Package 'CalibrationCurves'

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Author De Cock Bavo [aut, cre], Nieboer Daan [aut], Van Calster Ben [aut], Steyerberg Ewout [aut], Vergouwe Yvonne [aut]
Maintainer De Cock Bavo bavo .decock@kuleuven.be>
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.rcspline.plot

Internal function

Description

Adjusted version of the rcspline.plot function where only the output is returned and no plot is made

Usage

Index

```
.rcspline.plot(
 х,
 у,
 model = c("logistic", "cox", "ols"),
 xrange,
 event,
 nk = 5,
 knots = NULL,
 show = c("xbeta", "prob"),
 adj = NULL,
 xlab,
 ylab,
 ylim,
 plim = c(0, 1),
 plotcl = TRUE,
  showknots = TRUE,
 add = FALSE,
 plot = TRUE,
 subset,
 lty = 1,
 noprint = FALSE,
 smooth = FALSE,
```

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```
bass = 1,
main = "auto",
statloc
)
```

Arguments

a numeric predictor Χ a numeric response. For binary logistic regression, y should be either 0 or 1. y "logistic" or "cox". For "cox", uses the coxph.fit function with method="efron" model argument set. range for evaluating x, default is f and 1-f quantiles of x, where $f = \frac{10}{\max(n,200)}$ xrange and n the number of observations event event/censoring indicator if model="cox". If event is present, model is assumed to be "cox" nk number of knots knot locations, default based on quantiles of x (by rcspline.eval) knots show "xbeta" or "prob" - what is plotted on y-axis adj optional matrix of adjustment variables x-axis label, default is the "label" attribute of x xlab ylab y-axis label, default is the "label" attribute of y ylim y-axis limits for logit or log hazard plim y-axis limits for probability scale plotcl plot confidence limits show knot locations with arrows showknots add add this plot to an already existing plot logical to indicate whether a plot has to be made. FALSE suppresses the plot. plot subset subset of observations to process, e.g. sex == "male" lty line type for plotting estimated spline function noprint suppress printing regression coefficients and standard errors for model="logistic", plot grouped estimates with triangles. Each group contains m ordered observations on x. plot nonparametric estimate if model="logistic" and adj is not specified smooth bass smoothing parameter (see supsmu) main title, default is "Estimated Spline Transformation" main statloc location of summary statistics. Default positioning by clicking left mouse button

Value

list with components ('knots', 'x', 'xbeta', 'lower', 'upper') which are respectively the knot locations, design matrix, linear predictor, and lower and upper confidence limits

to suppress statistics.

where upper left corner of statistics should appear. Alternative is "11" to place below the graph on the lower left, or the actual x and y coordinates. Use "none" 4 auc.nonpara.mw

See Also

```
lrm, cph, rcspline.eval, plot, supsmu, coxph.fit, lrm.fit
```

auc.nonpara.mw

AUC Based on the Mann-Whitney Statistic

Description

Obtain the point estimate and the confidence interval of the AUC by various methods based on the Mann-Whitney statistic.

Usage

Arguments

x a vector of observations from class P.
y a vector of observations from class N.

conf. level confidence level of the interval. The default is 0.95.

method a method used to construct the CI. newcombe is the method recommended in

Newcombe (2006); pepe is the method proposed in Pepe (2003); delong is the method proposed in Delong et al. (1988); jackknife uses the jackknife method; bootstrapP uses the bootstrap with percentile CI; bootstrapBCa uses bootstrap with bias-corrected and accelerated CI. The default is newcombe. It

can be abbreviated.

nboot number of bootstrap iterations.

Details

The function implements various methods based on the Mann-Whitney statistic.

Value

Point estimate and lower and upper bounds of the CI of the AUC.

Note

The observations from class P tend to have larger values than that from class N.

This help-file is a copy of the original help-file of the function auc.nonpara.mw from the auRoc-package. It is important to note that, when using method="pepe", the confidence interval is computed as documented in Qin and Hotilovac (2008) and that this is different from the original function.

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References

Elizabeth R Delong, David M Delong, and Daniel L Clarke-Pearson (1988) Comparing the areas under two or more correlated receiver operating characteristic curves: a nonparametric approach. *Biometrics* **44** 837-845

Dai Feng, Giuliana Cortese, and Richard Baumgartner (2015) A comparison of confidence/credible interval methods for the area under the ROC curve for continuous diagnostic tests with small sample size. *Statistical Methods in Medical Research* DOI: 10.1177/0962280215602040

Robert G Newcombe (2006) Confidence intervals for an effect size measure based on the Mann-Whitney statistic. Part 2: asymptotic methods and evaluation. *Statistics in medicine* **25(4)** 559-573

Margaret Sullivan Pepe (2003) The statistical evaluation of medical tests for classification and prediction. *Oxford University Press*

Qin, G., & Hotilovac, L. (2008). Comparison of non-parametric confidence intervals for the area under the ROC curve of a continuous-scale diagnostic test. *Statistical Methods in Medical Research*, **17(2)**, pp. 207-21

CalibrationCurves

General information on the package and its functions

Description

Using this package, you can assess the calibration performance of your prediction model. That is, to which extent the predictions and correspond with what we observe empirically. To assess the calibration of model with a binary outcome, you can use the val.prob.ci.2 or the valProbggplot function. If the outcome of your prediction model is not binary but follows a different distribution of the exponential family, you can employ the genCalCurve function.

If you are not familiar with the theory and/or application of calibration, you can consult the vignette of the package. This vignette provides a comprehensive overview of the theory and contains a tutorial with some practical examples. Further, we suggest the reader to consult the paper on generalized calibration curves on arXiv. In this paper, we provide the theoretical background on the generalized calibration framework and illustrate its applicability with some prototypical examples of both statistical and machine learning prediction models that are well-calibrated, overfit and underfit.

Originally, the package only contained functions to assess the calibration of prediction models with a binary outcome. The details section provides some background information on the history of the package's development.

Details

Some years ago, Yvonne Vergouwe and Ewout Steyerberg adapted the function val.prob from the rms-package (https://cran.r-project.org/package=rms) into val.prob.ci and added the following functions to val.prob:

- Scaled Brier score by relating to max for average calibrated Null model
- · Risk distribution according to outcome

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- 0 and 1 to indicate outcome label; set with d1lab="..", d0lab=".."
- Labels: y axis: "Observed Frequency"; Triangle: "Grouped observations"
- · Confidence intervals around triangles
- A cut-off can be plotted; set x coordinate

In December 2015, Bavo De Cock, Daan Nieboer, and Ben Van Calster adapted this to val.prob.ci.2:

- Flexible calibration curves can be obtained using loess (default) or restricted cubic splines, with pointwise 95% confidence intervals. Flexible calibration curves are now given by default and this decision is based on the findings reported in Van Calster et al. (2016).
- Loess: confidence intervals can be obtained in closed form or using bootstrapping (CL.BT=T will do bootstrapping with 2000 bootstrap samples, however this will take a while)
- RCS: 3 to 5 knots can be used
 - the knot locations will be estimated using default quantiles of x (by rcspline.eval, see rcspline.plot and rcspline.eval)
 - if estimation problems occur at the specified number of knots (nr.knots, default is 5), the analysis is repeated with nr.knots-1 until the problem has disappeared and the function stops if there is still an estimation problem with 3 knots
- You can now adjust the plot through use of normal plot commands (cex.axis etcetera), and the size of the legend now has to be specified in cex.leg
- Label y-axis: "Observed proportion"
- Stats: added the Estimated Calibration Index (ECI), a statistical measure to quantify lack of calibration (Van Hoorde et al., 2015)
- Stats to be shown in the plot: by default we show the "abc" of model performance (Steyerberg et al., 2011). That is, calibration intercept (calibration-in-the-large), calibration slope and c-statistic. Alternatively, the user can select the statistics of choice (e.g. dostats=c("C (ROC)", "R2") or dostats=c(2,3).
- Vectors p, y and logit no longer have to be sorted

In 2023, Bavo De Cock (Campo) published a paper that introduces the generalized calibration framework. This framework is an extension of the logistic calibration framework to prediction models where the outcome's distribution is a member of the exponential family. As such, we are able to assess the calibration of a wider range of prediction models. The methods in this paper are implemented in the CalibrationCurves package.

The most current version of this package can always be found on https://github.com/BavoDC
and can easily be installed using the following code:
install.packages("devtools") # if not yet installed
require(devtools)
install_github("BavoDC/CalibrationCurves", dependencies = TRUE, build_vignettes = TRUE)

References

De Cock Campo, B. (2023). Towards reliable predictive analytics: a generalized calibration framework. arXiv:2309.08559, available at https://arxiv.org/abs/2309.08559.

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Steyerberg, E.W.Van Calster, B., Pencina, M.J. (2011). Performance measures for prediction models and markers: evaluation of predictions and classifications. *Revista Espanola de Cardiologia*, **64(9)**, pp. 788-794

Van Calster, B., Nieboer, D., Vergouwe, Y., De Cock, B., Pencina M., Steyerberg E.W. (2016). A calibration hierarchy for risk models was defined: from utopia to empirical data. *Journal of Clinical Epidemiology*, **74**, pp. 167-176

Van Hoorde, K., Van Huffel, S., Timmerman, D., Bourne, T., Van Calster, B. (2015). A spline-based tool to assess and visualize the calibration of multiclass risk predictions. *Journal of Biomedical Informatics*, **54**, pp. 283-93

genCalCurve

Calibration performance using the generalized calibration framework

Description

Function to assess the calibration performance of a prediction model where the outcome's distribution is a member of the exponential family (De Cock Campo, 2023). The function plots the generalized calibration curve and computes the generalized calibration slope and intercept.

Usage

```
genCalCurve(
 у,
  yHat,
  family,
  plot = TRUE,
  Smooth = FALSE,
  GLMCal = TRUE,
  lwdIdeal = 2,
  colIdeal = "gray",
  ltyIdeal = 1,
  lwdSmooth = 1,
  colSmooth = "blue",
  ltySmooth = 1,
  argzSmooth = alist(degree = 2),
  lwdGLMCal = 1,
  colGLMCal = "red",
  ltyGLMCal = 1,
  AddStats = T,
 Digits = 3,
  cexStats = 1,
  lwdLeg = 1.5,
  Legend = TRUE,
  legendPos = "bottomright",
  xLim = NULL,
  yLim = NULL,
```

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```
posStats = NULL,
  confLimitsSmooth = c("none", "bootstrap", "pointwise"),
  confLevel = 0.95,
  Title = "Calibration plot",
  xlab = "Predicted value",
  ylab = "Empirical average"
  EmpiricalDistribution = TRUE,
  length.seg = 1,
)
```

Arguments

У a vector with the values for the response variable

yHat a vector with the predicted values

a description of the type of distribution and link function in the model. This can family

be a character string naming a family function, a family function or the result of

a call to a family function. (See family for details of family functions.)

plot logical, indicating if a plot should be made or not.

Smooth logical, indicating if the flexible calibration curve should be estimated. logical, indicating if the GLM calibration curve has to be estimated. GLMCa1

lwdIdeal the line width of the ideal line. colIdeal the color of the ideal line. ltyIdeal the line type of the ideal line.

1wdSmooth the line width of the flexible calibration curve. colSmooth the color of the flexible calibration curve.

the line type of the flexible calibration curve. 1tySmooth

argzSmooth arguments passed to loess.

1wdGLMCa1 the line width of the GLM calibration curve. the color of the GLM calibration curve. colGLMCal

ltyGLMCal the line type of the GLM calibration curve.

AddStats logical, indicating whether to add the values of the generalized calibration slope

and intercept to the plot.

Digits the number of digits of the generalized calibration slope and intercept.

the font size of the statistics shown on the plot. cexStats

the line width in the legend. lwdLeg

logical, indicating whether the legend has to be added. Legend

legendPos the position of the legend on the plot.

numeric vectors of length 2, giving the x and y coordinates ranges (see plot.window) xLim, yLim

posStats numeric vector of length 2, specifying the x and y coordinates of the statistics

(generalized calibration curve and intercept) printed on the plot. Default is NULL

which places the statistics in the top left corner of the plot.

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confLimitsSmooth

character vector to indicate if and how the confidence limits for the flexible calibration curve have to be computed. "none" omits the confidence limits, "bootstrap" uses 2000 bootstrap samples to calculate the 95% confidence lim-

its and "pointwise" uses the pointwise confidence limits.

confLevel the confidence level for the calculation of the pointwise confidence limits of the

flexible calibration curve.

Title the title of the plot

x-axis label, default is "Predicted value". xlab y-axis label, default is "Empirical average". ylab

EmpiricalDistribution

logical, indicating if the empirical distribution of the predicted values has to be

added to the bottom of the plot.

length.seg controls the length of the histogram lines. Default is 1.

arguments to be passed to plot, see par

Value

An object of type GeneralizedCalibrationCurve with the following slots:

call the matched call. ggPlot the ggplot object.

stats a vector containing performance measures of calibration.

cl.level the confidence level used.

Calibration contains the calibration intercept and slope, together with their confidence inter-

Cindex the value of the c-statistic, together with its confidence interval.

warningMessages

if any, the warning messages that were printed while running the function.

CalibrationCurves

The coordinates for plotting the calibration curves.

References

De Cock Campo, B. (2023). Towards reliable predictive analytics: a generalized calibration framework. arXiv:2309.08559, available at https://arxiv.org/abs/2309.08559.

Examples

```
library(CalibrationCurves)
library(mgcv)
data("poissontraindata")
data("poissontestdata")
glmFit = glm(Y \sim ., data = poissontraindata, family = poisson)
```

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```
# Example of a well calibrated poisson prediction model
y00S = poissontestdata$Y
yHat = predict(glmFit, newdata = poissontestdata, type = "response")
genCalCurve(y00S, yHat, family = "poisson", plot = TRUE)

# Example of an overfit poisson prediction model
gamFit = gam(Y ~ x1 + x3 + x1:x3 + s(x5), data = poissontraindata, family = poisson)
yHat = as.vector(predict(gamFit, newdata = poissontestdata, type = "response"))
genCalCurve(y00S, yHat, family = "poisson", plot = TRUE)

# Example of an underfit poisson prediction model
glmFit = glm(Y ~ x2, data = poissontraindata, family = poisson)
y00S = poissontestdata$Y
yHat = predict(glmFit, newdata = poissontestdata, type = "response")
genCalCurve(y00S, yHat, family = "poisson", plot = TRUE)
```

LibraryM

Function to load multiple packages at once

Description

Function to load multiple packages at once

Usage

```
LibraryM(...)
```

Arguments

... the packages that you want to load

Value

invisible NULL

Examples

LibraryM(CalibrationCurves)

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```
print.CalibrationCurve
```

Print function for a CalibrationCurve object

Description

Prints the call, confidence level and values for the performance measures.

Usage

```
## S3 method for class 'CalibrationCurve' print(x, ...)
```

Arguments

```
x an object of type CalibrationCurve, resulting from val.prob.ci.2.
```

... arguments passed to print

Value

The original CalibrationCurve object is returned.

See Also

```
val.prob.ci.2
```

```
print.GeneralizedCalibrationCurve
```

Print function for a GeneralizedCalibrationCurve object

Description

Prints the call, confidence level and values for the performance measures.

Usage

```
## S3 method for class 'GeneralizedCalibrationCurve' print(x, ...)
```

Arguments

```
x an object of type GeneralizedCalibrationCurve, resulting from genCalCurve.
```

... arguments passed to print

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Value

The original GeneralizedCalibrationCurve object is returned.

See Also

```
genCalCurve
```

```
print.ggplotCalibrationCurve
```

Print function for a ggplotCalibrationCurve object

Description

Prints the ggplot, call, confidence level and values for the performance measures.

Usage

```
## S3 method for class 'ggplotCalibrationCurve' print(x, ...)
```

Arguments

x an object of type ggplotCalibrationCurve, resulting from valProbggplot.

... arguments passed to print

Value

The original ggplotCalibrationCurve object is returned.

See Also

```
valProbggplot
```

simulateddata

Simulated data sets to illustrate the package functionality

Description

Both the traindata and testdata dataframe are synthetically generated data sets to illustrate the functionality of the package. The traindata has 1000 observations and the testdata has 500 observations. The same settings were used to generate both data sets.

Usage

```
data(traindata)
data(testdata)
```

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Format

```
y the binary outcome variable
x1 covariate 1
x2 covariate 2
x3 covariate 3
x4 covariate 4
```

Details

See the examples for how the data sets were generated.

Examples

```
# The data sets were generated as follows
set.seed(1782)
# Simulate training data
nTrain
        = 1000
         = c(0.1, 0.5, 1.2, -0.75, 0.8)
Χ
         = replicate(4, rnorm(nTrain))
p0true = binomial()$linkinv(cbind(1, X) %*% B)
         = rbinom(nTrain, 1, p0true)
colnames(X) = paste0("x", seq_len(ncol(X)))
traindata = data.frame(y, X)
# Simulate validation data
nTest = 500
       = replicate(4, rnorm(nTest))
p0true = binomial()$linkinv(cbind(1, X) %*% B)
        = rbinom(nTest, 1, p0true)
colnames(X) = paste0("x", seq_len(ncol(X)))
testdata = data.frame(y, X)
```

simulatedpoissondata Simulated data sets to illustrate the package functionality

Description

Both the traindata and testdata dataframe are synthetically generated data sets to illustrate the functionality of the package. The traindata has 5000 observations and the testdata has 1000 observations. The same settings were used to generate both data sets.

Usage

```
data(poissontraindata)
data(poissontestdata)
```

Format

```
y the poisson distributed outcome variable x1 covariate 1 x2 covariate 2 x3 covariate 3 x4 covariate 4 x5 covariate 5
```

Details

See the examples for how the data sets were generated.

Examples

```
# The data sets were generated as follows
library(MASS)
library(magrittr)
ScaleRange <- function(x, xmin = -1, xmax = 1) {
xRange = range(x)
(x - xRange[1]) / diff(xRange) * (xmax - xmin) + xmin
set.seed(144)
p = 5
N = 1e6
n = 5e3
n00S = 1e3
S = matrix(NA, 5, 5)
rho = c(0.025, 0, 0, 0.05, 0.075, 0, 0, 0.025, 0, 0)
S[upper.tri(S)] = rho
S[lower.tri(S)] = t(S)[lower.tri(S)]
diag(S) = 1
Matrix::isSymmetric(S)
X = mvrnorm(N, rep(0, p), Sigma = S, empirical = TRUE)
X = apply(X, 2, ScaleRange)
B = c(-2.3, 1.5, 2, -1, -2, -1.5)
mu = poisson()$linkinv(cbind(1, X) %*% B)
Y = rpois(N, mu)
Df = data.frame(Y, X)
colnames(Df)[-1] %<>% tolower()
set.seed(2)
DfS = Df[sample(1:nrow(Df), n, FALSE), ]
Df00S = Df[sample(1:nrow(Df), n00S, FALSE), ]
poissontraindata = DfS
poissontestdata = Df00S
```

val.prob.ci.2

Calibration performance

Description

The function val.prob.ci.2 is an adaptation of val.prob from Frank Harrell's rms package, https://cran.r-project.org/package=rms. Hence, the description of some of the functions of val.prob.ci.2 come from the the original val.prob.

The key feature of val.prob.ci.2 is the generation of logistic and flexible calibration curves and related statistics. When using this code, please cite: Van Calster, B., Nieboer, D., Vergouwe, Y., De Cock, B., Pencina, M.J., Steyerberg, E.W. (2016). A calibration hierarchy for risk models was defined: from utopia to empirical data. *Journal of Clinical Epidemiology*, **74**, pp. 167-176

Usage

```
val.prob.ci.2(
  p,
 у,
  logit,
  group,
 weights = rep(1, length(y)),
  normwt = FALSE,
  pl = TRUE,
  smooth = c("loess", "rcs", "none"),
  CL.smooth = "fill",
  CL.BT = FALSE,
  lty.smooth = 1,
  col.smooth = "black",
  lwd.smooth = 1,
  nr.knots = 5,
  logistic.cal = FALSE,
  lty.log = 1,
  col.log = "black",
  lwd.log = 1,
  xlab = "Predicted probability",
 ylab = "Observed proportion",
  xlim = c(-0.02, 1),
 ylim = c(-0.15, 1),
 m,
  g,
  cuts,
  emax.lim = c(0, 1),
  legendloc = c(0.5, 0.27),
  statloc = c(0, 0.85),
  dostats = TRUE,
  cl.level = 0.95,
```

```
method.ci = "pepe",
  roundstats = 2,
  riskdist = "predicted",
  cex = 0.75,
  cex.leg = 0.75,
  connect.group = FALSE,
  connect.smooth = TRUE,
  g.group = 4,
  evaluate = 100,
 nmin = 0,
 d0lab = "0",
 d1lab = "1",
  cex.d01 = 0.7,
  dist.label = 0.04,
  line.bins = -0.05,
  dist.label2 = 0.03,
  cutoff,
  las = 1,
  length.seg = 1,
 y.intersp = 1,
 lty.ideal = 1,
  col.ideal = "red",
  lwd.ideal = 1,
  allowPerfectPredictions = FALSE,
 argzLoess = alist(degree = 2),
)
```

Arguments

р	predicted probability
У	vector of binary outcomes
logit	predicted log odds of outcome. Specify either p or logit.
group	a grouping variable. If numeric this variable is grouped into g.group quantile groups (default is quartiles). Set group=TRUE to use the group algorithm but with a single stratum for val.prob.
weights	an optional numeric vector of per-observation weights (usually frequencies), used only if group is given.
normwt	set to TRUE to make weights sum to the number of non-missing observations.
pl	TRUE to plot the calibration curve(s). If FALSE no calibration curves will be plotted, but statistics will still be computed and outputted.
smooth	"loess" generates a flexible calibration curve based on loess, "rcs" generates a calibration curves based on restricted cubic splines (see rcs and rcspline.plot), "none" suppresses the flexible curve. We recommend to use loess unless N is large, for example N>5000. Default is "loess".
CL.smooth	"fill" shows pointwise 95% confidence limits for the flexible calibration curve with a gray area between the lower and upper limits, TRUE shows pointwise

95% confidence limits for the flexible calibration curve with dashed lines, FALSE suppresses the confidence limits. Default is "fill". CL.BT TRUE uses confidence limits based on 2000 bootstrap samples, FALSE uses closed form confidence limits. Default is FALSE. lty.smooth the linetype of the flexible calibration curve. Default is 1. col.smooth the color of the flexible calibration curve. Default is "black". lwd.smooth the line width of the flexible calibration curve. Default is 1. nr.knots specifies the number of knots for rcs-based calibration curve. The default as well as the highest allowed value is 5. In case the specified number of knots leads to estimation problems, then the number of knots is automatically reduced to the closest value without estimation problems. logistic.cal TRUE plots the logistic calibration curve, FALSE suppresses this curve. Default is if logistic.cal=TRUE, the linetype of the logistic calibration curve. Default is lty.log col.log if logistic.cal=TRUE, the color of the logistic calibration curve. Default is "black". lwd.log if logistic.cal=TRUE, the line width of the logistic calibration curve. Default xlab x-axis label, default is "Predicted Probability". ylab y-axis label, default is "Observed proportion". xlim, ylim numeric vectors of length 2, giving the x and y coordinates ranges (see plot.window) If grouped proportions are desired, average no. observations per group If grouped proportions are desired, number of quantile groups g cuts If grouped proportions are desired, actual cut points for constructing intervals, e.g. c(0, .1, .8, .9, 1) or seq(0, 1, by=.2)Vector containing lowest and highest predicted probability over which to comemax.lim pute Emax. legendloc if p1=TRUE, list with components x, y or vector c(x, y) for bottom right corner of legend for curves and points. Default is c(.50, .27) scaled to lim. Use locator(1) to use the mouse, FALSE to suppress legend. statloc the "abc" of model performance (Steverberg et al., 2011)-calibration intercept, calibration slope, and c statistic-will be added to the plot, using statloc as the upper left corner of a box (default is c(0,.85)). You can specify a list or a vector. Use locator(1) for the mouse, FALSE to suppress statistics. This is plotted after the curve legends. dostats specifies whether and which performance measures are shown in the figure. TRUE shows the "abc" of model performance (Steyerberg et al., 2011): calibration intercept, calibration slope, and c-statistic. TRUE is default. FALSE suppresses the presentation of statistics in the figure. A c() list of specific stats shows the specified stats. The key stats which are also mentioned in this paper are "C (ROC)" for the c statistic, "Intercept" for the calibration intercept, "Slope" for the calibration slope, and "ECI" for the estimated calibra-

tion index (Van Hoorde et al, 2015). The full list of possible statistics is taken

	from val.prob and augmented with the estimated calibration index: "Dxy", "C (ROC)", "R2", "D", "D:Chi-sq", "D:p", "U", "U:Chi-sq", "U:p", "Q", "Brier", "Intercept", "Slope", "Emax", "Brier scaled", "Eavg", "ECI". These statistics are always returned by the function.
cl.level	if dostats=TRUE, the confidence level for the calculation of the confidence intervals of the calibration intercept, calibration slope and c-statistic. Default is $\emptyset.95$.
method.ci	method to calculate the confidence interval of the c-statistic. The argument is passed to auc.nonpara.mw from the auRoc-package and possible methods to compute the confidence interval are "newcombe", "pepe", "delong" or "jackknife". Bootstrap-based methods are not available. The default method is "pepe" and here, the confidence interval is the logit-transformation-based confidence interval as documented in Qin and Hotilovac (2008). See auc.nonpara.mw for more information on the other methods.
roundstats	specifies the number of decimals to which the statistics are rounded when shown in the plot. Default is 2.
riskdist	Use "calibrated" to plot the relative frequency distribution of calibrated probabilities after dividing into 101 bins from lim[1] to lim[2]. Set to "predicted" (the default as of rms 4.5-1) to use raw assigned risk, FALSE to omit risk distribution. Values are scaled so that highest bar is 0.15*(lim[2]-lim[1]).
cex, cex.leg	controls the font size of the statistics (cex) or plot legend (cex.leg). Default is 0.75
connect.group	Defaults to FALSE to only represent group fractions as triangles. Set to TRUE to also connect with a solid line.
connect.smooth	Defaults to TRUE to draw smoothed estimates using a line. Set to FALSE to instead use dots at individual estimates
g.group	number of quantile groups to use when group is given and variable is numeric.
evaluate	number of points at which to store the lowess-calibration curve. Default is 100. If there are more than evaluate unique predicted probabilities, evaluate equally-spaced quantiles of the unique predicted probabilities, with linearly interpolated calibrated values, are retained for plotting (and stored in the object returned by val.prob.
nmin	applies when group is given. When nmin > 0 , val.prob will not store coordinates of smoothed calibration curves in the outer tails, where there are fewer than nmin raw observations represented in those tails. If for example nmin=50, the plot function will only plot the estimated calibration curve from a to b , where there are 50 subjects with predicted probabilities $< a$ and $> b$. nmin is ignored when computing accuracy statistics.
d0lab, d1lab	controls the labels for events and non-events (i.e. outcome y) for the histograms. Defaults are d1lab="1" for events and d0lab="0" for non-events.
cex.d01	controls the size of the labels for events and non-events. Default is 0.7.
dist.label	controls the horizontal position of the labels for events and non-events. Default is 0.04.
line.bins	controls the horizontal (y-axis) position of the histograms. Default is -0.05.

dist.label2 controls the vertical distance between the labels for events and non-events. De-

fault is 0.03.

cutoff puts an arrow at the specified risk cut-off(s). Default is none.

las controls whether y-axis values are shown horizontally (1) or vertically (0).

length.seg controls the length of the histogram lines. Default is 1.

y.intersp character interspacing for vertical line distances of the legend (legend)

lty.ideal linetype of the ideal line. Default is 1.

col.ideal controls the color of the ideal line on the plot. Default is "red". lwd.ideal controls the line width of the ideal line on the plot. Default is 1.

allowPerfectPredictions

Logical, indicates whether perfect predictions (i.e. values of either 0 or 1) are allowed. Default is FALSE, since we transform the predictions using the logit transformation to calculate the calibration measures. In case of 0 and 1, this results in minus infinity and infinity, respectively. if allowPerfectPredictions

= TRUE, 0 and 1 are replaced by 1e-8 and 1 - 1e-8, respectively.

argzLoess a list with arguments passed to the loess function

... arguments to be passed to plot, see par

Details

When using the predicted probabilities of an uninformative model (i.e. equal probabilities for all observations), the model has no predictive value. Consequently, where applicable, the value of the performance measure corresponds to the worst possible theoretical value. For the ECI, for example, this equals 1 (Edlinger et al., 2022).

Value

An object of type CalibrationCurve with the following slots:

call the matched call.

stats a vector containing performance measures of calibration.

cl.level the confidence level used.

Calibration contains the calibration intercept and slope, together with their confidence inter-

vals.

Cindex the value of the c-statistic, together with its confidence interval.

warningMessages

if any, the warning messages that were printed while running the function.

CalibrationCurves

The coordinates for plotting the calibration curves.

Note

In order to make use (of the functions) of the package auRoc, the user needs to install JAGS. However, since our package only uses the auc.nonpara.mw function which does not depend on the use of JAGS, we therefore copied the code and slightly adjusted it when method="pepe".

References

Edlinger, M, van Smeden, M, Alber, HF, Wanitschek, M, Van Calster, B. (2022). Risk prediction models for discrete ordinal outcomes: Calibration and the impact of the proportional odds assumption. *Statistics in Medicine*, **41(8)**, pp. 1334–1360

Qin, G., & Hotilovac, L. (2008). Comparison of non-parametric confidence intervals for the area under the ROC curve of a continuous-scale diagnostic test. *Statistical Methods in Medical Research*, **17(2)**, pp. 207-21

Steyerberg, E.W., Van Calster, B., Pencina, M.J. (2011). Performance measures for prediction models and markers: evaluation of predictions and classifications. *Revista Espanola de Cardiologia*, **64(9)**, pp. 788-794

Van Calster, B., Nieboer, D., Vergouwe, Y., De Cock, B., Pencina M., Steyerberg E.W. (2016). A calibration hierarchy for risk models was defined: from utopia to empirical data. *Journal of Clinical Epidemiology*, **74**, pp. 167-176

Van Hoorde, K., Van Huffel, S., Timmerman, D., Bourne, T., Van Calster, B. (2015). A spline-based tool to assess and visualize the calibration of multiclass risk predictions. *Journal of Biomedical Informatics*, **54**, pp. 283-93

Examples

```
# Load package
library(CalibrationCurves)
set.seed(1783)
# Simulate training data
      = replicate(4, rnorm(5e2))
p0true = binomial()$linkinv(cbind(1, X) %*% c(0.1, 0.5, 1.2, -0.75, 0.8))
       = rbinom(5e2, 1, p0true)
Df
       = data.frame(y, X)
# Fit logistic model
FitLog = lrm(y \sim ., Df)
# Simulate validation data
Xval = replicate(4, rnorm(5e2))
p0true = binomial()$linkinv(cbind(1, Xval) %*% c(0.1, 0.5, 1.2, -0.75, 0.8))
yval = rbinom(5e2, 1, p0true)
Pred = binomial()$linkinv(cbind(1, Xval) %*% coef(FitLog))
# Default calibration plot
val.prob.ci.2(Pred, yval)
# Adding logistic calibration curves and other additional features
val.prob.ci.2(Pred, yval, CL.smooth = TRUE, logistic.cal = TRUE, lty.log = 2,
 col.log = "red", lwd.log = 1.5)
val.prob.ci.2(Pred, yval, CL.smooth = TRUE, logistic.cal = TRUE, lty.log = 9,
col.log = "red", lwd.log = 1.5, col.ideal = colors()[10], lwd.ideal = 0.5)
```

valProbggplot

Calibration performance: ggplot version

Description

The function valProbggplot is an adaptation of val.prob from Frank Harrell's rms package, https://cran.r-project.org/package=rms. Hence, the description of some of the functions of valProbggplot come from the the original val.prob.

The key feature of valProbggplot is the generation of logistic and flexible calibration curves and related statistics. When using this code, please cite: Van Calster, B., Nieboer, D., Vergouwe, Y., De Cock, B., Pencina, M.J., Steyerberg, E.W. (2016). A calibration hierarchy for risk models was defined: from utopia to empirical data. *Journal of Clinical Epidemiology*, **74**, pp. 167-176

Usage

```
valProbggplot(
  р,
 у,
  logit,
  group,
 weights = rep(1, length(y)),
  normwt = FALSE,
  pl = TRUE,
  smooth = c("loess", "rcs", "none"),
  CL.smooth = "fill",
  CL.BT = FALSE,
  lty.smooth = 1,
  col.smooth = "black",
  lwd.smooth = 1,
  nr.knots = 5,
  logistic.cal = FALSE,
  lty.log = 1,
  col.log = "black",
  lwd.log = 1,
  xlab = "Predicted probability",
 ylab = "Observed proportion",
  xlim = c(-0.02, 1),
 ylim = c(-0.15, 1),
 m,
  g,
  cuts,
  emax.lim = c(0, 1),
  legendloc = c(0.5, 0.27),
  statloc = c(0, 0.85),
  dostats = TRUE,
  cl.level = 0.95,
```

```
method.ci = "pepe",
 roundstats = 2,
  riskdist = "predicted",
  size = 3,
  size.leg = 5,
  connect.group = FALSE,
  connect.smooth = TRUE,
 g.group = 4,
 evaluate = 100,
 nmin = 0,
 d0lab = "0",
 d1lab = "1",
  size.d01 = 5,
 dist.label = 0.01,
 line.bins = -0.05,
 dist.label2 = 0.04,
  cutoff,
  length.seg = 0.85,
 lty.ideal = 1,
  col.ideal = "red",
 lwd.ideal = 1,
 allowPerfectPredictions = FALSE,
 argzLoess = alist(degree = 2)
)
```

Arguments

р	predicted probability
У	vector of binary outcomes
logit	predicted log odds of outcome. Specify either p or logit.
group	a grouping variable. If numeric this variable is grouped into g.group quantile groups (default is quartiles). Set group=TRUE to use the group algorithm but with a single stratum for val.prob.
weights	an optional numeric vector of per-observation weights (usually frequencies), used only if group is given.
normwt	set to TRUE to make weights sum to the number of non-missing observations.
pl	TRUE to plot the calibration curve(s). If FALSE no calibration curves will be plotted, but statistics will still be computed and outputted.
smooth	"loess" generates a flexible calibration curve based on loess, "rcs" generates a calibration curves based on restricted cubic splines (see rcs and rcspline.plot), "none" suppresses the flexible curve. We recommend to use loess unless N is large, for example N>5000. Default is "loess".
CL.smooth	"fill" shows pointwise 95% confidence limits for the flexible calibration curve with a gray area between the lower and upper limits, TRUE shows pointwise 95% confidence limits for the flexible calibration curve with dashed lines, FALSE suppresses the confidence limits. Default is "fill".

CL.BT	TRUE uses confidence limits based on 2000 bootstrap samples, FALSE uses closed form confidence limits. Default is FALSE.
lty.smooth	the linetype of the flexible calibration curve. Default is 1.
col.smooth	the color of the flexible calibration curve. Default is "black".
lwd.smooth	the line width of the flexible calibration curve. Default is 1.
nr.knots	specifies the number of knots for rcs-based calibration curve. The default as well as the highest allowed value is 5. In case the specified number of knots leads to estimation problems, then the number of knots is automatically reduced to the closest value without estimation problems.
logistic.cal	TRUE plots the logistic calibration curve, FALSE suppresses this curve. Default is FALSE.
lty.log	if $logistic.cal=TRUE$, the linetype of the logistic calibration curve. Default is 1.
col.log	if $logistic.cal=TRUE$, the color of the $logistic$ calibration curve. Default is "black".
lwd.log	if $logistic.cal=TRUE$, the line width of the logistic calibration curve. Default is 1.
xlab	x-axis label, default is "Predicted Probability".
ylab	y-axis label, default is "Observed proportion".
xlim, ylim	numeric vectors of length 2, giving the x and y coordinates ranges (see $xlim$ and $ylim$).
m	If grouped proportions are desired, average no. observations per group
g	If grouped proportions are desired, number of quantile groups
cuts	If grouped proportions are desired, actual cut points for constructing intervals, e.g. $c(0, .1, .8, .9, 1)$ or $seq(0, 1, by=.2)$
emax.lim	Vector containing lowest and highest predicted probability over which to compute Emax.
legendloc	if pl=TRUE, list with components x,y or vector $c(x,y)$ for bottom right corner of legend for curves and points. Default is $c(.50, .27)$ scaled to lim. Use locator(1) to use the mouse, FALSE to suppress legend.
statloc	the "abc" of model performance (Steyerberg et al., 2011)-calibration intercept, calibration slope, and c statistic-will be added to the plot, using statloc as the upper left corner of a box (default is $c(0,.85)$). You can specify a list or a vector. Use locator(1) for the mouse, FALSE to suppress statistics. This is plotted after the curve legends.
dostats	specifies whether and which performance measures are shown in the figure. TRUE shows the "abc" of model performance (Steyerberg et al., 2011): calibration intercept, calibration slope, and c-statistic. TRUE is default. FALSE suppresses the presentation of statistics in the figure. A c() list of specific stats shows the specified stats. The key stats which are also mentioned in this paper are "C (ROC)" for the c statistic, "Intercept" for the calibration intercept, "Slope" for the calibration slope, and "ECI" for the estimated calibration index (Van Hoorde et al, 2015). The full list of possible statistics is taken

from val. prob and augmented with the estimated calibration index: "Dxy", "C (ROC)", "R2", "D", "D:Chi-sq", "D:p", "U", "U:Chi-sq", "U:p", "Q", "Brier", "Intercept", "Slope", "Emax", "Brier scaled", "Eavg", "ECI". These statistics are always returned by the function. cl.level if dostats=TRUE, the confidence level for the calculation of the confidence intervals of the calibration intercept, calibration slope and c-statistic. Default is 0.95. method.ci method to calculate the confidence interval of the c-statistic. The argument is passed to auc.nonpara.mw from the auRoc-package and possible methods to compute the confidence interval are "newcombe", "pepe", "delong" or "jackknife". Bootstrap-based methods are not available. The default method is "pepe" and here, the confidence interval is the logit-transformation-based confidence interval as documented in Qin and Hotilovac (2008). See auc.nonpara.mw for more information on the other methods. roundstats specifies the number of decimals to which the statistics are rounded when shown in the plot. Default is 2. riskdist Use "calibrated" to plot the relative frequency distribution of calibrated probabilities after dividing into 101 bins from lim[1] to lim[2]. Set to "predicted" (the default as of rms 4.5-1) to use raw assigned risk, FALSE to omit risk distribution. Values are scaled so that highest bar is 0.15*(lim[2]-lim[1]). controls the font size of the statistics (size) or plot legend (size.leg). Default size, size.leg is 3 and 5, respectively. connect.group Defaults to FALSE to only represent group fractions as triangles. Set to TRUE to also connect with a solid line. connect.smooth Defaults to TRUE to draw smoothed estimates using a line. Set to FALSE to instead use dots at individual estimates g.group number of quantile groups to use when group is given and variable is numeric. evaluate number of points at which to store the lowess-calibration curve. Default is 100. If there are more than evaluate unique predicted probabilities, evaluate equally-spaced quantiles of the unique predicted probabilities, with linearly interpolated calibrated values, are retained for plotting (and stored in the object returned by val.prob. applies when group is given. When nmin > 0, val.prob will not store coornmin dinates of smoothed calibration curves in the outer tails, where there are fewer than nmin raw observations represented in those tails. If for example nmin=50, the plot function will only plot the estimated calibration curve from a to b, where there are 50 subjects with predicted probabilities < a and > b. nmin is ignored when computing accuracy statistics. d0lab, d1lab controls the labels for events and non-events (i.e. outcome y) for the histograms. Defaults are dllab="1" for events and d@lab="0" for non-events. size.d01 controls the size of the labels for events and non-events. Default is 5. dist.label controls the horizontal position of the labels for events and non-events. Default is 0.01. line.bins controls the horizontal (y-axis) position of the histograms. Default is -0.05.

dist.label2 controls the vertical distance between the labels for events and non-events. De-

fault is 0.03.

cutoff puts an arrow at the specified risk cut-off(s). Default is none. length.seg controls the length of the histogram lines. Default is 0.85.

lty.ideal linetype of the ideal line. Default is 1.

col.ideal controls the color of the ideal line on the plot. Default is "red".

lwd.ideal controls the line width of the ideal line on the plot. Default is 1.

allowPerfectPredictions

Logical, indicates whether perfect predictions (i.e. values of either 0 or 1) are allowed. Default is FALSE, since we transform the predictions using the logit transformation to calculate the calibration measures. In case of 0 and 1, this results in minus infinity and infinity, respectively. if allowPerfectPredictions

= TRUE, 0 and 1 are replaced by 1e-8 and 1 - 1e-8, respectively.

argzLoess a list with arguments passed to the loess function

Details

When using the predicted probabilities of an uninformative model (i.e. equal probabilities for all observations), the model has no predictive value. Consequently, where applicable, the value of the performance measure corresponds to the worst possible theoretical value. For the ECI, for example, this equals 1 (Edlinger et al., 2022).

Value

An object of type ggplotCalibrationCurve with the following slots:

call the matched call.
ggPlot the ggplot object.

stats a vector containing performance measures of calibration.

cl.level the confidence level used.

Calibration contains the calibration intercept and slope, together with their confidence inter-

vals.

Cindex the value of the c-statistic, together with its confidence interval.

warningMessages

if any, the warning messages that were printed while running the function.

CalibrationCurves

The coordinates for plotting the calibration curves.

Note

In order to make use (of the functions) of the package auRoc, the user needs to install JAGS. However, since our package only uses the auc.nonpara.mw function which does not depend on the use of JAGS, we therefore copied the code and slightly adjusted it when method="pepe".

References

Edlinger, M, van Smeden, M, Alber, HF, Wanitschek, M, Van Calster, B. (2022). Risk prediction models for discrete ordinal outcomes: Calibration and the impact of the proportional odds assumption. *Statistics in Medicine*, **41**(8), pp. 1334–1360

Qin, G., & Hotilovac, L. (2008). Comparison of non-parametric confidence intervals for the area under the ROC curve of a continuous-scale diagnostic test. *Statistical Methods in Medical Research*, **17(2)**, pp. 207-21

Steyerberg, E.W., Van Calster, B., Pencina, M.J. (2011). Performance measures for prediction models and markers: evaluation of predictions and classifications. *Revista Espanola de Cardiologia*, **64(9)**, pp. 788-794

Van Calster, B., Nieboer, D., Vergouwe, Y., De Cock, B., Pencina M., Steyerberg E.W. (2016). A calibration hierarchy for risk models was defined: from utopia to empirical data. *Journal of Clinical Epidemiology*, **74**, pp. 167-176

Van Hoorde, K., Van Huffel, S., Timmerman, D., Bourne, T., Van Calster, B. (2015). A spline-based tool to assess and visualize the calibration of multiclass risk predictions. *Journal of Biomedical Informatics*, **54**, pp. 283-93

Examples

```
# Load package
library(CalibrationCurves)
set.seed(1783)
# Simulate training data
      = replicate(4, rnorm(5e2))
p0true = binomial()$linkinv(cbind(1, X) %*% c(0.1, 0.5, 1.2, -0.75, 0.8))
       = rbinom(5e2, 1, p0true)
Df
       = data.frame(y, X)
# Fit logistic model
FitLog = lrm(y \sim ., Df)
# Simulate validation data
Xval = replicate(4, rnorm(5e2))
p0true = binomial()$linkinv(cbind(1, Xval) %*% c(0.1, 0.5, 1.2, -0.75, 0.8))
yval = rbinom(5e2, 1, p0true)
Pred = binomial()$linkinv(cbind(1, Xval) %*% coef(FitLog))
# Default calibration plot
valProbggplot(Pred, yval)
# Adding logistic calibration curves and other additional features
valProbggplot(Pred, yval, CL.smooth = TRUE, logistic.cal = TRUE, lty.log = 2,
 col.log = "red", lwd.log = 1.5)
valProbggplot(Pred, yval, CL.smooth = TRUE, logistic.cal = TRUE, lty.log = 9,
col.log = "red", lwd.log = 1.5, col.ideal = colors()[10], lwd.ideal = 0.5)
```

%<=%

%<=%	Infix operator to run background jobs
------	---------------------------------------

Description

This infix operator can be used to create a background job in RStudio/Posit and, once completed, the value of rhs is assigned to lhs.

Usage

```
lhs %<=% rhs
```

Arguments

1hs the object that the rhs value is assigned to

rhs the value you want to assign to lhs

Value

prints the ID of the background job in the console and, once completed, the value of lhs is assigned to rhs

Examples

```
# Can only be executed in Rstudio
## Not run: x %<=% rnorm(1e7)</pre>
```

%{}%

Infix operator to run background jobs

Description

This infix operator can be used to create a background job for a block of code in RStudio/Posit and, once completed, all objects created in the block of code are imported into the global environment.

Usage

```
lhs %{}% rhs
```

Arguments

1hs not used, see details and examplesrhs the block of code that you want to run

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Details

You can use this infix operator in two different ways. Either you set the left-hand side to NULL or you use the syntax `%{}%` ({BlockOfCode})

Value

prints the ID of the background job in the console and, once completed, the objects created in the block of code are imported into the global environment

Examples

```
# Can only be executed in Rstudio
## Not run:
NULL %{}% {
    x = rnorm(1e7)
    y = rnorm(1e7)
}
`%{}%` ({
    x = rnorm(1e7)
    y = rnorm(1e7)
}
## End(Not run)
```

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