Package 'adsoRptionCV'

June 3, 2025

Type Package

Title Cross-Validation Methods for Adsorption Isotherm Models

Version 0.1.0

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Description Provides cross-
validation tools for adsorption isotherm models, supporting both linear and non-linear forms.
Current methods cover commonly used isotherms including the Freundlich, Lang-
muir, and Temkin models.
This package implements K-fold and leave-one-out cross-
validation (LOOCV) with optional clustering-based
fold assignment to preserve underlying data structures during validation. Model predictive per-
formance is assessed
using mean squared error (MSE), with optional graphical visualization of fold-
wise MSEs to support intuitive evaluation of model accuracy.
This package is intended to facilitate rigorous model validation in adsorption studies and aid re-
searchers in selecting robust isotherm models.
For more details, see Montgomery et al. (2012) <isbn: 978-0-470-54281-1>, Lu-
mumba et al. (2024) <doi:10.11648/j.ajtas.20241305.13>, and Yates et al. (2022) <doi:10.1002/ecm.1557>.

License GPL-3

Encoding UTF-8

Imports stats, nls2, graphics

Suggests testthat

Config/testthat/edition 3

RoxygenNote 7.3.2

NeedsCompilation no

Repository CRAN

Date/Publication 2025-06-03 13:00:06 UTC

Contents

`cv_freundlichLM` *Cross-Validation for Freundlich Isotherm Linear Model with Clustering-based Fold Assignment*

Description

Performs K-fold or leave-one-out cross-validation (LOOCV) on the linearized Freundlich isotherm model: log(Qe) = log(KF) + (1/n) * log(Ce) Evaluates predictive performance using Mean Squared Error (MSE). Optionally displays a barplot of fold-wise MSEs. Optionally uses clustering-based fold assignment to preserve data structure.

Arguments

`Ce`	Numeric vector of equilibrium concentrations (Ce). Must be positive.
`Qe`	Numeric vector of amounts adsorbed (Qe). Must be positive and same length as Ce.
`K`	Integer. Number of folds to use in K-fold CV (default is 10). Ignored if loocv = TRUE.
`seed`	Integer. Random seed for reproducibility (default is 123).
`loocv`	Logical. If TRUE, performs leave-one-out cross-validation (overrides K).
`plot`	Logical. If TRUE, displays a barplot of fold MSEs (default is FALSE).
`use_clustering`	Logical. If TRUE, assigns folds using k-means clustering on the data (default FALSE).

Value

A list with the following components:

mean_mse The average mean squared error across all folds.

fold_mse A numeric vector of MSEs for each fold.

Author(s)

Paul Angelo C. Manlapaz

References

Montgomery, D.C., Peck, E.A., & Vining, G.G. (2012). Introduction to Linear Regression Analysis, 5th ed. Wiley.

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
cv_freundlichLM(Ce, Qe, K = 5, seed = 123, plot = TRUE, use_clustering = TRUE)
cv_freundlichLM(Ce, Qe, loocv = TRUE, plot = TRUE)
```

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cv_freundlichNLM *Cross-Validation for Freundlich Isotherm Non-Linear Model with Clustering-based Fold Assignment*

Description

Performs K-fold or leave-one-out cross-validation (LOOCV) on the non-linear Freundlich isotherm model: Qe = KF * Ce^(1/n) Fits a non-linear model of Qe versus Ce using non-linear least squares (nls2). Evaluates predictive performance using Mean Squared Error (MSE). Optionally displays a barplot of fold-wise MSEs. Optionally uses clustering-based fold assignment to preserve data structure.

Arguments

`Ce`	Numeric vector of equilibrium concentrations (Ce). Must be positive.
`Qe`	Numeric vector of amounts adsorbed (Qe). Must be positive and same length as Ce.
`K`	Integer. Number of folds to use in K-fold CV (default is 10). Ignored if loocv = TRUE.
`seed`	Integer. Random seed for reproducibility (default is 123).
`loocv`	Logical. If TRUE, performs leave-one-out cross-validation (overrides K).
`plot`	Logical. If TRUE, displays a barplot of fold MSEs (default is FALSE).
`use_clustering`	Logical. If TRUE, assigns folds using k-means clustering on the data (default FALSE).

Value

A list with the following components:

mean_mse The average mean squared error across all folds.

fold_mse A numeric vector of MSEs for each fold.

Author(s)

Paul Angelo C. Manlapaz

References

Montgomery, D.C., Peck, E.A., & Vining, G.G. (2012). Introduction to Linear Regression Analysis, 5th ed. Wiley.

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
cv_freundlichNLM(Ce, Qe, K = 5, seed = 123, plot = TRUE, use_clustering = TRUE)
cv_freundlichNLM(Ce, Qe, loocv = TRUE, plot = TRUE)
```

---

cv_langmuirLM1 *Cross-Validation for Langmuir Isotherm First Linear Model with Clustering-based Fold Assignment*

Description

Performs K-fold or leave-one-out cross-validation (LOOCV) on the linearized Langmuir isotherm model (Form 1): Ce / Qe = 1 / (Qmax * b) + Ce / Qmax This corresponds to a linear regression of Ce / Qe versus Ce. Evaluates predictive performance using Mean Squared Error (MSE). Optionally displays a barplot of fold-wise MSEs. Optionally uses clustering-based fold assignment to preserve data structure.

Arguments

`Ce`	Numeric vector of equilibrium concentrations (Ce). Must be positive.
`Qe`	Numeric vector of amounts adsorbed (Qe). Must be positive and same length as Ce.
`K`	Integer. Number of folds to use in K-fold CV (default is 10). Ignored if loocv = TRUE.
`seed`	Integer. Random seed for reproducibility (default is 123).
`loocv`	Logical. If TRUE, performs leave-one-out cross-validation (overrides K).
`plot`	Logical. If TRUE, displays a barplot of fold MSEs (default is FALSE).
`use_clustering`	Logical. If TRUE, assigns folds using k-means clustering on the data (default FALSE).

Value

A list with the following components:

mean_mse The average mean squared error across all folds.

fold_mse A numeric vector of MSEs for each fold.

Author(s)

Paul Angelo C. Manlapaz

References

Montgomery, D.C., Peck, E.A., & Vining, G.G. (2012). Introduction to Linear Regression Analysis, 5th ed. Wiley.

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
cv_langmuirLM1(Ce, Qe, K = 5, seed = 123, plot = TRUE, use_clustering = TRUE)
cv_langmuirLM1(Ce, Qe, loocv = TRUE, plot = TRUE)
```

---

cv_langmuirLM2 *Cross-Validation for Langmuir Isotherm Second Linear Model with Clustering-based Fold Assignment*

Description

Performs K-fold or leave-one-out cross-validation (LOOCV) on the linearized Langmuir isotherm model (Form 2): 1 / Qe = (1 / (Qmax * b)) * (1 / Ce) + 1 / Qmax This corresponds to a linear regression of 1 / Qe versus 1 / Ce. Evaluates predictive performance using Mean Squared Error (MSE). Optionally displays a barplot of fold-wise MSEs. Optionally uses clustering-based fold assignment to preserve data structure.

Arguments

`Ce`	Numeric vector of equilibrium concentrations (Ce). Must be positive.
`Qe`	Numeric vector of amounts adsorbed (Qe). Must be positive and same length as Ce.
`K`	Integer. Number of folds to use in K-fold CV (default is 10). Ignored if loocv = TRUE.
`seed`	Integer. Random seed for reproducibility (default is 123).
`loocv`	Logical. If TRUE, performs leave-one-out cross-validation (overrides K).
`plot`	Logical. If TRUE, displays a barplot of fold MSEs (default is FALSE).
`use_clustering`	Logical. If TRUE, assigns folds using k-means clustering on the data (default FALSE).

Value

A list with the following components:

mean_mse The average mean squared error across all folds.

fold_mse A numeric vector of MSEs for each fold.

Author(s)

Paul Angelo C. Manlapaz

References

Montgomery, D.C., Peck, E.A., & Vining, G.G. (2012). Introduction to Linear Regression Analysis, 5th ed. Wiley.

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
cv_langmuirLM2(Ce, Qe, K = 5, seed = 123, plot = TRUE, use_clustering = TRUE)
cv_langmuirLM2(Ce, Qe, loocv = TRUE, plot = TRUE)
```

---

cv_langmuirLM3 *Cross-Validation for Langmuir Isotherm Third Linear Model with Clustering-based Fold Assignment*

Description

Performs K-fold or leave-one-out cross-validation (LOOCV) on the linearized Langmuir isotherm model (Form 3): Qe = Qmax - (1 / b) * (Qe / Ce) This corresponds to a linear regression of Qe versus Qe / Ce. Evaluates predictive performance using Mean Squared Error (MSE). Optionally displays a barplot of fold-wise MSEs. Optionally uses clustering-based fold assignment to preserve data structure.

Arguments

`Ce`	Numeric vector of equilibrium concentrations (Ce). Must be positive.
`Qe`	Numeric vector of amounts adsorbed (Qe). Must be positive and same length as Ce.
`K`	Integer. Number of folds to use in K-fold CV (default is 10). Ignored if loocv = TRUE.
`seed`	Integer. Random seed for reproducibility (default is 123).
`loocv`	Logical. If TRUE, performs leave-one-out cross-validation (overrides K).
`plot`	Logical. If TRUE, displays a barplot of fold MSEs (default is FALSE).
`use_clustering`	Logical. If TRUE, assigns folds using k-means clustering on the data (default FALSE).

Value

A list with the following components:

mean_mse The average mean squared error across all folds.

fold_mse A numeric vector of MSEs for each fold.

Author(s)

Paul Angelo C. Manlapaz

References

Montgomery, D.C., Peck, E.A., & Vining, G.G. (2012). Introduction to Linear Regression Analysis, 5th ed. Wiley.

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
cv_langmuirLM3(Ce, Qe, K = 5, seed = 123, plot = TRUE, use_clustering = TRUE)
cv_langmuirLM3(Ce, Qe, loocv = TRUE, plot = TRUE)
```

---

cv_langmuirLM4 *Cross-Validation for Langmuir Isotherm Fourth Linear Model with Clustering-based Fold Assignment*

Description

Performs K-fold or leave-one-out cross-validation (LOOCV) on the linearized Langmuir isotherm model (Form 4): Qe / Ce = b * Qmax - b * Qe This corresponds to a linear regression of Qe / Ce versus Qe. Evaluates predictive performance using Mean Squared Error (MSE). Optionally displays a barplot of fold-wise MSEs. Optionally uses clustering-based fold assignment to preserve data structure.

Arguments

`Ce`	Numeric vector of equilibrium concentrations (Ce). Must be positive.
`Qe`	Numeric vector of amounts adsorbed (Qe). Must be positive and same length as Ce.
`K`	Integer. Number of folds to use in K-fold CV (default is 10). Ignored if loocv = TRUE.
`seed`	Integer. Random seed for reproducibility (default is 123).
`loocv`	Logical. If TRUE, performs leave-one-out cross-validation (overrides K).
`plot`	Logical. If TRUE, displays a barplot of fold MSEs (default is FALSE).
`use_clustering`	Logical. If TRUE, assigns folds using k-means clustering on the data (default FALSE).

Value

A list with the following components:

mean_mse The average mean squared error across all folds.

fold_mse A numeric vector of MSEs for each fold.

Author(s)

Paul Angelo C. Manlapaz

References

Montgomery, D.C., Peck, E.A., & Vining, G.G. (2012). Introduction to Linear Regression Analysis, 5th ed. Wiley.

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
cv_langmuirLM4(Ce, Qe, K = 5, seed = 123, plot = TRUE, use_clustering = TRUE)
cv_langmuirLM4(Ce, Qe, loocv = TRUE, plot = TRUE)
```

---

cv_langmuirNLM *Cross-Validation Analysis for Langmuir Isotherm Non-linear Model with Clustering-based Fold Assignment*

Description

Performs K-fold or leave-one-out cross-validation (LOOCV) on the Langmuir isotherm non-linear model: Qe = (Qmax * Ce) / (b + Ce) where Qmax is the maximum adsorption capacity and b is the Langmuir constant. Supports optional clustering-based fold assignment and visualization of fold MSEs.

Arguments

`Ce`	Numeric vector of equilibrium concentrations (Ce). Must be positive.
`Qe`	Numeric vector of amounts adsorbed (Qe). Must be positive and same length as Ce.
`K`	Integer. Number of folds to use in K-fold CV (default is 10). Ignored if loocv = TRUE.
`seed`	Integer. Random seed for reproducibility (default is 123).
`loocv`	Logical. If TRUE, performs leave-one-out cross-validation (overrides K).
`plot`	Logical. If TRUE, displays a barplot of fold MSEs (default is FALSE).
`use_clustering`	Logical. If TRUE, assigns folds using k-means clustering on the data (default FALSE).

Value

A list with the following components:

mean_mse The average mean squared error across all folds.

fold_mse A numeric vector of MSEs for each fold.

Author(s)

Paul Angelo C. Manlapaz

References

Montgomery, D.C., Peck, E.A., & Vining, G.G. (2012). Introduction to Linear Regression Analysis, 5th ed. Wiley.

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
cv_langmuirNLM(Ce, Qe, K = 5, seed = 123, plot = TRUE, use_clustering = TRUE)
cv_langmuirNLM(Ce, Qe, loocv = TRUE, plot = TRUE)
```

---

cv_temkinLM *Cross-Validation for Temkin Isotherm Linear Model with Clustering-based Fold Assignment*

Description

Performs K-fold or leave-one-out cross-validation (LOOCV) on the Temkin isotherm linear model: Qe = B * log(A) + B * log(Ce) This corresponds to a linear regression of Qe versus log(Ce). Evaluates predictive performance using Mean Squared Error (MSE). Optionally displays a barplot of fold-wise MSEs. Optionally uses clustering-based fold assignment to preserve data structure.

Arguments

`Ce`	Numeric vector of equilibrium concentrations (Ce). Must be positive.
`Qe`	Numeric vector of amounts adsorbed (Qe). Must be positive and same length as Ce.
`K`	Integer. Number of folds to use in K-fold CV (default is 10). Ignored if loocv = TRUE.
`seed`	Integer. Random seed for reproducibility (default is 123).
`loocv`	Logical. If TRUE, performs leave-one-out cross-validation (overrides K).
`plot`	Logical. If TRUE, displays a barplot of fold MSEs (default is FALSE).
`use_clustering`	Logical. If TRUE, assigns folds using k-means clustering on the data (default FALSE).

Value

A list with the following components:

mean_mse The average mean squared error across all folds.

fold_mse A numeric vector of MSEs for each fold.

Author(s)

Paul Angelo C. Manlapaz

References

Montgomery, D.C., Peck, E.A., & Vining, G.G. (2012). Introduction to Linear Regression Analysis, 5th ed. Wiley.

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
cv_temkinLM(Ce, Qe, K = 5, seed = 123, plot = TRUE, use_clustering = TRUE)
cv_temkinLM(Ce, Qe, loocv = TRUE, plot = TRUE)
```

---

cv_temkinNLM *Cross-Validation for Temkin Isotherm Non-Linear Model with Clustering-based Fold Assignment*

Description

Performs K-fold or leave-one-out cross-validation (LOOCV) on the non-linear Temkin isotherm model: Qe = (RT / bT) * log(AT * Ce) Fits a non-linear model of Qe versus Ce using non-linear least squares (nls2). Evaluates predictive performance using Mean Squared Error (MSE). Optionally displays a barplot of fold-wise MSEs. Optionally uses clustering-based fold assignment to preserve data structure.

Arguments

`Ce`	Numeric vector of equilibrium concentrations (Ce). Must be positive.
`Qe`	Numeric vector of amounts adsorbed (Qe). Must be positive and same length as Ce.
`Temp`	Numeric scalar. Temperature in Kelvin. Must be positive.
`K`	Integer. Number of folds to use in K-fold CV (default is 10). Ignored if loocv = TRUE.
`seed`	Integer. Random seed for reproducibility (default is 123).
`loocv`	Logical. If TRUE, performs leave-one-out cross-validation (overrides K).
`plot`	Logical. If TRUE, displays a barplot of fold MSEs (default is FALSE).
`use_clustering`	Logical. If TRUE, assigns folds using k-means clustering on the data (default FALSE).

Value

A list with the following components:

mean_mse The average mean squared error across all folds.

fold_mse A numeric vector of MSEs for each fold.

Author(s)

Paul Angelo C. Manlapaz

References

Montgomery, D.C., Peck, E.A., & Vining, G.G. (2012). Introduction to Linear Regression Analysis, 5th ed. Wiley.

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
cv_temkinNLM(Ce, Qe, Temp = 298, K = 5, seed = 123, plot = TRUE, use_clustering = TRUE)
cv_temkinNLM(Ce, Qe, Temp = 298, loocv = TRUE, plot = TRUE)
```

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