in simultaneous tests for non-inferiority of the three doses versus the active control by including the placebo. Following Pigeot et al. (2003), the hypotheses can succinctly be formulated as $H_{0i} : (\mu_j - \mu_2)/(\mu_1 - \mu_2) \leq 0.9$ versus $H_{1i} : (\mu_j - \mu_2)/(\mu_1 - \mu_2) > 0.9$, $j = 3,4,5$, where μ_i, $i = 1,\ldots,5$ denote the means for the active control, placebo, dose 50, dose 100 and dose 150, consecutively. In this example, the non-inferiority margins are all set to 0.9.

```
> data("AP")
> NC <- rbind(N1 = c(0, -1, 1, 0, 0),
+             N2 = c(0, -1, 0, 1, 0),
+             N3 = c(0, -1, 0, 0, 1))
> DC <- rbind(D1 = c(1, -1, 0, 0, 0),
+             D2 = c(1, -1, 0, 0, 0),
+             D3 = c(1, -1, 0, 0, 0))
> ap.test <- simtest.ratio(pre_post ~
+     treatment, data = AP, Num.Contrast = NC,
+     Den.Contrast = DC, Margin.vec = 0.9,
+     alternative = "greater")
> ap.test

Alternative hypotheses: Ratios greater
 than margins

      margin estimate statistic
N1/D1    0.9    5.306    2.9812
N2/D2    0.9    4.878    2.7152
N3/D3    0.9    1.969    0.7236
      p.value.raw p.value.adj
N1/D1    0.001554    0.004429
N2/D2    0.003505    0.009799
N3/D3    0.234952    0.451045
```

By using the command `summary(ap.test)`, one can get further information — for example, the correlation matrix under the null hypotheses and the critical point (equi-coordinate percentage point of the multivariate t-distribution).

Simultaneous Confidence Intervals

Unlike in multiple testing, in simultaneous estimation of the ratios $\gamma_j = \boldsymbol{c}_j'\boldsymbol{\mu}/\boldsymbol{d}_j'\boldsymbol{\mu},\ j = 1,\ldots,r$, the joint distribution of the associated t-statistics follows a multivariate t-distribution with a correlation matrix that depends on the unknown ratios. This means that the critical points that are required for confidence interval construction depend on these unknown parameters. There are various methods of dealing with this problem. They are (i) using the unadjusted intervals (Fieller confidence intervals without multiplicity adjustments); (ii) Bonferroni (Fieller intervals with simple Bonferroni adjustments); (iii) a method called MtI which consists of replacing the unknown correlation matrix of the multivariate t-distribution by an identity matrix of the same dimension according to Sidak and Slepian inequalities (Hochberg and Tamhane, 1987) for two- and one-sided confidence intervals, respectively; and (iv) plug-in (plugging the maximum likelihood estimates of the ratios into the unknown correlation matrix). The latter method is known to have good simultaneous coverage probabilities and hence it is set as a default method in the R functions to be introduced. For details regarding these methodologies, we refer to Dilba et al. (2006a).

The `sci.ratio` function is used to construct simultaneous CIs for ratios of linear combinations of treatment means in a one-way ANOVA model. Several standard contrast types (e.g., Dunnett, Tukey, sequence, and many others) are implemented in this function. The default contrast is many-to-one comparisons (Dunnett type) with the mean of the first level of the factor (in alpha-numeric order) taken as the denominator of the ratios. In addition, this function has an option for user-defined contrast matrices.

Example 3. Recall the data from the multi-dose experiment in Example 2 above. Now, suppose that the interest is to calculate simultaneous lower 95% confidence limits for the ratios of the three doses and the active control to the placebo. Noting that placebo is the second level in the alpha-numeric order of the treatments, we use the following R code to calculate the limits.

```
> ap.sci <- sci.ratio(pre_post ~
+     treatment, data = AP, type = "Dunnett",
+     base = 2, alternative = "greater",
+     method = "MtI")
```

The graph of the confidence intervals can be obtained by applying the plot function to the object in which the confidence interval estimates are stored, see Figure 1.

```
> plot(ap.sci)
```

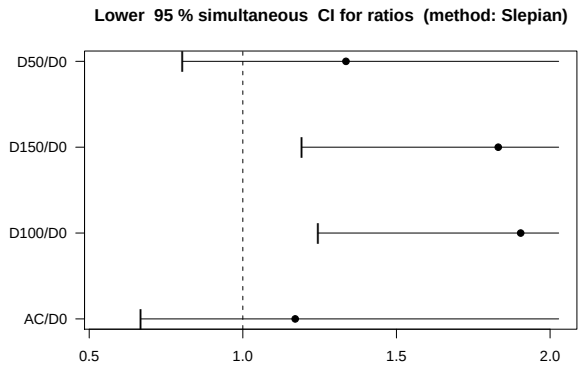

Figure 1: Graphical visualization of the `ap.sci` object.

The `sci.ratio.gen` function is a more general function that can construct simultaneous confidence intervals for ratios of linear combinations of coefficients in the general linear model. For this function, it is necessary to specify the vector of responses, the design matrix, and the numerator and denominator contrast matrices.

Example 4. Consider the problem of simultaneously estimating relative potencies in a multiple slope ratio assay. Jensen (1989) describes an experiment in which three preparations are compared to a control. The response variable (Y) is pantothenic acid content of plant tissues. The model is $Y_{ij} = \alpha + \beta_i X_{ij} + \epsilon_{ij}$, $i = 0,1,2,3$; $j = 1,\ldots,n_i$, where the X_{ij}s are the dose levels and $i = 0$ refers to the control group. The vector of regression coefficients is $(\alpha, \beta_0, \beta_1, \beta_2, \beta_3)'$. Now using the data in Table 5 of Jensen (1989), the interest is to construct simultaneous CIs for β_i/β_0, $i = 1,2,3$. The function `sci.ratio.gen` needs the response vector Y and the design matrix X as an input.

```
> data(SRAssay)
> Y <- SRAssay[, "Response"]
> X <- model.matrix(Response ~ Treatment:Dose,
+     data = SRAssay)
> NC <- matrix(c(0, 0, 1, 0, 0,
+                0, 0, 0, 1, 0,
+                0, 0, 0, 0, 1),
+       nrow = 3, byrow = TRUE)
> DC <- matrix(c(0, 1, 0, 0, 0,
+                0, 1, 0, 0, 0,
+                0, 1, 0, 0, 0),
+       nrow = 3, byrow = TRUE)
> s.ratio <- sci.ratio.gen(Y, X,
+     Num.Contrast = NC, Den.Contrast = DC)
> s.ratio

Two-sided 95 % simultaneous confidence
 intervals for ratios:


   estimate  lower  upper
C1   1.1217 1.0526 1.1964
C2   0.7193 0.6603 0.7805
C3   0.7537 0.6942 0.8157
```

Using the command `summary(s.ratio)`, one can also get further details regarding the fitted regression model, the contrast matrices and an estimate of the correlation matrix (when the plug-in method is used). The estimate of the correlation matrix used for critical point calculation can also be obtained as

```
> s.ratio[["CorrMat.est"]]

          [,1]      [,2]      [,3]
[1,] 1.0000000 0.4083451 0.4260802
[2,] 0.4083451 1.0000000 0.3767098
[3,] 0.4260802 0.3767098 1.0000000
```

Note that by choosing the option for method as 'Sidak', one gets the results reported by Jensen (1989).

Before closing this section, we give two important remarks.

i) According to the Slepian inequality (Hochberg and Tamhane, 1987), it is appropriate to use the MtI method for estimating one-sided simultaneous confidence limits only when all the elements of the correlation matrix are non-negative. Therefore, if some of the (estimated) correlations are negative, `sci.ratio` and `sci.ratio.gen` functions report a warning message about the inappropriateness of the MtI method.

ii) In simultaneous CI estimation (using either `sci.ratio` or `simtest.ratio.gen`), one may encounter the case where some of the contrasts in the

denominators of the ratios are not significantly different from zero. In this situation, NSD (standing for "non-significant denominator") will be printed. For instance, in Example 2 above, since there is no significant difference between the placebo and the active control, one gets NSD in constructing the related simultaneous CIs for the three ratios.

Sample Size Calculation

Consider the design of a special problem in simultaneous comparison of $m \geq 2$ treatments with a control for non-inferiority (or superiority), where the margins are expressed as a percentage of the mean of the control group. For sample size calculation, we implement a method based on normal approximation to the exact method which involves inversion of a univariate (multivariate) non-central t-distribution (see Dilba et al. (2006b) for details on the exact method). Given the number of comparisons (`m`), the non-inferiority (superiority) margin (`rho`), the power (`Power`), the coefficient of variation of the control group (`CV0`), the percentage (of the mean of the control group) to be detected (`rho.star`), the family-wise type-I error rate (`alpha`), and the kind of power to be controlled (by default minimal power), the function `n.ratio` calculates the sample size required in a balanced design.

Example 5. Suppose that we have a response variable where large response values indicate better treatment benefits. The following R code calculates the sample size required per treatment in designing a non-inferiority trial with four treatment arms (including the control).

```
> n.ratio(m = 3, rho = 0.7, Power = 0.8,
+     CV0 = 0.5, rho.star = 0.95,
+     alpha = 0.05, Min.power = TRUE)

 Number of observations per treatment =  52
         Total number of observations = 208
```

If the aim is to control the complete power, we set `Min.power` to `FALSE`.

For the two-sample design ($m = 1$), the sample sizes required in the non-inferiority trials discussed by Laster and Johnson (2003) can be calculated as a special case.

Remarks

We conclude by giving some general remarks regarding the four basic functions in the **mratios** package.

- In two-sample ratio problems with homogeneous variances, `t.test.ratio` is a special case of `simtest.ratio` and `sci.ratio`.
- The `simtest.ratio` function with all the elements of the vector of margins equal to 1 gives the same result as the analysis based on the difference of treatment means. Thus, the difference-based test is a special case of the ratio-based test with the thresholds set to 1.
- The `sci.ratio` function is a special case of `sci.ratio.gen` for the one-way layout.

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Working with Unknown Values

The gdata package

by Gregor Gorjanc

Introduction

Unknown or missing values can be represented in various ways. For example SAS uses . (dot), while R uses NA, which we can read as Not Available. When we import data into R, say via read.table or its derivatives, conversion of blank fields to NA (according to read.table help) is done for logical, integer, numeric and complex classes. Additionally, the na.strings argument can be used to specify values that should also be converted to NA. Inversely, there is an argument na in write.table and its derivatives to define value that will replace NA in exported data. There are also other ways to import/export data into R as described in the *R* Data Import/Export manual (R Development Core Team, 2006). However, all approaches lack the possibility to define unknown value(s) for some particular column. It is possible that an unknown value in one column is a valid value in another column. For example, I have seen many datasets where values such as 0, -9, 999 and specific dates are used as column specific unknown values.

This note describes a set of functions in package **gdata**[1] (Warnes , 2006): isUnknown, unknownToNA and NAToUnknown, which can help with testing for unknown values and conversions between unknown values and NA. All three functions are generic (S3) and were tested (at the time of writing) to work with: integer, numeric, character, factor, Date, POSIXct, POSIXlt, list, data.frame and matrix classes.

Description with examples

The following examples show simple usage of these functions on numeric and factor classes, where value 0 (beside NA) should be treated as an unknown value:

```
> library("gdata")
> xNum <- c(0, 6, 0, 7, 8, 9, NA)
> isUnknown(x=xNum)
[1] FALSE FALSE FALSE FALSE FALSE FALSE
    TRUE
```

The default unknown value in isUnknown is NA, which means that output is the same as is.na — at least for atomic classes. However, we can pass the argument unknown to define which values should be treated as unknown:

```
> isUnknown(x=xNum, unknown=0)
[1] TRUE FALSE  TRUE FALSE FALSE FALSE
    FALSE
```

This skipped NA, but we can get the expected answer after appropriately adding NA into the argument unknown:

```
> isUnknown(x=xNum, unknown=c(0, NA))
[1] TRUE FALSE  TRUE FALSE FALSE FALSE
    TRUE
```

Now, we can change all unknown values to NA with unknownToNA. There is clearly no need to add NA here. This step is very handy after importing data from an external source, where many different unknown values might be used. Argument warning=TRUE can be used, if there is a need to be warned about "original" NAs:

```
> xNum2 <- unknownToNA(x=xNum, unknown=0)
[1] NA  6 NA  7  8  9 NA
```

Prior to export from R, we might want to change unknown values (NA in R) to some other value. Function NAToUnknown can be used for this:

```
> NAToUnknown(x=xNum2, unknown=999)
[1] 999   6 999   7   8   9 999
```

Converting NA to a value that already exists in x issues an error, but force=TRUE can be used to overcome this if needed. But be warned that there is no way back from this step:

```
> NAToUnknown(x=xNum2, unknown=7,
              force=TRUE)
[1] 7 6 7 7 8 9 7
```

Examples below show all peculiarities with class factor. unknownToNA removes unknown value from levels and inversely NAToUnknown adds it with a warning. Additionally, "NA" is properly distinguished from NA. It can also be seen that the argument unknown in functions isUnknown and unknownToNA need not match the class of x (otherwise factor should be used) as the test is internally done with %in%, which nicely resolves coercing issues.

```
> xFac <- factor(c(0, "BA", "RA", "BA",
                   NA, "NA"))
[1] 0    BA   RA   BA   <NA> NA
Levels: 0 BA NA RA
> isUnknown(x=xFac)
[1] FALSE FALSE FALSE FALSE  TRUE FALSE
> isUnknown(x=xFac, unknown=0)
[1]  TRUE FALSE FALSE FALSE FALSE FALSE
> isUnknown(x=xFac, unknown=c(0, NA))
[1]  TRUE FALSE FALSE FALSE  TRUE FALSE
```

[1] package version 2.3.1

```
> isUnknown(x=xFac, unknown=c(0, "NA"))
[1]  TRUE FALSE FALSE FALSE FALSE  TRUE
> isUnknown(x=xFac, unknown=c(0, "NA", NA))
[1]  TRUE FALSE FALSE FALSE  TRUE  TRUE

> xFac <- unknownToNA(x=xFac, unknown=0)
[1] <NA> BA   RA   BA   <NA> NA
Levels: BA NA RA
> xFac <- NAToUnknown(x=xFac, unknown=0)
[1] 0  BA RA BA 0  NA
Levels: 0 BA NA RA
Warning message:
new level is introduced: 0
```

These two examples with classes `numeric` and `factor` are fairly simple and we could get the same results with one or two lines of R code. The real benefit of the set of functions presented here is in `list` and `data.frame` methods, where `data.frame` methods are merely wrappers for `list` methods.

We need additional flexibility for `list`/`data.frame` methods, due to possibly having multiple unknown values that can be different among `list` components or `data.frame` columns. For these two methods, the argument `unknown` can be either a `vector` or `list`, both possibly named. Of course, greater flexibility (defining multiple unknown values per component/column) can be achieved with a `list`.

When a `vector`/`list` object passed to the argument `unknown` is not named, the first value/component of a `vector`/`list` matches the first component/column of a `list`/`data.frame`. This can be quite error prone, especially with `vectors`. Therefore, I encourage the use of a `list`. In case `vector`/`list` passed to argument `unknown` is named, names are matched to names of `list` or `data.frame`. If lengths of `unknown` and `list` or `data.frame` do not match, recycling occurs.

The example below illustrates the application of the described functions to a list which is composed of previously defined and modified numeric (`xNum`) and factor (`xFac`) classes. First, function `isUnknown` is used with `0` as an unknown value. Note that we get `FALSE` for `NA`s as has been the case in the first example.

```
> xList <- list(a=xNum, b=xFac)
$a
[1]  0  6  0  7  8  9 NA

$b
[1] 0  BA RA BA 0  NA
Levels: 0 BA NA RA
> isUnknown(x=xList, unknown=0)
$a
[1] TRUE FALSE  TRUE FALSE FALSE FALSE
    FALSE

$b
[1] TRUE FALSE FALSE FALSE  TRUE FALSE
```

We need to add `NA` as an unknown value. However, we do not get the expected result this way!

```
> isUnknown(x=xList, unknown=c(0, NA))
$a
[1] TRUE FALSE  TRUE FALSE FALSE FALSE
    FALSE

$b
[1] FALSE FALSE FALSE FALSE FALSE FALSE
```

This is due to matching of values in the argument `unknown` and components in a `list`; i.e., `0` is used for component `a` and `NA` for component `b`. Therefore, it is less error prone and more flexible to pass a `list` (preferably a named list) to the argument `unknown`, as shown below.

```
> xList1 <- unknownToNA(x=xList,
+    unknown=list(b=c(0, "NA"), a=0))
$a
[1] NA  6 NA  7  8  9 NA

$b
[1] <NA> BA   RA   BA   <NA> <NA>
Levels: BA RA
```

Changing `NA`s to some other value (only one per component/column) can be accomplished as follows:

```
> NAToUnknown(x=xList1,
+    unknown=list(b="no", a=0))
$a
[1] 0 6 0 7 8 9 0

$b
[1] no BA RA BA no no
Levels: BA no RA

Warning message:
new level is introduced: no
```

A named component `.default` of a `list` passed to argument `unknown` has a special meaning as it will match a component/column with that name and any other not defined in `unknown`. As such it is very useful if the number of components/columns with the same unknown value(s) is large. Consider a wide `data.frame` named `df`. Now `.default` can be used to define unknown value for several columns:

```
> df <- unknownToNA(x=df,
+                   unknown=(.default=0,
+                            col1=999,
+                            col2="unknown"))
```

If there is a need to work only on some components/columns you can of course "skip" columns with standard R mechanisms, i.e., by subsetting `list` or `data.frame` objects:

```
> cols <- c("col1", "col2")
> df[, cols] <- unknownToNA(x=df[, cols],
+    unknown=(col1=999,
+             col2="unknown"))
```

Summary

Functions `isUnknown`, `unknownToNA` and `NAToUnknown` provide a useful interface to work with various representations of unknown/missing values. Their use is meant primarily for shaping the data after importing to or before exporting from R. I welcome any comments or suggestions.

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A New Package for Fitting Random Effect Models

The npmlreg package

by Jochen Einbeck, John Hinde, and Ross Darnell

Introduction

Random effects have become a standard concept in statistical modelling over the last decades. They enter a wide range of applications by providing a simple tool to account for such problems as model misspecification, unobserved (latent) variables, unobserved heterogeneity, and the like. One of the most important model classes for the use of random effects is the generalized linear model. Aitkin (1999) noted that "the literature on random effects in generalized linear models is now extensive," and this is certainly even more true today.

However, most of the literature and the implemented software on generalized linear mixed models concentrates on a normal random effect distribution. An approach that avoids specifying this distribution parametrically was provided by Aitkin (1996a), using the idea of 'Nonparametric Maximum Likelihood' (NPML) estimation (Laird, 1978). The random effect distribution can be considered as an unknown mixing distribution and the NPML estimate of this is a finite discrete distribution. This can be determined by fitting finite mixture distributions with varying numbers of support points, where each model is conveniently fitted using a straightforward EM algorithm.

This approach is implemented in GLIM4 (Aitkin and Francis, 1995). Despite being a quite powerful tool, the current GLIM-based software is computationally limited and the GLIM system is no longer widely used. Though the alternatives C.A.MAN (Böhning et al., 1992) and the Stata program `gllamm` (Skrondal and Rabe-Hesketh, 2004) cover parts of GLIMs capacities (in the latter case based on Newton-Raphson instead of EM), no R implementation of NPML estimation existed. The package **npmlreg** (Einbeck et al., 2006), which we wish to introduce to the R community in this article, is designed to fill this gap.

NPML estimation

Assume there is given a set of explanatory vectors $x_1, \ldots, x_n$ and a set of observations $y_1, \ldots, y_n$ sampled from an exponential family distribution[1] $f(y_i|\beta, \phi_i)$ with dispersion[2] parameter ϕ_i. In a generalized linear model, predictors and response are assumed to be related through a link function h,

$$\mu_i \equiv E(y_i|\beta, \phi_i) = h(\eta_i) \equiv h(x_i'\beta),$$

and the variance $Var(y_i|\beta, \phi_i) = \phi_i v(\mu_i)$ depends on a function $v(\mu_i)$ which is entirely determined by the choice of the particular exponential family. However, often the actual variance in the data is larger than the variance according to this strict mean-variance relationship. This effect is commonly called overdispersion, reasons for which might be, e.g., correlation in the data or important explanatory variables not included in the model. In order to account for additional unexplained variability of the individual observations, a random effect z_i with density $g(z)$ is in-

[1] In the present implementation, Gaussian, Poisson, Binomial, and Gamma distributed responses are supported

[2] For binomial and Poisson models, $\phi_i \equiv 1$. For Gaussian and Gamma models, the dispersion may be specified as constant, i.e., $\phi_i \equiv \phi$, or as depending on the observation i. The theory in this section is provided for the most general case, i.e., variable dispersion.

cluded into the linear predictor

$$\eta_i = x_i'\beta + z_i.$$

The likelihood can be approximated by a finite mixture

$$L = \prod_{i=1}^{n} \int f(y_i|z_i, \beta, \phi_i) g(z_i)\, dz_i \approx \prod_{i=1}^{n} \left\{ \sum_{k=1}^{K} f_{ik} \pi_k \right\},$$

where $f_{ik} = f(y_i|z_k, \beta, \phi_k)$, z_k are the mass points and π_k their masses. The score equations, obtained by setting the partial derivatives of the log-likelihood $\ell = \log L$ equal to zero,

$$\frac{\partial \ell}{\partial z_k} = 0, \quad \frac{\partial \ell}{\partial \beta} = 0, \quad \frac{\partial \ell}{\partial \phi_k} = 0,$$

turn out to be weighted versions of the single-distribution score equations, with weights $w_{ik} = \pi_k f_{ik} / \sum_l \pi_l f_{il}$.

The weights w_{ik} can be interpreted as posterior probabilities that the observation y_i comes from component k. The score equation for the mixture proportions,

$$\frac{\partial \ell - \lambda(\sum \pi_k - 1)}{\partial \pi_k} = 0,$$

gives the ML estimate $\hat{\pi}_k = \frac{1}{n} \sum_i w_{ik}$, which can be nicely interpreted as the average posterior probability for component k. The parameters β, z_k and π_k can now be simultaneously estimated by the EM algorithm, whereby the missing information is the component membership of the observations:

E-Step Adjust weights $w_{ik} = P(\text{obs. } i \text{ comes from comp. } k)$

M-Step Update parameter estimates fitting a weighted GLM with weights w_{ik}.

As starting values for the EM algorithm one uses Gauss-Hermite integration points and masses. The location of these starting points can be scaled inwards or outwards by means of a tuning parameter `tol`, which is by default set to 0.5.

This procedure, and its straightforward extension to random coefficient models, is implemented in the function `alldist`, while variance component models can be fitted with `allvc`; see Aitkin et al. (2005), pp 474ff and 485ff for details.

The function `alldist`

The main functions of this package are `alldist` and `allvc`, the names of which were adapted from the homonymous macros in GLIM4. The functions can be used in a similar manner to the R function `glm`.

As an example for `alldist`, we consider data from a study on lung cancer mortality presented in Tsutakawa (1985). The data were recorded in the 84 largest Missouri cities from 1972-1981 and give the number of lung cancer deaths of males aged 45-54 as well as the city sizes[3]. The data were analyzed by Tsutakawa (1985) and Aitkin (1996b), both authors considering logit models of type

$$\log \frac{p_i}{1 - p_i} = z_i,$$

where z_i is a random effect associated with the $i-$th city and p_i is its associated mortality rate. While Tsutakawa fitted a Poisson model with a normal random effect, Aitkin opted for a binomial model with an unspecified random effect distribution. We follow Aitkin and will leave the random effect unspecified, but as lung cancer death is a rather rare event (the crude rate does not exceed 0.03 in any of the cities), it seems natural to work with Poisson models. Hence, one can write $\log(p_i) = z_i$, or equivalently, in terms of the means $\mu_i = n_i p_i$,

$$\log(\mu_i) = \log(n_i) + z_i,$$

where the logarithm of the city sizes n_i appears as an offset. The two-point solution is then obtained via the function `alldist`, using the same notation as for a usual `glm` fit, except that the random term and the number of mass points `k=2` have also to be specified. The resulting object (which we name, say, `missouri.np2`) is of class '`glmmNPML`' and its printed output is given by

```
> print(missouri.np2)

Call:  alldist(formula = Deaths ~1, random =
 ~1, family = poisson(link = "log"), data =
 missouri, k = 2, offset = log(Size))

Coefficients:
 MASS1   MASS2
-4.844  -4.232

Mixture proportions:
    MASS1      MASS2
0.8461624  0.1538376
-2 log L:          355.3
```

One minor difference to a `glm` output is that the disparity ($-2 \log L$) is displayed instead of the deviance, but the latter one is immediately obtained via

```
> missouri.np2$dev
 [1] 92.49207,
```

which is slightly better than the deviance 93.10 reported in Aitkin (1996b) for the corresponding two-mass point binomial logit model fitted with GLIM4. As also observed by Aitkin, the disparity does not

[3] The data set `missouri` is part of this R package

fall significantly when increasing the number of mass points further.

Empirical Bayes predictions (generally, $h(x_i'\hat{\beta} + \hat{z}_i)$ for the number of deaths per city can be obtained by the use of `fitted(missouri.np2)`, or equivalently, `missouri.np2$fitted.values`, or equivalently, `predict(missouri.np2, type="response")`. Dividing this quantity by `missouri$Size`, one obtains estimated or 'shrunken' rates which can be compared to the 6th column in Table 4, Aitkin (1996b). The shrunken rates are less variable than the crude rates and hence are useful for small area estimation problems. The posterior probabilities w_{ik} can be obtained from the fitted model (in analogy to the 8th and 9th column of Table 4, Aitkin, 1996b), via the component `$post.prob`. Further, 'posterior intercepts' for the construction of 'league tables' are stored in component `$post.int` — see Sofroniou et al. (2006) for an example of their application.

Methods for most generic functions that are applied to fitted model objects, such as `update()`, `coefficients()`, `residuals()`, `fitted()`, `summary()`, `predict()` and `plot()`, have been defined for the `glmmNPML` class. In some cases (the first four generic functions listed above) the default method is used; in other cases (the last three generics) explicit methods are provided. The `plot()` function offers four different plots: (i) disparity vs. EM iterations; (ii) EM trajectories; (iii) Empirical Bayes predictions vs. true response; and (iv) posterior probabilities against the residuals of the fixed part of the GLM fit in the last EM iteration. Plots (i) and (ii) are generated by default when running `alldist` and are depicted in Fig. 1 for the model fitted above.

One observes that the EM trajectories converge essentially to the fixed part residuals of cities no. 4 and 84 (in Tsutakawa's list), which have populations of 54155 and 22514, respectively, being much larger than the majority of the other cities with only several hundreds of inhabitants (For the very interested, the numerical values associated with the disparity plot and the EM trajectories, as well as the residuals plotted vertically in the latter plot, are available in component `$Misc`).

This was a simple example without any covariates. In general an arbitrary number of fixed effects can be specified, and the random component can be an intercept (∼1) or a single variable giving a model with a random slope *and* random intercept.

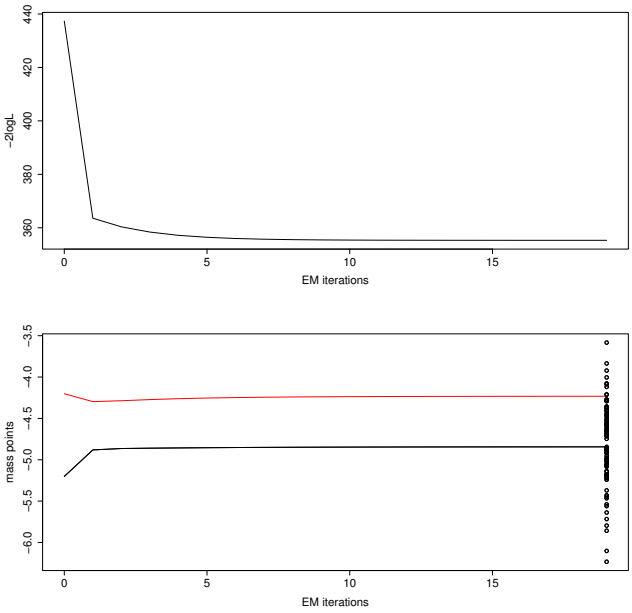

Figure 1: Top: Disparity ($-2\log L$) trend; bottom: EM trajectories. The vertical dots in the latter plot are the residuals of the fixed part of the fitted random effect model (Note that these residuals are not centered around 0, in contrast to the residuals of a simple fixed effect model. The plotted residuals, generally $h^{-1}(y_i) - x_i'\hat{\beta}$, represent the random effect distribution and are on the same scale as the mass points).

The function `allvc`

The function `alldist` is designed to fit simple overdispersion models (i.e., one has a random effect on the individual observations). However, often one wishes to introduces *shared* random effects, e.g. for students from the same class or school, for the same individual observed repeatedly over time (longitudinal data), or in small area estimation problems. This leads to variance component models, which can be fitted in **npmlreg** using the function `allvc`. As an example, let us consider the Oxford boys data from Brush and Harrison (1990), which were analyzed with NPML using GLIM4 by Aitkin et al. (2005).

The data set is part of the R package **nlme** (Pinheiro et al., 2005) and contains the heights of 26 boys, measured in Oxford on nine occasions over two years. The boys, indexed by the factor `Subject`, represent the upper level (primary sampling units, PSU), and the particular measurements at different time points correspond to the lower-level units (secondary sampling units, SSU).

As suggested by (Aitkin et al., 2005, p. 495), we fit a Gaussian model with unspecified random effect distribution and $K = 7$ mass points,

```
(Oxboys.np7 <- allvc(height ~ age, random =
~1|Subject, data = Oxboys, k=7))$disparity
[1] 1017.269
```

which confirms the GLIM4 result. Aitkin et al. state that for all models using $K > 7$ the fitted mass points 'are duplicated with the same total mass as in lower-dimension models', and hence consider this 7- mass point model as 'sufficiently complex'. However, fitting for comparison a simple linear mixed model with function `lmer` in package **lme4** (Bates and Sarkar, 2006)

```
(fm1 <- lmer(height ~ age + (1|Subject),
data = Oxboys, method = "ML"))
```

gives the `MLdeviance`, i.e., disparity, of 940.569. As this model is based on a normal random effect distribution, NPML should be superior to this, or at least competitive with it. Therefore, we went on fitting models with $K = 8$ and $K = 9$ mass points, yielding

```
 (Oxboys.np8 <- allvc(height ~ age, random =
 ~1|Subject, data = Oxboys, k=8))$disparity
 [1] 931.3752
(Oxboys.np9 <- allvc(height ~ age, random =
 ~1|Subject, data = Oxboys, k=9,
 tol=0.3))$disparity
 [1]  916.0921
```

For both models, all mass points are indeed distinct. For instance, for the 9-mass point model one has

```
       Estimate  Std. Error
age     6.523719 0.05094195
MASS1 130.200174 0.16795344
MASS2 138.416628 0.09697325
MASS3 143.382397 0.09697225
MASS4 147.350113 0.07511877
MASS5 150.954327 0.06857400
MASS6 153.869256 0.11915344
MASS7 156.178153 0.09676418
MASS8 159.521550 0.16795354
MASS9 164.883640 0.11876372
```

This increased performance compared to the GLIM code is due to the installation of a 'damping' mechanism in the first cycles of the EM algorithm; see Einbeck and Hinde (2006) for details.

Further increase of K does not yield major drops in disparity, so we continue to work with nine mass points, and extend the model by allowing the linear trend to vary across boys. The function call then takes the form

```
 (Oxboys.np9s <- allvc(height ~ age, random =
  ~age|Subject, data = Oxboys, k = 9,
  tol=0.3))
```

The difference in disparities is

```
> Oxboys.np9$disparity - Oxboys.np9s$disparity
[1] 102.1071
```

on

```
>  Oxboys.np9$df.res - Oxboys.np9s$df.res
[1] 8
```

degrees of freedom, showing clear heterogeneity in the slope.

Summary

We have introduced the R package **npmlreg**, which is in some parts a simple translation from the corresponding GLIM4 code, but, in other parts, contains substantial extensions and methodological improvements. In particular, we mention the possibility to fit Gamma models and to work with dispersion parameters varying smoothly over components, and, as already noted, the installation of a damping procedure. We note finally that for the sake of comparability all implemented features are also available for Gaussian Quadrature instead of NPML (leaving the z_k and π_k fixed and equal to Gauss-Hermite integration points and masses). The R package is available on CRAN. Future developments will include 3-level models and multicategory responses.

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Augmenting R with Unix Tools

Andrew Robinson

This article describes a small collection of Unix command-line tools that can be used to augment R. I introduce:

`make` which after judicious preparation will allow one-word execution of large-scale simulations, all the way from compilation of source code to construction of a PDF report;

`screen` which will permit remote monitoring of program execution progress with automatic protection against disconnection; and

`mail` which will allow automatic alerting under error conditions or script completion.

These programs will be part of the default installations of many flavours of Unix-like operating systems. Although these tools have many different applications, each is very useful for running R remotely on a Unix-like operating system, which is the focus of their usage in this article.

Regardless of what kind of computer is on your own desk, you may find these tools useful; they do not require you to be running a BSD or GNU/Linux on your own machine.

R and `screen`

It is sometimes necessary to run R code that executes for long periods of time upon remote machines. This requirement may be because the local computing resources are too slow, too unstable, or have insufficient memory.

For example, I have recently completed some simulations that took more than a month on a reasonably fast cluster of Linux computers. I developed, trialed, and profiled my code on my local, not-particularly-fast, computer. I then copied the scripts and data to a more powerful machine provided by my employer and ran the simulations on R remotely on that machine. To get easy access to the simulations whilst they ran, I used `screen`.

`screen` is a so-called terminal multiplexor, which allows us to create, shuffle, share, and suspend command line sessions within one window. It provides protection against disconnections and the flexibility to retrieve command line sessions remotely. `screen` is particularly useful for R sessions that are running on a remote machine.

We might use the following steps to invoke R within `screen`:

1. log in remotely via secure shell,

2. start `screen`,
3. start R,
4. `source` our script with `echo=TRUE`,
5. detach the screen session, using `Ctrl-a d`, and
6. log out.

The R session continues working in the background, contained within the `screen` session. If we want to revisit the session to check its progress, then we

1. log in remotely via secure shell,
2. start `screen -r`, which recalls the unattached session,
3. examine the saved buffer; scrolling around, copying and pasting as necessary,
4. detach the screen session, using `Ctrl-a d`, and
5. log out.

This approach works best if examining the buffer is informative, which requires that the R script be written to provide readable output or flag its progress every so often. I find that the modest decrease in speed of looping is more than compensated by a cheerful periodic reminder, say every 1000^{th} iteration, that everything is still working and that there are only n iterations left to run. I have also been experimenting with various algorithms for R to use the elapsed time, the elapsed number of simulations, and the number of simulations remaining, to estimate the amount of time left until the run is complete.

`screen` offers other advantages. You can manage several screens in one window, so editing a script remotely using, say, `emacs`, and then sourcing the script in the remote R session in another screen, is quick and easy. If you lose your connection, the session is kept alive in the background, and can be re-attached, using `screen -r` as above. If you have forgotten to detach your session you can do so forcibly from another login session, using `screen -dr`. You can change the default history/scrollback buffer length, and navigate the buffer using intuitive keystrokes. Finally, you can share a `screen` session with other people who are logged in to the same machine. That is, each user can type and see what the other is typing, so a primitive form of online collaboration is possible.

So, running an R session in `screen` provides a simple and robust way to allow repeated access to a simulation or a process.

More information about `screen` can be found from `http://www.gnu.org/software/screen/`, or `man screen`.

R and `mail`

It is very useful to be able to monitor an R session that is running remotely. However, it would also be useful if the session could alert us when the script has completed, or when it has stopped for some reason, including some pre-determined error conditions. We can use `mail` for this purpose, if the computer is running an appropriate mail server, such as `sendmail`.

`mail` is an old email program, small enough to be included by default on most Unix-like systems, and featureless enough to be almost universally ignored by users in favour of other programs, such as `mutt`, or those with shiny graphical user interfaces. However, `mail` does allow us to send email from the command line. And, R can do pretty much anything that can be done from the command line[1]. Of course, a small amount of fiddling is necessary to make it work. A simple function will help[2]. This function will fail if any of the arguments contain single or double quotes. So, craft your message carefully.

```
mail <- function(address, subject, message) {
  system(paste("echo '", message,
  "' | mail -s '", subject,
  "' ", address, sep=""))
}
```

We can now send mail from R via, for example,

```
mail("andrewr", "Test", "Hello world!")
```

You can place calls to this function in strategic locations within your script. I call it at the end of the script to let me know that the simulations are finished, and I can collect the results at my leisure. In order to have R let us know when it has stopped, we can use a function like this:

```
alert <- function() {
      mail("andrewr", "Stopped", "Problem")
      browser()
}
```

then in our script we call

```
options(error = alert)
```

Now in case of an error, R will send an email and drop into the browser, to allow detailed follow-up. If you have more than one machine running, then calling `hostname` via `system`, and pasting that into the subject line, can be helpful.

Alternatively, you can use `mutt` with exactly the same command line structure as `mail`, if `mutt` is installed on your system. An advantage of `mutt` is that it uses the MIME protocol for binary attachments. That would enable you to, say, attach to your email the PDF that your script has just created with `Sweave` and `pdflatex`, or the *cvs* file that your script creates,

[1] In theory, it can do everything, I suppose. I haven't tried.
[2] Caveat: this function is written to work on bash version 3.1.17. Your mileage may vary.

or even the relevant objects saved from the session, neatly packaged and compressed in a `*.RData` object.

Different flavours of Unix `mail` are available. You can find out more about yours by `man mail`.

R and `make`

I have recently been working on bootstrap tests of a model-fitting program that uses maximum likelihood to fit models with multivariate normal and t distributions. The program is distributed in FORTRAN, and it has to be compiled every time that it is run with a new model. I wanted to use a studentized bootstrap for interval estimates, gather up all the output, and construct some useful tables and graphics.

So, I need to juggle FORTRAN files, FORTRAN executables, R source files, Sweave files, PDFs, and so on. R does a great job preparing the input files, calling the executable (using `system()`), and scooping up the output files. However, to keep everything in sync, I use `make`.

Although it is commonly associated with building executable programs, `make` can control the conversion of pretty much any file type into pretty much any other kind of file type. For example, `make` can be told how to convert a FORTRAN source file to an executable, and it will do so if and when the source file changes. It can be told how and when to run an R source file, and then how and when to call Sweave upon an existing file, and then how and when to create a PDF from the resulting LaTeX file.

The other advantage that `make` offers is splitting large projects into chunks. I use Sweave to bind my documentation and analysis tightly together. However, maintaining the link between documentation and analysis can be time-consuming. For example, when documenting a large-scale simulation, I would rather not run the simulation every time I correct a spelling mistake.

One option is to tweak the number of runs. `make` provides a flexible infrastructure for testing code, as we can pass parameters, such as the number of runs to perform, to R. For example, with an appropriate Makefile, typing `make test` at the operating system prompt will run the entire project with only 20 simulations, whereas typing `make` will run the project with 2000 simulations.

Another option is to split the project into two parts: the simulation, and the analysis, and run only the second, unless important elements change in the first. Again, this sort of arrangement can be constructed quite easily using `make`.

For example, I have an R source file called `sim.r` that controls the simulations and produces a .RData object called `output.RData`. The content is:

```
randoms <- runif(reps)
save.image("output.RData")
```

I also have a Sweave file called `report.rnw` which provides summary statistics (and graphics, not included here) for the runs. The content is:

```
\documentclass{article}
\begin{document}
<<>>=
load("output.RData")
@
We performed \Sexpr{reps} simulations.
\end{document}
```

The latter file often requires tweaking, depending on the output. So, I want to separate the simulations and the report writing, and only run the simulations if I absolutely have to. Figure 1 is an example Makefile that takes advantage of both options noted above. All the files referenced here are assumed to be held in the same directory as the Makefile, but of course they could be contained in subdirectories, which is generally a neater strategy.

I do not actually need `make` to do these tasks, but it does simplify the operation a great deal. One advantage is that `make` provides conditional execution without me needing to fiddle around to see what has and has not changed. If I now edit `report.rnw`, and type `make`, it won't rerun the simulation, it will just recompile `report.rnw`. On the other hand, if I make a change to `sim.r`, or even run `sim.r` again (thus updating the `.RData` object), `make` will rerun everything. That doesn't seem very significant here, but it can be when you're working on a report with numerous different branches of analysis.

The other advantage (which my Makefile doesn't currently use) is that it provides wildcard matching. So, if I have a bunch of Sweave files (one for each chapter, say) and I change only one of them, then `make` will identify which one has changed and which ones depend on that change, and recompile only those that are needed. But I don't have to produce a separate line in the Makefile for each file.

Also, the Makefile provides implicit documentation for the flow of operations, so if I need to pass the project on to someone else, all they need to do is call `make` to get going.

More information on `make` can be found from `http://www.gnu.org/software/make/`.

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```
## Hashes indicate comments.  Use these for documentation.
## Makefiles are most easily read from the bottom up, the first time!

# 'make' is automatically interpreted as 'make report.pdf'.

# Update report.pdf whenever report.tex changes, by running this code.

report.pdf : report.tex
        ( \
        \pdflatex report.tex; \
        while \grep -q "Rerun to get cross-references right." report.log;\
        do \
                \pdflatex report.tex; \
        done \
        )

# Update report.tex whenever report.rnw *or* output.RData changes,
# by running this code.

report.tex : report.rnw output.RData
        echo "Sweave(\"report.rnw\")" | R --no-save --no-restore

# Update output.RData whenever sim.r changes, by running this code.

output.RData : sim.r
        echo "reps <- 2000; source(\"sim.r\")" | R --no-save --no-restore

#########################################################################

## The following section tells make how to respond to specific keywords.

.PHONY: test full neat clean

# 'make test' cleans up, runs a small number of simulations,
# and then constructs a report

test:
        make clean;
        echo "reps <- 10; source(\"sim.r\")" | R --no-save --no-restore;
        make

# 'make full' cleans up and runs the whole project from scratch

full :
        make clean;
        make

# 'make neat' cleans up temporary files - useful for archiving

neat :
        rm -fr *.txt *.core fort.3 *~ *.aux *.log *.ps *.out

# 'make clean' cleans up all created files.

clean :
        rm -fr *.core fort.3 *~ *.exe *.tex *.txt *.lof *.lot *.tex \
                *.RData *.ps *.pdf *.aux *.log *.out *.toc *.eps
```

Figure 1: The contents of a Makefile. Note that all the indenting is done by means of tab characters, not spaces. This Makefile has been tested for both GNU make and BSD make.

POT: Modelling Peaks Over a Threshold

by Mathieu Ribatet

The Generalised Pareto Distribution (**GPD**) is the limiting distribution of normalised excesses over a threshold, as the threshold approaches the endpoint of the variable (Pickands, 1975). The **POT** package contains useful tools to perform statistical analysis for peaks over a threshold using the GPD approximation.

There is many packages devoted to the extreme value theory (**evd**, **ismev**, **evir**, ...); however, the **POT** package is specialised in peaks over threshold analysis. Moreover, this is currently the only one which proposes many estimators for the GPD. A user's guide (as a package vignette) and two demos are also included in the package.

Asymptotic Approximation

Let $X_1, \ldots, X_n$ be a series of *i.id.* random variables with common distribution function F. Let $M_n = \max\{X_1, \ldots, X_n\}$. Suppose there exists constants $a_n > 0$ and b_n such that:

$$\mathbb{P}\left[\frac{M_n - b_n}{a_n} \leq z\right] \longrightarrow G(z), \quad n \to +\infty$$

for $z \in \mathbb{R}$ and where G is a non degenerate distribution function. Then, for $i = 1, \ldots, n$, we have:

$$\mathbb{P}\left[X_i \leq z | X_i > u\right] \longrightarrow H(z), \quad u \to u_{\text{end}} \qquad (1)$$

with

$$H(y) = 1 - \left(1 + \xi\frac{y-\mu}{\sigma}\right)_+^{-1/\xi},$$

where (μ, σ, ξ) are the location, scale and shape parameters respectively, $\sigma > 0$ and $z_+ = \max(z, 0)$ and u_{end} is the right end-point of the variable X_i.

It is usual to fit the GPD to excesses over a (high enough) threshold. Thus we suppose that the asymptotic result given by equation (1) is (approximately) true for the threshold of interest.

Application: Ardières River at Beaujeu

The `ardieres` data frame containing flood discharges (in $m^3 \cdot s^{-1}$) over a period of 33 years of the Ardières river at Beaujeau (FRANCE) is included in the package. There are `NA` values in year 1994 as a flood event damaged record instrumentation. We use this dataset as an example for a typical univariate analysis. First, we have to "extract" independent events from the time series and select a suitable threshold such that asymptotic approximation in equation (1) is good enough.

```
library("POT")
data("ardieres")
tmp <- clust(ardieres, 0.85, tim.cond = 7/365,
             clust.max = TRUE)
par(mfrow=c(2,2))
mrlplot(tmp["obs"], xlim = c(0.85, 17))
diplot(tmp, u.range = c(0.85, 17))
tcplot(tmp["obs"], u.range = c(0.85, 17))
```

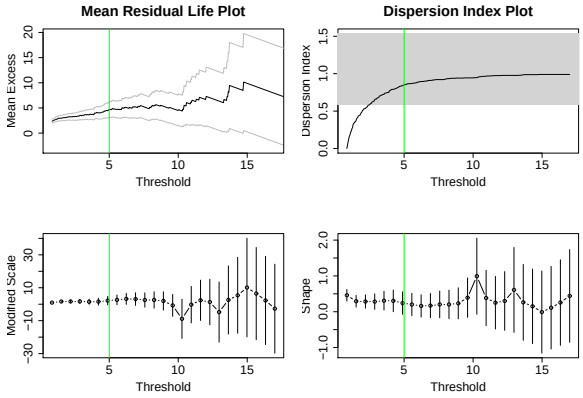

Figure 1: Tools for the threshold selection

The threshold selection stage is a compromise between bias and variance. On one hand, if a too high threshold is selected, the bias decreases as the asymptotic approximation in equation (1) is good enough while the variance increases as there is not enough data above this threshold. On the other hand, by taking a lower threshold, the variance decreases as the number of observations is larger and the bias increases as the asymptotic approximation becomes poorer.

According to Fig. 1, a threshold around five $m^3 \cdot s^{-1}$ should be a "good compromise". Indeed, the mean residual life plot is "linear" on the range $(5, 7)$; for thresholds greater than 5, the dispersion index estimates are "near" the theoretical value 1; and both modified scale and shape estimates seem to be constant on the range $(5, 9)$. Thus, we select only independent values above this threshold by invoking:

```
events <- clust(ardieres, u = 5,
    tim.cond = 7/365, clust.max = TRUE)
```

We can fit the GPD to those excesses according several estimators by setting the `method` option. There is currently 7 estimators: Moments `"moments"`, Unbiased and Biased Probability Weighted Moments `"pwmu"`, `"pwmb"`, Minimum Density Power Divergence `"mdpd"`, medians `"med"`, Pickands `"pickands"`

and Maximum Likelihood (the default) `"mle"` estimators. References for these estimators can be found in (Pickands, 1975; Hosking and Wallis, 1987; Coles, 2001; Peng and Welsh, 2001) and (Juárez and Schucany, 2004). For example, if we want to fit the GPD using the unbiased probability weighted moment estimator:

```
obs <- events[,"obs"]
pwmu <- fitgpd(obs, thresh = 5, "pwmu")
```

Here is the scale and shape parameter estimates of the GPD for the 7 estimators implemented.

```
       scale     shape
mle 2.735991 0.2779359
mom 2.840792 0.2465661
pwmu 2.668368 0.2922964
pwmb 2.704665 0.2826697
mdpd 2.709254 0.2915759
med 2.135882 0.8939585
pick 2.328240 0.6648158
```

By invoking:

```
par(mfrow=c(2,2))
plot(pwmu, npy=2.63)
```

we obtain Fig. 2 which depicts graphic tools for model diagnostic. Profile likelihood confidence intervals can also be computed, even for return levels see Fig. 3, with:

```
gpd.pfrl(mle, 0.995, range = c(20, 120),
         conf = 0.95)
```

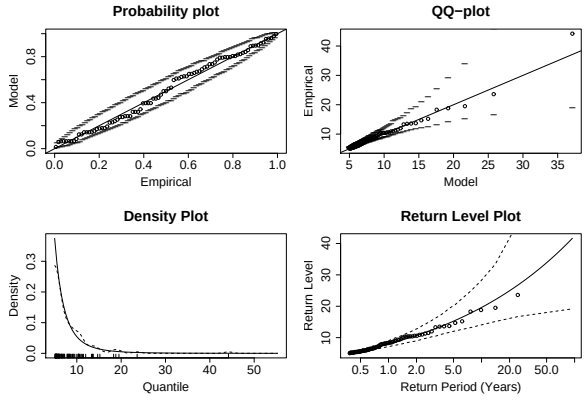

Figure 2: Graphic tools for model diagnostic.

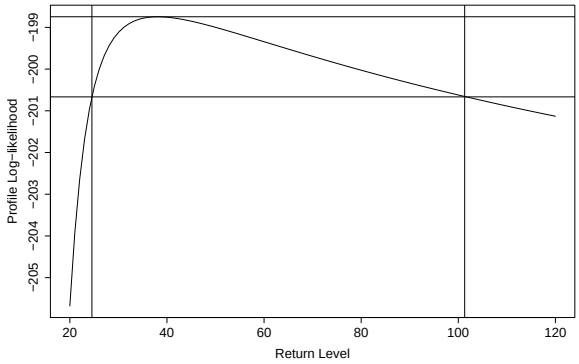

Figure 3: 95% profile confidence interval for the return level associated to non exceedance probability 0.995.

Miscellaneous Features

The **POT** package can also:

- simulate and compute density, quantile and distribution functions for the GPD;
- fit the GPD with a varying threshold using MLE;
- fit the GPD with held fixed parameters using MLE;
- perform analysis of variance for two nested models;
- estimate the extremal index using two estimators;
- display a L-Moment plot (Hosking and Wallis, 1997);
- compute sample L-moments;
- convert non exceedance probabilities to return periods and vice-versa;
- compute "averaged" time series using an average mobile window.

Currently, most of the package developments are devoted to bivariate peaks over threshold. For this purpose, the **POT** package can also:

- fit a bivariate GPD using 6 parametric dependence functions;
- fit a first order Markov chain with a fixed extreme value dependence structure to all threshold exceedances;
- simulate first order Markov chains with a fixed extreme value dependence structure;
- plot the Pickands' dependence and the spectral density functions.

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Backtests

by Kyle Campbell, Jeff Enos, Daniel Gerlanc and David Kane

Introduction

The **backtest** package provides facilities for exploring portfolio-based conjectures about financial instruments (stocks, bonds, swaps, options, et cetera). For example, consider a claim that stocks for which analysts are raising their earnings estimates perform better than stocks for which analysts are lowering estimates. We want to examine if, on average, stocks with raised estimates have higher future returns than stocks with lowered estimates and whether this is true over various time horizons and across different categories of stocks. Colloquially, "backtest" is the term used in finance for such tests.

Background

To demonstrate the capabilities of the **backtest** package we will consider a series of examples based on a single real-world data set. StarMine[1] is a San Fransisco research company which creates quantitative equity models for stock selection. According to the company:

> StarMine Indicator is a 1-100 percentile ranking of stocks that is predictive of future analyst revisions. StarMine Indicator improves upon basic earnings revisions models by:
>
> - Explicitly considering management guidance.
> - Incorporating SmartEstimates, StarMine's superior estimates constructed by putting more weight on the most accurate analysts.
> - Using a longer-term (forward 12-month) forecast horizon (in addition to the current quarter).
>
> StarMine Indicator is positively correlated to future stock price movements. Top-decile stocks have annually outperformed bottom-decile stocks by 27 percentage points over the past ten years across all global regions.

These ranks and other attributes of stocks are in the `starmine` data frame, available as part of the **backtest** package.

```
> data("starmine")
> names(starmine)

 [1] "date"       "id"         "name"
 [4] "country"    "sector"     "cap.usd"
 [7] "size"       "smi"        "fwd.ret.1m"
[10] "fwd.ret.6m"
```

`starmine` contains selected attributes such as sector, market capitalisation, country, and various measures of return for a universe of approximately 6,000 securities. The data is on a monthly frequency from January, 1995 through November, 1995. The number of observations varies over time from a low of 4,528 in February to a high of 5,194 in November.

```
      date count
1995-01-31  4593
1995-02-28  4528
1995-03-31  4569
1995-04-30  4708
1995-05-31  4724
1995-06-30  4748
1995-07-31  4878
1995-08-31  5092
1995-09-30  5185
1995-10-31  5109
1995-11-30  5194
```

[1] See www.starmine.com for details.

The smi column contains the StarMine Indicator score for each security and date if available. Here is a sample of rows and columns from the data frame:

```
      date          name fwd.ret.1m fwd.ret.6m smi
1995-01-31   Lojack Corp       0.09        0.8  96
1995-02-28  Raymond Corp       0.05        0.1  85
1995-02-28   Lojack Corp       0.08        0.7  90
1995-03-31   Lojack Corp       0.15        1.0  49
1995-08-31 Supercuts Inc      -0.11       -0.5  57
1995-10-31   Lojack Corp      -0.40       -0.2  22
1995-11-30   Lojack Corp       0.20        0.4  51
```

Most securities (like LoJack above) have multiple entries in the data frame, each for a different date. The row for Supercuts indicates that, as of the close of business on August 31, 1995, its smi was 57. During the month of September, its return (i.e., fwd.ret.1m) was -11%.

A simple backtest

Backtests are run by calling the function backtest to produce an object of class backtest.

```
> bt <- backtest(starmine, in.var = "smi",
+     ret.var = "fwd.ret.1m")
```

starmine is a data frame containing all the information necessary to conduct the backtest. in.var and ret.var identify the columns containing the input and return variables, respectively. backtest splits observations into 5 (the default) quantiles, or "buckets," based on the value of in.var. Lower (higher) buckets contain smaller (larger) values of in.var. Each quantile contains an approximately equal number of observations. This backtest creates quantiles according to values in the smi column of starmine.

```
  [1,21]  (21,40]  (40,59]  (59,82] (82,100]
    6765     6885     6642     6600     6496
```

backtest calculates the average return within each bucket. From these averages we calculate the spread, or the difference between the average return of the highest and lowest buckets.

Calling summary on the resulting object of class backtest reports the in.var, ret.var, and by.var used. We will use a by.var in later backtests.

```
> summary(bt)

Backtest conducted with:

1 in.var: smi;
1 ret.var: fwd.ret.1m;
and no by.var.

         low     2     3    4  high spread
pooled 0.011 0.013 0.016 0.02 0.032  0.021
```

This backtest is an example of a *pooled* backtest. In such a backtest, we assume that all observations are exchangeable. This means that a quantile may contain observations for any stock and from any date. Quantiles may contain multiple observations for the same stock.

The backtest summary shows that the average return for the highest bucket was 3.2%. This value is the mean one month forward return of stocks with smi values in the highest quantile. As the observations are exchangeable, we use every observation in the starmine data frame with a non-missing smi value. This means that the returns for LoJack from both 1995-01-31 and 1995-02-28 would contribute to the 3.2% mean of the high bucket.

The backtest suggests that StarMine's model predicted performance reasonably well. On average, stocks in the highest quantile returned 3.2% while stocks in the lowest quantile returned 1.1%. The spread of 2.1% suggests that stocks with high ratings perform better than stocks with low ratings.

Natural backtests

A *natural* backtest requires that the frequency of returns and observations be the same.

A natural backtest approximates the following implementation methodology: in the first period form an equal weighted portfolio with long positions in the stocks in the highest quantile and short positions in the stocks in the lowest quantile. Each stock has an equal weight in the portfolio; if there are 5 stocks on the long side, each stock has a weight of 20%. Subsequently rebalance the portfolio every time the in.var values change. If the observations have a monthly frequency, the in.var values change monthly and the portfolio must be rebalanced accordingly. When the in.var values change, rebalancing has the effect of exiting positions that have left the top and bottom quantiles and entering positions that have entered the top and bottom quantiles. If the data contains monthly observations, we will form 12 portfolios per year.

To create a simple natural backtest, we again call backtest using fwd.ret.1m. This is the only return value in starmine for which we can construct a natural backtest of smi.

```
> bt <- backtest(starmine, id.var = "id",
+     date.var = "date", in.var = "smi",
+     ret.var = "fwd.ret.1m", natural = TRUE)
```

Natural backtests require a date.var and id.var, the names of the columns in the data frame containing the dates of the observations and unique security identifiers, respectively. Calling summary displays the results of the backtest:

```
> summary(bt)
```

```
Backtest conducted with:

1 in.var: smi;
1 ret.var: fwd.ret.1m;
and no by.var.

              low      2      3       4   high spread
1995-01-31  0.003  0.011  0.003 -0.0001  0.019  0.016
1995-02-28 -0.008 -0.003  0.003  0.0072  0.013  0.021
1995-03-31  0.029  0.017  0.013  0.0225  0.037  0.008
1995-04-30 -0.002 -0.003  0.002 -0.0054  0.005  0.007
1995-05-31  0.010  0.013  0.019  0.0228  0.044  0.034
1995-06-30  0.072  0.059  0.057  0.0708  0.101  0.030
1995-07-31  0.033  0.030  0.034  0.0323  0.052  0.018
1995-08-31 -0.004  0.006  0.017  0.0119  0.024  0.028
1995-09-30 -0.055 -0.030 -0.031 -0.0219 -0.014  0.041
1995-10-31  0.030  0.032  0.040  0.0430  0.038  0.008
1995-11-30  0.013  0.016  0.021  0.0294  0.037  0.024
MEAN        0.011  0.014  0.016  0.0193  0.032  0.021

average turnover: 0.5
mean spread: 0.02
sd spread: 0.01
raw sharpe ratio: 2
```

Focus on the mean return of the highest quantile for 1995-02-28 of 1.3%. `backtest` calculated this value by first computing the 5 quantiles of the input variable `smi` over all observations in `starmine`. Among the observations that fall into the highest quantile, those with date 1995-02-28 contribute to the mean return of 1.3%. It is important to note that the input variable quantiles are computed over the whole dataset, as opposed to within each category that may be defined by a `date.var` or `by.var`.

The bottom row of the table contains the mean quantile return over all dates. On account of the way we calculate quantile means, a single stock will have more effect on the quantile mean if during that month there are fewer stocks in the quantile. Suppose that during January there are only 2 stocks in the low quantile. The return of a single stock in January will account for $\frac{1}{22}$ of the quantile mean. This is different than a pooled backtest where every observation within a quantile has the same weight. In a natural backtest, the weight of a single observation depends on the number of observations for that period.

Calling `summary` yields information beyond that offered by the `summary` method of a pooled backtest. The first piece of extra information is average turnover. Turnover is the percentage of the portfolio we would have to change each month if we implemented the backtest as a trading strategy. For example, covering all the shorts and shorting new stocks would yield a turnover of 50% because we changed half the portfolio. We trade stocks when they enter or exit the extreme quantiles due to `in.var` changes. On average, we would turn over 50% of this portfolio each month.

The second piece of extra information is mean spread. The spread was positive each month, so on average the stocks with the highest `smi` values outperformed the stocks with the lowest `smi` values. On average, stocks in the highest quantile outperformed stocks in the lowest quantile by 2%. The third piece of extra information, the standard deviation of spread, is 1%. The spread varied from month to month, ranging from a low of close to 0% to a high of over 4%.

We define the fourth piece of extra information, raw (non-annualized) Sharpe ratio, as $\frac{\text{return}}{\text{risk}}$. We set return equal to mean spread return and use the standard deviation of spread return as a measure of risk.

More than one `in.var`

`backtest` allows for more than one `in.var` to be tested simultaneously. Besides using `smi`, we will test market capitalisation in dollars, `cap.usd`. This is largely a nonsense variable since we do not expect large cap stocks to outperform small cap stocks — if anything, the reverse is true historically.

```
> bt <- backtest(starmine, id.var = "id",
+     date.var = "date", in.var = c("smi",
+         "cap.usd"), ret.var = "fwd.ret.1m",
+     natural = TRUE)
```

Because more than one `in.var` was specified, only the spread returns for each `in.var` are displayed, along with the summary statistics for each variable.

```
> summary(bt)

Backtest conducted with:

2 in.vars: smi, cap.usd;
1 ret.var: fwd.ret.1m;
and no by.var.

              smi cap.usd
1995-01-31 0.016 -0.0138
1995-02-28 0.021  0.0017
1995-03-31 0.008 -0.0023
1995-04-30 0.007 -0.0052
1995-05-31 0.034 -0.0568
1995-06-30 0.030 -0.0143
1995-07-31 0.018 -0.0008
1995-08-31 0.028  0.0051
1995-09-30 0.041  0.0321
1995-10-31 0.008  0.0127
1995-11-30 0.024  0.0029

summary stats for in.var = smi:
average turnover: 0.5
mean spread: 0.02
sd spread: 0.01
raw sharpe ratio: 2

summary stats for in.var = cap.usd:
average turnover: 0.1
mean spread: -0.004
sd spread: 0.02
raw sharpe ratio: -0.2
```

Viewing the results for the two input variables side-by-side allows us to compare their performance easily. As we expected, `cap.usd` as an input variable did not perform as well as `smi` over our backtest period. While `smi` had a positive return during each month, `cap.usd` had a negative return in 6 months and a negative mean spread. In addition, the spread returns for `cap.usd` were twice as volatile as those of `smi`.

There are several plotting facilities available in `backtest` that can help illustrate the difference in performance between these two signals. These plots can be made from a natural backtest with any number of input variables. Below is a bar chart of the monthly returns of the two signals together:

```
> plot(bt, type = "return")
```

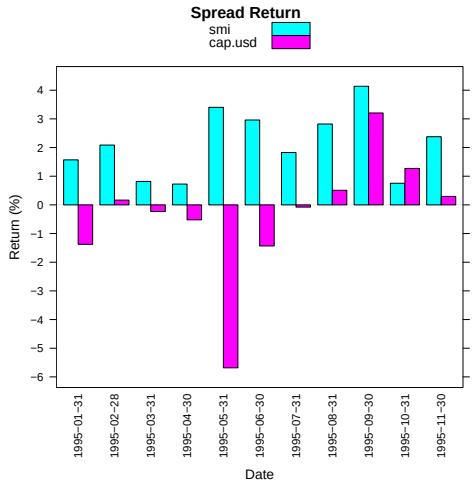

Figure 1: Monthly return spreads.

Returns for `smi` were consistently positive. Returns for `cap.usd` were of low quality, but improved later in the period. `cap.usd` had a particularly poor return in June. We can also plot cumulative returns for each input variable as shown in Figure 2.

The top region in this plot shows the cumulative return of each signal on the same return scale, and displays the total return and worst drawdown of the entire backtest period. The bottom region shows the cumulative return of the individual quantiles over time. We can see that `smi`'s top quantile performed best and lowest quantile performed worst. In contrast, `cap.usd`'s lowest quantile was its best performing.

Though it is clear from the summary above that `smi` generated about 5 times as much turnover as `cap.usd`, a plot is available to show the month-by-month turnover of each signal, see Figure 3. This chart shows that the turnover of `smi` was consistently around 50% with lower turnover in September and October, while the turnover of `cap.usd` was consistently around 10%.

```
> plot(bt.save, type = "cumreturn.split")
```

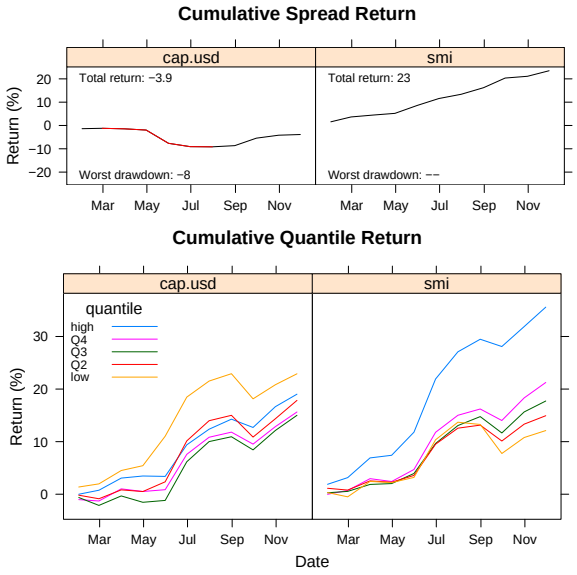

Figure 2: Cumulative spread and quantile returns.

```
> plot(bt, type = "turnover")
```

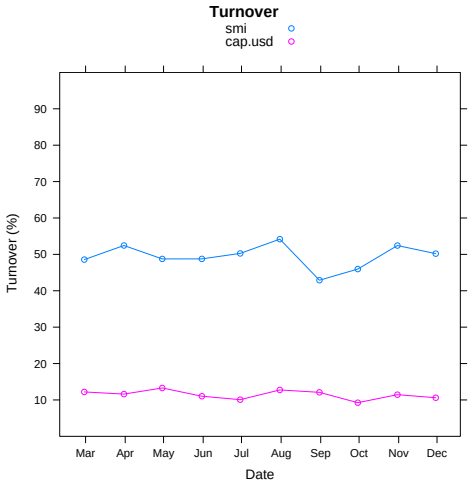

Figure 3: Monthly turnover.

Using `by.var`

In another type of backtest we can look at quantile spread returns *by* another variable. Specifying `by.var` breaks up quantile returns into categories defined by the levels of the `by.var` column in the input data frame. Consider a backtest of `smi` by `sector`:

```
> bt <- backtest(starmine, in.var = "smi",
+      ret.var = "fwd.ret.1m",
+      by.var = "sector")

> summary(bt)

Backtest conducted with:
```

```
1 in.var: smi;
1 ret.var: fwd.ret.1m;
and by.var: sector.

         low     2     3     4 high spread
Durbl 0.0063 0.007 0.009 0.007 0.01  0.004
Enrgy 0.0152 0.014 0.017 0.019 0.04  0.024
HiTec 0.0237 0.016 0.026 0.029 0.05  0.024
Hlth  0.0395 0.036 0.021 0.038 0.05  0.006
Manuf 0.0005 0.005 0.014 0.009 0.02  0.022
Money 0.0190 0.024 0.021 0.026 0.04  0.017
NoDur 0.0036 0.010 0.010 0.019 0.03  0.025
Other 0.0045 0.006 0.015 0.017 0.02  0.017
Shops 0.0020 0.004 0.005 0.017 0.03  0.026
Telcm 0.0277 0.014 0.022 0.023 0.03  0.005
Utils 0.0128 0.021 0.013 0.016 0.02  0.007
```

This backtest categorises observations by the quantiles of `smi` and the levels of `sector`. The highest spread return of 2.6% occurs in `Shops`. Since `smi` quantiles were computed before the observations were split into groups by `sector`, however, we can not be sure how much confidence to place in this result. There could be very few observations in this sector or one of the top and bottom quantiles could have a disproportionate number of observations, thereby making the return calculation suspect. `counts` provides a simple check.

```
> counts(bt)

$smi
       low    2    3    4 high
Durbl  348  349  261  231  223
Enrgy  246  250  158  130   64
HiTec  647  660  824 1004 1432
Hlth   380  377  410  464  424
Manuf 1246 1265 1279 1395 1576
Money  959 1265 1244 1095  875
NoDur  615  563  528  441  371
Other 1034  940  784  760  710
Shops  870  714  710  697  548
Telcm  186  177  140  129   95
Utils  152  245  252  198  130
```

While there seems to be an adequate number of observations in `Shops`, it is important to note that there are approximately 60% more observations contributing to the mean return of the lowest quantile than to the mean return of the highest quantile, 870 versus 548. Overall, we should be more confident in results for `Manuf` and `Money` due to their larger sample sizes. We might want to examine the result for `HiTec` more closely, however, since there are more than twice the number of observations in the highest quantile than the lowest.

`by.var` can also be numeric, as in this backtest using `cap.usd`:

```
> bt <- backtest(starmine,
+     in.var = "smi", ret.var = "fwd.ret.1m",
+     by.var = "cap.usd",
+     buckets = c(5, 10))

> summary(bt)

Backtest conducted with:

1 in.var: smi;
1 ret.var: fwd.ret.1m;
and by.var: cap.usd.

        low      2      3     4  high spread
low  0.0105 0.0139 0.0236 0.028 0.038  0.028
2    0.0078 0.0093 0.0216 0.025 0.046  0.038
3    0.0186 0.0072 0.0167 0.031 0.034  0.016
4    0.0124 0.0142 0.0139 0.013 0.038  0.026
5    0.0080 0.0124 0.0087 0.010 0.025  0.017
6    0.0126 0.0121 0.0191 0.021 0.026  0.013
7    0.0080 0.0070 0.0160 0.019 0.034  0.026
8    0.0050 0.0181 0.0101 0.014 0.027  0.022
9    0.0104 0.0153 0.0167 0.014 0.028  0.018
high 0.0156 0.0207 0.0133 0.023 0.026  0.011
```

Since `cap.usd` is numeric, the observations are now split by two sets of quantiles. Those listed across the top are, as before, the input variable quantiles of `smi`. The row names are the quantiles of `cap.usd`. The `buckets` parameter of `backtest` controls the number of quantiles. The higher returns in the lower quantiles of `cap.usd` suggests that `smi` performs better in small cap stocks than in large cap stocks.

Multiple return horizons

Using `backtest` we can also analyse the performance of a signal relative to multiple return horizons. Below is a backtest that considers one month and six month forward returns together:

```
> bt <- backtest(starmine, in.var = "smi",
+     buckets = 4, ret.var = c("fwd.ret.1m",
+         "fwd.ret.6m"))

> summary(bt)

Backtest conducted with:

1 in.var: smi;
2 ret.vars: fwd.ret.1m, fwd.ret.6m;
and no by.var.

             low     2     3 high spread
fwd.ret.1m 0.011 0.015 0.018 0.03  0.019
fwd.ret.6m 0.112 0.121 0.142 0.17  0.059
```

The performance of `smi` over these two return horizons tells us that the power of the signal degrades after the first month. Using six month forward return, `fwd.ret.6m`, the spread is 6%. This is only 3 times larger than the 2% spread return in the first month despite covering a period which is 6 times longer. In other words, the model produces 2% spread returns in the first month but only 4% in the 5 months which follow.

Conclusion

The **backtest** package provides a simple collection of tools for performing portfolio-based tests of financial conjectures. A much more complex package, **portfolioSim**, provides facilities for historical portfolio performance analysis using more realistic assumptions. Built on the framework of the **portfolio**[2] package, **portfolioSim** tackles the issues of risk exposures and liquidity constraints, as well as arbitrary portfolio construction and trading rules. Above all, the flexibility of R itself allows users to extend and modify these packages to suit their own needs. Before reaching that level of complexity, however, **backtest** provides a good starting point for testing a new conjecture.

Bibliography

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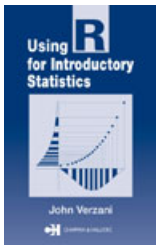
Review of John Verzani's Book Using R for Introductory Statistics

Andy Liaw



To the best of my knowledge, this book is the first of its kind: a *standalone* introductory statistics textbook that integrates R throughout. The advantages should be obvious: Students would not need to purchase a supplement that covers the software, in addition to the main textbook (although the author states in the Preface that the book should also be useful as an accompaniment for a standard introductory text). That the software is freely available is a big bonus. Moreover, the book covers basic descriptive statistics before any probability models are mentioned. For students that are less mathematically inclined, this should make materials easier to absorb. (The author states in the Preface that the book aims at classes that are based on pre-calculus skills.)

The book contains 12 chapters. The first four chapters of the book cover descriptive statistics, both numerical and graphical, from general introduction (Chapter 1), through univariate and bivariate data (Chapters 2 and 3) to multivariate data (Chapter 4). Each chapter covers both categorical and numerical data. The author chose to treat two independent samples as bivariate data and several independent samples as multivariate data, which I think is a bit unusual. Chapter 5 covers probability models. Chapter 6 covers simulations, setting up for the topics on inference in the chapters that follow. Chapters 7 and 8 cover confidence intervals and significance tests, respectively. Chapter 9 discusses the χ^2 tests for the multinomial distribution, the test for independence, and goodness-of-fit tests such as Kolmogorov-Smirnov and Shapiro-Wilk. Chapter 10 covers both simple and multiple linear regression. Chapter 11 covers one- and two-way ANOVA as well as ANCOVA. Chapter 12 covers logistic and nonlinear regression. There are also five appendices that cover various aspects of R (installation, GUI, teaching with R, graphics, programming). Throughout the book, examples of R usage are interspersed among the main text, and some sections devoted to R topics are introduced as the need arises (e.g., in Chapter 6, Simulations, Section 6.2 covers `for()` loops). Data used as examples were drawn from a wide variety of areas. Exercises are given at the end of sections (rather than chapters). The book also has an accompanying add-on package, `UsingR` (available on CRAN), which contains data sets and some functions used in the book. The book also has a web site that contains answers to selected problems, the `UsingR` package for various platforms (including one for S-PLUS), as well as errata.

Several ideas presented in the book deserve accolades (e.g., covering EDA before introducing probability models, coverage of robust/resistant methods, thorough integration of R into the materials). However, there are also drawbacks. The most glaring one is the fact that many rather technical terms are used before they are introduced or explained, and some are not sufficiently elaborated. (E.g., "density" is first used to show how a kernel density estimate can be added to a histogram, but no explanation was given for what a density is or what it means.) In my teaching experience, one of the most difficult (but absolutely essential) concepts for students to grasp is the

[2]See Enos and Kane (2006) for an introduction to the **portfolio** package.

idea of the sampling distribution of a statistic, yet this did not receive nearly the attention I believe it deserves. The discussion of scatterplot smoothing (Section 3.4.7, "Trend lines") gave a minimal description of what smoothers are available in base R, such as smoothing splines, loess, and Friedman's supersmoother. I would be surprised if students in intro stat courses are not completely bewildered by such a minimal description. This will make it harder for some students to follow the text along on their own.

Some people might be interested in learning how to do basic data analysis using R. As these people are not among the intended audience, this book may not serve them as nicely as others, because the R-specific topics are scattered throughout the book in bits and pieces, each making its entrance as the statistical topic being covered requires it.

Now, some real nit-picking on more esoteRic things: The author seems to use "library" and "package" interchangeably, which could make some R users cringe. Also, on page 8, the virtue of using `<-` is touted, but the author still decides to use `=` for the book, without explanation. I also found the mention of the (evil?) `<<-` wholely unnecessary: The author said that it may be useful in programming R, yet personally I have not used it in the years I have been programming R. At the level the book is intended, I believe the students would be better served by its exclusion.

In summary, I like the structure of the book very much. However, the various problems mentioned above keep me from giving it a whole-hearted recommendation as a standalone text. It may serve well as a supplementary text for a more standard introductory Statistics textbook (*a la* Peter Dalgaard's "Introductory Statistics with R").

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DSC 2007

by Hadley Wickham

The fifth "Directions in Statistical Computing" conference was held in sunny Auckland, New Zealand, 8–10 February 2007. Despite the distant location, over 80 attendees from around the world made it to the conference, to enjoy the interesting talks, fabulous weather and the great food and drink of Auckland, including a fantastic ocean-side conference dinner.

The five key note speakers presented five quite different looks at the future of statistical computing:

- Ross Ihaka (re-)explored the use of LISP as a computational backend to R. He said, repeatedly, that this was just for fun, and will not be the next R (Q?)
- L. Fraser Jackson demonstrated the use of J (an open source grand child of APL) for statistics. A very concise and powerful language.
- Patrick Wessa gave an interesting talk about costs of the current scientific publishing framework and how we can do better.
- Olivia Lau discussed **zelig**, a modeling framework for R, which provides a common structure for modeling functions, making it easier for users and developers.
- Duncan Temple Lang talked how about a more composable object orientated R core (the code, not the people) would make it easier to experiment and explore new ideas, and continue to keep R relevant for the future.

A complete programme and abstracts are available on the conference website, `http://www.stat.auckland.ac.nz/dsc-2007/`. Conference papers will be published in a special issue of *Computational Statistics*.

A big round of thanks goes to the organizing committee, Paul Murrell, Ross Ihaka, David Scott and Thomas Yee, for such a great conference, as well as to Sharon Walker and Suryashobha Herle for feeding the hungry attendees.

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New Journal: Annals of Applied Statistics

Bradley Efron, Stanford University, USA

The Annals of Applied Statistics, newest journal from the Institute of Mathematical Statistics, began accepting papers on November 1, 2006. Computational statistics is an area of particular interest. Please visit the journal website at `http://www.imstat.org/aoas` for further information.

Forthcoming Events: useR! 2007

by Dianne Cook

The first North American useR! will be held at Iowa State University, Ames, Iowa, August 8–10, 2007, which will be a week after JSM'07.

This follows successful meetings in Vienna, Austria, in 2006 and 2004, and also Directions in Statistical Computing (DSC) meetings in Auckland, NZ (Feb 2007), Seattle (2005), and Vienna (1999, 2001, 2003). Information about the meeting can be found at `http://www.useR2007.org/` or by emailing `useR2007@iastate.edu`.

The important dates to remember are:

- April 23, 2007: Deadline for paper submission, with referees comments returned by April 30.
- May 1, 2007: Early registration ends
- June 30: Poster abstract submission ends
- August 8, 2007: useR! 2007 begins!

We look forward to meet you in Ames!

On behalf of the organizing committee:
Diane Cook
Department of Statistics
Iowa State University
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Changes in R 2.5.0

by the R Core Team

User-visible changes

- `apropos(x)` and `find(x)` now both only work for character `x`, and hence drop all non-standard evaluation behaviour.
- Data frames can have 'automatic' row names which are not converted to dimnames by `as.matrix()`. (Consequently, e.g., `t()` for such data frames has `NULL` column names.) This change leads to memory reductions in several places, but can break code which assumes character dimnames for data frames derived from matrices.

  No existing R object is regarded as having 'automatic' row names, and it may be beneficial to recreate such objects via `read.table()` or `data.frame()`.
- Using `$` on an atomic vector now raises a warning, as does use on an S4 class for which a method has not been defined.
- The Unix-alike readline terminal interface now does command-completion for R objects, incorporating the functionality formerly in package **rcompletion** by Deepayan Sarkar. This can be disabled by setting the environment variable `R_COMPLETION` to `FALSE` when starting R (e.g., in '∼/.Renviron').

New features

- `abbreviate()` no longer has an 8191 byte limit on the size of strings it can handle.
- `abs(x)` now returns integer for integer or logical arguments.
- `apropos()` has a new argument `ignore.case` which defaults to `TRUE`, potentially matching more than previously, thanks to a suggestion by Seth Falcon.
- `args()`, `str()` and `print()` now give the argument lists of primitive functions.
- `as.matrix()` gains the `...` argument that several packages have assumed it always had (and S-PLUS has).
- Manipulation of integers as roman numerals via `as.roman()` in package **utils**.

- `attr()` no longer treats `name = NA_character_` as meaning `name = "NA"`.
- `binom.test()` now allows a 'fuzz' for calculated integer values in its `x` and `n` arguments.
- `boxplot(*, notch = TRUE)` now warns when notches are outside hinges; related to PR#7690.
- New function `callCC()` providing a downward-only version of Scheme's call with current continuation.
- `capabilities()` now has a `profmem` entry indicating whether R has been compiled with memory profiling.
- `colnames<-()` and `rownames<-()` now handle data frames explicitly, so calling `colnames<-` on a data frame no longer alters the representation of the row names.
- `commandArgs()` has a new `trailingOnly` argument to be used in conjunction with '`--args`'.
- `contour()` now passes graphical parameters in `...` to `axis()` and `box()`.
- New data set `crimtab` on Student (1908)'s 3000 criminals.
- `cut.default()` has a new argument `ordered_result`.
- `.deparseOpts()` has two new options: `keepNA` to ensure that different types (logical, integer, double, character and complex) of `NA`s are distinguished, and `S_compatible` to suppress the use of R-specific features such as 123L and to deparse integer values of a double vector with a trailing decimal point.

  The `keepInteger` option now uses the suffix `L` rather than `as.integer()` where possible (unless all entries are `NA` or `S_compatible` is also set).

  Other deparse options can now be added to `all` (which has not for some time actually switched on all options).

  Integer sequences `m:n` are now deparsed in that form.
- `deparse()` and `dput()` now include `keepInteger` and `keepNA` in their defaults for the `control` argument.
- `detach()` now takes another argument, `unload`, which indicates whether or not to unload the package and then only cleans up the S4 methods if the package successfully unloads.
- There are new constants `NA_integer_`, `NA_real_`, `NA_complex_` and `NA_character_` to denote `NA`s of those types, and they will be used in deparsing in place of `as.integer(NA)` etc unless `.deparseOpts()` includes `S_compatible`.
- `dev.print()` now recognizes `screen devices` as all those with an enabled display list, rather than a hard-coded set.
- Objects of class `difftime` are now handled more flexibly. The units of such objects can now be accessed via a `units()` function, which also has a replacement form, and there are conversion methods to and from numeric, which also allow the specification of units. Objects of this class can also be stored in data frames now. A `format()` method has been added, and the print method was revised.
- New function `environmentName()` to give the print name of environments such as '`namespace:base`'. This is now used by `str()`.
- New function `env.profile()` provides R level access to summary statistics on environments. In a related patch, `new.env()` now allows the user to specify an initial size for a hashed environment.
- `file()` can read the X11 clipboard selection as `"X11_clipboard"` on suitable X11-using systems.
- `file("stdin")` is now recognized, and refers to the process's stdin file stream whereas `stdin()` refers to the console. These may differ, for example for a GUI console, an embedded application of R or if '`--file=`' has been used.
- `file_test()` is now also available in package **utils**. (It is now private in package **tools**.)
- `file.show()` gains an `encoding` argument.
- New functions `formatUL()` and `formatOL()` in package **utils** for formatting unordered (`itemize`) and ordered (`enumerate`) lists.
- The statistics reported when `gcinfo(TRUE)` are now of the amounts used (in Mb) and not of the amounts free (which are not really relevant when there are no hard limits, only gc trigger points).
- New function `get_all_vars()` to retrieve all the (untransformed) variables that the default method of `model.frame()` would use to create the model frame.
- `interaction()` has a new argument `lex.order`.

- `initialize()` (in **methods**) now tries to be smarter about updating the new instance in place, thereby reducing copying.

- `install.packages(dependencies = NA)` is a new default, which is to install essential dependencies when installing from repositories to a single library. As a result of this change, `update.packages()` will install any new dependencies of the packages it is updating (alongside the package in the same library tree).

  If `lib` is not specified or is specified of length one and the chosen location is not a writable directory, `install.packages()` offers to create a personal library directory for you if one does not already exist, and to install there.

- `is.atomic`, `is.call`, `is.character`, `is.complex`, `is.double` (= `is.real`), `is.environment`, `is.expression`, `is.function`, `is.integer`, `is.list`, `is.logical`, `is.null`, `is.object`, `is.pairlist`, `is.recursive`, `is.single` and `is.symbol` (= `is.name`) are no longer internally S3 generic, nor can S4 methods be written for them.

  The `factor` methods of `is.integer` and `is.numeric` have been replaced by internal code.

- Added `is.raw()` for completeness.

- `l10n_info()` also reports if the current locale is Latin-1.

- `levels<-()`, `names()` and `names<-()` now dispatch internally for efficiency and so no longer have S3 default methods.

- `.libPaths()` now does both tilde and glob expansion.

- Functions `lm()`, `glm()` `loess()`, `xtabs()` and the default method of `model.frame()` coerce their `formula` argument (if supplied) to a formula.

- `max()`, `min()` and `range()` now work with character vectors.

- `message()` has a new argument `appendLF` to handle messages with and without newlines. There is a new message class `packageStartupMessage` that can be suppressed separately.

- A new function, `method.skeleton()` writes a skeleton version of a call to `setMethod()` to a file, with correct arguments and format, given the name of the function and the method signature.

- `mode<-` and `storage.mode<-` do slightly less copying.

- `nls.control(* , printEval = FALSE, warnOnly = FALSE)` are two new options to help better analyze (non-)convergence of `nls()`, thanks to Kate Mullen.

  `nls()` and `summary(nls())` now contain more information and also print information about convergence.

- `options(device = )` now accepts a function object as well as the name of a function.

- `pdf()` supports new values for `paper` of `'"US"'` (same as `'"letter"'`), `'"a4r"'` and `'"USr"'` (the latter two meaning rotated to landscape). `postscript()` also accepts `paper = "US"`.

- `persp()` now respects the graphical pars `cex.axis`, `cex.lab`, `font.axis` and `font.lab`.

- New faster internal functions `pmax.int()` and `pmin.int()` for inputs which are atomic vectors without classes (called by `pmax`/`pmin` where applicable).

  `pmin`/`pmax` are now more likely to work with classed objects: they work with `POSIXlt` datetimes, for example.

- `postscript()` now by default writes grey colors (including black and white) via `setgray`, which gives more widely acceptable output. There are options to write pure RGB, CMYK or gray via the new argument `colormodel`.

- `rbind.data.frame()` now ignores all zero-row inputs, as well as zero-column inputs (which it used to do, undocumented). This is because `read.table()` can create zero-row data frames with `NULL` columns, and those cannot be extended.

- `readChar()` and `writeChar()` can now work with a raw vector.

- `read.table()`, `write.table()` and allies have been moved to package **utils**.

- `rgb()` now accepts the red, green and blue components in a single matrix or data frame.

- New utility function `RShowDoc()` in package **utils** to find and display manuals and other documentation files.

- New `.row_names_info()` utility function finds the number of rows efficiently for data frames; consequently, `dim.data.frame()` has become very fast for large data frames with 'automatic' row names.

- `RSiteSearch()` now also allows to search postings of the 'R-devel' mailing list.

- `screeplot()` is now (S3) generic with a default method, thanks to a patch from Gavin Simpson.
- Experimental `verbose` argument for `selectMethod()`. Might be replaced later by a better interface for method selection inspection.
- Added links to source files to the parsing routines, so that `source()` can now echo the original source and comments (rather than deparsing). This affects `example()` and `Sweave()` as well.
- `stack()` and `unstack()` have been moved to package **utils**.
- `strptime()` now sets the 'tzone' attribute on the result if `tz != ""`.
- `str.default()` typically prints fewer entries of logical vectors.
- The `RweaveLatex` driver for `Sweave()` now supports two new options: `expand=FALSE`, to show chunk references in the output, and `concordance=TRUE`, to output the concordance between input and output lines.
- `system()` now takes the same set of arguments on all platforms, with those which are not applicable being ignored with a warning. Unix-alikes gain `input` and `wait`, and Windows gains `ignore.stderr`.
- `system.time()` and `proc.time()` now return an object of class `proc_time` with a `print()` method that returns a POSIX-like format with names.
- `Sys.getenv()` has a new argument `unset` to allow unset and set to `""` to be distinguished (if the OS does). The results of `Sys.getenv()` are now sorted (by name).
- New function `Sys.glob()`, a wrapper for the POSIX.2 function `glob(3)` to do wildcard expansion (on systems which have it, plus an emulation on Windows).
- `Sys.setenv()` is a new (and preferred) synonym for `Sys.putenv()`. The internal C code uses the POSIX-preferred `setenv` rather than `putenv` where the former is available.
- New function `Sys.unsetenv()` to remove environment variables (on systems where `unsetenv` is implemented or `putenv` can remove variables, such as on Windows).
- `text()`, `mtext()`, `strheight()`, `strwidth()`, `legend()`, `axis()`, `title()`, `pie()`, `grid.text()` and `textGrob()` all attempt to coerce non-language annotation objects (in the sense of `is.object`) to character vectors. This is principally intended to cover factors and POSIXt and Date objects, and is done via the new utility function `as.graphicsAnnot()` in package **grDevices**.
- `tk_select.list()` in package **tcltk** now chooses the width to fit the widest item.
- `retracemem()` and `untracemem()` are now primitives for efficiency and so migrate from **utils** to **base**.
- `union()`, `intersect()`, `setdiff()` and `setequal()` now coerce their arguments to be vectors (and they were documented only to apply to vectors).
- `uniroot()` now works if the zero occurs at one of the ends of the interval (suggestion of Tamas Papp).
- There is a new function `View()` for viewing matrix-like objects in a spreadsheet, which can be left up whilst R is running.
- New function `withVisible()` allows R level access to the visibility flag.
- `zip.file.extract()` has been moved to package **utils**.
- A few more cases of subassignment work, e.g., *raw*`[]` `<-` *list* and *vector*`[]` `<-` *expression*, with suitable coercion of the LHS.
- There is a warning if a '\' is used unnecessarily in a string when being parsed., e.g., '`\.`' where probably '`\\.`' was intended. ('`\.`' is valid, but the same as '`.`'.) Thanks to Bill Dunlap for the suggestion.
- Introduced the suffix `L` for integer literals to create integer rather than numeric values, e.g., `100L`, `0x10L`, `1e2L`.
- Set the parser to give verbose error messages in case of syntax errors.
- The class `LinearMethodsList` has been extended and will be used to create list versions of methods, derived from the methods tables (environments). The older recursive `MethodsList` class will be deprecated (by the release of 2.5.0 if possible).
- There are more flexible ways to specify the default library search path. In addition to `R_LIBS` and `.Library`, there are `.Library.site` (defaults to 'R_HOME/site-library') and `R_LIBS_USER` (defaults to a platform- and version-specific directory in '~/R'). See `?.libPaths` for details.

- LAPACK has been updated to version 3.1.0. This should cause only small changes to the output, but do remember that the sign of eigenvectors (and principal components) is indeterminate.
- PCRE has been updated to version 7.0.
- Several functions handle row names more efficiently:
  - `read.table()` and `read.DIF()` make use of integer row names where appropriate, and avoid at least one copy in assigning them.
  - `data.frame()` and the standard `as.data.frame()` methods avoid generating long dummy row names and then discarding them.
  - `expand.grid()` and `merge()` generate compact 'automatic' row names.
  - `data.matrix()` and `as.matrix.data.frame()` have a new argument 'rownames.force' that by default drops 'automatic' row names.
- *data_frame*`[i, j]` is substantially more memory-efficient when only a small part of the data frame is selected, especially when (part of) a single column is selected.
- Command-line R (and 'Rterm.exe' under Windows) accepts the options '`-f` *filename*', '`--file=`*filename*' and '`-e` *expression*' to follow other script interpreters. These imply '`--no-save`' unless '`--save`' is specified.
- Invalid bytes in character strings in an MBCS now deparse/print in the form '`\xc1`' rather than '`<c1>`', which means they can be parsed/scanned.
- Printing functions (without source attributes) and expressions now preserves integers (using the `L` suffix) and `NA`s (using `NA_real_` etc where necessary).
- The 'internal' objects `.helpForCall`, `.tryHelp` and `topicName` are no longer exported from **utils**.
- The internal regex code has been upgraded to glibc 2.5 (from 2.3.6).
- Text help now attempts to display files which have an `encoding` section in the specified encoding via `file.show()`.
- R now attempts to keep track of character strings which are known to be in Latin-1 or UTF-8 and print or plot them appropriately in other locales. This is primarily intended to make it possible to use data in Western European languages in both Latin-1 and UTF-8 locales. Currently `scan()`, `read.table()`, `readLines()`, `parse()` and `source()` allow encodings to be declared, and console input in suitable locales is also recognized.

  New function `Encoding()` can read or set the declared encodings for a character vector.
- There have been numerous performance improvements to the data editor on both Windows and X11. In particular, resizing the window works much better on X11.

Deprecated & defunct

- `symbol.C()` and `symbol.For()` are defunct, and have been replaced by wrappers that give a warning.
- Calling a builtin function with an empty argument is now always an error.
- The autoloading of `ts()` is defunct.
- The undocumented reserved word `GLOBAL.ENV` has been removed. (It was yet another way to get the value of the symbol `.GlobalEnv`.)
- The deprecated behaviour of `structure()` in adding a class when specifying with `tsp` or `levels` attributes is now defunct.
- `unix()` is now finally defunct, having been deprecated for at least seven years.
- `Sys.putenv()` is now deprecated in favour of `Sys.setenv()`, following the POSIX recommendation.
- Building R with '`--without-iconv`' is deprecated.
- Using `$` on an atomic vector is deprecated (it was previously valid and documented to return `NULL`).
- The use of `storage.mode<-` for other than standard types (and in particular for value `"single"`) is deprecated: use `mode<-` instead.

Installation

- A suitable iconv (e.g., from glibc or GNU libiconv) is required. For 2.5.x only you can build R without it by configuring using '`--without-iconv`'.
- There is support again for building on AIX (tested on 5.2 and 5.3) thanks to Ei-ji Nakama.

- Autoconf 2.60 or later is used to create `configure`. This makes a number of small changes, and incorporates the changes to the detection of a C99-compliant C compiler backported for 2.4.1.
- Detection of a Java development environment was added such that packages don't need to provide their own Java detection.

  `R CMD javareconf` was updated to look for the corresponding Java tools as well.
- Added workaround for reported non-POSIX `sh` on OSF1. (PR#9375)
- `make install-strip` now works, stripping the executables and also the shared libraries and modules on platforms where `libtool` knows how to do so.
- Building R as a shared library and standalone nmath now installs pkg-config files 'libR.pc' and 'libRmath.pc' respectively.
- Added test for insufficiently complete implementation of sigaction.

C-level facilities

- Functions `str2type`, `type2char` and `type2str` are now available in 'Rinternals.h'.
- Added support for Objective C in R and packages (if available).
- `R_ParseVector()` has a new 4th argument `SEXP srcfile` allowing source references to be attached to the returned expression list.
- Added `ptr_R_WriteConsoleEx` callback which allows consoles to distinguish between regular output and errors/warnings. To ensure backward compatibility it is only used if `ptr_R_WriteConsole` is set to `NULL`.

Utilities

- Additional `Sweave()` internal functions are exported to help writing new drivers, and `RweaveLatexRuncode()` is now created using a helper function (all from a patch submitted by Seth Falcon).
- The following additional flags are accessible from `R CMD config`: `OBJC`, `OBJCFLAGS`, `JAR`, `JAVA`, `JAVAC`, `JAVAH`, `JAVA_HOME`, `JAVA_LIBS`
- `R CMD build` now takes the package name from the 'DESCRIPTION' file and not from the directory. (PR#9266)
- `checkS3methods()` (and hence `R CMD check`) now checks agreement with primitive internal generics, and checks for additional arguments in methods where the generic does not have a `...` argument.

  `codoc()` now knows the argument lists of primitive functions.
- `R CMD INSTALL` and `R CMD REMOVE` now use as the default library (if '`-l`' is not specified) the first library that would be used if R were run in the current environment (and they run R to find it).
- There is a new front-end 'Rscript' which can be used for `#!` scripts and similar tasks. See `help("Rscript")` and 'An Introduction to R' for further details.
- `R CMD BATCH` (not Windows) no longer prepends '`invisible(options(echo = TRUE))`' to the input script. This was the default unless '`--slave`' is specified and the latter is no longer overridden.

  On all OSes it makes use of the '`-f`' argument to R, so `file("stdin")` can be used from `BATCH` scripts.

  On all OSes it reports `proc.time()` at the end of the script unless `q()` is called with options to inhibit this.
- `R CMD INSTALL` now prepends the installation directory (if specified) to the library search path.
- Package installation now re-encodes R files and the 'NAMESPACE' file if the 'DESCRIPTION' file specifies an encoding, and sets the encoding used for reading files in preparing for `LazyData`. This will help if a package needs to be used in (say) both Latin-1 and UTF-8 locales on different systems.
- `R CMD check` now reports on non-ASCII strings in datasets. (These are a portability issue, which can be alleviated by marking their encoding: see 'Writing R Extensions'.)
- `Rdiff` now converts CRLF endings in the target file, and converts UTF-8 single quotes in either to ASCII quotes.
- New recommended package **codetools** by Luke Tierney provides code-analysis tools. This can optionally be used by `R CMD check` to detect problems, especially symbols which are not visible.
- `R CMD config` now knows about LIBnn .

- New recommended package **rcompgen** by Deepayan Sarkar provides support for command-line completion under the Unix terminal interface (provided readline is enabled) and the Windows Rgui and Rterm front ends.

Bug fixes

- `gc()` can now report quantities of 'Vcells' in excess of 16Gb on 64-bit systems (rather than reporting `NA`).
- Assigning class `factor` to an object now requires it has integer (and not say double) codes.
- `structure()` ensures that objects with added class `factor` have integer codes.
- The `formula` and `outer` attributes of datasets `ChickWeight`, `CO2`, `DNase`, `Indometh`, `Loblolly`, `Orange` and `Theoph` now have an empty environment and not the environment used to dump the datasets in the package.
- Dataset `Seatbelts` now correctly has class `c("mts", "ts")`.
- `str()` now labels classes on data frames more coherently.
- Several 'special' primitives and .Internals could return invisibly if the evaluation of an argument led to the visibility flag being turned off. These included `as.character()`, `as.vector()`, `call()`, `dim()`, `dimnames()`, `lapply()`, `rep()`, `seq()` and `seq_along()`. Others (e.g., `dput()` and `print.default()`) could return visibly when this was not intended.
- Several primitives such as `dim()` were not checking the number of arguments supplied before method dispatch.
- Tracing of primitive functions has been corrected. It should now be the case that tracing either works or is not allowed for all primitive functions. (Problems remain if you make a primitive into a generic when it is being traced. To be fixed later.)
- `max.col()` now omits infinite values in determining the relative tolerance.
- `R CMD Sweave` and `R CMD Stangle` now respond to '`--help`' and '`--version`' like other utilities.
- `.libPaths()` adds only existing directories (as it was documented to, but could add non-directories).
- `setIs()` and `setClassUnion()` failed to find some existing subclasses and produced spurious warnings, now fixed.
- `data.frame()` ignored `row.names` for 0-column data frames, and no longer treats an explicit `row.names=NULL` differently from the default value.
- `identical()` looked at the internal structure of the `row.names` attribute, and not the value visible at R level.
- `abline(reg)` now also correctly works with intercept-only `lm` models, and `abline()` warns more when it's called illogically.
- `warning()` was truncating messages at `getOption("warning.length") - 1` (not as documented), with no indication. It now appends `[... truncated]`.
- Stangle/Sweave were throwing spurious warnings if options `result` or `strip.white` were unset.
- `all.equal()` was ignoring `check.attributes` for list and expression targets, and checking only attributes on raw vectors. Logical vectors were being compared as if they were numeric, (with a mean difference being quoted).
- Calculating the number of significant digits in a number was itself subject to rounding errors for digits $\geq$ 16. The calculation has been changed to err on the side of slightly too few significant digits (but still at least 15) rather than far too many. (An example is `print(1.001, digits=16)`.)
- `unlink()` on Unix-alikes failed for paths containing spaces.
- `substr()` and friends treated `NA` `start` or `stop` incorrectly.
- `merge(x, y, all.y = TRUE)` would sometimes incorrectly return logical columns for columns only in `y` when there were no common rows.
- `read.table(fn, col.names=)` on an empty file returned `NULL` columns, rather than `logical(0)` columns (which is what results from reading a file with just a header).
- `grid.[xy]axis(label=logical(0))` failed.
- `expression()` was unnecessarily duplicating arguments.
- `as.expression(`*list*`)` returned a single-element expression vector, which was not compatible with S: it now copies lists element-by-element.

- `supsmu(periodic = TRUE)` could segfault. (PR#9502, detection and patch by Bill Dunlap.)
- `pmax/pmin` called with only logical arguments did not coerce to numeric, although they were documented to do so (as `max/min` do).
- `methods()` did not know that `cbind()` and `rbind()` are internally generic.
- `dim(x) <- NULL` removed the names of `x`, but this was always undocumented. It is not clear that it is desirable but it is S-compatible and relied on, so is now documented.
- `which(x, arr.ind = TRUE)` did not return a matrix (as documented) if `x` was an array of length 0.
- C-level `duplicate()` truncated `CHARSXP`s with embedded nuls.
- Partial matching of attributes was not working as documented in some cases if there were more than two partial matches or if 'names' was involved.
- `data(package=character(0))` was not looking in '`./data`' as documented.
- `summary.mlm()` failed if some response names were `""` (as can easily happen if `cbind()` is used).
- The `postscript()` and `pdf()` drivers shared an encoding list but used slightly different formats. This caused problems if both were used with the same non-default encoding in the same session. (PR#9517)
- The data editor was not allowing `Inf`, `NA` and `NaN` to be entered in numerical columns. It was intended to differentiate between empty cells and `NA`s, but did not do so: it now does so for strings.
- `supsmu()` could segfault if all cases had non-finite values. (PR#9519)
- `plnorm(x, lower.tail=FALSE)` was returning the wrong tail for $x \leq 0$. (PR#9520)
- `which.min()` would not report a minimum of `+Inf`, and analogously for `which.max()`. (PR#9522)
- `R CMD check` could fail with an unhelpful error when checking Rd files for errors if there was only one file and that had a serious error. (PR#9459)
- `try()` has been reimplemented using `tryCatch()` to solve two problems with the original implementation: (i) `try()` would run non-NULL `options("error")` expressions for errors within a try, and (ii) `try()` would catch user interrupts.
- `str(obj)` could fail when `obj` contained a dendrogram.
- Using *data_frame*`[, `*last_column*`] <- NULL` failed (PR#9565).
- `choose(n, k)` could return non-integer values for integer `n` and small `k` on some platforms.
- `nclass.scott(x)` and `nclass.FD(x)` no longer return `NaN` when `var(x)` or `IQR(x)` (respectively) is zero.

  `hist()` now allows `breaks = 1` (which the above patch will return), but not `breaks = Inf` (which gave an obscure error).
- `strptime("%j")` now also works for the first days of Feb-Dec. (PR#9577)
- `write.table()` now recovers better if `file` is an unopened connection. (It used to open it for both the column names and the data.)
- Fixed bug in `mosaicplot(sort=)` introduced by undocumented change in R 2.4.1 (changeset r39655).
- `contr.treatment(n=0)` failed with a spurious error message. (It remains an error.)
- `as.numeric()` was incorrectly documented: it is identical to `as.double()`.
- `jitter(rep(-1, 3))` gave `NaN`s. (PR#9580)
- `max.col()` was not random for a row of zeroes. (PR#9542)
- `ansari.test(conf.int=TRUE, exact=FALSE)` failed.
- `trace()` now works on S3 registered methods, by modifying the version in the S3 methods table.
- `rep(length=1, each=0)` segfaulted.
- `postscript()` could overflow a buffer if used with a long `command` argument.
- The internal computations to copy complete attribute lists did not copy the flag marking S4 objects, so the copies no longer behaved like S4 objects.
- The C code of `nlminb()` was altering a variable without duplicating it. (This did not affect `nlminb()` but would have if the code was called from a different wrapper.)
- `smooth(kind = "3RS3R")` (the current default) used `.C(DUP = FALSE)` but altered its input argument. (This was masked by duplication in `as.double()`.)

- The signature for the predefined S4 method for `as.character()` was missing `...`.
- `readBin(raw_vector)` could read beyond the end of the vector when size-changing was involved.
- The C entry point `PrintValue` (designed to emulate auto-printing) would not find `show()` for use on S4 objects, and did not have the same search path (for `show()`, `print()` and `print()` methods) as auto-printing. Also, auto-printing and `print()` of S4 objects would fail to find `show` if the methods namespace was loaded but the package was not attached (or otherwise not in the search path).
- `print()` (and auto-printing) now recognize S4 objects even when **methods** is not loaded, and print a short summary rather than dump the internal structure.

Changes on CRAN

by Kurt Hornik

New contributed packages

ARES Allelic richness estimation, with extrapolation beyond the sample size. Generates an allelic richness accumulation curve. This curve shows the expected number of unique alleles in a population when taking a sample of individuals. The function `aresCalc` takes a binary data matrix as input, showing the presence of alleles per individual, and gives an accumulation curve (mean with 95% confidence bounds) back. The function `aresPlot` can be used to plot the output from `aresCalc`. By Emiel van Loon and Scott Davis.

BayHaz Bayesian Hazard Rate Estimation: a suite of R functions for Bayesian estimation of smooth hazard rates via Compound Poisson Process (CPP) priors. By Luca La Rocca.

BiasedUrn Biased Urn model distributions. Statistical models of biased sampling in the form of univariate and multivariate non-central hypergeometric distributions, including those of Wallenius and Fisher (also called extended hypergeometric distribution). By Agner Fog.

BootCL Bootstrapping test for chromosomal localization. By Eun-Kyung Lee, Samsun Sung, and Heebal Kim.

Brobdingnag Very large numbers in R. Real numbers are held using their natural logarithms, plus a logical flag indicating sign. The package includes a vignette that gives a step-by-step introduction to using S4 methods. By Robin K. S. Hankin.

CCA Canonical correlation analysis. Provides a set of functions that extend the `cancor` function with new numerical and graphical outputs. It also include a regularized extension of the canonical correlation analysis to deal with data sets with more variables than observations. By Ignacio González and Sébastien Déjean.

CreditMetrics Functions for calculating the CreditMetrics risk model. By Andreas Wittmann.

DAAGxtras Data sets and functions additional to **DAAG**, used in additional exercises for the book "Data Analysis and Graphics Using R" by J. H. Maindonald and W. J. Brain (2007, 2nd edn.), and for laboratory exercises prepared for a 'Data Mining' course. By John Maindonald.

GenABEL genome-wide association analysis between quantitative or binary traits and SNPs. By Yurii Aulchenko.

GeoXp Interactive exploratory spatial data analysis. A tool for researchers in spatial statistics, spatial econometrics, geography, ecology etc., allowing to link dynamically statistical plots with elementary maps. By Christine Thomas-Agnan, Yves Aragon, Anne Ruiz-Gazen, Thibault Laurent, and Laurianne Robidou.

HydroMe Estimation of the parameters in infiltration and water retention models by curve-fitting method. The models considered are those that are commonly used in soil science. By Christian Thine Omuto.

IPSUR Data sets and functions accompanying the book "Introduction to Probability and Statistics Using R" by G. Andy Chang and G. Jay Kerns (in progress). By G. Jay Kerns with contributions by Theophilius Boye, adapted from the work of John Fox et al.

InfNet Simulation of epidemics in a network of contacts. The simulations consider SIR epidemics with events in continuous time (exponential inter-event times). It can consider a structure of local networks and has an option to visualize it with the animator called SoNIA (`http://www.stanford.edu/group/sonia/`). By Lilia Ramirez Ramirez and Mary Thompson.

JointModeling Joint modeling of mean and dispersion through two interlinked GLMs or GAMs. By Mathieu Ribatet and Bertrand Iooss.

NMMAPSlite NMMAPS Data Lite. Provides remote access to daily mortality, weather, and air pollution data from the National Morbidity, Mortality, and Air Pollution Study for 108 U.S. cities (1987–2000); data are obtained from the Internet-based Health and Air Pollution Surveillance System (iHAPSS). By Roger D. Peng.

NRAIA Data sets from the book "Nonlinear Regression Analysis and Its Applications" by D. M. Bates and D. G. Watts (1998), John Wiley and Sons. By Douglas Bates.

PKtools Unified computational interfaces for pop PK. By M. Suzette Blanchard.

PhySim Phylogenetic tree simulation based on a virth death model. Functions are provided to model a lag-time to speciation and extract sister species ages. By Jason T. Weir, Dolph Schluter.

PresenceAbsence Presence-absence model evaluation. Includes functions for calculating threshold dependent measures such as confusion matrices, pcc, sensitivity, specificity, and Kappa, and produces plots of each measure as the threshold is varied. Can also optimize threshold choice, and plot the threshold independent ROC curves along with the associated AUC By Elizabeth Freeman.

RJDBC Provides access to databases through the JDBC interface, implementing R's DBI interface using JDBC as a back-end. This allows R to connect to any DBMS that has a JDBC driver. By Simon Urbanek.

RLadyBug Analysis of small scale infectious disease data using stochastic Susceptible-Exposed-Infectious-Recovered (SEIR) models. By Michael Hoehle and Ulrike Feldmann.

RaschSampler A Rasch sampler for sampling binary matrices with fixed margins. By Reinhold Hatzinger, Patrick Mair, and Norman Verhelst.

Rcmdr.HH Rcmdr support for the introductory course at Temple University, which spends time on several topics that are not yet in the R Commander. By Richard M. Heiberger, with contributions from Burt Holland.

Rserve A binary R server which acts as a socket server (TCP/IP or local sockets) allowing binary requests to be sent to R. Every connection has a separate workspace and working directory. Client-side implementations are available for popular languages such as C/C++ and Java, allowing any application to use facilities of R without the need of linking to R code. Supports remote connection, user authentication and file transfer. A simple R client is included as well. By Simon Urbanek.

SLmisc Miscellaneous functions for analysis of gene expression data at SIRS-Lab GmbH. By Matthias Kohl.

SMPracticals Data sets and a few functions for use with the practicals outlined in Appendix A of the book "Statistical Models" by A. Davison (2003), Cambridge University Press. The practicals themselves can be found at `http://statwww.epfl.ch/davison/SM/`. By Anthony Davison.

SNPmaxsel Asymptotic methods related to maximally selected statistics, with applications to SNP data. By Anne-Laure Boulesteix.

Snowball Snowball stemmers. By Kurt Hornik.

SpherWave Spherical wavelets and SW-based spatially adaptive methods. Carries out spherical wavelet transform developed Li (1999) and Oh (1999), and implements wavelet thresholding approaches proposed by Oh and Li (2004). By Hee-Seok Oh and Donghoh Kim.

Synth Causal inference using the synthetic control group method of Abadie and Gardeazabal (2003) and Abadie, Diamond, Hainmueller (2007). By Alexis Diamond and Jens Hainmueller.

TRAMPR Matching of terminal restriction fragment length polymorphism (TRFLP) profiles between unknown samples and a database of knowns. Facilitates the analysis of many unknown profiles at once, and provides tools for working directly with electrophoresis output through to generating summaries suitable for community analyses with R's rich set of statistical functions. Also resolves the issues of multiple TRFLP profiles within a species, and shared TRFLP profiles across species. By Rich FitzJohn and Ian Dickie.

VGAM Vector generalized linear and additive models, and associated models (Reduced-Rank VGLMs, Quadratic RR-VGLMs, Reduced-Rank VGAMs). Fits many models and distribution by maximum likelihood estimation (MLE) or penalized MLE. Also fits constrained ordination models in ecology. By Thomas W. Yee.

WWGbook Functions and data sets for the book "Linear Mixed Models: A Practical Guide Using Statistical Software" by B. T. West, K. B. Welch, and A. T. Galecki (2006), Chapman

Hall / CRC Press. By Shu Chen and Andrzej Galecki.

WeedMap Map of weed intensity. Compute spatial predictions from exact count and a covariate. By Gilles Guillot.

ZIGP Adapt and analyze Zero Inflated Generalized Poisson (ZIGP) regression models. By Vinzenz Erhardt.

adimpro Adaptive smoothing of digital images via the Propagation Separation approach by Polzehl and Spokoiny (2006). By Karsten Tabelow and Joerg Polzehl.

agricolae Statistical Procedures for Agricultural Research. These functions are currently utilized by the International Potato Center Research (CIP), the Statistics and Informatics Instructors and the Students of the Universidad Nacional Agraria La Molina Peru, and the Specialized Master in "Bosques y Gestión de Recursos Forestales" (Forest Resource Management). Contains functionality for the statistical analysis of experimental designs applied specially for field experiments in agriculture and plant breeding. By Felipe de Mendiburu.

analogue Analogue methods for palaeoecology. Fits modern analogue technique transfer function models for prediction of environmental data from species data. Also performs analogue matching, a related technique used in palaeoecological restoration. By Gavin L. Simpson.

arm Data analysis using regression and multilevel/hierarchical models. By Andrew Gelman, Yu-Sung Su, Jennifer Hill, Maria Grazia Pittau, Jouni Kerman, and Tian Zheng.

arrayMissPattern Exploratory analysis of missing patterns for microarray data. By Eun-kyung Lee and Taesung Park.

bbmle Modifications and extensions of the **stats4** `mle` code. By Ben Bolker, modifying code by Peter Dalgaard and other R-core members.

bcp Bayesian Change Point. An implementation of the Barry and Hartigan (1993) product partition model for the standard change point problem using Markov Chain Monte Carlo. By Chandra Erdman.

binGroup Evaluation and experimental design for binomial group testing. By Frank Schaarschmidt.

cgh Analysis of microarray comparative genome hybridization data using the Smith-Waterman algorithm. By Tom Price.

classifly Exploration of classification models in high dimensions, implementing methods for understanding the division of space between groups. See `http://had.co.nz/classifly` for more details. By Hadley Wickham.

clustTool GUI for clustering data with spatial information. By Matthias Templ.

clusterGeneration Random cluster generation (with specified degree of separation). By Weiliang Qiu and Harry Joe.

clusterSim Searching for optimal clustering procedure for a data set. By Marek Walesiak Andrzej Dudek.

cobs99 Constrained B-splines – outdated 1999 version. By Pin T. Ng and Xuming He; R port by Martin Maechler.

corrgram Plot correlograms. By Kevin Wright.

distrDoc Documentation for packages **distr**, **distrEx**, **distrSim**, and **distrTEst**. By Florian Camphausen, Matthias Kohl, Peter Ruckdeschel, and Thomas Stabla.

drm Likelihood-based marginal regression and association modeling for repeated, or otherwise clustered, categorical responses using dependence ratio as a measure of the association. By Jukka Jokinen.

elrm Exact Logistic Regression via MCMC. By David Zamar, Jinko Graham, and Brad McNeney.

emdbook Data sets and auxiliary functions for the book "Ecological Models and Data" by B. Bolker (in progress). By Ben Bolker.

epicalc Epidemiological calculator. By Virasakdi Chongsuvivatwong.

fEcofin Selected economic and financial data for teaching financial engineering and computational finance. By Diethelm Wuertz and many others.

fame Interface for the FAME time series database. Includes FAME storage and retrieval function, as well as functions and S3 classes for time indexes and time indexed series, which are compatible with FAME frequencies. By Jeff Hallman.

filehashSQLite Simple key-value database using SQLite as the backend. By Roger D. Peng.

gamlss.dist Extra distributions for GAMLSS modeling. By Mikis Stasinopoulos and Bob Rigby with contributions from Calliope Akantziliotou and Raydonal Ospina.

glmc Fits generalized linear models where the parameters are subject to linear constraints. The model is specified by giving a symbolic description of the linear predictor, a description of the error distribution, and a matrix of constraints on the parameters. By Sanjay Chaudhuri, Mark S. Handcock, and Michael S. Rendall.

heplots Visualizing Tests in Multivariate Linear Models. Represents sums-of-squares-and-products matrices for linear hypotheses and for error using ellipses (in two dimensions) and ellipsoids (in three dimensions). By John Fox, Michael Friendly, and Georges Monette.

homtest A collection of homogeneity tests and other stuff for hydrological applications. By Alberto Viglione.

ibdreg A method to test genetic linkage with covariates by regression methods with response IBD sharing for relative pairs. Accounts for correlations of IBD statistics and covariates for relative pairs within the same pedigree. By Jason P. Sinnwell and Daniel J. Schaid.

kernelPop Spatially explicit population genetic simulations. Creates an individual-based population genetic simulation in discrete time, where individuals have spatial coordinates, with dispersal governed by mixtures of Weibull and normal pdfs. Simulates diploid and haploid inheritance. Allows the development of null distributions of genotypes for complex demographic scenarios. By Allan Strand and James Niehaus.

klin Implements efficient ways to evaluate and solve equations of the form $Ax = b$, where A is a Kronecker product of matrices. Also includes functions to solve least squares problems of this type. By Tamas K Papp.

knnflex A more flexible KNN implementation which allows the specification of the distance used to calculate nearest neighbors (euclidean, binary, etc.), the aggregation method used to summarize response (majority class, mean, etc.) and the method of handling ties (all, random selection, etc.). Additionally, continuous responses are handled. By Atina Dunlap Brooks.

languageR Data sets and functions for the book "Analyzing Linguistic Data: A practical introduction to Statistics" by R. H. Baayen (2006), Cambridge University Press. By R. H. Baayen.

lss Accelerated failure time model to right censored data based on least-squares principle. By Lin Huang and Zhezhen Jin.

mFilter Several time series filters useful for smoothing and extracting trend and cyclical components of a time series. Currently, Christiano-Fitzgerald, Baxter-King, Hodrick-Prescott, Butterworth, and trigonometric regression filters are included in the package. By Mehmet Balcilar.

meboot Maximum entropy density based dependent data bootstrap for time series. An algorithm is provided to create a population of time series (ensemble) without assuming stationarity. By Hrishikesh D. Vinod and Javier López-de-Lacalle.

memisc Miscellaneous tools for data management, including tools for preparing (especially social science) survey data, conducting simulation studies, and presentation of results of statistical analyses. By Martin Elff.

mixstock Functions for mixed stock analysis. By Ben Bolker.

mixtools Tools for analyzing mixture models. By Ryan Elmore, Tom Hettmansperger, David Hunter, Hoben Thomas, Fengjuan Xuan, and Derek Young.

mlCopulaSelection Use numerical maximum likelihood to choose and fit a bivariate copula model (from a library of 40 models) to the data. By Jesus Garcia and Veronica Gonzalez-Lopez.

msgcop Semiparametric Bayesian Gaussian copula estimation, treating the univariate marginal distributions as nuisance parameters in Hoff (2006). Also provides a semiparametric imputation procedure for missing multivariate data. By Peter Hoff.

muS2RC S-PLUS to R compatibility for package **muStat**. By Knut M. Wittkowski and Tingting Song.

muStat Prentice Rank Sum Test and McNemar Test. Performs Wilcox rank sum test, Kruskal rank sum test, Friedman rank sum test and McNemar test. By Knut M. Wittkowski and Tingting Song.

muUtil A collection of utility functions for package **muStat**. By Knut M. Wittkowski and Tingting Song.

np Nonparametric kernel smoothing methods for mixed data types. By Tristen Hayfield and Jeffrey S. Racine.

nsRFA Tools for objective (non-supervised) applications of the Regional Frequency Analysis methods in hydrology. By Alberto Viglione.

pARtial (Partial) attributable risk estimates, corresponding variance estimates and confidence intervals. By Andrea Lehnert-Batar.

pmml Generate PMML for various models. The Predictive Modeling Markup Language (PMML) is a language for representing models, in an application independent way. Such models can then be loaded into other applications supporting PMML, such as Teradata Warehouse Miner and IBM's DB2. By Graham Williams.

popbio Construct and analyze projection matrix models from a demography study of marked individuals classified by age or stage. Covers methods described in the books "Matrix Population Models" by Caswell (2001) and "Quantitative Conservation Biology" by Morris and Doak (2002). By Chris Stubben and Brook Milligan.

portfolioSim Framework for simulating equity portfolio strategies. By Jeff Enos and David Kane, with contributions from Kyle Campbell.

prim Patient Rule Induction Method (PRIM) for estimating highest density regions in high-dimensional data. By Tarn Duong.

qgen Analysis of quantitative genetic data, especially helpful to perform parametric resampling of quantitative genetic data sets. By Thomas Fabbro.

rcdk Interface to the CDK libraries, a Java framework for cheminformatics. Allows to load molecules, evaluate fingerprints, calculate molecular descriptors and so on. By Rajarshi Guha.

rcompgen Generates potential completions for a given command snippet based on circumstantial evidence. By Deepayan Sarkar.

rcompletion Pseudo-intelligent TAB completion for R when run from a terminal, using the GNU Readline library. By Deepayan Sarkar.

relaxo Relaxed Lasso, a generalization of the Lasso shrinkage technique for linear regression. Both variable selection and parameter estimation is achieved by regular Lasso, yet both steps do not necessarily use the same penalty parameter. By Nicolai Meinshausen.

rggm Fitting Gaussian Graphical Models with robustified methods. By Masashi Miyamura.

rjacobi Compute Jacobi polynomials and Gauss-Jacobi quadrature related operations. By Paulo Jabardo.

sciplot Scientific graphs with error bars for data collected from one-way or higher factorial designs. By Manuel Morales.

signal A set of generally Matlab/Octave-compatible signal processing functions. Includes filter generation utilities, filtering functions, resampling routines, and visualization of filter models. By Tom Short.

smoothtail Smooth Estimation of the Generalized Pareto distribution shape parameter. By Kaspar Rufibach and Samuel Mueller.

snp.plotter Creates plots of p-values using single SNP and/or haplotype data, with options to display a linkage disequilibrium (LD) plot and the ability to plot multiple data sets simultaneously. By Augustin Luna and Kristin K. Nicodemus.

spsurvey Algorithms required for design and analysis of probability surveys such as those utilized by the U.S. Environmental Protection Agency's Environmental Monitoring and Assessment Program (EMAP). By Tom Kincaid and Tony Olsen, with contributions from Don Stevens, Christian Platt, Denis White, and Richard Remington.

staRt Inferenza classica con TI-83 Plus. Una libreria per utilizzare con semplicità le tecniche di statistica inferenziale presenti sulla calcolatrice scientifica grafica TI-83 Plus. By Fabio Frascati.

stashR A set of tools for administering shared repositories. By Sandy Eckel, and Roger D. Peng.

stochmod Stochastic Modeling: learning and inference algorithms for a variety of probabilistic models. By Artem Sokolov.

stream.net Functions with example data for creating, importing, attributing, analyzing, and displaying stream networks represented as binary trees. Capabilities include upstream and downstream distance matrices, stochastic network generation, segmentation of network into reaches, adding attributes to reaches with specified statistical distributions, interpolating reach attributes from sparse data, analyzing auto-correlation of reach attributes, and creating maps with legends of attribute data. Target applications include dynamic fish modeling. By Denis White.

svcm Fir 2-d and 3-d space-varying coefficient models to regular grid data using either a full B-spline tensor product approach or a sequential approximation. By Susanne Heim, with support from Paul Eilers, Thomas Kneib, and Michael Kobl.

tdm A tool for therapeutic drug monitoring. Can estimate individual pharmacokinetic parameters with one or more drug serum/plasma concentrations obtained from a single subject or multiple subjects, calculate a suggested dose with the target drug concentration or calculate a predicted drug concentration with a given dose. By Miou-Ting Chen, Yung-Jin Lee.

titan GUI to analyze mass spectrometric data on the relative abundance of two substances from a titration series. By Tom Price.

tkrgl TK widget tools for package **rgl**. By Duncan Murdoch and Ming Chen.

tm A framework for text mining applications within R. By Ingo Feinerer.

trip Access and manipulate spatial data for animal tracking. By Michael D. Sumner.

wombsoft Wombling Computation. Analyses individually geo-referenced multilocus genotypes for the inferences of genetic boundaries between populations. Based on the wombling method which estimates the systemic function by looking for the local variation of the allele frequencies. By Ameline Crida.

yaImpute Perform *k*-NN imputation. By Nicholas L. Crookston and Andrew O. Finley.

Other changes

- Package **micEcdat** was moved from the main CRAN section to the Archive.
- Package **SAGx** was removed from CRAN.

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R Foundation News

by Kurt Hornik

Donations and new members

Donations

Peter M Maksymuk (USA)

New benefactors

Schröder Investment Management Ltd., London, GB
Prediction Company, Santa Fe, New Mexico, USA

New supporting institutions

Ef-prime Inc., Tokyo, Japan

New supporting members

David Vonka (CZ)
Olivier Celhay (France)
Katarzyna Kopczewska (Poland)

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R News Referees 2006

by Torsten Hothorn

R News articles are peer-reviewed by external and independent experts. The editorial board members would like to take the opportunity to thank all referees who read and commented on submitted manuscripts during the last year. Much of the quality of R News publications is due to their invaluable and timely service. Thank you!

- Murray Aitkin
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