

Package ‘gWQS’

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Type Package

Title Generalized Weighted Quantile Sum Regression

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Description Fits Weighted Quantile Sum (WQS) regression (Carrico et al. (2014) <doi:10.1007/s13253-014-0180-3>), a random subset implementation of WQS (Curtin et al. (2019) <doi:10.1080/03610918.2019.1577971>) and a repeated hold-out validation WQS (Tanner et al. (2019) <doi:10.1016/j.mex.2019.11.008>) for continuous, binomial, multinomial, Poisson, quasi-Poisson and negative binomial outcomes.

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R topics documented:

gwqs	2
gwqs_barplot	6
summary.gwqs	8
wqs_data	12

Index	14
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gwqs

*Fitting Weighted Quantile Sum regression models***Description**

Fits Weighted Quantile Sum (WQS) regression (Carrico et al. (2014) doi: [10.1007/s132530140180-3](https://doi.org/10.1007/s132530140180-3)), a random subset implementation of WQS (Curtin et al. (2019) doi: [10.1080/03610918.2019.1577971](https://doi.org/10.1080/03610918.2019.1577971)) and a repeated holdout validation WQS (Tanner et al. (2019) doi: [10.1016/j.mex.2019.11.008](https://doi.org/10.1016/j.mex.2019.11.008)) for continuous, binomial, multinomial, Poisson, quasi-Poisson and negative binomial outcomes.

Usage

```
gwqs(formula, data, na.action, weights, mix_name, stratified, valid_var, b = 100,
      b1_pos = TRUE, b1_constr = FALSE, zero_infl = FALSE, q = 4,
      validation = 0.6, family = gaussian, signal = c("t2", "one", "abst", "expt"),
      rs = FALSE, n_vars = NULL,
      zilink = c("logit", "probit", "cloglog", "cauchit", "log"), seed = NULL,
      plan_strategy = "sequential",
      optim.method = c("BFGS", "Nelder-Mead", "CG", "SANN"),
      control = list(trace = FALSE, maxit = 2000, reltol = 1e-9), ...)
```

```
gwqsrh(formula, data, na.action, weights, mix_name, stratified, valid_var, rh = 100,
        b = 100, b1_pos = TRUE, b1_constr = FALSE, zero_infl = FALSE, q = 4,
        validation = 0.6, family = gaussian,
        signal = c("t2", "one", "abst", "expt"), rs = FALSE, n_vars = NULL,
        zilink = c("logit", "probit", "cloglog", "cauchit", "log"), seed = NULL,
        plan_strategy = "sequential",
        optim.method = c("BFGS", "Nelder-Mead", "CG", "SANN"),
        control = list(trace = FALSE, maxit = 2000, reltol = 1e-9), ...)
```

Arguments

formula	An object of class formula specifying the relationship to be tested. The wqs term must be included in formula, e.g. $y \sim wqs + \dots$. To test for an interaction term with a continuous variable a or for a quadratic term we can specify the formula as below: $y \sim wqs*a + \dots$ and $y \sim wqs + I(wqs^2) + \dots$, respectively.
data	The data.frame containing the variables to be included in the model.
na.action	<code>model.frame</code> . <code>na.omit</code> is the default.
weights	An optional vector of weights to be used in the fitting process. Should be NULL or a numeric vector.
mix_name	A character vector listing the variables contributing to a mixture effect.
stratified	The character name of the variable for which you want to stratify for. It has to be a factor.

valid_var	A character value containing the name of the variable that identifies the validation and the training dataset. You previously need to create a variable in the dataset which is equal to 1 for the observations you want to include in the validation dataset, equal to 0 for the observation you want to include in the training dataset (use 0 also for the validation dataset if you want to train and validate the model on the same data) and equal to 2 if you want to keep part of the data for the predictive model.
b	Number of bootstrap samples used in parameter estimation.
b1_pos	A logical value that determines whether weights are derived from models where the beta values were positive or negative.
b1_constr	A logical value that determines whether to apply positive (if b1_pos = TRUE) or negative (if b1_pos = FALSE) constraints in the optimization function for the weight estimation.
zero_infl	A logical value (TRUE or FALSE) that allows to fit a zero inflated model in case family = "poisson" or family = "negbin".
q	An integer to specify how mixture variables will be ranked, e.g. in quartiles (q = 4), deciles (q = 10), or percentiles (q = 100). If q = NULL then the values of the mixture variables are taken (these must be standardized).
validation	Percentage of the dataset to be used to validate the model. If validation = 0 then the test dataset is used as validation dataset too.
family	A character value that allows to decide for the glm: gaussian for linear regression, binomial for logistic regression "multinomial" for multinomial regression, poisson for Poisson regression, quasipoisson for quasi-Poisson regression, "negbin" for negative binomial regression.
signal	Character identifying the signal function to be used when the average weights are estimated. It can take values from "one" to apply the identity, "abst" to apply the absolute value of the t-statistic, "t2" to apply the squared value of the t-statistic, "expt" to apply the exponential of the t-statistic as signal function.
rs	A logic value. If rs = FALSE then the bootstrap implementation of WQS is performed. If rs = TRUE then the random subset implementation of WQS is applied (see the "Details" and the vignette for further information).
n_vars	The number of mixture components to be included at each random subset step. If rs = TRUE and n_vars = NULL then the square root of the number of elements in the mixture is taken.
zilink	Character specification of link function in the binary zero-inflation model (you can choose among "logit", "probit", "cloglog", "cauchit", "log").
seed	An integer value to fix the seed, if it is equal to NULL no seed is chosen.
plan_strategy	A character value that allows to choose the evaluation strategies for the plan function. You can choose among "sequential", "transparent", "multisession", "multicore", "multiprocess", "cluster" and "remote" (see plan help page for more details).
optim.method	A character identifying the method to be used by the <code>optim</code> function (you can choose among "BFGS", "Nelder-Mead", "CG", "SANN", "BFGS" is the default). See optim for details.

control	The control list of optimization parameters. See <code>optim</code> for details.
...	Additional arguments to be passed to the function
rh	Number of repeated holdout validations. This option is only available for <code>gwqsrh</code> function.

Details

gwQS uses the `glm` function in the **stats** package to fit the linear, logistic, the Poisson and the quasi-Poisson regression, while the `glm.nb` function from the **MASS** package is used to fit the negative binomial regression respectively. The `nlm` function from the **stats** package was used to optimize the log-likelihood of the multinomial regression.

The `optim` optimization function is used to estimate the weights at each bootstrap step.

The `seed` argument specifies a fixed seed through the `set.seed` function.

The `rs` term allows to choose the type of methodology between the bootstrap implementation (WQSBS) or the random subset implementation (WQSRS) of the WQS. The first method performs `b` bootstrapped samples to estimate the weights while the second creates `b` randomly-selected subset of the total predictor set. For further details please see the vignette ("How to use gwQS package") and the references below.

Value

gwqs return the results of the WQS regression as well as many other objects and datasets.

fit	The object that summarizes the output of the WQS model, reflecting a linear, logistic, multinomial, Poisson, quasi-Poisson or negative binomial regression depending on how the <code>family</code> parameter was specified. The summary function can be used to call and print fit data (not for multinomial regression).
final_weights	<code>data.frame</code> containing the final weights associated to each chemical.
conv	Indicates whether the solver has converged (0) or not (1 or 2).
bres	Matrix of estimated weights, mixture effect parameter estimates and the associated standard errors, statistics and p-values estimated for each bootstrap iteration.
wqs	Vector containing the wqs index for each subject.
qi	List of the cutoffs used to divide in quantiles the variables in the mixture
bindex	List of vectors containing the rownames of the subjects included in each bootstrap dataset.
tindex	Vector containing the rows used to estimate the weights in each bootstrap.
vindex	Vector containing the rows used to estimate the parameters of the final model.
y_wqs_df	<code>data.frame</code> containing the dependent variable values adjusted for the residuals of a fitted model adjusted for covariates (original values when <code>family = binomial</code> or "multinomial") and the wqs index estimated values.
family	The family specified.

call	The matched call.
formula	The formula supplied.
mix_name	The vector of variable names used to identify the elements in the mixture.
q	The method used to rank variables included in the mixture.
n_levels	The number of levels of the of the dependent variable when a multinomial regression is ran.
zero_infl	If a zero inflated model was ran (TRUE) or not (FALSE)
zilink	The chosen link function when a zero inflated model was ran.
levelnames	The name of each level when a multinomial regression is ran.
data	The data used in the WQS analysis.
objfn_values	The vector of the b values of the objective function corresponding to the optima values
optim_messages	The vector of character strings giving any additional information returned by the optimizer, or NULL.
gwqslist	List of the output from the rh WQS models.
coefmat	Matrix containing the parameter estimates from each repeated holdout WQS model.
wmat	Matrix containing the weight estimates from each repeated holdout WQS model.

Author(s)

Stefano Renzetti, Paul Curtin, Allan C Just, Ghalib Bello, Chris Gennings

References

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Statistics - Simulation and Computation. doi: [10.1080/03610918.2019.1577971](https://doi.org/10.1080/03610918.2019.1577971).

Tanner EM, Bornehag CG, Gennings C. Repeated holdout validation for weighted quantile sum regression. *MethodsX*. 2019 Nov 22;6:2855-2860. doi: [10.1016/j.mex.2019.11.008](https://doi.org/10.1016/j.mex.2019.11.008).

See Also

[glm](#), [glm.nb](#), [multinom](#), [zeroinfl](#).

Examples

```
# we save the names of the mixture variables in the variable
# "toxic_chems"
toxic_chems = names(wqs_data)[1:34]

# To run a linear model and save the results in the variable
# "results". This linear model (family = gaussian) will
# rank/standardize variables in deciles (q = 10), perform a
# 40/60 split of the data for training/validation
# (validation = 0.6), and estimate weights over 2 bootstrap
# samples (b = 2; in practical applications at least 100
# bootstraps should be used). Weights will be derived from
# mixture effect parameters that are positive (b1_pos = TRUE).
# A unique seed was specified (seed = 2016) so this model will
# be reproducible, and plots describing the variable weights
# and linear relationship will be generated as output
# (plots = TRUE). In the end tables describing the weights
# values and the model parameters with the respectively
# statistics are generated in the plots window (tables = TRUE):
results = gwqs(yLBX ~ wqs, mix_name = toxic_chems,
              data = wqs_data, q = 10, validation = 0.6,
              b = 2, b1_pos = TRUE, b1_constr = FALSE,
              family = gaussian, seed = 2016)

# to test the significance of the covariates
summary(results)
```

gwqs_barplot

Plots and tables functions

Description

Functions that allow to generate plots and tables helping in visualizing and summarise Weighted Quantile Sum (WQS) regression results.

Usage

```

gwqs_barplot(object, tau, ...)

gwqs_scatterplot(object, ...)

gwqs_fitted_vs_resid(object, sumtype = c("norm", "perc"), ...)

gwqs_levels_scatterplot(object, ...)

gwqs_ROC(object, newdata, sumtype = c("norm", "perc"), ...)

gwqsrh_boxplot(object, tau, ...)

gwqs_summary_tab(object, sumtype = c("norm", "perc"), ...)

gwqs_weights_tab(object, ...)

selectdatavars(data, na.action, formula, mix_name, ...)

gwqs_rank(data, mix_name, q)

```

Arguments

object	An object of class "gwqs" as returned by gwqs.
tau	A number identifying the cutoff for the significant weights. If tau is missing then reciprocal of the number of elements in the mixture is considered. To avoid printing the threshold line set tau = NULL.
...	Further arguments to be passed to the function.
sumtype	Type of summary statistic to be used: "norm" takes the mean of the estimated parameters on the validation sets and the 95 as the parameters estimates and the 2.5, 97.5 percentiles as CI. This option is only available for objects of class gwqsrh.
newdata	A data frame in which to look for variables with which to predict and generate the ROC curve.
data	Dataset from which you want to select the variables you are interested in.
na.action	Allows to choose what action has to be taken to deal with NAs.
formula	Formula used in the model to specify the dependent and independent variables.
mix_name	Vector containing element names included in the mixture.
q	An integer to specify how mixture variables will be ranked, e.g. in quartiles (q = 4), deciles (q = 10), or percentiles (q = 100).

Details

The gwqs_barplot, gwqs_scatterplot, gwqs_fitted_vs_resid, gwqs_levels_scatterplot, gwqs_ROC and gwqsrh_boxplot functions produce five figures through the [ggplot](#) function.

The `gwqs_summary_tab` and `gwqs_weights_tab` functions produce two tables in the viewer pane through the use of the `kable` and `kable_styling` functions.

The `gwqs_barplot`, `gwqs_scatterplot` plots are available for all family types while `gwqs_fitted_vs_resid` is not available when `family = binomial` or "multinomial". `gwqs_levels_scatterplot` plot is only available when `family = "multinomial"` and `gwqs_ROC` when `family = binomial`. All these plots can also be applied to the objects of class `gwqsrh`. For these objects an additional plot is available through the function `gwqs_boxplot`.

The `gwqs_rank` function allows to split the variables selected through the vector `mix_name` in quantiles (depending by the value assigned to `q`).

Value

All the plot functions print the output in the Plots pane while the table functions print the output in the Viewer pane.

<code>Qm</code>	The matrix containing the quantiled variables of the elements included in the mixture.
<code>qi</code>	A list of vectors containing the cut points used to determine the quantiled variables.

Author(s)

Stefano Renzetti, Paul Curtin, Allan C Just, Ghalib Bello, Chris Gennings

Examples

```
toxic_chems = names(wqs_data)[1:34]
results = gwqs(yLBX ~ wqs, mix_name = toxic_chems, data = wqs_data, q = 4, validation = 0.6,
              b = 1, b1_pos = TRUE, b1_constr = FALSE, family = gaussian)

# barplot
gwqs_barplot(results)

# scatterplot
gwqs_scatterplot(results)

# fitted values vs residuals scatterplot
gwqs_fitted_vs_resid(results)
```

summary.gwqs

Methods for gwqs objects

Description

Methods for extracting information from fitted Weighted Quantile Sum (WQS) regression model objects of class "gwqs".

Usage

```
## S3 method for class 'gwqs'
summary(object, ...)

## S3 method for class 'gwqsrh'
summary(object, sumtype = c("norm", "perc"), ...)

## S3 method for class 'gwqs'
print(x, digits = max(3L, getOption("digits") - 3L), ...)

## S3 method for class 'gwqsrh'
print(x, digits = max(3L, getOption("digits") - 3L), ...)

## S3 method for class 'summary.gwqs'
print(x, digits = max(3L, getOption("digits") - 3L), ...)

## S3 method for class 'summary.gwqsrh'
print(x, digits = max(3L, getOption("digits") - 3L), ...)

## S3 method for class 'gwqs'
predict(
  object,
  newdata,
  type = c("link", "response", "prob", "count", "zero", "class", "probs", "terms"),
  ...
)

## S3 method for class 'gwqsrh'
predict(
  object,
  newdata,
  sumtype = c("norm", "perc"),
  type = c("link", "response", "prob", "count", "zero", "class", "probs", "terms"),
  ...
)

## S3 method for class 'gwqs'
coef(object, ...)

## S3 method for class 'gwqsrh'
coef(object, sumtype = c("norm", "perc"), ...)

## S3 method for class 'gwqs'
vcov(object, model = c("full", "count", "zero"), ...)

## S3 method for class 'gwqsrh'
vcov(object, model = c("full", "count", "zero"), ...)
```

```

## S3 method for class 'gwqs'
fitted(object, type = c("prob", "response"), ...)

## S3 method for class 'gwqsrh'
fitted(object, sumtype = c("norm", "perc"), type = c("prob", "response"), ...)

## S3 method for class 'gwqs'
residuals(
  object,
  type = c("deviance", "pearson", "working", "response", "partial"),
  ...
)

## S3 method for class 'gwqsrh'
residuals(
  object,
  sumtype = c("norm", "perc"),
  type = c("pearson", "response"),
  ...
)

```

Arguments

object, x	An object of class "gwqs" as returned by gwqs.
...	Further arguments to be passed.
sumtype	Type of summary statistic to be used: "norm" takes the mean of the estimated parameters on the validation sets and the 95 as the parameters estimates and the 2.5, 97.5 percentiles as CI. This option is only available for objects of class gwqsrh.
digits	The number of significant digits to use when printing.
newdata	Optionally, a data frame in which to look for variables with which to predict. If omitted, the original observations are used.
type	Character specifying the type of predictions, fitted values or residuals, respectively. For details see below.
model	Character specifying for which component of the model the variance-covariance matrix should be extracted when zero_infl = TRUE.

Details

A set of standard extractor functions for fitted model objects is available for objects of class "gwqs", including methods to the generic functions print and summary which print the estimated coefficients along with some further information. As usual, the summary method returns an object of class "summary.gwqs" containing the relevant summary statistics which can subsequently be printed using the associated print method.

The methods for `coef` and `vcov` by default return a single vector of coefficients (a matrix when `family = "multinomial"`) and their associated covariance matrix, respectively. By setting the `model` argument, the estimates for the corresponding model components can be extracted.

Both the `fitted` and `predict` methods can compute fitted responses. The latter sets the default on the scale of the linear predictors; the alternative "response" is on the scale of the response variable. Thus for a default binomial model the default predictions are of log-odds (probabilities on logit scale) and `type = "response"` gives the predicted probabilities. `Type` can be equal to "prob", "count" or "zero" when `zero_infl = T` to estimate the predicted density (i.e., probabilities for the observed counts), the predicted mean from the count component (without zero inflation) and the predicted probability for the zero component. `Type = "class"` allow to predict the dependent variable categories when `family = "multinomial"`. The "terms" option returns a matrix giving the fitted values of each term in the model formula on the linear predictor scale.

The `residuals` method allows to extract model residuals from the objects of class "gwqs".

Value

All these methods return the classic output as for the corresponding `glm`, `glm.nb`, `multinom` and `zeroinfl` classes. Only the `predict` method gives a different output made of the following values.

<code>df_pred</code>	A data.frame containing the dependent variable and the predicted values.
<code>Q</code>	The matrix containing the new dataset quantiled variables of the elements included in the mixture.
<code>qi</code>	A list of vectors containing the cut points used to determine the quantiled variables.
<code>wqs</code>	The vector containing the wqs index built on the new dataset.

Author(s)

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Examples

```
toxic_chems = names(wqs_data)[1:34]
set.seed(1234)
rws <- sample(1:500, 150)
results = gwqs(yLBX ~ wqs, mix_name = toxic_chems, data = wqs_data[-rws,], q = 4, validation = 0.6,
               b = 1, b1_pos = TRUE, b1_constr = FALSE, family = gaussian)

# to test the significance of the covariates
summary(results)

# extract regression coefficients
coef(results)

# estimate variance-covariance matrix
vcov(results)

# estimate fitted values
fitted(results)

# estimate regression residuals
residuals(results)
```

```
# estimate predicted values on the left part of wqs_data
pred_res <- predict(results, wqs_data[rws,])
pred_res$df_pred
```

wqs_data

Exposure concentrations of 34 PCB (simulated dataset)

Description

We created the 'wqs_data' dataset to show how to use this function. These data reflect 59 exposure concentrations simulated from a distribution of 34 PCB exposures and 25 phthalate biomarkers measured in subjects participating in the NHANES study (2001-2002). Additionally, 8 outcome measures were simulated applying different distributions and fixed beta coefficients to the predictors. In particular 'y' and 'yLBX' were simulated from a normal distribution, 'ybin' and 'ybinLBX' from a binomial distribution, 'ymultinom' and 'ymultinomLBX' from a multinomial distribution and 'ycount' and 'ycountLBX' from a Poisson distribution. The regression coefficients used to generate the outcomes 'yLBX', 'ybinLBX' and 'ycountLBX' were set to:

LBX105LA = 0.3

LBX138LA = 0.6

LBX157LA = 0.2

LBXD02LA = 0.45

LBXD04LA = 0.15

LBXF06LA = 0.3

LBXF07LA = 0.45

then the following terms were added to generate the variables 'y', 'ybin' and 'ycount':

URXMC1 = 0.15

URXMOH = 0.45

URXP02 = 0.2

URXP10 = 0.3

URXUCR = 0.2

All the remaining coefficients were set to 0.

The coefficients to generate 'ymultinomLBX' were set as below:

level B:

LBX138LA = 0.8

LBXD04LA = 0.2

level C:

LBX105LA = 0.4

LBX157LA = 0.3

LBXD02LA = 0.6

LBXF06LA = 0.4

LBXF07LA = 0.6

and the following terms were added for 'ymultinom':

level B:

URXMC1 = 0.2

URXP02 = 0.3

URXP10 = 0.4

URXUCR = 0.3

level C:

URXMOH = 0.6

The 'sex' variable was also simulated to allow to adjust for a covariate in the model. This dataset can thus be used to test the 'gWQS' package by analyzing the mixed effect of the 59 simulated PCBs on the continuous, binary or count outcomes, with adjustments for covariates.

Usage

wqs_data

Format

A data frame with 500 rows and 68 variables

Details

y continuous outcome generated considering all the predictors

yLBX continuous outcome generated considering only PCBs

ybin binary outcome generated considering all the predictors

ybinLBX binary outcome generated considering only PCBs

ymultinom multinomial outcome generated considering all the predictors

ymultinomLBX multinomial outcome generated considering only PCBs

ycount count outcome generated considering all the predictors

ycountLBX count outcome generated considering only PCBs

sex covariate, gender of the subject

LBX 34 exposure concentrations of PCB

URX 25 exposure concentrations of phthalates ...

Index

* datasets

wqs_data, 12

coef, 10
coef.gwqs (summary.gwqs), 8
coef.gwqsrh (summary.gwqs), 8

fitted.gwqs (summary.gwqs), 8
fitted.gwqsrh (summary.gwqs), 8

ggplot, 7
glm, 6
glm.nb, 6
gwqs, 2
gwqs_barplot, 6
gwqs_fitted_vs_resid (gwqs_barplot), 6
gwqs_levels_scatterplot (gwqs_barplot), 6
gwqs_rank (gwqs_barplot), 6
gwqs_ROC (gwqs_barplot), 6
gwqs_scatterplot (gwqs_barplot), 6
gwqs_summary_tab (gwqs_barplot), 6
gwqs_weights_tab (gwqs_barplot), 6
gwqsrh (gwqs), 2
gwqsrh_boxplot (gwqs_barplot), 6

kable, 8
kable_styling, 8

model.frame, 2
multinom, 6

optim, 3, 4

plan, 3
predict, 11
predict.gwqs (summary.gwqs), 8
predict.gwqsrh (summary.gwqs), 8
print.gwqs (summary.gwqs), 8
print.gwqsrh (summary.gwqs), 8
print.summary.gwqs (summary.gwqs), 8
print.summary.gwqsrh (summary.gwqs), 8

residuals, 11
residuals.gwqs (summary.gwqs), 8
residuals.gwqsrh (summary.gwqs), 8

selectdatavars (gwqs_barplot), 6
summary.gwqs, 8
summary.gwqsrh (summary.gwqs), 8

vcov, 10
vcov.gwqs (summary.gwqs), 8
vcov.gwqsrh (summary.gwqs), 8

wqs_data, 12

zeroinfl, 6