Package: PoolDilutionR (via r-universe)

October 18, 2024

Type Package

Title Calculate Gross Biogeochemical Flux Rates from Isotope Pool Dilution Data

Version 1.0.0

Description Pool dilution is a isotope tracer technique wherein a biogeochemical pool is artifically enriched with its heavy isotopologue and the gross productive and consumptive fluxes of that pool are quantified by the change in pool size and isotopic composition over time. This package calculates gross production and consumption rates from closed-system isotopic pool dilution time series data. Pool size concentrations and heavy isotope (e.g., 15N) content are measured over time and the model optimizes production rate (P) and the first order rate constant (k) by minimizing error in the model-predicted total pool size, as well as the isotopic signature. The model optimizes rates by weighting information against the signal:noise ratio of concentration and heavy- isotope signatures using measurement precision as well as the magnitude of change over time. The calculations used here are based on von Fischer and Hedin (2002) <doi:10.1029/2001GB001448> with some modifications.

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Encoding UTF-8

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Config/testthat/edition 3

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Author Kendalynn A. Morris [cre, aut] (<https://orcid.org/0000-0002-0388-6965>), Ben Bond-Lamberty [ctb] (<https://orcid.org/0000-0001-9525-4633>)

Maintainer Kendalynn A. Morris <kendalynn.morris@gmail.com>

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`frac_k_default` *Retrieve default k fractionation value for a pool*

Description

Retrieve default k fractionation value for a pool

Usage

```
frac_k_default(pool)
```

Arguments

`pool`	Name of pool, character

Value

The default entry for `pool` listed in `pdr_fractionation`.

Examples

```
frac_k_default("CH4")
```

frac_P_default *Retrieve default P fractionation value for a pool*

Description

Retrieve default P fractionation value for a pool

Usage

```
frac_P_default(pool)
```

Arguments

pool	Name of pool, character

Value

The default entry for pool listed in pdr_fractionation.

Examples

```
frac_P_default("CH4")
```

Morris2023 *Example time series data from a methane dilution pool experiment.*

Description

Sequential measurements of methane concentration and isotopic signature were taken using a Picarro G2920 with a Small Sample Introduction module. This instrument provides gas concentrations in ppm and signatures in delta-13C, here we provide those data converted into volume of methane and atom percent.

Usage

```
Morris2023
```

Format

id Sample ID, a factor

time_days time in days between measurements, starting at 0

cal12CH4ml ml of 12C-CH4 at each timestep

cal13CH4ml ml of 13C-CH4 at each timestep

AP_obs atom percent 13C-CH4 at each timestep

pdr_cost *Cost function between observed and predicted pools*

Description

Cost function between observed and predicted pools

Usage

```
pdr_cost(
  params,
  time,
  m,
  n,
  m_prec,
  ap_prec,
  P,
  k,
  pool = "CH4",
  frac_P = frac_P_default(pool),
  frac_k = frac_k_default(pool),
  log_progress = NULL
)
```

Arguments

params	Named list holding optimizer-assigned values for parameters
time	Vector of numeric time values; first should be zero
m	Observed total pool size, same length as time
n	Observed pool size of heavy isotope, same length as time
m_prec	Instrument precision for pool size, expressed as a standard deviation
ap_prec	Instrument precision for atom percent, expressed as a standard deviation
P	production rate, unit pool size/unit time
k	first-order rate constant for consumption, 1/unit time
pool	Name of pool; see pdr_fractionation
frac_P	Fractionation value for production; see pdr_fractionation
frac_k	Fractionation value for consumption; see pdr_fractionation
log_progress	An optional logging function

Value

Returns a cost metric summarizing the difference between the predicted and observed m (total pool size) and AP (atom percent).

Note

This implements Equations 12-14 from von Fischer and Hedin (2002).

Author(s)

K.A. Morris & B. Bond-Lamberty

Examples

```
m <- c(10, 8, 6, 5, 4, 3)
n <- c(1, 0.7, 0.6, 0.4, 0.3, 0.2)
pdr_cost(params = list(P = 0.5, k = 0.3), time = 0:5, m, n, m_prec = 0.001, ap_prec = 0.01)
```

---

pdr_estimate_k0 *Estimate initial k from heavy isotope concentration data*

Description

Estimate initial k from heavy isotope concentration data

Usage

```
pdr_estimate_k0(time, n, frac_k, quiet = FALSE)
```

Arguments

time	Vector of numeric time values (e.g. days); first should be zero
n	Observed heavy isotope (as a volume), same length as time
frac_k	Fractionation: 13C consumption as a fraction of 12C consumption
quiet	Suppress output message, logical

Value

Initial estimate of k0 (consumption rate constant)

Examples

```
pdr_estimate_k0(1:5, c(1, 0.9, 0.7, 0.65, 0.4), frac_k = 0.98)
```

pdr_fractionation *P and k fractionation values*

Description

A compendium of possible production (P) and consumption (k) fractionation values, by pool.

Usage

```
pdr_fractionation
```

Format

Pool Name of pool (gas or solid)

frac_P Fractionation value of production (P)

frac_k Fractionation value of consumption (k)

Default Default for this pool? Logical

Source Source paper or URL

Note

Currently there is only one set of fractionation values available, from von Fischer and Hedin (2002, 10.1029/2001GB001448).

pdr_optimize *Optimize production and consumption parameters for pool dilution data*

Description

Optimize production and consumption parameters for pool dilution data

Usage

```
pdr_optimize(
  time,
  m,
  n,
  m_prec,
  ap_prec,
  P,
  k,
  params_to_optimize = c("P", "k"),
  pool = "CH4",
```

```
  frac_P = NULL,
  frac_k = NULL,
  other_params = list(),
  cost_fn = pdr_cost,
  prediction_fn = pdr_predict,
  include_progress = FALSE,
  quiet = FALSE
)
```

Arguments

time	Vector of numeric time values (e.g. days); first should be zero
m	Observed total pool size (as a volume), same length as time
n	Observed heavy isotope (as a volume), same length as time
m_prec	Instrument precision for pool size, expressed as a standard deviation
ap_prec	Instrument precision for atom percent, expressed as a standard deviation
P	production rate, unit gas/unit time
k	first-order rate constant for consumption, 1/unit time
params_to_optimize	Named vector of parameters ("P", "k", "frac_P", and/or "frac_k") to optimize against observations
pool	Name of pool to use when looking up fractionation values if they are not supplied; see pdr_fractionation
frac_P	Fractionation value for production; see pdr_fractionation
frac_k	Fractionation value for consumption; see pdr_fractionation
other_params	Other parameters pass on to optim
cost_fn	Cost function to use; the default is pdr_cost
prediction_fn	Prediction function that the cost function will use; the default is pdr_predict
include_progress	Include detailed optimizer progress data in output?
quiet	Suppress output messages, logical

Value

The output of optim.

Note

Currently there is only one set of fractionation values available in pdr_fractionation, from von Fischer and Hedin (2002, 10.1029/2001GB001448).

See Also

pdr_optimize_df

Examples

```
tm <- 0:5
m <- c(10, 8, 6, 5, 4, 3)
n <- c(1, 0.7, 0.6, 0.4, 0.3, 0.2)
m_prec <- 0.001
ap_prec <- 0.01

# Optimize values for P (production) and k (consumption), provide starting values for P and k
pdr_optimize(time = tm, m, n, m_prec, ap_prec, P = 0.5, k = 0.3)
# If we don't provide a value for k, it can be estimated from the data
pdr_optimize(tm, m, n, m_prec, ap_prec, P = 0.5)
# Hold k and frac_k constant (ie., k = estimated k0, frac_k = default value), optimize P and frac_P
pdr_optimize(tm, m, n, m_prec, ap_prec, P = 0.5, params_to_optimize = c("P", "frac_P"))
# Optimize only k (provide P and exclude from params_to_optimize)
pdr_optimize(tm, m, n, m_prec, ap_prec, P = 0.5, params_to_optimize = "k")
# Optimize only k, bounding its possible values
op <- list(lower = c("k" = 0.2), upper = c("k" = 0.3))
pdr_optimize(tm, m, n, m_prec, ap_prec, 0.5, 0.27, params_to_optimize = "k", other_params = op)
```

`pdr_optimize_df` *Optimize production and consumption parameters for pool dilution data*

Description

Optimize production and consumption parameters for pool dilution data

Usage

```
pdr_optimize_df(...)
```

Arguments

`...`	Parameters to be passed on to `pdr_optimize`

Value

The output of `pdr_optimize` summarized in a data frame, with one line per parameter estimates (`P`, `k`, `frac_P`, and/or `frac_k`).

See Also

`pdr_optimize`

Examples

```
tm <- 0:5
m <- c(10, 8, 6, 5, 4, 3)
n <- c(1, 0.7, 0.6, 0.4, 0.3, 0.2)
m_prec <- 0.001
ap_prec <- 0.01
# Optimize values for P (production) and k (consumption)
pdr_optimize_df(time = tm, m, n, m_prec, ap_prec, P = 0.5, k = 0.3)
```

`pdr_predict` *Predict total pool, heavy isotope pool, and atom percent*

Description

Predict total pool, heavy isotope pool, and atom percent

Usage

```
pdr_predict(
  time,
  m0,
  n0,
  P,
  k,
  pool = "CH4",
  frac_P = frac_P_default(pool),
  frac_k = frac_k_default(pool)
)
```

Arguments

`time`	Vector of numeric time values (e.g. days); first should be zero
`m0`	total pool size at time zero, as a volume
`n0`	pool size of heavy isotope at time zero, as a volume
`P`	production rate, unit gas/unit time
`k`	first-order rate constant for consumption, 1/unit time
`pool`	Name of pool; see `pdr_fractionation`
`frac_P`	Fractionation value for production; see `pdr_fractionation`
`frac_k`	Fractionation value for consumption; see `pdr_fractionation`

Value

Returns a data frame with `mt`, `nt`, and `AP_pred` (atom percent) for each time step

Note

This is Eq. 11 from von Fischer and Hedin 2002 with a few modifications.

Author(s)

K.A. Morris & B. Bond-Lamberty

Examples

```
pdr_predict(time = 0:5, m0 = 10, n0 = 1, P = 0.5, k = 0.3)
```

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