

# Package ‘CalibrationCurves’

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**Type** Package

**Title** Calibration Performance

**Version** 2.0.1

**Description** Plots calibration curves and computes statistics for assessing calibration performance. See De Cock Campo (2023) <[arXiv:2309.08559](https://arxiv.org/abs/2309.08559)> and Van Calster et al. (2016) <[doi:10.1016/j.jclinepi.2015.12.005](https://doi.org/10.1016/j.jclinepi.2015.12.005)>.

**License** GPL (>= 3)

**LazyData** TRUE

**Depends** R (>= 3.5.0), rms, ggplot2

**Imports** grDevices, graphics, methods, stats, utils, survival, Hmisc, bookdown

**Suggests** knitr, rmarkdown, mgcv, MASS, magrittr, Matrix

**RoxygenNote** 7.2.3

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**VignetteBuilder** knitr

**URL** <https://bavodc.github.io/websiteCalibrationCurves/>

**NeedsCompilation** no

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.rcspline.plot	<i>Internal function</i>
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### Description

Adjusted version of the [rcspline.plot](#) function where only the output is returned and no plot is made

### Usage

```
.rcspline.plot(
  x,
  y,
  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,
  m,
  smooth = FALSE,
  bass = 1,
  main = "auto",
  statloc
)
```

### Arguments

x	a numeric predictor
y	a numeric response. For binary logistic regression, y should be either 0 or 1.
model	"logistic" or "cox". For "cox", uses the <code>coxph.fit</code> function with <code>method="efron"</code> argument set.
xrange	range for evaluating x, default is $f$ and $1-f$ quantiles of x, where $f = \frac{10}{\max(n,200)}$ and $n$ the number of observations
event	event/censoring indicator if <code>model="cox"</code> . If event is present, model is assumed to be "cox"
nk	number of knots
knots	knot locations, default based on quantiles of x (by <a href="#">rcspline.eval</a> )
show	"xbeta" or "prob" - what is plotted on y-axis
adj	optional matrix of adjustment variables
xlab	x-axis label, default is the "label" attribute of x
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
showknots	show knot locations with arrows
add	add this plot to an already existing plot
plot	logical to indicate whether a plot has to be made. FALSE suppresses the plot.
subset	subset of observations to process, e.g. <code>sex == "male"</code>
lty	line type for plotting estimated spline function
noprint	suppress printing regression coefficients and standard errors
m	for <code>model="logistic"</code> , plot grouped estimates with triangles. Each group contains $m$ ordered observations on x.
smooth	plot nonparametric estimate if <code>model="logistic"</code> and <code>adj</code> is not specified
bass	smoothing parameter (see <code>supsmu</code> )
main	main title, default is "Estimated Spline Transformation"
statloc	location of summary statistics. Default positioning by clicking left mouse button where upper left corner of statistics should appear. Alternative is "ll" to place below the graph on the lower left, or the actual x and y coordinates. Use "none" to suppress statistics.

### 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

### 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**

```
auc.nonpara.mw(x, y, conf.level=0.95,  
               method=c("newcombe", "pepe", "delong",  
                        "jackknife", "bootstrapP", "bootstrapBCa"),  
               nboot)
```

**Arguments**

<code>x</code>	a vector of observations from class P.
<code>y</code>	a vector of observations from class N.
<code>conf.level</code>	confidence level of the interval. The default is 0.95.
<code>method</code>	a method used to construct the CI. <code>newcombe</code> is the method recommended in Newcombe (2006); <code>pepe</code> is the method proposed in Pepe (2003); <code>delong</code> is the method proposed in Delong et al. (1988); <code>jackknife</code> uses the jackknife method; <code>bootstrapP</code> uses the bootstrap with percentile CI; <code>bootstrapBCa</code> uses bootstrap with bias-corrected and accelerated CI. The default is <code>newcombe</code> . It can be abbreviated.
<code>nboot</code>	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.

## 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

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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 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 `val.Probplot` 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

- 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.legend`
- 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>.

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

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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(  
  y,  
  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,
```

```

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

<code>y</code>	a vector with the values for the response variable
<code>yHat</code>	a vector with the predicted values
<code>family</code>	a description of the type of distribution and link function in the model. This can be a character string naming a family function, a family function or the result of a call to a family function. (See <code>family</code> for details of family functions.)
<code>plot</code>	logical, indicating if a plot should be made or not.
<code>Smooth</code>	logical, indicating if the flexible calibration curve should be estimated.
<code>GLMCal</code>	logical, indicating if the GLM calibration curve has to be estimated.
<code>lwdIdeal</code>	the line width of the ideal line.
<code>colIdeal</code>	the color of the ideal line.
<code>ltyIdeal</code>	the line type of the ideal line.
<code>lwdSmooth</code>	the line width of the flexible calibration curve.
<code>colSmooth</code>	the color of the flexible calibration curve.
<code>ltySmooth</code>	the line type of the flexible calibration curve.
<code>argzSmooth</code>	arguments passed to <code>loess</code> .
<code>lwdGLMCal</code>	the line width of the GLM calibration curve.
<code>colGLMCal</code>	the color of the GLM calibration curve.
<code>ltyGLMCal</code>	the line type of the GLM calibration curve.
<code>AddStats</code>	logical, indicating whether to add the values of the generalized calibration slope and intercept to the plot.
<code>Digits</code>	the number of digits of the generalized calibration slope and intercept.
<code>cexStats</code>	the font size of the statistics shown on the plot.
<code>lwdLeg</code>	the line width in the legend.
<code>Legend</code>	logical, indicating whether the legend has to be added.
<code>legendPos</code>	the position of the legend on the plot.
<code>xLim, yLim</code>	numeric vectors of length 2, giving the x and y coordinates ranges (see <code>plot.window</code> )
<code>posStats</code>	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.



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 limits 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
xlab	x-axis label, default is "Predicted value".
ylab	y-axis label, default is "Empirical average".
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 <code>plot</code> , see <code>par</code>

### Value

An object of type `GeneralizedCalibrationCurve` with the following slots:

call	the matched call.
ggPlot	the <code>ggplot</code> 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 intervals.
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 ~ ., data = poissontraindata, family = poisson)
```

```
# 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)
```

---

`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](#)

**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)
```

**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
B = c(0.1, 0.5, 1.2, -0.75, 0.8)
X = replicate(4, rnorm(nTrain))
p0true = binomial()$linkinv(cbind(1, X) %*% B)
y = rbinom(nTrain, 1, p0true)
colnames(X) = paste0("x", seq_len(ncol(X)))
traindata = data.frame(y, X)
```

```
# Simulate validation data
nTest = 500
X = replicate(4, rnorm(nTest))
p0true = binomial()$linkinv(cbind(1, X) %*% B)
y = 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,
  y,
  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

<code>p</code>	predicted probability
<code>y</code>	vector of binary outcomes
<code>logit</code>	predicted log odds of outcome. Specify either <code>p</code> or <code>logit</code> .
<code>group</code>	a grouping variable. If numeric this variable is grouped into <code>g.group</code> quantile groups (default is quartiles). Set <code>group=TRUE</code> to use the group algorithm but with a single stratum for <code>val.prob</code> .
<code>weights</code>	an optional numeric vector of per-observation weights (usually frequencies), used only if <code>group</code> is given.
<code>normwt</code>	set to <code>TRUE</code> to make <code>weights</code> sum to the number of non-missing observations.
<code>pl</code>	<code>TRUE</code> to plot the calibration curve(s). If <code>FALSE</code> no calibration curves will be plotted, but statistics will still be computed and outputted.
<code>smooth</code>	"loess" generates a flexible calibration curve based on <code>loess</code> , "rcs" generates a calibration curves based on restricted cubic splines (see <code>rcs</code> and <code>rcspline.plot</code> ), "none" suppresses the flexible curve. We recommend to use <code>loess</code> unless <code>N</code> is large, for example <code>N&gt;5000</code> . Default is "loess".
<code>CL.smooth</code>	"fill" shows pointwise 95% confidence limits for the flexible calibration curve with a gray area between the lower and upper limits, <code>TRUE</code> shows pointwise 95% confidence limits for the flexible calibration curve with dashed lines, <code>FALSE</code> suppresses the confidence limits. Default is "fill".
<code>CL.BT</code>	<code>TRUE</code> uses confidence limits based on 2000 bootstrap samples, <code>FALSE</code> uses closed form confidence limits. Default is <code>FALSE</code> .
<code>lty.smooth</code>	the linetype of the flexible calibration curve. Default is 1.
<code>col.smooth</code>	the color of the flexible calibration curve. Default is "black".
<code>lwd.smooth</code>	the line width of the flexible calibration curve. Default is 1.
<code>nr.knots</code>	specifies the number of knots for <code>rcs</code> -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.
<code>logistic.cal</code>	<code>TRUE</code> plots the logistic calibration curve, <code>FALSE</code> suppresses this curve. Default is <code>FALSE</code> .
<code>lty.log</code>	if <code>logistic.cal=TRUE</code> , the linetype of the logistic calibration curve. Default is 1.
<code>col.log</code>	if <code>logistic.cal=TRUE</code> , the color of the logistic calibration curve. Default is "black".



lwd.log	if <code>logistic.cal=TRUE</code> , 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 <a href="#">plot.window</a> )
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. <code>c(0, .1, .8, .9, 1)</code> or <code>seq(0, 1, by=.2)</code>
emax.lim	Vector containing lowest and highest predicted probability over which to compute <code>E<sub>max</sub></code> .
legendloc	if <code>pl=TRUE</code> , list with components <code>x</code> , <code>y</code> or vector <code>c(x, y)</code> for bottom right corner of legend for curves and points. Default is <code>c(.50, .27)</code> scaled to <code>lim</code> . Use <code>locator(1)</code> to use the mouse, <code>FALSE</code> 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 <code>statloc</code> as the upper left corner of a box (default is <code>c(0,85)</code> ). You can specify a list or a vector. Use <code>locator(1)</code> for the mouse, <code>FALSE</code> to suppress statistics. This is plotted after the curve legends.
dostats	specifies whether and which performance measures are shown in the figure. <code>TRUE</code> shows the "abc" of model performance (Steyerberg et al., 2011): calibration intercept, calibration slope, and c-statistic. <code>TRUE</code> is default. <code>FALSE</code> suppresses the presentation of statistics in the figure. A <code>c()</code> 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 <a href="#">val.prob</a> 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", "E <sub>max</sub> ", "Brier scaled", "Eavg", "ECI". These statistics are always returned by the function.
cl.level	if <code>dostats=TRUE</code> , 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 <a href="#">auc.nonpara.mw</a> from the <code>auRoc</code> -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 <a href="#">auc.nonpara.mw</a> 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 $\text{lim}[1]$ to $\text{lim}[2]$ . 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 $0.15 * (\text{lim}[2] - \text{lim}[1])$ .
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. Default 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 ( <a href="#">legend</a> )
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 <a href="#">loess</a> function
...	arguments to be passed to <a href="#">plot</a> , see <a href="#">par</a>

## 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:

<code>call</code>	the matched call.
<code>stats</code>	a vector containing performance measures of calibration.
<code>cl.level</code>	the confidence level used.
<code>Calibration</code>	contains the calibration intercept and slope, together with their confidence intervals.
<code>Cindex</code>	the value of the c-statistic, together with its confidence interval.
<code>warningMessages</code>	if any, the warning messages that were printed while running the function.
<code>CalibrationCurves</code>	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
X      = replicate(4, rnorm(5e2))
p0true = binomial()$linkinv(cbind(1, X) %*% c(0.1, 0.5, 1.2, -0.75, 0.8))
y      = rbinom(5e2, 1, p0true)
Df     = data.frame(y, X)

# Fit logistic model
FitLog = lrm(y ~ ., 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(
  p,
```

```
y,  
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

p	predicted probability
y	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 <a href="#">loess</a> , "rcs" generates a calibration curves based on restricted cubic splines (see <a href="#">rcs</a> and <a href="#">rcspline.plot</a> ), "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 <a href="#">xlim</a> and <a href="#">ylim</a> ).
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. <code>c(0, .1, .8, .9, 1)</code> or <code>seq(0, 1, by=.2)</code>
emax.lim	Vector containing lowest and highest predicted probability over which to compute Emax.
legendloc	if <code>pl=TRUE</code> , list with components <code>x, y</code> or vector <code>c(x, y)</code> for bottom right corner of legend for curves and points. Default is <code>c(.50, .27)</code> scaled to <code>lim</code> . Use <code>locator(1)</code> to use the mouse, <code>FALSE</code> 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 <code>statloc</code> as the upper left corner of a box (default is <code>c(0,.85)</code> ). You can specify a list or a vector. Use <code>locator(1)</code> for the mouse, <code>FALSE</code> to suppress statistics. This is plotted after the curve legends.
dostats	specifies whether and which performance measures are shown in the figure. <code>TRUE</code> shows the "abc" of model performance (Steyerberg et al., 2011): calibration intercept, calibration slope, and c-statistic. <code>TRUE</code> is default. <code>FALSE</code> suppresses the presentation of statistics in the figure. A <code>c()</code> 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 <a href="#">val.prob</a> 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 <code>dostats=TRUE</code> , the confidence level for the calculation of the confidence intervals of the calibration intercept, calibration slope and c-statistic. Default is <code>0.95</code> .
method.ci	method to calculate the confidence interval of the c-statistic. The argument is passed to <a href="#">auc.nonpara.mw</a> from the <code>auRoc</code> -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 <a href="#">auc.nonpara.mw</a> 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 <code>lim[1]</code> to <code>lim[2]</code> . Set to "predicted" (the default as of rms 4.5-1) to use raw assigned risk, <code>FALSE</code> to omit risk distribution. Values are scaled so that highest bar is $0.15 * (\text{lim}[2] - \text{lim}[1])$ .

size, size.leg	controls the font size of the statistics (size) or plot legend (size.leg). Default 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.
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.
size.d01	controls the size of the labels for events and non-events. Default is 5.
dist.label1	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. Default 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 <a href="#">loess</a> 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:

<code>call</code>	the matched call.
<code>ggPlot</code>	the <code>ggplot</code> object.
<code>stats</code>	a vector containing performance measures of calibration.
<code>cl.level</code>	the confidence level used.
<code>Calibration</code>	contains the calibration intercept and slope, together with their confidence intervals.
<code>Cindex</code>	the value of the c-statistic, together with its confidence interval.
<code>warningMessages</code>	if any, the warning messages that were printed while running the function.
<code>CalibrationCurves</code>	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
X      = replicate(4, rnorm(5e2))
p0true = binomial()$linkinv(cbind(1, X) %*% c(0.1, 0.5, 1.2, -0.75, 0.8))
y      = rbinom(5e2, 1, p0true)
Df     = data.frame(y, X)

# Fit logistic model
FitLog = lrm(y ~ ., 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)
```

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