Package 'TOU'

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Type Package

Title Transformed Ornstein-Uhlenbeck Model for Adsorption Kinetics

Version 0.1.0

Description

Estimates the parameters of a Transformed Ornstein-Uhlenbeck (TOU) stochastic model for adsorption data and also the parameters of the related pseudo-n-order (PNO) model, such as the maximum adsorption capacity (qe), the adsorption rate constant (kn) and the order of the model (n).

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Encoding UTF-8

RoxygenNote 7.1.2

Imports DEoptim (>= 2.2-6), ggplot2 (>= 3.3.5), Rdpack

RdMacros Rdpack

NeedsCompilation no

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draw.model.tou   *A plot with the experimental data and the Transformed Ornstein-Uhlenbeck (TOU) model.*

Description

Plots the experimental data and the fitted TOU model.

Usage

```
draw.model.tou(x, time.unit = NULL, adsorption.unit = NULL)
```

Arguments

x   a tou object.

time.unit   an optional label indicating the unit name for the time, the allowed labels are
                    "seconds", "minutes" and "hours".

adsorption.unit
                    a label indicating for unit name for the adsorption, the allowed labels are "mg/g"
                    and "mg/mmol".

Value

a plot with the experimental data and the fitted TOU model.

Examples

```
# an example with one trajectory of experimental adsorption
observed.time <- c(0, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 150, 200,
                    250, 300)
observed.values <- c(0, 1.684, 2.341, 2.581, 2.842, 2.890, 2.959, 3.042,
                        3.083, 3.043, 3.017, 2.954, 2.996, 2.886, 2.844)
observed.process <- cbind(observed.time, observed.values)
# fitting the model without any fixed parameters
result <- fit.model.tou(w=observed.process)
# default units time in minutes and default units adsorption in mg/g
draw.model.tou(result)
# changing units time to seconds and units adsorption to mg/mmol
draw.model.tou(result, time.unit="seconds", adsorption.unit="mg/mmol")

observed.time <- c(0, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 150, 200,
                    250, 300)
observed.values.1 <- c(0, 1.684, 2.341, 2.581, 2.842, 2.890, 2.959, 3.042,
                        3.083, 3.043, 3.017, 2.954, 2.996, 2.886, 2.844)
observed.values.2 <- c(0, 1.618, 2.217, 2.571, 2.763, 2.841, 2.866, 2.898,
                        2.935, 2.973, 2.906, 2.919, 2.910, 3.012, 3.071)
observed.values.3 <- c(0, 1.596, 2.333, 2.611, 2.750, 2.731, 2.829, 2.838,
                        2.864, 2.884, 2.886, 2.911, 2.896, 2.877, 2.969)
observed.processes <- cbind(observed.time, observed.values.1,
```

```
                              observed.values.2, observed.values.3)
# fitting the model without any fixed parameters
result <- fit.model.tou(w=observed.processes)
draw.model.tou(result)
```

---

fit.model.tou   *Estimation of Transformed Ornstein-Uhlenbeck model for adsorption kinetics.*

Description

This function finds the best values for the parameters of the pseudo-n-order (PNO) model and its related Transformed Ornstein-Uhlenbeck (TOU) model. It also provides information about some goodness of fit measures.

This function allows to freely estimate the parameters of the TOU model by fixing some parameters of the related pseudo-n-order (PNO) model, such as the maximum adsorption capacity (qe), the adsorption rate constant (kn) and the order of the model (n).

Usage

```
fit.model.tou(w, qe = NULL, kn = NULL, n = NULL)
```

Arguments

w   a matrix with the observed values. The first column has the observed times and the following columns have the observed values of the dependent variable, one column per experimental trajectory.

qe   an optional scalar indicating a fixed value for the parameter qe.

kn   an optional scalar indicating a fixed value for the parameter kn.

n   an optional scalar indicating a fixed value for the parameter n.

Details

This package is based on the methodology provided by (Rodríguez-Narciso et al. 2021) and it is designed to model the adsorption kinetics of removal of contaminants such as dyes, metal ions, fluorides, cyanides, arsenates, arsenites, antibiotics, hormones, etc. from an aqueous phase by several materials. In this case, the only limiting factor in the decrease of pollutant concentration is adsorption on the surface of the adsorbent and does not exclude the existence of intraparticle and film diffusion phenomena.

This function provides the following parameters: the maximum adsorption (qe), the value of the fractional-order kinetics (n), the adsorption rate constant (kn), the parameter related to the reaction order n of the kinect process (a), rate constant (lambda), the rate constant related to the variance of the Brownian motion (sigma), the variance of the long term kinetics (tau), the time needed to reach half of the maximum adsorption (t.half.qe) and the time needed to reach the maximum adsorption (t.reach.qe). The goodness of fit measures provided for this function are the loglikelihood of the model (logLikelihood), the coefficient of determination (R2), the mean squared error (MSE) and the normalized standard deviation (delta.q).

Value

a list with the estimated parameters and the goodness of fit measures.

References

Rodríguez-Narciso S, Lozano-Álvarez JA, Salinas-Gutiérrez R, Castañeda-Leyva N (2021). "A Stochastic Model for Adsorption Kinetics." *Adsorption Science & Technology*, **2021**, 1–21. doi: 10.1155/ 2021/5522581.

Examples

```
# an example with one trajectory of experimental adsorption
observed.time <- c(0, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 150, 200,
                   250, 300)
observed.values <- c(0, 1.684, 2.341, 2.581, 2.842, 2.890, 2.959, 3.042,
                      3.083, 3.043, 3.017, 2.954, 2.996, 2.886, 2.844)
observed.process <- cbind(observed.time, observed.values)
# fitting the model without any fixed parameters
result <- fit.model.tou(w=observed.process)
print(result)
# fitting the model with a fixed value for the parameter qe
result <- fit.model.tou(w=observed.process, qe=2.9)
print(result)
# fitting the model with fixed values for the parameters qe and n
result <- fit.model.tou(w=observed.process, qe=2.9, n=1.2)
print(result)

# an example with three trajectories of experimental adsorption
observed.time <- c(0, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 150, 200,
                   250, 300)
observed.values.1 <- c(0, 1.684, 2.341, 2.581, 2.842, 2.890, 2.959, 3.042,
                        3.083, 3.043, 3.017, 2.954, 2.996, 2.886, 2.844)
observed.values.2 <- c(0, 1.618, 2.217, 2.571, 2.763, 2.841, 2.866, 2.898,
                        2.935, 2.973, 2.906, 2.919, 2.910, 3.012, 3.071)
observed.values.3 <- c(0, 1.596, 2.333, 2.611, 2.750, 2.731, 2.829, 2.838,
                        2.864, 2.884, 2.886, 2.911, 2.896, 2.877, 2.969)
observed.processes <- cbind(observed.time, observed.values.1,
                            observed.values.2, observed.values.3)
# fitting the model with a fixed value for the parameter n
result <- fit.model.tou(w=observed.processes, n=1.21)
print(result)
# fitting the model with fixed values for the parameters qe, kn and n
result <- fit.model.tou(w=observed.processes, qe=2.95, kn=0.07, n=1.21)
print(result)
```

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