What's in 'rgr 1.1.13' ?

1. Statistical graphics functions:

gx.hist	Displays histograms using a variety of bin width selection methods.
cnpplt	Displays a normal cumulative percent probability (CPP) plot.
gx.cnpplts	Displays up to nine CPP plots in a single display, these may be either data subsets or variables.
gx.cnpplts.setup	Permits the user to define the symbols and their colours for the up to nine data sets to be plotted with gx.cnpplts.
gx.ecdf	Displays an empirical cumulative distribution function (ECDF).
gx.mf	Displays an empirical log-log concentration-number (C-N) plot.
gx.ks.test	Displays two ECDFs in a single display and carries out a Kolmogorov-Smirnov test for the two populations being drawn from the same underlying population.
bxplot	Displays a horizontal Tukey boxplot or a box-and-whisker plot.
shape	Displays a combination of a histogram, Tukey boxplot or a box-and-whisker plot, ECDF and CPP on a single screen/page.
shape.alt	Displays a combination of a histogram, ECDF, CPP and log-log C-N plot on a single screen/page.
inset	Displays a combination of a histogram and a CPP plot, together with some summary statistics, for use as an inset on a geochemical map.
inset.exporter	A version of 'inset' for use in a production environment where the graphics file is saved as defined by the user for later map production.
bwplots	Displays vertical box-and-whisker plots for a single variable subdivided into various subsets (groups or factors).
bwplots.by.var	Uses 'bwplot' to plot different variables (elements) side-by-side.
tbplots	Displays vertical Tukey boxplots for a single variable subdivided into various subsets (groups or factors).
tbplots.by.var	Uses 'tbplot' to plot different variables (elements) side-by-side.

All the above functions permit both normal arithmetic and logarithmic scaling, and user-defined axis labelling and titling. The 'bwplot' and 'tbplot' functions permit the groups (factors) to be ordered (left-to-right) and labelled as defined by the user.

2. Mapping and XY Plotting functions:

Mapping:

map.eda7	Displays a map using symbols that correspond to a Tukey boxplot, i.e. lower near and far outliers, in the lower whisker, in the mid 50%, in the upper whisker, etc.
map.eda8	Displays a map using symbols to indicate the magnitude of a variable (element) subdivided by the 2^{nd}, 5^{th}, 25^{th}, 50^{th}, 75^{th}, 95^{th} and 98^{th} percentiles.
map.tags	Displays a map of posted values.

map.z	Displays a map using circles that increase in diameter with magnitude of the variable (element) being plotted. The rate of increase of symbol size may be user-defined.
caplot	Displays a concentration-area (C-A) plot to assess whether the data are spatially multifractal. The data may be optionally log-transformed, and the interpolated estimates may be accumulated in either direction.

The above functions require that the R library packages 'MASS' and 'akima' (caplot only) be available at run-time. All the above functions require that rectangular coordinates are available for the data points, and permit user-defined axis labelling, titling, and symbol colour and scaling.

Note: the EDA mapping functions are not provided to replace a full mapping or GIS package, but to provide a 'quick-look' in order to appreciate the spatial distribution of the data and to support threshold (upper limit of geochemical background) selection.

Plotting:

xyplot.eda7	Displays a X-Y plot using symbols for the third that correspond to a Tukey boxplot, i.e. lower near and far outliers, in the lower whisker, in the mid 50%, in the upper whisker, etc.
xyplot.eda8	Displays a X-Y plot using symbols for the third variable to indicate the magnitude of the third variable variable (element) subdivided by the 2^{nd}, 5^{th}, 25^{th}, 50^{th}, 75^{th}, 95^{th} and 98^{th} percentiles.
xyplot.tags	Displays a X-Y plot of the posted values of a third variable.
xyplot.z	Displays a X-Y plot using circles that increase in diameter with magnitude of the third variable (element) being plotted. The rate of increase of symbol size may be user-defined.

3. Summary statistics functions:

gx.stats	Computes and displays summary statistics as for 'inset', and serves as a stats 'sub-engine' for various summary statistics functions..
gx.summary1	Displays a concise one-line summary statistics report.
gx.summary.mat	Displays a concise one-line summary statistics report for selected columns of a data frame or matrix.
gx.summary.groups	Displays a concise one-line summary statistics report for data subsets grouped by factor name in a data frame or matrix.
gx.summary2	Displays a five-line summary statistics report.
fences	Computes and displays the various estimates of background range discussed in Reimann, Filzmoser & Garrett, 2005.

fences.summary
: A version of 'fences' for when it is required to estimate background ranges for various subsets (groups or factors) of a variable (element) and to save them in a user-named tab delimited 'txt' file for later inspection with a spreadsheet program, e.g., Excel™.

framework.summary
: Computes summary statistics for various data subsets (groups or factors), e.g., EcoProvinces, Great Soil Groups, Lithological units, etc., of a variable (element) and saves them in a user-named 'csv' file for later inspection with a spreadsheet program, e.g., Excel™, or importation into other software.

gx.fractile
: Estimate the fractile for a specified quantile of a distribution.

gx.fractile
: Estimate the quantile for a specified fractile of a distribution.

gx.ngr.skew
: Estimate the skewness of a data set.

4. Bivariate and Multivariate functions:

gx.pearson
: Estimates the Pearson product moment correlation correlations for a matrix or columns of a data frame. The coefficients are displayed in the upper triangle and the significance of them not being due to chance (Ho: coefficient = 0) is displayed in the lower triangle.

gx.spearman
: Estimates the Spearman rank correlation correlations for a matrix or columns of a data frame. The coefficients are displayed in the upper triangle and the significance of them not being due to chance (Ho: coefficient = 0) is displayed in the lower triangle.

gx.sm
: Estimates a matrix of the robust ilr stabilities and log-ratio medians for a matrix or columns of a data frame of parts of a compositional data set; displaying them in the upper and lower triangles of the matrix, respectively.

gx.vm
: Estimates an Aitchison Variability Matrix for a matrix or columns of a data frame of parts of a compositional data set, with the variances and means of the log–ratios in the upper and lower triangles, respectively.

gx.pairs4parts
: Displays a graphical matrix of log10 scaled x-y plots in the upper triangle and boxplots of the ilr transforms in the lower triangle for the parts of a compositional matrix. The robust ilr stability for each x-y pair is displayed as the boxplot title.

gx.plot2parts
: Displays a panel of four plots for a pair of parts from a compositional data set. The displays consist of a log10 scaled x-y plot, a boxplot of the corresponding values of ilr(x,y) annotated with the robust ilr stability measure, and sequential index and ECDF plots of the ilr values.

gx.rma
: Estimates the coefficients of the Reduced Major Axis (RMA) for quantifying the relationship between two independent variables, such as analyses of the same samples by two independent methods. Confidence bounds are estimated for the coefficients to assist in determining if they are significantly different from (0,1). Optionally plots the data, the 1:1 line and the RMA.

wtd.sums
: Computes weighted sums (see Garrett and Grunsky, 2001) for a set of user defined variables and their 'relative importances'.

gx.scores	Function to compute scores on the basis of threshold estimates for a set of user defined variables. Optionally weights, including negatives, may be applied in score computation.
gx.2dproj	Computes 2-d projections of p-space data via the Sammon non-linear mapping, metric or non-metric multidimensional scaling, or projection pursuit procedures. Closed compositional, geochemical, data is accommodated through an optional ilr log-ratio transformation. A log transformation and a variety of data normalization procedures are available as pre-processing options for open, non-compositional, data sets. Optionally individual rows of the input matrix may be trimmed in a graphical adaptive interactive trimming (GAIT) procedure.
gx.2dproj.plot	Displays the results saved from function gx.2dproj.
gx.mva	Undertakes a R-Q Principal Components Analysis (PCA) and estimates Mahalanobis distances using classical covariance estimation procedures.
gx.mva.closed	As above but for closed, compositional data. Estimates classical statistics following an ilr transform, then back-transforms to the clr form for the PCA.
gx.md.gait	Undertakes a graphical adaptive interactive trimming (GAIT) procedure based on Mahalanobis distance estimation for multivariate outlier detection and the selection of clean 'reference' data subsets for use by gx.mv.alloc.
gx.md.gait.closed	As for gx.md.gait, but specifically for closed compositional, geochemical, data. The data are isometrically log-ratio (ilr) transformed for computational purposes, and then back transformed to the centred log-ratio (clr) basis for subsequent processing by gx.mvalloc.closed.
gx.md.plot	Displays Chi-square plots for the Mahalanobis distances saved from either gx.mva, gx.mva.closed, gx.robmva, gx.robmva.closed or gx.md.gait.
gx.md.print	Displays tables of all individuals and/or saves the tables as a 'csv' file, or individuals whose predicted probabilities of group membership fall below a user-defined cut-off value, i.e. multivariate outliers.
gx.md.display	Displays tables of all individuals and/or saves the tables as a 'csv' file, or individuals whose predicted probabilities of group membership fall below a user-defined cut-off value, i.e. multivariate outliers, together with additional variables from the source data frame or matrix. The saved '.csv' file can be imported into a spreadsheet program for report preparation.
gx.mvalloc	A typicality, Mahalanobis distance, based allocation procedure where an individual may be classified into one of up to nine 'reference', geochemical 'background', groups. If typicality, group membership, in all reference groups falls below a used defined cut-off, probability, those individuals are identified as outliers, 'anomalies', and allocated to an 'outlier' group. The allocations are made on the assumption that the reference group covariances are heteroscedastic, i.e. are of different sizes, shapes and orientations

gx.mvalloc.closed

As for gx.mvalloc, but specifically for closed compositional, geochemical data. The reference groups have to have been generated by gx.md.gait.closed or gx.robmva.closed, both of which return an inverse of the robust clr covariance matrix required by the allocation procedure. The input data are clr transformed prior to use in typicality estimations.

gx.mvalloc.print

Displays lists of all individuals and/or saves the list as a 'csv' file, or lists only individuals whose predicted probabilities of group membership fall below a user-defined cut-off value, i.e. multivariate outliers.

gx.lm.vif Estimates the variance inflation factor as a measure of collinearity in the independent (predictor) variables of a linear model.

gx.robmva Undertakes a R-Q Principal Components Analysis (PCA) and estimates Mahalanobis distances using robust covariance estimation procedures. Options include the minimum covariance determinant (MCD), minimum volume ellipsoid (MVE) procedures, and the use of user-defined weights – not necessarily just zero or one.

gx.robmva.closed

As above but for closed, compositional data. Estimates robust statistics following an ilr transform, then back-transforms to the clr form for the PCA.

gx.rotate Undertakes a Kaiser Varimax rotation on the PCs saved from either gx.mva, gx.mva.closed, gx.robmva or gx.robmva.closed.

gx.rqpca.screeplot

Displays a scree plot for the results of a PCA saved from either gx.mva, gx.mva.closed, gx.robmva or gx.robmva.closed.

gx.rqpca.loadplot

Displays a graphic where the loadings above some critical value, 'crit', are plotted for each PC in a space proportional to the variability that each PC contributes to the total data variability.

gx.rqpca.plot Displays R-Q bi-plots for the results of a PCA saved from either gx.mva, gx.mva.closed, gx.robmva, gx.robmva.closed, or gx.rotate.

gx.rqpca.print Displays tables of the loadings of each variable on each PC, and scores of the individuals on the PCs. Optionally the percentage contribution of each variable to the variability of each PC may be displayed.

gx.rqpca.save Saves tables of the loadings of each variable on each PC, and scores of the individuals on the PCs as .csv files.

gx.adjr2 Calculates adjusted R^2 values for multiple regression (linear) models taking into account the number of cases (individuals) and independent (predictor) variables.

Function gx.2dproj requires R library packages 'MASS' and 'fastICA' be available at run-time.

5. QA/QC support functions:

ad.plot1	Plots the results of analytical duplicate analyses as percentage differences relative to their means, as relative standard deviations (RSDs) against either the order of the analyses, the duplicate means, or the ratio of the duplicate means to the detection limit of the analytical method. Optionally a tolerance line (red) may be plotted.
ad.plot2	Similar to 'ad.plot1' but for use where the duplicates are stored as 1 to n values of x1 followed by 1 to n values of x2, or as alternating rows of x1 and x2 values.
ad.plot3	Plots the results of analytical duplicate analyses as ratios against their means with log scaling. The mean and standard deviation of the ratios are estimated and 95% confidence limits for the data are added to the plot.
ad.plot4	Similar to 'ad.plot3' but for use where the duplicates are stored as 1 to n values of x1 followed by 1 to n values of x2, or as alternating rows of x1 and x2 values.
anova1	Computes a random effects model ANOVA (Analysis of Variance) on a set of duplicate measurements to determine if the analytical, or combined sampling and analytical (within) variability is significantly smaller than the variability between the duplicates. For use where the n duplicates are stored as x1 and x2 in n rows.
anova2	Similar to 'anova1' but for use where the duplicates are stored as 1 to n values of x1 followed by 1 to n values of x2, or as alternating rows of x1 and x2 values.
crm.plot	Plots the results of Control Reference Material (CRM) analyses against the order of the analyses. Optionally (a) red tolerance line(s) may be plotted.
crm.plot.new	A version of crm.plot that facilitates the addition of new CRM determinations to the plot.
gx.triples.aov	Computes a random effects model ANOVA and estimates the variance components for a staggered 3-level design of field and analytical triplicates to simultaneously evaluate the significance and relative magnitude of 'regional', local sampling and analytical variability.
gx.triples.fgx	Computes two random effects model ANOVAs to estimate the regional representivity of the 'triples' in the context of the total regional survey variability and the equivalence of the variability of the two field duplicates.
thplot1	Displays a Thompson-Howarth plot for duplicate measurements to visually inspect them as a part of the QA/QC process. A target precision may be entered to aid visual data inspection. For use where the n duplicates are stored as x1 and x2 in n rows.
thplot2	Similar to 'thplot1' but for use where the duplicates are stored as 1 to n values of x1 followed by 1 to n values of x2, or as alternating rows of x1 and x2 values.

All of 'anova1', 'anova2', 'gx.triples.aov' and 'gx.triple.fgx' provide for an optional log-transformation of the data in order to meet homogeneity of variance and normality requirements.

6. Data conditioning functions:

ltdl.fix	Replaces less-than-detection values recorded as –x with x/2 or NA, a code to represent no information, i.e. blank. Optionally zero values and/or coded values, e.g., -9999, may be set to a NA.
ltdl.fix.df	Performs a 'ltdl.fix', see above, on a data frame, any factor variables are transferred to the new data frame.
remove.na	Removes any NAs from a vector or matrix, reporting on the number of NA values, or NA containing matrix rows, removed and the number of remaining rows and columns for a matrix.
gx.subset	Extracts a subset of rows from a data frame on the basis of a criterion supplied by the user, returning a new data frame.
logit	Computes the logit transformation for a vector of zero to one proportions representing a compositional data set.
expit	Computes the inverse-logit transformation so that the results of computations undertaken on logit-transformed proportions can be returned to the original proportions.
alr	Computes additive log-ratios for a matrix in order to remove the effects of data closure.
clr	Computes centred log-ratios for a matrix in order to remove the effects of data closure.
ilr	Computes isometric log-ratios for a matrix in order to remove the effects of data closure.
orthonorm	Computes orthornormal back-transformation to the clr form from a matrix resulting from the processing of ilr transformed data.
rng	Computes range transformations on the columns of a matrix.

7. Utility functions:

alts2dups	Takes sequentially arranged duplicate analyses and builds a matrix with 'number of duplicate' rows and two columns.
df.test	Determines if a specific data frame is available (attached) or exists in the work space. If it does, the names of the variables are displayed together with dimensions of the data frame.
where.na	Identifies any positions in a vector or matrix containing NAs, and can be used to remove any NAs from a data vector or matrix.
ilr.stab	Computes and displays the robust ilr stability for 2 parts of a composition.
gx.sort	Displays a sorted, or reverse sorted, data frame or matrix on the value of a specified column.
gx.sort.df	Displays a sorted data frame on the basis of any combination of numeric or factor variables in any combination of ascending or descending orders.
gx.t.test	Perform a t-test for equality of means when the mean, standard deviation and the size of the two populations are known.
gx.hypergeom	Estimate the probability that anomaly (above threshold sites) locations are informative, i.e. coincide with an expected model along transects or traverses (see Stanley, 2003).

gx.runs	Carry out a Wald-Wolfowitz, Runs, test for pattern coherence along transects and traverses.
display.lty	Displays the available line types and colours.
display.marks	Displays the available plotting symbols.
display.ascii.o	Displays the octal numbers corresponding to the Windows Latin 1 font, these are required when inserting symbols such as µ or ° into an axis label or title.
display.rainbow	Displays the 36 colours of the "rainbow" palette.
syms.pfunc	Displays the effect of changing the parameter 'p', which controls the rate of change of circular symbol size, in the 'edamap' function.

Notes:

Data frames are a data management feature of the S and R languages, they accommodate row and column names, real numbers, factor variables and NAs. NAs are a S and R language feature for identifying data items for which there is no information, as such they are a 'special code' for 'blanks' in a data file.

The boxes of Tukey boxplots, box-and-whisker plots and histograms are infilled in grey (8) from the palette displayed in 'display.lty', alternate colours may be selected from that palette. The "rainbow" palette is used for symbol colours in 'map.eda7', 'map.eda8', 'xyplot.eda7' and 'xyplot.eda8' the user may select alternate colours from this palette if required.

The above list of 99 functions only includes those directly accessible by a user, it does not include nine (9) functions that 'lurk in the basement' and are used as 'engines' to achieve the desired graphical and tabular displays.

A history of package changes is provided below:

Changes since 'rgr 1.0.3'

rgr 1.0.4' was a maintenance release built with R 2.12.0, no new functions were added. Minor changes were made to functions caplot, edamap and framework.stats. Two utility functions were removed, display.alts and display.ascii.d.

The release was required to bring the help, Rd, files into conformity with the new parsing rules for R 2.11. Some other text changes were made to the help files for shape and fences.summary.

Changes since 'rgr 1.0.4'

'rgr 1.0.5' was built with R 2.12.0 and includes a number of additional functions for the display of univariate data, QA/QC and utility functions. The names of the 'map' functions and dftest were changed to achieve better internal consistency in naming. Some multivariate or pseudo-multivariate functions were added, these carry out various log-ratio transformations to remove the closure effect from compositional (constant sum) data, to compute Pearson and Spearman correlation coefficients and their significance, and to compute weighted sums.

Changes since 'rgr 1.0.5'

'rgr 1.1.0' was built with R 2.12.0. At the maintenance level it includes some corrections of 'typos' in the help file, and a correction to Reduced Major Axis slope estimation (gx.rma). A function is now present to identify the locations of any NAs in a data vector or matrix. The major additions to version 1.1.0 are functions for multivariate exploratory data analysis. These include:

1. 2-d projections of p-space data using Sammon's non-linear mapping and multidimensional scaling. Unfortunately the Friedman and Rafsky implementation of minimum spanning tree 'planing' is not available in the R version of the Venables and Ripley 'MASS' Library;
2. Both classical and robust estimation implementations of R-Q Principal Components Analysis (PCA) and the estimation of Mahalanobis distances. Options for robust estimation include the minimum covariance determinant and minimum volume ellipsoid procedures, and user-supplied weight – not necessarily 0 or 1. A function is provided for the Kaiser Varimax rotation, as are functions for the display of the various results;
3. A robust estimation procedure for undertaking a PCA and the computation of Mahalanobis distances specifically for closed, compositional, data;
4. A graphical adaptive interactive trimming (GAIT) procedure based on Mahalanobis distance estimation for multivariate outlier detection and the selection of clean 'reference', in the applied geochemical context 'background', data subsets. Two functions are provided for the display of the GAIT results, one permits saving the results as a '.csv' file;
5. A Mahalanobis distance based multivariate allocation procedure employing predicted probabilities of reference (geochemical 'background') group memberships, i.e. typicalities. Atypical individuals whose membership falls below a user-defined cut-off in any of the reference groups are identified as 'unallocated' for further inspection. The allocations are made on the assumption that the reference group covariances are heteroscedastic, i.e. are of different sizes, shapes and orientations. The results may be displayed and/or saved as a '.csv' file; and
6. Two utility functions for linear modelling exercises are included, for estimating variance inflation factors and computing adjusted R^2 values. However, in the latter context, the use of Akaike's Information Criterion, available in the R {stats} library, is recommended.

Changes since 'rgr 1.1.0'

'rgr 1.1.1' was built with R 2.12.0. At the maintenance level it includes corrections of 'typos' in the help files, and changes in the names of functions bwplot, bwplot.by.var, tbplot and tbplot.by.var to bwplots, bwplots.by.var, tbplots and tbplots.by.var. These changes were made to avoid a conflict with function bwplot in the display package 'lattice' with the function of the same name in 'rgr', the 's' was added to the related function names for the sake of consistency. Other changes include:

1. The additions of Kruskal's non-metric multidimensional scaling procedure and a projection pursuit procedure based on the fastICA function; and

2. The addition of two functions, gx.md.gait.closed and gx.mvalloc.closed, together with a modification to gx.rob.mva closed. These additions/changes facilitate the investigation of closed data sets using Mahalanobis distance based procedures. Function gx.mvalloc.closed now requires the inverse of the reference data covariance matrix. This is achieved by back-transforming the inverse of the ilr transformed covariance matrix used for robust estimation in functions gx.md.gait.closed and gx.robmva.closed to the clr basis.
3. The addition of two functions to display the results of Principal Components Analyses, functions gx.rqpca.print and gx.rqpca.loadplot. The former displays tables of the PC loadings and scores of the individuals on the PCs, in addition, the percentage contribution of each variable to the variability of each PC may be displayed. The latter function displays a graphic where the loadings above some critical value, 'crit', set by default to an absolute loading of 0.3, are plotted for each PC in a space proportional to the variability that each PC contributes to the total data variability.

Issues that remain to be addressed in future releases of 'rgr'are:

1. The provision of the Friedman and Rafsky 'planing' tool for visualizing p-space data in 2-d for function gx.2dproj;
2. The correction of any errors in the scripts or help files (manual) as they are identified; and
3. The addition of 'useful' display functions as they are identified and/or developed.

Changes since 'rgr 1.1.1'

'rgr 1.1.2' was built with R 2.12.0. This is primarily a maintenance and enhancement release consisting of:

1. Corrections to the help files;
2. Minor changes to the formats of the summary statistics tables;
3. Some 'bullet proofing' was added to the summary statistics functions for instances where a data (sub)set contained no valid data, i.e. all NAs, or consisted of a single non-NA value;
4. The addition of legends to the map.* and xyplot.* functions;
5. The addition of estimation of fences following a logit transform, that recognizes the closed nature of geochemical analytical data, to functions fences and fences.summary. This required functions to be added for the logit and inverse-logit (expit) transformations; and
6. Three additional test data sets: sind.mat2open - to save repetitive matrix preparation in the examples; ogrady.mat2open - for investigating the closed nature of lithogeochemical data; and fix.test.asis – an alternate result from read.table usage.

Changes since 'rgr 1.1.2'

'rgr 1.1.3' was built with R 2.12.0. This is primarily a maintenance and enhancement release consisting of:

1. The addition of four functions (2 graphical) for the bivariate study of parts of a compositional data set, and the inclusion of a function to compute an Aitchison Variability Matrix;
2. A change to the output format of function fences.summary to improve display of the resulting saved tab delimited 'txt' file with a spreadsheet program; and
3. Corrections to the help files.

Changes since 'rgr 1.1.3'

'rgr 1.1.4' was built with R 2.14.1. This version is the same as rgr 1.1.3 except for a 'bug' fix to function tbplots and a change to the documentation for tbplots. Now requesting that the Tukey boxplot fences be based on logarithmically transformed data also results in logarithmic scaling being used for the boxplots. The 'bug' was that under certain circumstances the request for logarithmically based fences with a logarithmically scale plot failed, with the result that arithmetic fences were plotted.

Changes since 'rgr 1.1.4'

'rgr 1.1.5' was built with R 2.14.1. This version includes three functions for QA/QC support that graphically display the results of analytical duplicate and Control Reference Material (CRM) analyses.

Changes since 'rgr 1.1.5'

'rgr 1.1.6' was built with R 2.15.0. This version includes enhancements to the QA/QC support functions introduced in 'rgr 1.1.5'. A bug fix in function bwplots (ylim was not working correctly), and the reintroduction of function gx.mva.closed, now based on internal clr and ilr transform, similar to gx.robmva.closed. A number of cosmetic changes have been made to the output of the 'fences' functions, and where possible default file names are generated for saved .txt or .csv files where necessary if file names have not been specified or are present as blanks.

Changes since 'rgr 1.1.6'

'rgr 1.1.7' was built with R 2.15.0. This version includes a change to the QA/QC support functions ad.plot1 and ad.plot2 to facilitate multiple plots on a page, changes to the output tables in gx.rqpca.print, and some cosmetic changes to the manual.

Changes since 'rgr 1.1.7'

'rgr 1.1.8' was built with R 2.15.0. A new function, gx.scores, to support geochemical exploration has been introduced. Scores are computed on the basis of ratios of excedence of values relative to supplied threshold estimates. A data dependent bug related to the estimation of 95% confidence intervals on the median has been fixed; and some cosmetic changes have been made to the 'mva' functions. The eigenvalues as percentages of their sum are now displayed, together with the variance of the PC scores. This later facilitates choosing high variance robust PC scores for inspection.

Changes since 'rgr 1.1.8'

'rgr 1.1.9' was built with R 2.15.0. Version 1.1.9 is essentially the same software as version 1.1.8. Output format change has been made to functions gx.pairs4parts and df.test, and changes have been made to the hypertext and printed manuals for many functions. Version 1.1.9 was required to honour the licensing for package akima, which is licensed for not-for-profit use only and is called by only one 'rgr' function, caplot. Therefore 'rgr' now suggests akima, rather than

depends on as in previous versions of 'rgr'. As a result 'rgr' continues to be licensed under GPL-2.

Changes since 'rgr 1.1.9'

'rgr 1.1.10' was built with R 3.1.2. Version 1.1.10 includes four new functions to support QA/QC: two for plotting duplicate measurements as ratios, ad.plot3 and ad.plot4; one that permits new data to be added to a Shewart plot for Control Reference Materials, crm.plot.new; and one for rearranging sequentially stored duplicate analyses into a 'N by 2' matrix, alts2dups. Functions ltdl.fix and ltdl.fix.df have an extra option for replacing negative values used to indicate < Detection Limit values with NAs. A bug has been fixed in gx.summary.mat so that data frames can be processed as stated in the help file. Additional output concerning the variance of robust PCA scores has been added, and changes have been made to the PCA bi-plot function, gx.rqpca.plot, to facilitate customizing the display. Changes have been made to the gx.2dproj function to include an optional ilr log-ratio transformation and permit individuals to be trimmed in a GAIT procedure, and enhancements for the display of individual sample identifiers or input matrix row numbers have been added to gx.2dproj.plot. The new functions are fully documented. A major revision of the help files, documentation and manual, has been undertaken with appropriate updates, formatting and grammatical and typographic corrections.

Changes since 'rgr 1.1.10'

'rgr 1.1.11' was built with R 3.1.3. Changes and additions were made to gx.rma to: 1) Avoid a call to R cor, as if either package zCompositions or package NADA (also called from zCompositions) is loaded there is a potential conflict as NADA has a function cor; 2) to facilitate preparation of an equi-scaled x-y plot with the addition of the 1:1 line, and optionally the Reduced Major Axis for the preparation of Youden plots; and, 3) to facilitate accepting data for the two independent variables as a matrix from alts2dups for preparing Youden plots. The function, alts2dups, has been added to prepare N by 2 matrices of data stored sequentially to support QA/QC tasks. Minor changes have been made to functions gx.summary and gx.triples.aov concerning process flow and formatting, respectively; and a fix has been made to function gx.scores to replace NAs in the output with zeros to support post-calculation plotting. Changes and extra options have been implemented for shape, gx.rqpca.plot, the map.* and xyplot.* functions, and gx.md.print and gx.md.display. Defaults have been provided for all functions that save .csv or .txt files to save the files in the Working Directory. New functions, gx.ngr.summary, gx.ngr.stats and gx.ngr.skew, for preparing National Geochemical Reconnaissance style summary statistics tables have been added that export .csv files for import into a spreadsheet program to support report preparation. Revisions of the help files, documentation and manual, have been undertaken with appropriate updates, formatting and grammatical and typographic corrections.

Changes since 'rgr 1.1.11'

'rgr 1.1.12' was built with R 3.1.3. Further changes have been made to gx.rma to enable adding the coefficients of the Reduced Major Axis (Orthogonal Regression) and the result of the test for

a (0,1) intercept and slope to the plot. Function ad.plot3, and therefore ad.plot4, has been modified so that the default is a plot of ratios vs. their means, not as previously their order in the input file; and to plot the mean ratio and the 95% limits of the range of the data about the mean ratio. An additional function, gx.t.test, has been added to support QA/QC studies of Control Reference Material data that tests the hypothesis of equal means for two populations whose means, standard deviations and sizes are know. Users may find other more general uses for the function.

Changes since 'rgr 1.1.12'

'rgr 1.1.13' was built with R 3.1.3. A function, gx.mf, to display log-log empirical concentration-number plots has been added. This is called by function caplot to prepare concentration-area displays, and by a new function, shape.alt, that replaces the Tukey boxplot or box-and-whisker plot, in function shape with an empirical concentration-number plot to assist in the investigation of data sets for multifractality. Function gx.mf may also be executed directly to generate a screen/page size single display. The defaults for the histogram display function, gx.hist, have been modified. For data sets of size ≤500 and >500 the robust Scott (1979) and Friedman & Diaconis (1981) rules, respectively, are used. Alternately the user may specify either of these rules or the Sturges (Scott, 1992) rule, see the appropriate help files for details. Appropriate, and other, revisions of the help file and manual have been made.

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