## Release notes

Lobry, J.R. Necşulea, A. Palmeira, L. Penel, S. July 4, 2017

## Introduction

The release notes are listed in reverse chronological order: most recent on top.

# 3.4 series (JUL 2017)

### release 3.4-0

- New test file kaks-torture.fasta and corresponding dataset kaksTorture to check results of function kaks().
- Function read.alignment() can now handle legacy fasta format with commented lines starting with a semicolon.
- Function kaks() has gained a new argument rmgap to control gap removal option.
- As pointed by e-mail on 27-JUN-2017 by Sylvain Charlat the function kaks() could return non-finite values especially with short sequences. This is no more the case and a routine test checks now that computing the  $K_a$  and  $K_s$  values between all possible pairs of codons doesn't yield non-finite values.
- The routine check in the documentation of the kaks() function with data(AnoukResult) is active again.

## 3.3 series

#### release 3.3-6

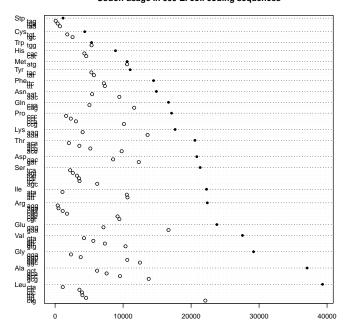
- Outdated URL in the documentation of function oriloc() were fixed.
- Addition of packagename\_init.c and modifications for registered routines.

## release 3.3-4

• As pointed by e-mail on 14-OCT-2016 by Christine Oger there was a bug in the function dotchart.uco() yielding points with an excessive size. This now fixed, for instance:

```
data(ec999)
ec999.uco <- rowSums(sapply(ec999, uco, index="eff"))
dotchart.uco(ec999.uco, main = "Codon usage in 999 E. coli coding sequences")</pre>
```

#### Codon usage in 999 E. coli coding sequences



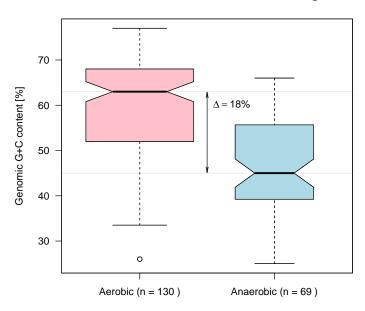
## release 3.3-3

- As requested by Kurt Hornik on 12-OCT-2016 the name seqinR was changed to seqinr in the CITATION file.
- New dataset gc02 that was used in Naya et al [20]. For instance to show the dramatic effect of aerobiosis on genomic G+C content in bacteria:

```
data(gc02)
vby <- function(...) as.vector(by(...))
first <- function(x) as.character(x[1])
GCbyGenus <- with(gc02, data.frame(
   Genus = vby(Genus, Genus, first),
   GC = vby(GC, Genus, mean),
   aerobiosis = vby(aerobiosis, Genus, first),
   n.species = vby(GC, Genus, length)))</pre>
```

```
with(GCbyGenus, {
  mybxp <- boxplot(GC~aerobiosis, xaxt = "n", yaxt = "n", ann = FALSE,
      names = c(paste("Aerobic (n =", sum(aerobiosis == "Aerobic"), ")"),
      paste("Anaerobic (n =", sum(aerobiosis == "Anaerobic"), ")")),
      varwidth = TRUE, notch = TRUE)
  y1 <- median(GC[aerobiosis == "Anaerobic"])
  y2 <- median(GC[aerobiosis == "Aerobic"])
  arrows(1.5, y1, 1.5, y2, code = 3, angle = 10, length = 0.1)
  abline(h = y1, col = grey(0.9))
  abline(h = y2, col = grey(0.9))
  text(1.5, 60, bquote(paste(Delta == .(y2 - y1), "%")), pos = 4)
  bxp(mybxp, varwidth = TRUE, notch = TRUE, add = TRUE,
      main = paste("Distribution of G+C content in", length(GC), "bacterial genera"),
      las = 1, ylab = "Genomic G+C content [%]", boxfill = c("pink", "lightblue"))}
)</pre>
```

#### Distribution of G+C content in 199 bacterial genera



• New dataset gcT that was used in [4]. For instance to reproduce figure 2:

```
data(gcT)
with(gcT[["genus"]], plot(Topt, GC, las = 1,
   main ="Figure 2 from Galtier & Lobry 1997 (n = 224 genera)",
   xlab = "Optimal growth temperature [C]", ylab = "Genomic G+C content [%]"))
```

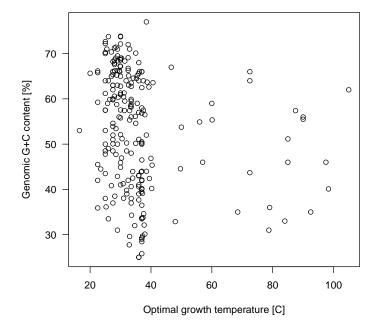


Figure 2 from Galtier & Lobry 1997 (n = 224 genera)

## release 3.3-2

• As pointed by e-mail on 04-OCT-2016 by Paulo Jorge Moura Pinto da Costa Dias three new genetic code were missing. They are now included.

## release 3.3-1

## release 3.3-0 in memoriam 2016-07-14

- Function extractseqs() has gained an extra argument zlib defaulting to FALSE so that it can be used on any platform. This follows from a request by Sam Borstein on 10-JUL-2016 on how to extract D-loop/control region in mitochondrial genomes. An example is now given in the FAQ.
- Function read.alignment() has been modified according to Matthew Krause in order to read abreviated path like '~login/alignment.txt' as filename. The C source code as been modified as well according to Matthew Krause in order to avoid problems due to corrupted or empty files.

## 3.2 series

#### release 3.2-0

- Images have been inserted in the documentation for datasets aacost, chargaff, m16j, waterabs and for the function dia.db.growth().
- Function gb2fasta() now uses a local file example.
- As pointed out by e-mail on 11-JUN-2016 by Haruo Suzuki a call to AA-stat() function may yield uninformative warning messages. The culprit is the computePI() function. This is now fixed.
- As from seqinR 3.2-0 we are switching to a lazy sticky scheme for seqinR release numbers. Release 3.2-x means that seqinR was checked against R release 3.2-y. In short, we are trying to follow R major revision numbers. This does not mean that you need a brand new version of R to run seqinR, for instance at this point (2016-06-17) you need at least R version 2.10.0 that was released in 2009. This new numbering scheme is just a matter of convenience.

## 3.1 series

#### release 3.1-5

- As pointed out by e-mail on 30-MAY-2016 by Haruo Suzuki a call to getLength(ec999) yielded spurious output and many warnings. This is now fixed.
- As pointed out by e-mail on 30-MAY-2016 by Haruo Suzuki there was a bug in the documentation of the functions recstat(), draw.recstat(), test.co.recstat() and test.li.recstat(). They were all looking for data in a package seqinr2 that doesn't exist. This is now fixed and the dontrun directive has been removed to detect automatically any further problem.
- As pointed out by e-mail on 25-MAY-2016 by Haruo Suzuki the read.fasta() function can import sequences directly from *local* gzipped files. A new smallAA.fasta.gz file has been added to document this in the examples of the read.fasta() function. This is however no more true if you try to read directly the sequences from a compressed file accessed via its URL. A workaround now given in the manual is to use a construct like read.fasta(gzcon(url(myurl))).
- As pointed out by e-mail on 12-MAY-2016 by Haruo Suzuki the documentation for the rho() function was misleading because in the refered article
   [9] the statistic was computed from the sequence concatenated with its inverted complement. This is now fixed.

#### release 3.1-4

- As pointed out by e-mail on 27-APRIL-2016 by Matthias Döring, R and Y were not correctly implemented in the comp() function. This is now fixed.
- As suggested by e-mail on 23-DECEMBER-2014 by Matt Huska, ade4 package has been switched from "Depends" to "Imports" in the DESCRIP-TION file.

#### release 3.1-1

• Removal of zlib code and headers with help from Prof. Ripley

#### release 3.1-0

• As suggested by e-mail on 19-NOVEMBER-2014 by Tang Chin Cheung, examples involving the query() function have been modified according to the new features of R-3.1.2. Indeed since R-3.1.2 it is not possible to change an object belonging to the global environment from a package, as spotted by e-mail on 4-NOVEMBER-2014 by T.J. Agin.

## 3.0 series

#### release 3.0-11

- In query(), NS=taxon\_name and NK=keyword\_name are now documented. The manual was also updated.
- The broken default link in get.db.growth() has been fixed so that now dia.db.growth() works as well.
- Function write.fasta() has gained an as.string argument so that it can handle sequences provided as strings instead of vectors of single character.

#### release 3.0-10

• As pointed out by e-mail on 5-MAY-2014 by Jan-Hendrik Troesemeier, the read.alignment() function was sending segfault with non-mase data. This is now fixed in the src/alignment.c source according to Jan-Hendrik Troesemeier suggestion.

## release 3.0-9

• As suggested by e-mail on 17-JANUARY-2014 by Peter Hraber, the dist.alignment() function include a new option for nucleotide sequences: if set to 1, gaps will be counted in the identity measure. (in case there is a gap aligned with and a non-gap, the number of difference is incremented.).

#### release 3.0-7

- As pointed out by e-mail on 04-OCTOBER-2013 by Jeremy Shearman, the comp() function was misleading when N's (instead of n's) were present in the sequence. This is now fixed.
- As pointed out by e-mail on 29-MAY-2013 by Domenico Cozzetto, the read.alignment() function was chopping sequence names after the first space. This is now fixed for FASTA, CLUSTAL and MASE formats.

#### release 3.0-6

- As pointed out by e-mail on 13-AUGUST-2012 by Grabor Grothendieck, the pipe caracter was not correctly processed in stresc() function. This is now fixed.
- As suggested by e-mail on 8-FEBRUARY-2012 by Juanjo Abellan, the kaks() function has been modified: new verbose option for display values of L0,L2,L4,A0,A2,A4,B0,B2,B4 has been added.

#### release 3.0-5

• As pointed out by e-mail on 3-FEBRUARY-2012 by Dave Gerrard, the consensus() function returns NA for all invariant sites when threshold is 1. Changing 'superior' into 'superior or equal' in the consenus function fixed this bug.

#### release 3.0-0

• As pointed out by Leonor Palmeira on the rpourlesnuls diffusion list on 20-MAY-2010 there was no constructor for objects of class alignment. There is now a as.alignment() function.

## 2.0 series

- As pointed out by Avril Coghlan on the seqinR diffusion list on 17-MAR-2010 there was a bug in the getAnnot() function. This is now fixed.
- As suggested by Avril Coghlan on the seqinR diffusion list on 02-MAR-2010 the function rho() has gained a wordsize argument.
- The argument word in function count() is now more explicitly called wordsize.
- The example section in file read.alignment.Rd has gained a new quality control sanity check.

- The File argument that was deprecated since seqinR release 1.1-3 in function read.alignment() is no more valid. Just use file instead.
- As pointed by Darren Obbard on the seqinr diffusion list on 05-MAR-2010 there was a memory leak problem when calling the read.alignment() function with the fasta format. This is now fixed for the fasta format, but the remaining formats have not been checked for this problem.

#### release 2.0-8

- As pointed by Oliver Clay and Lionel Guy on the sequin diffusion list on 19-FEB-2010 there was a bug in getSequence.list() function that confused write.fasta() when all sequences were of the same length (a similar bug was reported by Yann Lesecque on 30-MAR-2009 for the getTrans() function). This is now fixed.
- The message printed when function where.is.this.acc() fails to find a database with a given accession number for a sequence is now completed to warn the user that (s)he may have supplied a sequence name instead of a genuine accession number.
- The title in the documentation for the function write.fasta() was changed to make clear that more than one sequence can be written at once. The function now does not return anything instead of NULL previously. The argument file.out was moved to the left so that it is easier now to use it by position during function call.

- A new utility function where.is.this.acc() was introduced to loop over all availabale ACNUC databases to look for a given sequence accession number. This is useful when you have a sequence accession number and you don't know in which database it is present. The documentation of the function choosebank() was also changed to make a link to this function. As suggested by Avril Coghlan, the function has an argument stopAt-First defaulting to TRUE that stops the search at the first database found with the given accession number.
- As pointed out 05 Nov 2009 by Darren Obbard on the sequin diffusion list the argument forceToLower = FALSE in function comp() was not honored. This is now fixed and a new sanity check was added in the example section of the documentation of the function.
- Documentation for the function uco() for codon usage table computation was updated with new bibliographical references [18, 31].
- As basic regular expressions are defunct since R 2.11, the extended argument in functions words.pos() and trimSpace() was no more necessary. It is now deleted.

#### release 2.0-6

- The old argument File in function read.fasta() that was deprecated since release 1.1-3 is no more valid. Just use file instead.
- New function stutterabif() to estimate stutter ratio.
- Function plotabif() has a new default value for its ylim argument: c(min(y), max(y)) now instead of c(0, max(y)) previously to help ploting data with a highly negative baseline.
- Function peakabif() now returns in addition an estimate of the baseline value.
- New utility baselineabif() to estimate the baseline value.
- There was time shift of one datapoint unit for the peak locations returned by the peakabif() function, this is now fixed and the documentation is more explicit for the units used.
- New utility function fastacc() to compute the number of alleles in common between a genetic profile and a database of genetic profiles.

#### release 2.0-5

- New utility function circle() to draw a circle.
- Two more examples of files to be imported with the readBins() and read-Panels() functions are now available in the abif folder: NGM\_Bins.txt and NGM\_Pa.txt, respectively.
- New function plotPanels() to plot amplicon size ranges of STR kits data.
- New utility function col2alpha() to add a transparency chanel to a standard R color.
- New ABIF example file samplefsa2ps.fsa used in the read.abif() function to reproduce figure 1A from [12].
- New function move() aliased as mv() to rename an object without deep copy.
- New function swap() to exchange two objects.

## release 2.0-4

• Configuration files to be imported by the readBins() function may have trailling tabulations, as for instance in the test file Prototype\_PowerPlex\_EP01\_Bins.txt for allele 9 at locus D3S1358 and for allele 14 at locus D12S391. This was a source of trouble during importation. This is now fixed and the above mentioned file is used as a quality control. A warning is now issued if the

number of columns in the data frame corresponding to a locus is not 4 as expected.

• Configuration files to be imported by the readPanels() function may have more than one tabulation separator between two data items in a way that could be different from one line to another one. There is an example of such a case in the test file Prototype\_PowerPlex\_EP01\_Pa.txt where locus D10S1248 and D22S1045 are followed by a single tabulation when all remaining loci are followed by two tabulations. This was a source of trouble during importation. This is now fixed by preprocessing the input so that all consecutive tabulations are replaced by a single one. The above mentioned test file is now used as a quality control.

- As pointed out on the seqinr diffusion list on 23-APR-2009 by Darren Obbard there was an obscure error message when function kaks() was called with an alignment such that the number of nucleotides was not a multiple of 3 after gap removal. This check was partial as an alignment with out-of-frame gaps but with a total number of gaps multiple of 3 was not detected. The new behaviour is that if at least one non ACGT base is found in a codon, then the whole codon is forced to a gap codon (--). The documentation of the function has been clarified accordingly, and a new alignment file DarrenObbard.fasta added in the sequences folder to check this new behaviour.
- Function readBins() is now more tolerant when there is an extra column with possibly empty fields in data by forcing the fill argument of read.table() function to TRUE.
- As pointed out by e-mail on 30-MAR-2009 by Yann Lesecque there was a
  bug in the getTrans() function: when applied to a list of sequences with
  all the same length the returned result was a matrix instead of a list. This
  is now fixed.
- New utility functions readPanels() and readBins() to import data from GeneMapper configuration files. Four example files are now in the abif folder.
- Function peakabif() now returns the heights and surfaces of peaks in addition to their location.
- New utility function al2bp() to convert a forensic microsatellite allele name into its length in base pairs. Conventions used to name forensic microsatellite alleles (STR) are described in Bar et al. (1994) [1]. The name 9.3 means for instance that there are 9 repetitions of the complete base oligomer and an incomplete repeat with 3 bp.

#### release 2.0-2

- New ABIF format related functions: plotabif() to plot electrophoregrams with optonial internal size standard and optional allelic ladder, peakabif() to locate peaks in electrophoregrams, plotladder() to display an observed allelic ladder.
- New datasets gs500liz for size standards, identifiler for allelic ladder names, ECH for allelic ladder raw data and JLO for forensic genetic profile raw data. The last one is now used as a quality check for the read.abif() function.
- A new folder called abif has been created under the inst folder. The purpose of this folder is to contain examples of files in ABIF format so that the results of the read.abif() function can be checked against expected results for quality check. It contains for now two duplicated genetic profiles and two allelic ladders from the same batch experiment.

#### release 2.0-1

- The useless itemize in the argument section of documentation file stresc.Rd is now deleted.
- In function words.pos() the default value for parameter extended was changed from FALSE to TRUE to avoid warnings.
- New experimental function read.abif() to import files in ABIF format (\*.fsa, (\*.ab1).

- New draft chapter about making RISA in silico added.
- Objects from class qaw created after a call to the query() function have gained a new generic print method to focus on the most important information: number of sequences in the list, list type and the corresponding request.
- Function query() now allows a missing listname argument. In this case, list1 is used to store the result.
- Function autosocket() has been changed to behave more friendly with outdated R versions. This is essentially a backward compatibility issue that will not be maintained in the future. The function autosocket() works hard to check that everything is OK with the last opened database, especially with the socket infos available in banknameSocket\$socket thru its summary() generic. In old R versions (e.g. 2.6.2) this was returning socket instead of sockconn for the class, yielding an error in seqinR 1.1-7. The old result is now allowed but a warning is issued.

The 2.0 series started in summer 2008 along with the moving of the seqinr sources on R-forge.

## 1.1 series

- As suggested by Kurt Hornik two extra cr in the documentation file for ec999 were deleted.
- Function read.fasta() has gained four new arguments (viz. bfa, sizeof.longlong, endian, apply.mask) to read DNA binary fasta files in MAQ format.
   There is a new ct.bfa file in the sequences folder to check for the MAQ format reading.
- New dataset pK for the values for the side chain of charged amino acids from various sources compiled by Joanna Kiraga [11].
- Function words.pos() has gained new arguments that are passed to regexpr() including the dot-dot-dot argument in case of need in the future. The documentation has been modified to better explain the difference with the standard gregexpr() function.
- As pointed by e-mail on 28 May 2008 by Kim Milferstedt a function to compute the consensus for a set of aligned sequences would be helpful. There is now a function consensus() aliased to con() for this. The input is either an object from class alignment or a matrix of characters. The output is either a consensus sequence (using the majority rule, the majority rule with a threshold, or IUPAC symbols for RNA and DNA sequences) or a profile, that is a matrix with the count of each possible character at each position in the alignment.
- In the documentation of the read.alignment() function a link was added to the read.nexus() function from the ComPairWise package [26].
- New function bma() to find the IUPAC symbol corresponding to a nucleic sequence.
- New function as.matrix.alignment() to convert an alignment into a object of class matrix.
- The encoding of line ends in the example file test.mase is now an unix-like one
- As pointed by e-mail on 31 May 2008 by Marie Sémon there was no convenient function to compute the Codon Adaptation Index [29]. A new function cai() was introduced with the aim of reproducing exactly the results from the program codonW that was written by John Peden during

his PhD thesis [24] under the supervision of P.M. Sharp (the most authorative source for CAI computation). A new dataset caitab that was hard-encoded in codonW for the w values for some species (viz Escherichia coli, Bacillus subtilis, Saccharomyces cerevisiae) was added. Care was taken to credit original sources. The E. coli data that was uncredited is from [29]. The B. subtilis data that was uncredited is from [30] (see the note of caution in ?caitab before using this one directly to compute CAI in B. subtilis). The S. cerevisiae data that was credited to [28] dates back from [29]. A new text file scuco.txt produced by codonW was added in the sequences folder to check that the CAI results from cai() are consistents with thoses from codonW version 1.4.4 (03-MAR-2005). This legacy file is used in the example section of the cai() function.

#### release 1.1-6

- The construct get(getOption("device"))(width = 18, height = 11) that was used in the example section for data(prochlo) is no more valid since @ 2.8.0 (fall 2008). The example has been restricted to work only with X11, windows and quartz devices.
- As pointed by e-mail on 12 May 2008 by Indranuj Mukherjee there was a bug in the function oriloc(): when called with a gbk = NULL argument the function was trying to remove non-existent files, yielding an error. The bug has been fixed and the documentation of the function oriloc() has been extended to better explain how to use the arguments seq.fasta and gbk.
- A reference to [7] was missing in the documentation of function zscore() for the codon model.
- As suggested by e-mail on 11 Mar 2008 by Christian Gautier, the function count() has gained a new argument by to control the window step, allowing for instant to count dinucleotides in codon position III-I in a coding sequence. The example section of the function documentation has been extended to give an example of counting dinucleotides in position III-I.

```
alldinuclIIIpI <- s2c("NNaaNatNttNtgNgtNtcNctNtaNagNggNgcNcgNgaNacNccNcaNN")
(resIIIpI <- count(alldinuclIIIpI, word = 2, start = 2, by = 3))

aa ac ag at ca cc cg ct ga gc gg gt ta tc tg tt
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1

stopifnot(all( resIIIpI == 1))
```

• Function reverse.align() has gained two arguments forceDNAtolower = TRUE and forceAAtolower = FALSE that are passed to the functions used to read the sequences. There is now a new dataset revaligntest used to check the result in the example section of reverse.align().

- As pointed by e-mail on 21 Feb 2008 by Oliver Keatinge Clay function modifylist() failed to scan in GenBank FEATURES annotation lines. There is now a new function called prepgetannots(), aliased to pga(), that allows to set up the annotation lines to be scanned. Called with default arguments, this function turns on all annotation lines for scan. This function can also be used to set up partly the annotation lines to be returned by getAnnot().
- Function choosebank() has gained four arguments (server, blocking, open, encoding) that are passed to socketConnection(). The value of the argument verbose is now passed to clientid() which knows now how to handle it. The encoding argument was introduced to fix a localization bug on Mac OS X which symptom was a cryptic error message in if (res[1] != "0") { after a call to choosebank(). The culprit was an option(encoding = "latin1") that was set up before the call to choosebank() who called socketConnection() with its default encoding = getOption("encoding"), preventing readLines() to read from the socket. The bug was fixed by opening the socket with the native encoding, which is the current default.
- As pointed by e-mail on 15 Jan 2008 by Stefanie Hartmann, the argument frame in function count() was misleading for someone with a molecular biology background. The argument has been replaced by start. The old argument name is maintained as an alias for backward compatibility. The example section has been extended to give an example with the complete human mitochondrion sequence, the corresponding fasta file (humanMito.fasta) has been added in the sequences directory.

#### release 1.1-5

Minor release to fix mainly problems in the documentation.

- The argument section was empty in autosocket.Rd.
- The details section was empty in countfreelists.Rd and draw.oriloc.Rd.
- The value section was empty in gbk2g2.Rd. The corresponding function was changed to use a local file for the demo.
- The description section was missing in getFrag.Rd, getLength.Rd, get-Name.Rd, getSequence.Rd.
- Documentation of the function dia.bactgensize() to plot the distribution of bacterial genome size from GOLD data has been ammended to credit sources [13, 2, 15, 14]. It has gained a new argument maxgensize defaulting to 20000 to remove outliers. It has also gained a new argument source for the file to look for raw data, defaulting to an (outdated) local copy so that the function can be called even when there is no internet connection.

## release 1.1-4 (10-Dec-2007)

Minor release to fix problems found by Kurt Hornik.

- In the DESCRIPTION file License: GPL (>= 2) instead of License: GPL version 2 or newer.
- The files inst/doc/src/mainmatter/acnuc\_sockets.rnw .tex with non-portable file names were changed to acnucsocket.rnw and acnucsocket.tex.

- There is a new chapter to explain how to set up a local ACNUC server on Unix-like platforms.
- New dataset m16j to make a GC skew plot as in [17].
- New dataset waterabs giving the absorption of light by water. This dataset was compiled by Palmeira [22] from [16, 25].
- Generic functions getAnnot(), getFrag(), getKeyword(), getLength(), getLocation(), getName(), getSequence() and getTrans() have gained methods to handle objects from class list and qaw.
- Functions getAttributsocket() and getNumber.socket() are now deprecated, a warning is issued.
- There is a new appendix in which all the examples protected by a dontrun statement are forced to be executed.
- Function read.fasta() now supports comment lines starting by a semicolon character in FASTA files. An example of such a file is provided in sequences/legacy.fasta. The argument File is now deprecated. There is a new argument seqonly to import just the sequences without names, annotations and coercion attempts. There is a new argument strip.desc to remove the leading '>' character in annotations (as in function read-FASTA from the Biostrings package [21]). The FASTA file example some-ORF.fsa from Biostrings is also added for comparisons.
- Function GC() has gained a new argument NA.GC defaulting to NA to say what should be returned when the GC content cannot be computed from data (for instance with a sequence like NNNNNNNNNNNNNN). The argument oldGC is now deprecated and a warning is issued. Functions GC1(), GC2(), GC3() are now simple wrappers for the more general GCpos() function. The new argument frame allows to take the frame into account for CDS.
- Function read.alignment() has gained a new argument forceToLower defaulting to TRUE to force lower case in the character of the sequence (this is for a smoother interaction with the package ape). The argument

File is now deprecated and a warning is issued when used instead of file. The example in the function kaks() has been corrected to avoid this warning when reading the example files.

- New low level utility function acnucclose() and quitacnuc() to close an ACNUC server. These functions are called by closebank() so that a simple call to it should be enough.
- New low level utility function clientid() to send the client ID to an ACNUC server.
- New low level utility function countfreelists() to get the number of free lists available in an ACNUC server.
- New low level utility function knowndbs() and its shortcut kdb() to get a description of databases known by an ACNUC server.
- New low level utility function autosocket() to get the socket connection to the last opened ACNUC database.
- New function countsubseqs() to get the number of subsequences in an ACNUC list.
- New function savelist() to save sequence names or accession numbers from an ACNUC list into a local file.
- New function ghelp() to get help from an ACNUC server.
- New function modifylist() to modify a previously existing ACNUC list
  by selecting sequences either by length, either by date, either for the presence of a given string in annotations.
- New low level function getlistate() to ask for information about an ACNUC list.
- New low level function setlistname() to set the name of a list from an ACNUC server.
- New function residuecount() to count the total number of residues (nucleotides or aminoacids) in all sequences of an ACNUC list of specified rank.
- New function isenum() and its shortcut isn() to get the ACNUC number of a sequence from its name or accession number.
- New function prettyseq() to get a text representation of a sequence from an ACNUC server.
- New function gfrag() to extract sequence identified by name or by number from an ACNUC server.

- The details of the socket connection are no more stored in the slot socket for objects of class seqAcnucWeb: this slot is now deleted. As a consequence, the argument socket in function as.SeqAcnucWeb() has been removed and there is now a new argument socket = "auto" in functions getAnnot(), getFrag(), geyKeyword(), getLocation(), and getSequence(). The default value "auto" means that the details of the socket connection are taken automatically when necessary from the last opened bank. The size of local lists of sequences is reduced by about a third now as compared to the previous version.
- New function print.seqAcnucWeb() to print objects from class seqAcnucWeb.
- Internal function parser.socket() has been optimized and is about four times faster now. This decreases the time needed by the query() function.

#### release 1.1-2

- New function trimSpace() to remove leading and trailing spaces in string vectors.
- Function splitseq() is no more based on substring(), it is now more efficient for long sequences.
- A sanity check test was added in the documentation file for the function syncodons().
- The way this manual is produced is now documented in the doc/src/template/ folder.
- A bug in function oriloc() was reported on 23 Jul 2007 by Michael Kube: using directly genBank files was no more possible. The culprit was gbk2g2() that turns genBank files into glimmer files version 2 when oriloc() default is to use version 3 files. The glimmer.version argument is now forced to 2 when working with genBank files to fix this problem.
- Function zscore() has now a new argument exact (which is only effective for the option model = base). This argument, when set to TRUE allows for the exact analytical computation of the zscore under this model, instead of the approximation for large sequences. It is set to FALSE by default for backward compatibility.

#### release 1.1-1

• A bug was reported by Sylvain Mousset on 14 Jul 2007 in function dist.alignment(): when called with sequences in lower case letters, some sequences were modified. This should no more be the case:

- The CITATION file has been updated so that now citation("seqinr") returns the full complete reference for the package seqinR.
- Non ASCII characters in documentation (\*.Rd) files have been removed. Declaration of the encoding as latin1 when necessary is now present. The updated documentation files are: dinucl.Rd, gb2fasta.Rd, get.ncbi.Rd, lseqinr.Rd, n2s.Rd, prochlo.Rd, s2c.Rd, SeqAcnucWeb.Rd, SeqFrag.Rd, toyaa.Rd, words.pos.Rd, words.Rd, zscore.Rd.
- Function GC() and by propagation functions GC1(), GC2() and GC3() have gained a new argument oldGC allowing to compute the G+C content as in releases up to 1.0-6 included. The code has been also modified to avoid divisions by zero with very small sequences.
- New function rot13() that returns the ROT-13 encoding of a string of characters.

## 1.0 series

- A new *experimental* function extractseqs() to download sequences thru zlib compressed sockets from an ACNUC server is released. Preliminary tests suggest that working with about 100,000 CDS is possible with a home ADSL connection. See the manual for some system.time() examples.
- As pointed by e-mail on 16 Nov 2006 by Emmanuel Prestat the URL used in dia.bactgensize() was no more available, this has been fixed in the current version.
- As pointed by e-mail on 16 Nov 2006 by Guy Perrière, the function oriloc() was no more compatible with glimmer 3.0 outputs. The function has gained a new argument glimmer.version defaulting to 3, but the value 2 is still functional for backward compatibility with old glimmer outputs.

<sup>&</sup>lt;sup>1</sup>Glimmer is a program to predict coding sequences in microbial genomes [27, 3].

- As pointed by e-mail on 24 Oct 2006 by Lionel Guy (http://pbil.univ-lyon1.fr/seqinr/seqinrhtmlannuel/03/0089.html) there was no default value for the as.string argument in the getSequence.SeqFastadna(). A default FALSE value is now present for backward compatibility with older code.
- New utility vectorized function stresc() to escape LATEX special characters present in a string.
- New low level function readsmj() available.
- A new function readfirstrec() to get the record count of the specified ACNUC index file is now available.
- Function getType() called without arguments will now use the default ACNUC database to return available subsequence types.
- Function read.alignment() now also accepts file in addition to File as argument.
- A new function rearranged.oriloc() is available. This method, based on oriloc(), can be used to detect the effect of the replication mechanism on DNA base composition asymmetry, in prokaryotic chromosomes.
- New function extract.breakpoints(), used to extract breakpoints in rearranged nucleotide skews. This function uses the segmented package to define the position of the breakpoints.
- New function draw.rearranged.oriloc() available, to plot nucleotide skews on artificially rearranged prokaryotic chromosomes.
- New function gbk2g2.euk() available. Similarly to gbk2g2(), this function extracts the coding sequence annotations from a GenBank format file. This function is specifically designed for eukaryotic sequences, *i.e.* with introns. The output file will contain the coordinates of the exons, along with the name of the CDS to which they belong.
- After an e-mail by Marcelo Bertalan on 26 Mar 2007, a bug in oriloc()
  when the gbk argument was NULL was found and fixed by Anamaria
  Necsulea.
- Functions translate() and getTrans() have gained a new argument NAstring to represent untranslatable amino- acids, defaulting to character "X"
- There was a typo for the total number of printed bases in the ACNUC books [5, 6]: 474,439 should be 526,506.
- Function invers() has been deleted.

- Functions translate(), getTrans() and comp() have gained a new argument ambiguous defaulting to FALSE allowing to handle ambiguous bases. If TRUE, ambiguous bases are taken into account so that for instance GGN is translated to Gly in the standard genetic code.
- New function amb() to return the list of nucleotide matching a given IU-PAC nucleotide symbol.
- Function count() has gained a new argument alphabet so that oligopeptides counts are now possible. Thanks to Gabriel Valiente for this suggestion. The functions zscore(), rho() and summary.SeqFastadna() have also an argument alphabet which is forwarded to count().

#### release 1.0-6

Release 1.0-6 is a minor release to fix a problem found and solved by Kurt Hornik (namely a change from SET\_ELEMENT to SET\_STRING\_ELT in C code for s2c() in file util.c). The few changes are as follows.

- More typographical option for the output LATEX table of tablecode() are now available to outline deviations from the standard genetic code (see example in the appendix "genetic codes" of the manual).
- A new dataset aaindex extracted from the aaindex database [10, 32, 19] is now available. It contains a list of 544 physicochemical and biological properties for the 20 amino-acids
- The default value for argument dia is now FALSE in function tablecode().
- The example code for data(chargaff) has been changed.

- A new function dotPlot() is now available.
- A new function crelistfromclientdata() is now available to create a list on the server from a local file of sequence names, sequence accession numbers, species names, or keywords names.
- A new function pmw() to compute the molecular weight of a protein is now available.
- A new function reverse.align() contributed by Anamaria Necşulea is now available to align CDS at the protein level and then reverse translate this at the nucleic acid level from a clustalw output. This can be done on the fly if clustalw is available on your platform.

- An undocumented behavior was reported by Guy Perrière for uco() when computing RSCU on sequences where an amino-acid is missing. There is now a new argument NA.rscu that allows the user to force the missing values to his favorite magic value.
- There was a bug in read.fasta(): some sequence names were truncated, this is now fixed (thanks to Marcus G. Daniels for pointing this). In order to be more consistent with standard functions such as read.table() or scan(), the file argument starts now with a lower case letter (file) in function read.fasta(), but the old-style File is still functional for forward-compatibility. There is a new logical argument in read.fasta() named as.string to allow sequences to be returned as strings instead of vector of single characters. The automatic conversion of DNA sequences into lower case letters can now be disabled with the new logical argument forceDNAtolower. It is also possible to disable the automatic attributes settings with the new logical argument set.attributes.
- A new function write.fasta() is now available.
- The function kaks () now forces character in sequences to upper case. This default behavior can be neutralized in order to save time by setting the argument forceUpperCase to FALSE.

- The scaling factor  $n_{\bullet \bullet}$  was missing in equation ??.
- The files louse.fasta, louse.names, gopher.fasta, gopher.names and ortho.fasta that were used for examples in the previous version of this document are no more downloaded from the internet since they are now distributed in the sequences/ folder of the package.
- An example of synonymous and non synonymous codon usage analysis was added to the vignette along with two toy data sets (toyaa and toycodon).
- A FAQ section was added to the vignette.
- A bug in getAnnot() when the number of lines was zero is now fixed.
- There is now a new argument, latexfile, in tablecode() to export genetic codes tables in a LATEX document, for instance table ?? and table ?? here.
- There is now a new argument, freq, in count() to compute word frequencies instead of counts.
- Function splitseq() has been entirely rewritten to improve speed.
- Functions computing the G+C content: GC(), GC1(), GC2(), GC3() were rewritten to improve speed, and their document files were merged to facilitate usage.

- The following new functions have been added:
  - syncodons() returns all synonymous codons for a given codon. Argument numcode specifies the desired genetic code.
  - ucoweight() returns codon usage bias on a sequence as the number of synonymous codons present in the sequence for each amino acid.
  - synsequence() generates a random coding sequence which is synonymous to a given sequence and has a chosen codon usage bias.
  - permutation() generates a new sequence from a given sequence, while maintaining some constraints from the given sequence such as nucleotide frequency, codon usage bias, ...
  - rho() computes the rho statistic on dinucleotides as defined in [8].
  - zscore() computes the zscore statistic on dinucleotides as defined in [23].
- Two datasets (dinucl and prochlo) were added to illustrate these new functions.

- The new package maintainer is Dr. Simon Penel, PhD, who has now a fixed position in the laboratory that issued seqinR (penel@biomserv.univ-lyon1.fr). Delphine Charif was successful too to get a fixed position in the same lab, with now a different research task (but who knows?). Thanks to the close vicinity of our pioneering maintainers the transition was sweet. The DESCRIPTION file of the seqinR package has been updated to take this into account.
- The reference paper for the package is now *in press*. We do not have the full reference for now, you may use citation("seqinr") to check if it is complete now:

```
citation("seqinr")
To cite seqinr in publications use:
   Charif, D. and Lobry, J.R. (2007)
Une entrée BibTeX pour les utilisateurs LaTeX est

@InCollection{,
    author = {D. Charif and J.R. Lobry},
    title = {Seqin{R} 1.0-2: a contributed package to the {R} project for statistical computing devoted to booktitle = {Structural approaches to sequence evolution: Molecules, networks, populations},
    year = {2007},
    editor = {U. Bastolla and M. Porto and H.E. Roman and M. Vendruscolo},
    series = {Biological and Medical Physics, Biomedical Engineering},
    pages = {207-232},
    address = {New York},
    publisher = {Springer Verlag},
    note = {{ISBN :} 978-3-540-35305-8},
```

- There was a bug when sending a gfrag request to the server for long (Mb range) sequences. The length argument was converted to scientific notations that are not understand by the server. This is now corrected and should work up the the Gb scale.
- The query() function has been improved by de-looping list element info request, there are now download at once which is much more efficient. For example, a query from a researcher-home ADSL connection with a list with about 1000 elements was 60 seconds and is now only 4 seconds (*i.e.* 15 times faster now).
- A new parameter virtual has been added to query() so that long lists can stay on the server without trying to download them automatically. A query like query(s\$socket,"allcds","t=cds", virtual = TRUE) is now possible.
- Relevant genetic codes and frames are now automatically propagated.
- SeqinR sends now its name and version number to the server.
- Strict control on ambiguous DNA base alphabet has been relaxed.
- Default value for parameter invisible of function query() is now TRUE.

## Session Informations

This part was compiled under the following @ environment:

- R version 3.4.0 (2017-04-21), x86\_64-apple-darwin15.6.0
- Locale: fr\_FR.UTF-8/fr\_FR.UTF-8/fr\_FR.UTF-8/C/fr\_FR.UTF-8/fr\_FR.UTF-8
- Running under: macOS Sierra 10.12.5
- Matrix products: default
- $\bullet \ \ BLAS: \verb|/Library/Frameworks/R.framework/Versions/3.4/Resources/lib/libRblas.0.dylib| \\$
- LAPACK: /Library/Frameworks/R.framework/Versions/3.4/Resources/lib/libRlapack.dylib
- Base packages: base, datasets, graphics, grDevices, grid, methods, stats, utils
- Other packages: ade4 1.7-6, ape 4.1, grImport 0.9-0, MASS 7.3-47, seqinr 3.4-0, tseries 0.10-41, XML 3.98-1.9, xtable 1.8-2
- Loaded via a namespace (and not attached): compiler 3.4.0, lattice 0.20-35, nlme 3.1-131, parallel 3.4.0, quadprog 1.5-5, quantmod 0.4-10, tools 3.4.0, TTR 0.23-1, xts 0.9-7, zoo 1.8-0

There were two compilation steps:

- @ compilation time was: Tue Jul 4 13:27:07 2017
- LATEX compilation time was: July 4, 2017

## References

- W. Bar, B. Brinkmann, P. Lincoln, W.R. Mayr, and U. Rossi. DNA recommendations. 1994 report concerning further recommendations of the DNA commission of the ISFH regarding PCR-based polymorphisms in STR (short tandem repeat) systems. *Int. J. Leg. Med.*, 107:159–160, 1994.
- [2] A. Bernal, U. Ear, and N. Kyrpides. Genomes online database (GOLD): a monitor of genome projects world-wide. *Nucleic Acids Research*, 29:126–127, 2001.
- [3] A.L. Delcher, D. Harmon, S. Kasif, O. White, and S.L. Salzberg. Improved microbial gene identification with GLIMMER. *Nucleic Acids Research*, 27:4636–4641, 1999.
- [4] N. Galtier and J.R. Lobry. Relationships between genomic G+C content, RNA secondary structures, and optimal growth temperature in prokaryotes. *Journal of Molecular Evolution*, 44:632–635, 1997.
- [5] C. Gautier, M. Gouy, M. Jacobzone, and R. Grantham. Nucleic acid sequences handbook. Vol. 1. Praeger Publishers, London, UK, 1982. ISBN 0-275-90798-8.
- [6] C. Gautier, M. Gouy, M. Jacobzone, and R. Grantham. Nucleic acid sequences handbook. Vol. 2. Praeger Publishers, London, UK, 1982. ISBN 0-275-90799-6.
- [7] C. Gautier, M. Gouy, and S. Louail. Non-parametric statistics for nucleic acid sequence study. *Biochimie*, 67:449–453, 1985.
- [8] S. Karlin and V. Brendel. Chance and statistical significance in protein and DNA sequence analysis. *Science*, 257:39–49, 1992.
- [9] S. Karlin and L.R. Cardon. Computational DNA sequence analysis. Annual Review of Microbiology, 48:619–654, 1994.
- [10] S. Kawashima and M. Kanehisa. AAindex: amino acid index database. *Nucleic Acids Res.*, 28:374–374, 2000.
- [11] J. Kiraga. Analysis and computer simulations of variability of isoelectric point of proteins in the proteomes. PhD thesis, University of Wrocław, 2008.
- [12] J. Krawczyk, A. Goesmann, R. Nolte, M. Werber, and B. Weisshaar. Trace2PS and FSA2PS: two software toolkits for converting trace and fsa files to PostScript format. Source Code for Biology and Medicine, 4:4, 2009.
- [13] N.C. Kyrpides. Genomes online database (GOLD 1.0): a monitor of complete and ongoing genome projects world-wide. *Bioinformatics*, 15:773–774, 1999.

- [14] K. Liolios, K. Mavrommatis, N. Tavernarakis, and N.C. Kyrpides. The genomes on line database (GOLD) in 2007: status of genomic and metagenomic projects and their associated metadata. *Nucleic Acids Research*, in press:D000–D000, 2008.
- [15] K. Liolios, N. Tavernarakis, P. Hugenholtz, and N.C. Kyrpides. The genomes on line database (GOLD) v.2: a monitor of genome projects worldwide. *Nucleic Acids Research*, 34:D332–D334, 2006.
- [16] R.A. Litjens, T.I. Quickenden, and C.G. Freeman. Visible and nearultraviolet absorption spectrum of liquid water. *Applied Optics*, 38:1216– 1223, 1999.
- [17] J.R. Lobry. Asymmetric substitution patterns in the two DNA strands of bacteria. *Molecular Biology and Evolution*, 13:660–665, 1996.
- [18] J.R. Lobry and D. Chessel. Internal correspondence analysis of codon and amino-acid usage in thermophilic bacteria. *Journal of Applied Genetics*, 44:235–261, 2003.
- [19] K. Nakai, A. Kidera, and M. Kanehisa. Cluster analysis of amino acid indices for prediction of protein structure and function. *Protein Eng.*, 2:93– 100, 1988.
- [20] H. Naya, H. Romero, A. Zavala, B. Alvarez, and H. Musto. Aerobiosis increases the genomic guanine plus cytosine content (GC%) in prokaryotes. *Journal of Molecular Evolution*, 55:260–264, 2002.
- [21] H. Pages, R. Gentleman, and S. DebRoy. *Biostrings: String objects representing biological sequences, and matching algorithms*, 2007. R package version 2.6.4.
- [22] L. Palmeira. Analyse et modélisation des dépendances entre sites voisins dans l'évolution des séquences d'ADN. PhD thesis, Université Claude Bernard Lyon I, 2007.
- [23] L. Palmeira, L. Guéguen, and J.R. Lobry. UV-targeted dinucleotides are not depleted in light-exposed prokaryotic genomes. *Molecular Biology and Evolution*, 23:2214–2219, 2006.
- [24] J.F. Peden. Analysis of codon usage. PhD thesis, University of Nottingham, 1999.
- [25] T.I. Quickenden and J.A. Irvin. The ultraviolet absorption spectrum of liquid water. *The Journal of Chemical Physics*, 72:4416–4428, 1980.
- [26] Trina E. Roberts. ComPairWise: Compare phylogenetic or population genetic data alignments, 2007. R package version 1.01.

- [27] S.L. Salzberg, A.L. Delcher, S. Kasif, and O. White. Microbial gene identification using interpolated Markov models. *Nucleic Acids Research*, 26:544–548, 1998.
- [28] P.M. Sharp and E. Cowe. Synonymous codon usage in *Saccharomyces cerevisiae*. Yeast, 7:657–678, 1991.
- [29] P.M. Sharp and W.-H. Li. The codon adaptation index a measure of directional synonymous codon usage bias, and its potential applications. *Nucleic Acids Research*, 15:1281–1295, 1987.
- [30] D.C. Shields and P.M. Sharp. Synonymous codon usage in *Bacillus subtilis* reflects both translational selection and mutational biases. *Nucleic Acids Research*, 15:8023–8040, 1987.
- [31] H. Suzuki, C.J. Brown, L.J. Forney, and E. Top. Comparison of correspondence analysis methods for synonymous codon usage in bacteria. *DNA Research*, 15:357–365, 2008.
- [32] K. Tomii and M. Kanehisa. Analysis of amino acid indices and mutation matrices for sequence comparison and structure prediction of proteins. *Pro*tein Eng., 9:27–36, 1996.