Package ‘gasfluxes’

August 6, 2018

Type Package
Title Greenhouse Gas Flux Calculation from Chamber Measurements
Version 0.4
Date 2018-08-04
Maintainer Roland Fuss <roland.fuss@thuenen.de>

BugReports https://bitbucket.org/ecoRoland/gasfluxes/issues

Description Functions for greenhouse gas flux calculation from chamber measurements.

License GPL (>= 2)
Depends R (>= 3.5.0)
Imports sfsmisc (>= 1.0), data.table (>= 1.9.4), MASS (>= 7.3), AICcmodavg (>= 2.0), stats, graphics, grDevices
Suggests testthat, knitr, rmarkdown
LazyData true
VignetteBuilder knitr, rmarkdown
RoxygenNote 6.1.0
NeedsCompilation no
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Repository CRAN
Date/Publication 2018-08-06 13:00:09 UTC

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**gasfluxes-package**

*Calculate greenhouse gas flux calculation from chamber measurements.*

**Description**

Gasfluxes provides functions for fitting non-linear concentration-time models as well as convenience functions for checking data and combining different calculation methods.

**Details**

The wrapper function for convenient flux calculation is `gasfluxes`. Several concentration-time models are implemented:

- **HMR.orig**: The original implementation of HMR.
- **HMR.fit**: A new implementation of HMR using partially linear least-squares. This is recommended over **HMR.orig**.
- **NDFE.fit**: An implementation of the NDFE model using partially linear least-squares.
- **lin.fit**: A simple linear model.
- **rlin.fit**: A simple linear model fit using robust regression.

---

**agg.fluxes**

*Accumulation of fluxes*

**Description**

Aggregate a time series of fluxes to a cumulative flux value.

**Usage**

```r
agg.fluxes(fluxes, datetimes, timeunit = "hours")
```
**erf**

**Arguments**

- fluxes: flux values
- datetimes: datetime values (POSIXct or POSIXlt)
- timeunit: the unit of time (denominator of the flux unit), supported are the explicit units supported by `difftime`

**Details**

The function uses linear interpolation. The unit of the cumulative flux is \([\text{fluxes}] \times \text{timeunit}\). NA values are removed and values sorted according to time order. If less than two non-NA value pairs are provided, NA is returned for the cumulative flux.

**Value**

A one-row data.frame with columns

- flux: the cumulative flux
- from: the start of the cumulation period
- to: the end of the cumulation period

The return value being a data.frame is useful, when the function is used for "split-apply-combine" type operations to calculate groupwise cumulated values, e.g., using package data.table.

**Examples**

```r
# Some random example data
datetimes <- Sys.time() + (1:20)/2*24*3600
set.seed(42)
fluxes <- rlnorm(20, 5)
agg.fluxes(fluxes, datetimes)
```

---

**erfc**

**Description**

This is the complementary error function.

**Usage**

```r
erfc(x)
```

**Arguments**

- x: a numeric vector
Value

A numeric vector, i.e., the erfc values.

---

fluxMeas  

Data from chamber N2O flux measurements.

---

Description

A dataset containing data from 1329 chamber N2O flux measurements.

Format

A data.table with 5300 rows and 5 variables:

- serie: ID of flux measurement
- V: Volume (normalized by area, i.e., the height in m)
- A: Area (always 1)
- time: closing time in h
- C: N2O concentration in mg N / m^3

Source

own data (anonymized by not including site and treatment information)

---

gasfluxes  

Flux calculation

---

Description

A wrapper function for convenient flux calculation.

Usage

gasfluxes(dat, .id = "ID", .V = "V", .A = "A", .times = "time", .C = "C", methods = c("linear", "robust linear", "HMR", "NDFE"), k_HMR = log(1.5), k_NDFE = log(0.01), verbose = TRUE, plot = TRUE, select, maxiter = 100, ...)


Arguments

dat  a data.frame or data.table with data from flux measurements.
.id  character vector specifying the columns to be used as ID, multiple ID columns are possible.
.V   character specifying the column containing chamber volume values.
.A   character specifying the column containing chamber area values.
.times character specifying the column containing chamber closing time values.
.C   character specifying the column containing concentration values.
.methods character: which methods to use for flux estimation. See details for available methods.
.k_HMR starting value for HMR.fit.
.k_NDFE starting value for NDFE.fit.
.verbose logical: print progress messages?
.plot create plots if TRUE (the default). The IDs are used as file names and should thus not include characters that are not allowed in file names, such as / or =. A directory "pics" is created in the working directory if it doesn’t exist. The plots are only intended to facilitate quick checking, not for publication quality graphs.
.select deprecated; please use function selectfluxes.
.maxiter see nls.control
... further parameters

Details

Available methods are

"linear":     lin.fit
"robust linear":  rlin.fit
"HMR":       HMR.fit
"original HMR":  HMR.orig
"NDFE":      NDFE.fit

Specifying other methods results in an error.

The default starting values for "HMR" and "NDFE", \( k = \log(\kappa) \) and \( \tau = \log(\tau) \), resp., assume that time is in hours. If you use a different time unit, you should adjust them accordingly. Note that nls is used internally by these functions and thus they should not be used with artificial "zero-residual" data.

The input data.frame or data.table should be in the following format:

<table>
<thead>
<tr>
<th>serie</th>
<th>V</th>
<th>A</th>
<th>time</th>
<th>C</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:</td>
<td>ID1</td>
<td>0.522625</td>
<td>1</td>
<td>0.00000000</td>
</tr>
<tr>
<td>2:</td>
<td>ID1</td>
<td>0.522625</td>
<td>1</td>
<td>0.33333333</td>
</tr>
<tr>
<td>3:</td>
<td>ID1</td>
<td>0.522625</td>
<td>1</td>
<td>0.66666667</td>
</tr>
</tbody>
</table>
However, more than one ID column are possible. E.g., the first ID column could be the plot and a second ID column could be the date. Keep in mind that the combination of IDs must be a unique identifier for each flux measurement.

Units of the output depend on input units. It’s recommended to use \([V] = \text{m}^3\), \([A] = \text{m}^2\), \([\text{time}] = \text{h}\), \([C] = \text{[mass or mol]/m}^3\), which results in \([f0] = \text{[mass or mol]/m}^2/\text{h}\). Since all algorithms use \(V/A\), \(A\) can be input as 1 and \(V\) as the chamber height.

**Value**

A data.table with the results of the flux calculation. See the documentation of the fitting functions for details. If a selection algorithm has been specified, the last columns are the selected flux estimate, the corresponding standard error and p-value and the method with which the selected flux was estimated.

**See Also**

`selectfluxes` for flux selection

**Examples**

```r
## Not run:
# compare result of original HMR with plinear HMR
data(fluxMeas)
res <- gasfluxes(fluxMeas[1:400,],
    .times = "time", .C = "C",
    methods = c("HMR", "original HMR"), verbose = TRUE)

# number of successful fits
res[, sum(is.na(HMR.kappa))]
res[, sum(is.na(original.HMR.kappa))]

# Do the results differ?
plot(res[["HMR.f0"]], res[["original.HMR.f0"]])
abline(0, 1)
```

```r
res <- gasfluxes(fluxMeas,
    .times = "time", .C = "C",
    methods = "HMR", verbose = TRUE)

# Error: time not sorted in flux ID ID556.
# Investigate the problem:
fluxMeas[serie %in% c("ID555", "ID556", "ID557")]
# serie   V   A  time   C
# 1: ID555 0.551625 1 0.000000 0.3884388
# 2: ID555 0.551625 1 0.3333333 0.4125270
# 3: ID555 0.551625 1 0.6666667 0.3714207
```
HMR fit

Description

Fit the HMR model using the Golub-Pereyra algorithm for partially linear least-squares models.

Usage

```r
HMR.fit(t, C, A = 1, V, serie = "", k = log(1.5), verbose = TRUE, plot = FALSE, maxiter = 100, ...)
```

Arguments

- `t` time values (usually in hours)
- `C` concentration values
- `A` area covered by the chamber
- `V` effective volume of the chamber
- `serie` id of the flux measurement
- `k` starting value for nls function
- `verbose` logical, TRUE prints message after each flux calculation
- `plot` logical, mainly intended for use in gasfluxes
- `maxiter` see nls.control
- `...` further parameters, currently none
Details

The HMR model (Pedersen et al., 2010) is \( C(t) = \phi + f_0 e^{-\kappa t} \). To ensure the lower bound \( \kappa > 0 \), the substitution \( \kappa = e^k \) is used. The resulting reparameterized model is then fit using \texttt{nls} with \texttt{algorithm = "plinear"}. This is computationally more efficient than the manual implementation in the HMR package and results in almost identical flux values. Flux standard errors and p-values differ strongly from those reported by the HMR package <= version 0.3.1, but are equal to those reported by later versions.

The default starting value \( k = \log(\kappa) \) assumes that time is in hours. If you use a different time unit, you should adjust it accordingly.

There have been demands to return the initial concentration as predicted by the model as this is useful for checking plausibility. However, this can be easily calculated from the parameters and the equation of the model by setting \( t = 0 \), i.e., \( C_0 = \phi + f_0 \).

Note that \texttt{nls} is used internally and thus this function should not be used with artificial "zero-residual" data.

Value

A list of

- \( f_0 \): flux estimate
- \( f_0.se \): standard error of flux estimate
- \( f_0.p \): p-value of flux estimate
- \( \kappa, \phi \): other parameters of the HMR model
- \( \text{AIC} \): Akaike information criterion
- \( \text{AICc} \): Akaike information criterion with small sample correction
- \( \text{RSE} \): residual standard error (sigma from \texttt{summary.nls})
- \( \text{diagnostics} \): error or warning messages

References


Examples

```r
# a single fit
library(HMR)
t <- c(0, 1/3, 2/3, 1)
C <- c(320, 341, 352, 359)
fit <- HMR.fit(t, C, 0.3, "a")
plot(C ~ t)
curve(fit$phi + fit$f0 * exp(-fit$kappa * x)/(fit$kappa * 0.3)),
from = 0, to = 1, add = TRUE)
# compare with fitting function from HMR package 0.3.1
fit <- HMR.fit1(t, C, 1, 0.3, "a",
ngrid = 1000, LR.always = FALSE, FollowHMR = TRUE,
JPG = FALSE, PS = FALSE, PHMR = FALSE, npred = 500,
```
HMR ориг

Фит HMR модель по алгоритму из пакета HMR.

**Описание**

Фитинг HMR модели по алгоритму из пакета HMR.

**Использование**

```r
HMR ориг(t, C, A = 1, V, serie = "", verbose = TRUE, ngrid = 1000,
plot = FALSE, ...)
```

**Аргументы**

- `t` — значения времени (обычно в часах)
- `C` — концентрация
- `A` — площадь, покрытая камерой
- `V` — эффективный объем камеры
- `serie` — идентификатор измерения потока
- `verbose` — логический, `TRUE` печатает сообщения после каждого расчета
- `ngrid` — увидите документацию HMR
- `plot` — логический, главным образом предназначен для использования в `gasfluxes`
- `...` — дополнительные параметры, в настоящее время нет
Details

The HMR model (Pedersen et al., 2010) is \( C(t) = \phi + f_0 e^{-\kappa t} \). The algorithm from the HMR package version 0.3.1 is used for fitting. Note that this is very inefficient and standard errors and p-values are over-estimated. \texttt{HMR.fit} is recommended instead and this function is only provided to be able to reproduce results obtained with older versions of the HMR package.

Value

A list of

- \( f_0 \) flux estimate
- \( f_0\.se \) standard error of flux estimate
- \( f_0\.p \) p-value of flux estimate
- kappa, phi other parameters of the HMR model
- AIC Akaike information criterion
- AICc Akaike information criterion with small sample correction
- diagnostics error or warning messages

Author(s)

Asger R. Pedersen for code copied from the not-exported HMR:::HMR.fit1 function, Roland Fuss

References


Examples

```r
# a single fit
t <- c(0, 1/3, 2/3, 1)
C <- c(320, 341, 352, 359)
print(fit <- HMR.orig(t, C, 1, 0.3, "a"))
plot(C ~ t)
curve((fit$phi + fit$f0 * exp(-fit$kappa * x)) / (-fit$kappa*0.3),
     from = 0, to = 1, add = TRUE)
```

lin.fit

\textit{Linear concentration - time model}

Description

Fit a linear model to concentration - time data.
**lin.fit**

Usage

```
lin.fit(t, C, A = 1, V, serie = "", verbose = TRUE, plot = FALSE, ...)
```

Arguments

- `t`: time values (usually in hours)
- `C`: concentration values
- `A`: area covered by the chamber
- `V`: effective volume of the chamber
- `serie`: id of the flux measurement
- `verbose`: logical, TRUE prints message after each flux calculation
- `plot`: logical, mainly intended for use in gasfluxes
- `...`: further parameters, currently none

Details

This is basically a wrapper of R’s OLS fitting facilities. For now `lm` (and methods for objects of class "lm") is used, but this may change to more efficient alternatives in later versions.

Value

A list of

- `f0`: flux estimate
- `f0.se`: standard error of flux estimate
- `f0.p`: p-value of flux estimate
- `C0`: estimated concentration at \( t = 0 \) (intercept)
- `AIC`: Akaike information criterion
- `AICc`: Akaike information criterion with small sample correction
- `RSE`: residual standard error (sigma from summary.nls)
- `r`: Pearson’s correlation coefficient
- `diagnostics`: error or warning messages

Examples

```
# a single fit
T <- c(0, 1/3, 2/3, 1)
C <- c(320, 341, 352, 359)
print(fit <- lin.fit(T, C, 1, 0.3, "a"))
plot(T ~ C)
curve((fit$f0/0.3 * x + fit$c0), from = 0, to = 1, add = TRUE)
```
NDFE.fit

Description

Fit the non-steady-state diffusive flux estimator model using the Golub-Pereyra algorithm for partially linear least-squares models.

Usage

NDFE.fit(t, C, A = 1, V, serie = "", k = log(0.01), verbose = TRUE, plot = FALSE, maxiter = 100, ...)

Arguments

- `t`: time values (usually in hours)
- `C`: concentration values
- `A`: area covered by the chamber
- `V`: effective volume of the chamber
- `serie`: id of the flux measurement
- `k`: starting value for nls function
- `verbose`: logical, TRUE prints message after each flux calculation
- `plot`: logical, mainly intended for use in gasflaxes
- `maxiter`: see nls.control
- `...`: further parameters, currently none

Details

The NDFE model (Livingston et al., 2006) is 
\[ C(t) = C_0 + f_0 \tau A V \left\{ \frac{2}{\sqrt{\pi}} \sqrt{t/\tau} + e^{t/\tau} \text{erfc}\left(\sqrt{t/\tau}\right) - 1 \right\}. \]

To ensure the lower bound \( \tau > 0 \), the substitution \( \tau = e^k \) is used. The resulting reparameterized model is then fit using nls with algorithm = "plinear".

Note that according to the reference the model is not valid for negative fluxes. Warning: This function does not check if fluxes are positive. It’s left to the user to handle negative fluxes.

The default starting value \( k = \log(\tau) \) assumes that time is in hours. If you use a different time unit, you should adjust it accordingly.

Note that nls is used internally and thus this function should not be used with artificial "zero-residual" data.
Value

A list of

- \( f_0 \) flux estimate
- \( f_0.se \) standard error of flux estimate
- \( f_0.p \) p-value of flux estimate
- \( C_0, \tau \) other parameters of the NDFE model
- \( \text{AIC} \) Akaike information criterion
- \( \text{AICC} \) Akaike information criterion with small sample correction
- \( \text{RSE} \) residual standard error (sigma from summary.nls)
- diagnostcics error or warning messages

References


Examples

```r
# a single fit
 t <- c(0, 1/3, 2/3, 1)
 C <- c(320, 340, 355, 362)
 print(fit <- NDFE.fit(t, C, 1, 0.3, "a"))
 plot(C ~ t)
 curve_coef <- function(x, tau) (x/x/tau)*exp(-x/x/tau)*erfc(sqrt(x/x/tau))-1)
 curve(\(\text{coef} \), from = 0, to = 1, add = TRUE)

# note that the flux estimate is very uncertain because
# there are no data points in the region of high curvature
```

---

**rlin.fit**

Robust linear concentration - time model

Description

Fit a linear model to concentration - time data using robust methods.

Usage

```r
rlin.fit(t, C, A = 1, V, serie = ",", verbose = TRUE, plot = FALSE,
...)
```
Arguments

t  time values (usually in hours)
C  concentration values
A  area covered by the chamber
V  effective volume of the chamber
serie  id of the flux measurement
verbose  logical, TRUE prints message after each flux calculation
plot  logical, mainly intended for use in gasfluxes
...  further parameters, currently none

Details

This is basically a wrapper of \texttt{rlm} using the Huber M estimator. This function never weights the first or last time point with zero with very few data points. However, there might exist "better" robust regression methods for flux estimation.

Value

A list of

f0  flux estimate
f0.se  standard error of flux estimate
f0.p  p-value of flux estimate
C0  estimated concentration at t = 0 (intercept)
weights  robustness weights
diagnostics  error or warning messages

Examples

# a single fit
t <- c(0, 1/3, 2/3, 1)
C <- c(320, 330, 315, 351)
print(fit <- rlin.fit(t, C, 1, 0.3, "a"))
plot(C ~ t)
curve((fit$f0/0.3 * x + fit$C0), from = 0, to = 1, add = TRUE)
selectfluxes

Select a flux estimate

Description

Selects the appropriate flux estimate from linear, robust linear and non-linear calculated fluxes.

Usage

selectfluxes(dat, select, f.detect = NULL, t.meas = NULL, ...)

Arguments

dat a data.table as returned by gasfluxes. The function modifies it by reference.
select character; specify a ruleset for selection of the final flux value, see details.
f.detect detection limit for HMR method. This can be determined by a simple simulation (see examples) or for four data points the approximation in Parkin et al. (2012) can be used.
t.meas a vector or single value giving the measurement time factor that relates to kappa.max. It is suggested to use the time difference between the first and last sample taken from the closed chamber. The unit should be consistent with the units of f.detect and kappa (e.g., h if kappa is in 1/h).

... further parameters

Details

Available selection algorithms currently are

"RF2011" The algorithm used, e.g., in Leiber-Sauheitl 2014 (doi:10.5194/bg-11-749-2014). This overwrites the methods parameter. The factor guarding against degenerate HMR fits can be set via the ellipsis as gfactor. Default is gfactor = 4. This method is not recommended any more and only provided for reproducibility of old results.

"RF2011new" The same rules as "RF2011", but using the improved fitting function for HMR, which results in larger SE and p-values. Thus, it is less likely to select the HMR result. This method is not recommended any more and only provided for reproducibility of old results.

"kappa.max" The selection algorithm restricts the use of HMR by imposing a maximal value for kappa "kappa.max", depending on the quotient of the linear flux estimate and the minimal detectable flux (f.detect), as well as the chamber closure time (t.meas). kappa.max = f.lin/f.detect/t.meas. This is currently the recommended algorithm.

Other selection algorithms could be implemented, but selection can always be done as a postprocessing step. E.g., if many data points are available for each flux measurement it is probably most sensible to use AICc.
selectfluxes

Value

A data.table with the with following columns added to the function input: selected flux estimate, the corresponding standard error and p-value and the method with which the selected flux was estimated. For the "kappa.max" method the "kappa.max" values are included. These columns are also added to the input data.table by reference.

References


Examples

```r
## Not run:
res <- gasfluxes(fluxMeas[1:499],
                  .times = "time", .C = "C",
                  methods = c("linear", "robust linear", "HMR"), verbose = FALSE, plot = FALSE)
selectfluxes(res, "RF2011new")
res[method == "HMR", .N] #2

### estimate f.detect by simulation ###
#ambient concentration:
C0 <- 320/1000 * 28 * 273.15 / 22.4 / (273.15 + 15) #mg N / m^3
#uncertainty of GC measurement:
sdGC <- 5/1000 * 28 * 273.15 / 22.4 / (273.15 + 15) #mg N / m^3
#create simulated concentrations corresponding to 1 hour flux measurements with zero fluxes:
set.seed(42)
sim <- data.frame(t = seq(0, 1, length.out = 4), C = rnorm(4e3, mean = C0, sd = sdGC),
                  id = rep(1:1e3, each = 4), A = 1, V = 0.52)
#fit HMR model:
simflux <- gasfluxes(sim, .id = "id", .times = "t", methods = c("HMR", "linear"), plot = FALSE)
simflux[, f0 := HMR.f0]
simflux[is.na(f0), f0 := linear.f0]
#dection limit as 97.5 % quantile (95 % confidence):
f.detect <- simflux[, quantile(f0, 0.975)] #0.03 mg N / m^2 / h

# example using the kappa.max (ref. Hueppi et al., 2018) with a single t.meas value
t.meas <- max(fluxMeas$time[1:499]) #1
selectfluxes(res, "kappa.max", f.detect = f.detect, t.meas = t.meas)
res[method == "HMR", .N] #11

# example using the kappa.max with a vector for t.meas
t.meas <- fluxMeas[1:499][, max(time), by = serie][["V1"]]
sim <- data.frame(t = sort(t.meas), .N = rep(1e3, nrow(t.meas)), .f = 1)
simflux <- gasfluxes(sim, .times = "t", methods = c("kappa.max", "HMR"), plot = FALSE)
res[method == "HMR", .N] # 10

## End(Not run)
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