Package 'ValCurvaR'

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Type Package

Title Validation of Analytical Calibration Curves

Version 0.1.0

Description Provides transparent tools for fitting and evaluating analytical calibration curves. Ordinary and weighted least squares fits are supported, together with lack-of-fit, heteroscedasticity and influence diagnostics, back-calculation, prediction uncertainty and publication-ready base graphics. The workflow is designed to support validation studies rather than rely on a single goodness-of-fit statistic. Methods follow Magnusson and Ornemark (2014) <https://www.eurachem.org/images/stories/Guides/pdf/MV_guide_2nd_ed_EN.pdf> and International Council for Harmonisation (2023) <https://database.ich.org/sites/default/files/ICH_Q2%28R2%29_Guideline_2023_1130_ErrorCorrection_2025.pdf>.

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URL https://github.com/isaquebrand/ValCurvaR

BugReports https://github.com/isaquebrand/ValCurvaR/issues

Encoding UTF-8

Imports graphics, grDevices, lmtest, nortest, outliers, stats

Suggests knitr, rmarkdown, testthat (>= 3.0.0)

VignetteBuilder knitr

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Config/roxygen2/version 8.0.0

NeedsCompilation no

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Repository CRAN

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Contents

`ajustar_curva` *Fit an analytical calibration curve*

Description

Fit an analytical calibration curve

Usage

```
ajustar_curva(
  dados,
  metodo = c("auto", "ols", "wls"),
  pesos = c("variancia_nivel", "1/x", "1/x2", "1/y", "1/y2")
)
```

Arguments

`dados`	Validated data from `validar_curva()` or a data frame with internal `.x` and `.y` columns.
`metodo`	One of `"auto"`, `"ols"` or `"wls"`.
`pesos`	WLS strategy. `"variancia_nivel"` uses the inverse experimental variance at each concentration; other choices are empirical alternatives.

Value

A `valcurva_fit` object.

analisar_sensibilidade *Evaluate the impact of suspicious observations without deleting them*

Description

Fits leave-one-out models solely for technical review. It never changes the original data or approves exclusion of a measurement.

Usage

```
analisar_sensibilidade(ajuste, observacoes = NULL)
```

Arguments

ajuste	A valcurva_fit object.
observacoes	Optional row numbers. By default, all observations flagged by Cook's distance, leverage, DFFITS, DFBETAS or studentized residuals are used.

Value

A data frame comparing each leave-one-out model with the original fit.

avaliar_adequacao *Evaluate calibration-curve adequacy against explicit criteria*

Description

No universal acceptance limits are imposed. Supply only the limits applicable to the analytical procedure, matrix, and intended range. A missing criterion is reported as not assessed rather than silently approved.

Usage

```
avaliar_adequacao(ajuste, criterios = list())
```

Arguments

ajuste	A valcurva_fit object.
criterios	A named list. Supported names are p_falta_ajuste_min, p_mandel_min, cv_max_percentual, and erro_relativo_retrocalculo_max_percentual.

Value

An object of class valcurva_adequacao with a criterion table, back-calculation table, and conclusion.

comparar_modelos *Compare OLS and WLS calibration models*

Description

Compare OLS and WLS calibration models

Usage

```
comparar_modelos(ols, wls)
```

Arguments

ols	An OLS valcurva_fit object.
wls	A WLS valcurva_fit object.

Value

A data frame intended as decision support, not an automatic approval.

dados_eurachem_a52 *Eurachem A5.2 calibration data*

Description

Fifteen individual absorbance measurements at five cadmium calibration levels. Values are transcribed from Table A5.2 of the Eurachem/CITAC uncertainty guide and are supplied in long format to preserve replicates.

Usage

```
dados_eurachem_a52()
```

Value

A data frame with concentracao_mg_L, replica, and absorbancia.

Examples

```
dados <- dados_eurachem_a52()
curva <- validar_curva(dados, concentracao_mg_L, absorbancia, replica)
ajuste <- ajustar_curva(curva, metodo = "ols")
grafico_calibracao(ajuste)
```

diagnosticar_curva *Calculate calibration-curve diagnostics*

Description

Calculate calibration-curve diagnostics

Usage

```
diagnosticar_curva(ajuste)
```

Arguments

ajuste	An object returned by ajustar_curva().

Value

A named list of diagnostic results.

gerar_relatorio_pdf *Generate a complete calibration-validation report in PDF*

Description

Generate a complete calibration-validation report in PDF

Usage

```
gerar_relatorio_pdf(
  ajuste,
  arquivo = file.path(tempdir(), "relatorio-calibracao.pdf"),
  titulo = "Relatorio de validacao da curva de calibracao",
  criterios = list(),
  quiet = TRUE
)
```

Arguments

ajuste	A valcurva_fit object.
arquivo	Output PDF path. By default, a temporary file is used so the function does not write to the user's working directory.
titulo	Title shown in the report.
criterios	Optional acceptance criteria forwarded to avaliar_adequacao().
quiet	Logical; suppress R Markdown progress messages.

Value

Invisibly, the normalized path to the generated PDF.

`grafico_calibracao` *Plot an analytical calibration diagram*

Description

Draws individual data, centroids, fitted line and 95% prediction limits in the visual language of the metrology article supplied for this project.

Usage

```
grafico_calibracao(ajuste, nivel = 0.95, ...)
```

Arguments

`ajuste`	A `valcurva_fit` object.
`nivel`	Confidence level for prediction limits.
`...`	Graphical parameters passed to `graphics::plot()`.

Value

Invisibly, a data frame used to draw the prediction curves.

`grafico_incerteza_predicao`
Plot inverse prediction uncertainty over the calibration range

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Description

Plot inverse prediction uncertainty over the calibration range

Usage

```
grafico_incerteza_predicao(ajuste, k = c(1, 2, 3, 4, 9, 16))
```

Arguments

`ajuste`	A `valcurva_fit` object.
`k`	Numeric vector of numbers of replicate measurements.

Value

Invisibly, plotted uncertainty data.

grafico_influencia *Plot Cook's distance and leverage against their screening limits*

Description

Plot Cook's distance and leverage against their screening limits

Usage

```
grafico_influencia(ajuste)
```

Arguments

ajuste	A valcurva_fit object.

Value

Invisibly, the influence diagnostics.

grafico_qq *Plot a normal Q-Q graph with a simulation envelope for residuals*

Description

Plot a normal Q-Q graph with a simulation envelope for residuals

Usage

```
grafico_qq(ajuste, nivel = 0.95, simulacoes = 999L, semente = NULL)
```

Arguments

ajuste	A valcurva_fit object.
nivel	Envelope coverage level.
simulacoes	Number of normal samples used to build the envelope.
semente	Optional seed for a reproducible envelope.

Value

Invisibly, data used to construct the graph.

grafico_residuos *Plot standardized residuals against concentration*

Description

Plot standardized residuals against concentration

Usage

```
grafico_residuos(ajuste)
```

Arguments

ajuste	A valcurva_fit object.

Value

Invisibly, residual diagnostic data.

grafico_variancia *Plot instrumental-response variability by concentration*

Description

Plot instrumental-response variability by concentration

Usage

```
grafico_variancia(ajuste)
```

Arguments

ajuste	A valcurva_fit object.

Value

Invisibly, the level summary.

painel_calibracao *Create the four-panel calibration figure*

Description

Create the four-panel calibration figure

Usage

```
painel_calibracao(ajuste, k = c(1, 2, 3, 4, 9, 16))
```

Arguments

ajuste	A valcurva_fit object.
k	Replicate counts for the uncertainty panel.

Value

Invisibly, ajuste.

relatorio_auditoria *Build an auditable calibration summary*

Description

Build an auditable calibration summary

Usage

```
relatorio_auditoria(ajuste, criterios = list())
```

Arguments

ajuste	A valcurva_fit object.
criterios	Optional criteria forwarded to avaliar_adequacao().

Value

A named list with model, diagnostics, adequacy assessment, and data.

`retrocalcular_concentracao` *Back-calculate concentration with GUM uncertainty propagation*

Description

The measurement model is `x = (y - a) / b`. The covariance of the fitted intercept (`a`) and slope (`b`) is retained explicitly in the combined uncertainty. It must not be discarded or treated as two independent inputs.

Usage

```
retrocalcular_concentracao(
  ajuste,
  sinal,
  k = 1L,
  u_sinal = NULL,
  nivel = 0.95,
  fator_cobertura = NULL
)
```

Arguments

`ajuste`	A `valcurva_fit` object.
`sinal`	Numeric vector of instrumental responses.
`k`	Number of replicate signals averaged for each result.
`u_sinal`	Standard uncertainty of each reported signal. If `NULL`, the residual standard deviation of the fit divided by `sqrt(k)` is used as a data-derived estimate.
`nivel`	Confidence level.
`fator_cobertura`	Optional coverage factor. If `NULL`, a two-sided Student t factor using the regression degrees of freedom is used. This keeps the correlated regression coefficients as one uncertainty block.

Value

A data frame with concentration, combined and expanded GUM uncertainty, and the individual variance contributions.

validar_curva *Validate analytical calibration data*

Description

Keeps the original measurements in long format. A horizontal table is also accepted: omit `sinal` and every numeric column other than `concentracao` is converted internally to a replicate column. Replicates must not be averaged before validation because they are needed for variance and lack-of-fit diagnostics.

Usage

```
validar_curva(dados, concentracao, sinal = NULL, replica = NULL)
```

Arguments

`dados`	A data frame.
`concentracao`	Concentration column, supplied bare or as a string.
`sinal`	Instrumental response column, supplied bare or as a string. Omit it for horizontal data with one numeric response column per replicate.
`replica`	Optional replicate identifier column.

Value

A `data.frame` with standard internal columns `.x`, `.y` and `.replica`.

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