Package 'eDITH'

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and Hydrology) model, which implements a mass balance of environmental DNA (eDNA) transport at a river network scale coupled with a species distribution model to obtain maps of species distribution. eDITH can work with both eDNA concentration (e.g., obtained via quantitative polymerase chain reaction) or metabarcoding (read count) data. Parameter estimation can be performed via Bayesian techniques (via the 'BayesianTools' package) or optimization algorithms. An interface to the 'DHARMa' package for posterior predictive checks is provided. See Carraro and Altermatt (2024) <doi:10.1111/2041-210X.14317> for a package introduction; Carraro et al. (2018) <doi:10.1073/pnas.1813843115> and Carraro et al. (2020) <doi:10.1038/s41467-020-17337-8> for methodological details. License MIT + file LICENSE **Encoding UTF-8 Depends** R (>= 3.6) Suggests knitr, rmarkdown, bookdown VignetteBuilder knitr URL https://lucarraro.github.io/eDITH/, https://github.com/lucarraro/eDITH BugReports https://github.com/lucarraro/eDITH/issues **Imports** Rcpp (>= 1.0.10), OCNet (>= 1.1.0), rivnet (>= 0.4.2), BayesianTools, LaplacesDemon, DHARMa, terra, fields LinkingTo Rcpp NeedsCompilation yes **Author** Luca Carraro [cre, aut], Florian Altermatt [aut], University of Zurich [cph, fnd] Maintainer Luca Carraro < luca.carraro@hotmail.it>

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Description

Runs the eDITH (eDNA Integrating Transport and Hydrology) model, which implements a mass balance of eDNA transport at a river network scale coupled with a species distribution model to obtain maps of species distribution. eDITH can work with both eDNA concentration (e.g., obtained via qPCR) or metabarcoding (read count) data. Parameter estimation can be performed via Bayesian techniques (via the BayesianTools package) or optimization algorithms. An interface to the DHARMa package for posterior predictive checks is provided.

Author(s)

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References

Carraro, L., Hartikainen, H., Jokela, J., Bertuzzo, E., and Rinaldo, A. (2018). Estimating species distribution and abundance in river networks using environmental DNA. Proceedings of the National Academy of Sciences of the United States of America, 115(46), 11724-11729. doi:10.1073/pnas.1813843115

Carraro, L., Maechler, E., Wuethrich, R., and Altermatt, F. (2020). Environmental DNA allows upscaling spatial patterns of biodiversity in freshwater ecosystems. Nature Communications, 11(1) doi:10.1038/s41467-020-17337-8

Carraro, L., Stauffer, J. B., and Altermatt, F. (2021). How to design optimal eDNA sampling strategies for biomonitoring in river networks. Environmental DNA, 3(1), 157-172. doi:10.1002/edn3.137

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Carraro, L., Blackman, R. C., and Altermatt, F. (2023). Modelling environmental DNA transport in rivers reveals highly resolved spatio-temporal biodiversity patterns. Scientific Reports, 13(1) doi:10.1038/s41598-023-35614-6

dataC

eDNA concentration data

Description

The dataset consists of triplicate eDNA measurements for each of the 24 sampling sites.

Usage

data(dataC)

Format

A data frame containing location of eDNA sampling sites for the river Wigger (dataC\$ID) and eDNA concentration values (dataC\$values) (in mol m-3) for a given taxon.

dataCD

eDNA concentration and direct observation data

Description

The dataset consists of triplicate eDNA measurements for each of the 24 sampling sites, plus 13 direct observation measurements.

Usage

data(dataCD)

Format

A data frame containing location of sampling sites for the river Wigger (dataCD\$ID), respective measured values (dataCD\$values) (in mol m-3 for eDNA samples; in m-2 for direct surveys) and data type (dataCD\$values) ("e" for eDNA samples; "d" for direct observations) for a given taxon.

dataRead

eDNA read number data

Description

The dataset consists of triplicate eDNA measurements for each of the 24 sampling sites.

Usage

```
data(dataRead)
```

Format

A data frame containing location of eDNA sampling sites for the river Wigger (dataRead\$ID) and eDNA read number values (dataRead\$values) for a given taxon.

eval_posterior_eDITH

Evaluate posterior predictions from an eDITH run

Description

Function that evaluates relevant quantities from a posterior sample of the parameters of an eDITH model

Usage

```
eval_posterior_eDITH(x, river, quant = 0.5)
```

Arguments

x List as produced by run_eDITH_BT.

river A river object generated via aggregate_river.

quant Vector of quantiles.

Value

The output list copies all objects of the input x list. The following objects are added:

p_quantile Selected quantiles (along rows) of the posterior distribution of production rates.

C_quantile Selected quantiles (along rows) of the posterior distribution of eDNA values

(concentrations or read numbers).

probDet_quantile

Selected quantiles (along rows) of the posterior distribution of detection proba-

bility.

p_mean Mean of the posterior distribution of production rates.

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C_mean Mean of the posterior distribution of eDNA values (concentrations or read num-

bers).

probDet_mean Mean of the posterior distribution of detection probability.

All of these objects are vectors of length river\$AG\$nNodes. However, if a custom likelihood was used in run_eDITH_BT, then probDet_quantile and probDet_mean are not evaluated, and are replaced by a vector of zero length.

Examples

```
library(rivnet)
data(wigger)
data(outSample)
out <- eval_posterior_eDITH(outSample, wigger)
plot(wigger, out$p_mean)</pre>
```

outSample

Posterior sample from fitted eDITH model

Description

It is produced via:

```
covariates <- data.frame(urban=wigger$SC$locCov$landcover_1, agriculture=wigger$SC$locCov$landcover_2
forest=wigger$SC$locCov$landcover_3, elev=wigger$AG$Z, log_drainageArea=log(wigger$AG$A))
set.seed(1)
outSample <- run_eDITH_BT(dataC, wigger, covariates, mcmc.settings=list(iterations=9e5, burnin = 6e5, message = TRUE, thin = 30))</pre>
```

Usage

```
data(outSample)
```

Format

A list.

```
posterior_pred_sim_eDITH
```

Predictive posterior simulations from an eDITH run

Description

This function performs predictive posterior simulations from a run of the eDITH model (via run_eDITH_BT). These can be used for diagnostics purposes, in particular to assess scaled (quantile) residuals via the DHARMa package.

Usage

```
posterior_pred_sim_eDITH(x, river, nParamSets = 10000, nDrawsPerParamSet = 10, verbose = FALSE)
```

Arguments

x List as produced by run_eDITH_BT.

river A river object generated via aggregate_river.

nParamSets Number of unique parameter sets sampled from the posterior distribution.

nDrawsPerParamSet

Number of simulations run per parameter set.

verbose Logical. Should updates be printed on the console?

Details

nParamSets can be higher than the number of unique parameter sets in the posterior distribution, since the sampling of posterior parameter sets is operated with replacement.

Value

A matrix with dimensions length(x\$data\$ID)-by-nParamSets*nDrawsPerParamSet. Each column is a predictive posterior simulation. Each row corresponds to a site where eDNA data were observed (corresponding to the entries of argument data in run_eDITH_BT. Matrix entries are eDNA values (either concentrations or read numbers) predicted by the model for a given predictive posterior simulation at a given observational site.

See Also

DHARMa.

Examples

```
library(DHARMa)
data(outSample)
data(wigger)
data(dataC)
pps <- posterior_pred_sim_eDITH(outSample, wigger, nParamSets = 1000)
# reduced nParamSets for illustrative purposes
sim.out <- createDHARMa(pps, dataC$values)
plot(sim.out)</pre>
```

run_eDITH_BT

Run eDITH with BayesianTools

Description

Function that runs a Bayesian sampler estimating parameters of an eDITH model

Usage

Arguments

data	eDNA data. Data frame containing columns ID (index of the AG node/reach where the eDNA sample was taken) and values (value of the eDNA measurement, expressed as concentration or number of reads).
river	A river object generated via aggregate_river.
covariates	Data frame containing covariate values for all river reaches. If NULL (default option), production rates are estimated via AEMs.
Z.normalize	Logical. Should covariates be Z-normalized?
use.AEM	Logical. Should eigenvectors based on AEMs be used as covariates? If covariates = NULL, it is set to TRUE. If TRUE and covariates are provided, AEM eigenvectors are appended to the covariates data frame.

n.AEM	Number of AEM eigenvectors (sorted by the decreasing respective eigenvalue) to be used as covariates. If par.AEM\$moranI = TRUE, this parameter is not used. Instead, the eigenvectors with significantly positive spatial autocorrelation are used as AEM covariates.
par.AEM	List of additional parameters that are passed to river_to_AEM for calculation of AEMs. In particular, par.AEM\$moranI = TRUE imposes the use of AEM covariates with significantly positive spatial autocorrelation based on Moran's I statistic.
no.det	Logical. Should a probability of non-detection be included in the model?
ll.type	Character. String defining the error distribution used in the log-likelihood formulation. Allowed values are norm (for normal distribution), 1norm (for lognormal distribution), nbinom (for negative binomial distribution) and geom (for geometric distribution). The two latter choices are suited when eDNA data are expressed as read numbers, while norm and 1norm are better suited to eDNA concentrations.
source.area	Defines the extent of the source area of a node. Possible values are "AG" (if the source area is the reach surface, i.e. length*width), "SC" (if the source area is the subcatchment area), or, alternatively, a vector with length river\$AG\$nodes.
mcmc.settings	List. It is passed as argument settings in runMCMC. Default is list(iterations = 2.7e6, burnin=1.8e6, message = TRUE, thin = 10).
likelihood	Likelihood function to be passed as likelihood argument to createBayesianSetup. If not specified, it is generated based on arguments no.det and ll.type. If a custom likelihood is specified, a custom prior must also be specified.
prior	Prior function to be passed as prior argument to createBayesianSetup. If not specified, it is generated based on the *.prior arguments provided. If a user-defined prior is provided, parameter names must be included in prior\$lower, prior\$upper (see example).
sampler.type	Character. It is passed as argument sampler in runMCMC.
tau.prior	List that defines the prior distribution for the decay time parameter tau. See details.
log_p0.prior	List that defines the prior distribution for the logarithm (in base 10) of the base- line production rate p0. See details. If covariates = NULL, this defines the prior distribution for the logarithm (in base 10) of production rates for all river reaches.
beta.prior	List that defines the prior distribution for the covariate effects beta. See details. If a single spec is provided, the same prior distribution is specified for all beta parameters. Alternatively, if spec (and the other arguments, if provided) is a vector with length equal to the number of covariates included, different prior distributions can be specified for the different beta parameters.
sigma.prior	List that defines the prior distribution for the standard deviation of the measurement error when 11.type is "norm" or "lnorm". It is not used if 11.type = "nbinom". See details.
omega.prior	List that defines the prior distribution for the overdispersion parameter omega of the measurement error when ll.type = "nbinom". It is not used if ll.type is "norm" or "lnorm". See details.

Cstar.prior List that defines the prior distribution for the Cstar parameter controlling the

probability of no detection. It is only used if no.det = TRUE. See details.

verbose Logical. Should console output be displayed?

Details

The arguments of the type *.prior consist in the lists of arguments required by dtrunc (except the first argument x).

By default, AEMs are computed without attributing weights to the edges of the river network. Use e.g. par.AEM = list(weight = "gravity") to attribute weights.

Value

A list with objects:

param_map Vector of named parameters corresponding to the maximum a posteriori esti-

mate. It is the output of the call to MAP.

p_map Vector of best-fit eDNA production rates corresponding to the maximum a pos-

teriori parameter estimate param_map. It has length equal to river\$AG\$nNodes.

C_map Vector of best-fit eDNA values (in the same unit as data\$values, i.e. concen-

trations or read numbers) corresponding to the maximum a posteriori parameter

estimate param_map. It has length equal to river\$AG\$nNodes.

probDet_map Vector of best-fit detection probabilities corresponding to the maximum a pos-

teriori parameter estimate param_map. It has length equal to river\$AG\$nNodes. If a custom likelihood is provided, this is a vector of null length (in which case the user should calculate the probability of detection independently, based

on the chosen likelihood).

cI Output of the call to getCredibleIntervals.

gD Output of the call to gelmanDiagnostics.

covariates Data frame containing input covariate values (possibly Z-normalized).

source.area Vector of source area values.

outMCMC Object of class mcmcSampler returned by the call to runMCMC.

Moreover, arguments 11.type (possibly changed to "custom" if a custom likelihood is specified), no.det and data are added to the list.

Examples

```
data(wigger)
data(dataC)
data(dataRead)

# reduce number of iterations for illustrative purposes
# (use default mcmc.settings to ensure convergence)
settings.short <- list(iterations = 1e3, thin = 10)
set.seed(1)
out <- run_eDITH_BT(dataC, wigger, mcmc.settings = settings.short)</pre>
```

```
library(rivnet)
# best-fit (maximum a posteriori) map of eDNA production rates
plot(wigger, out$p_map)
# best-fit map (maximum a posteriori) of detection probability
plot(wigger, out$probDet_map)
# compare best-fit vs observed eDNA concentrations
plot(out$C_map[dataC$ID], dataC$values,
xlab="Modelled (MAP) concentrations", ylab="Observed concentrations")
abline(a=0, b=1)
## fit eDNA read number data - use AEMs as covariates
out <- run_eDITH_BT(dataRead, wigger, ll.type = "nbinom",
par.AEM = list(weight = "gravity"),
mcmc.settings = settings.short) # use default mcmc.settings to ensure convergence
## use user-defined covariates
covariates <- data.frame(urban = wigger$SC$locCov$landcover_1,</pre>
                         agriculture = wigger$SC$locCov$landcover_2,
                         forest = wigger$SC$locCov$landcover_3,
                         elev = wigger$AG$Z,
                         log_drainageArea = log(wigger$AG$A))
out.cov <- run_eDITH_BT(dataC, wigger, covariates,</pre>
mcmc.settings = settings.short) # use default mcmc.settings to ensure convergence
# use user-defined covariates and AEMs
out.covAEM <- run_eDITH_BT(dataC, wigger, covariates,</pre>
use.AEM = TRUE, par.AEM = list(weight = "gravity"),
mcmc.settings = settings.short) # use default mcmc.settings to ensure convergence
# use AEMs with significantly positive spatial autocorrelation
out.AEM.moran <- run_eDITH_BT(dataC, wigger, use.AEM = TRUE,
par.AEM = list(weight = "gravity", moranI = TRUE),
mcmc.settings = settings.short) # use default mcmc.settings to ensure convergence
## use posterior sample to specify user-defined prior
library(BayesianTools)
data(outSample)
pp <- createPriorDensity(outSample$outMCMC)</pre>
# Important! add parameter names to objects lower, upper
names(pp$lower) <- names(pp$upper) <- colnames(outSample$outMCMC$chain[[1]])[1:8]</pre>
# the three last columns are for log-posterior, log-likelihood, log-prior
out.new <- run_eDITH_BT(dataC, wigger, covariates, prior = pp,
mcmc.settings = settings.short)
```

run_eDITH_BT_joint Run eDITH with BayesianTools based on joint eDNA and direct sampling data

Description

Function that runs a Bayesian sampler estimating parameters of an eDITH model fitted on both eDNA and direct sampling data.

Usage

```
run_eDITH_BT_joint(data, river, covariates = NULL, Z.normalize = TRUE,
           use.AEM = FALSE, n.AEM = NULL, par.AEM = NULL,
           no.det = FALSE, 11.type = "norm", source.area = "AG",
          mcmc.settings = NULL, likelihood = NULL, prior = NULL,
  sampler.type = "DREAMzs",
           tau.prior = list(spec="lnorm",a=0,b=Inf, meanlog=log(5),
                    sd=sqrt(log(5)-log(4))),
           log_p0.prior = list(spec="unif", min=-20, max=0),
           beta.prior = list(spec="norm",sd=1),
           sigma.prior = list(spec="unif",min=0,
                  max=max(data$values[data$type=="e"],
  na.rm = TRUE)),
           omega.prior = list(spec="unif",min=1,
                  max=10*max(data$values[data$type=="e"],
 na.rm = TRUE)),
           Cstar.prior = list(spec="unif", min=0,
                  max=max(data$values[data$type=="e"],
  na.rm = TRUE)),
           omega_d.prior = list(spec="unif", min=1,
                               max=10*max(c(0.11, data$values[data$type=="d"]),
na.rm = TRUE)),
           alpha.prior = list(spec="unif", min=0, max=1e6),
           verbose = FALSE)
```

Arguments

eDNA and direct observation data. Data frame containing columns ID (index of data

> the AG node/reach where the sample was taken), values (value of the eDNA or direct measurement) and type (equal to "e" for eDNA data and to "d" for direct observation data). eDNA values are expressed as concentration or number

of reads; direct observations are expressed as numbers of individuals.

river A river object generated via aggregate_river.

covariates Data frame containing covariate values for all river reaches. If NULL (default

option), production rates are estimated via AEMs.

Z.normalize Logical. Should covariates be Z-normalized?

use.AEM Logical. Should eigenvectors based on AEMs be used as covariates? If covariates = NULL, it is set to TRUE. If TRUE and covariates are provided, AEM eigenvectors are appended to the covariates data frame. n.AEM Number of AEM eigenvectors (sorted by the decreasing respective eigenvalue) to be used as covariates. If par. AEM\$moranI = TRUE, this parameter is not used. Instead, the eigenvectors with significantly positive spatial autocorrelation are used as AEM covariates. par.AEM List of additional parameters that are passed to river_to_AEM for calculation of AEMs. In particular, par. AEM\$moranI = TRUE imposes the use of AEM covariates with significantly positive spatial autocorrelation based on Moran's I statistic. no.det Logical. Should a probability of non-detection be included in the model? 11.type Character. String defining the error distribution used in the log-likelihood formulation. Allowed values are norm (for normal distribution), 1norm (for lognormal distribution), nbinom (for negative binomial distribution) and geom (for geometric distribution). The two latter choices are suited when eDNA data are expressed as read numbers, while norm and 1norm are better suited to eDNA concentrations. Defines the extent of the source area of a node. Possible values are "AG" (if the source.area source area is the reach surface, i.e. length*width), "SC" (if the source area is the subcatchment area), or, alternatively, a vector with length river\$AG\$nodes. mcmc.settings List. It is passed as argument settings in runMCMC. Default is list(iterations = 2.7e6, burnin=1.8e6, message = TRUE, thin = 10). likelihood Likelihood function to be passed as likelihood argument to createBayesianSetup. If not specified, it is generated based on arguments no. det and 11. type. If a custom likelihood is specified, a custom prior must also be specified. prior Prior function to be passed as prior argument to createBayesianSetup. If not specified, it is generated based on the *.prior arguments provided. If a userdefined prior is provided, parameter names must be included in prior\$lower, prior\$upper (see example). Character. It is passed as argument sampler in runMCMC. sampler.type List that defines the prior distribution for the decay time parameter tau. See tau.prior details. List that defines the prior distribution for the logarithm (in base 10) of the baselog_p0.prior line production rate p0. See details. If covariates = NULL, this defines the prior distribution for the logarithm (in base 10) of production rates for all river reaches. beta.prior List that defines the prior distribution for the covariate effects beta. See details. If a single spec is provided, the same prior distribution is specified for all beta parameters. Alternatively, if spec (and the other arguments, if provided) is a vector with length equal to the number of covariates included, different prior distributions can be specified for the different beta parameters. sigma.prior List that defines the prior distribution for the standard deviation of the measurement error when 11. type is "norm" or "lnorm". It is not used if 11. type = "nbinom". See details.

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List that defines the prior distribution for the overdispersion parameter omega of the measurement error when 11.type = "nbinom". It is not used if 11.type is "norm" or "lnorm". See details.
 Cstar.prior List that defines the prior distribution for the Cstar parameter controlling the probability of no detection. It is only used if no.det = TRUE. See details.
 Omega_d.prior Prior distribution for the overdispersion parameter for direct sampling density observations.
 alpha.prior Prior distribution for the inverse DNA shedding rate (i.e., the organismal density that sheds a unit eDNA value per unit time).

verbose Logical. Should console output be displayed?

Details

The arguments of the type *. prior consist in the lists of arguments required by dtrunc (except the first argument x).

By default, AEMs are computed without attributing weights to the edges of the river network. Use e.g. par.AEM = list(weight = "gravity") to attribute weights.

Value

A list with objects:

Vector of named parameters corresponding to the maximum a posteriori estiparam_map mate. It is the output of the call to MAP. Vector of best-fit eDNA production rates corresponding to the maximum a posp_map teriori parameter estimate param_map. It has length equal to river\$AG\$nNodes. C_{map} Vector of best-fit eDNA values (in the same unit as data\$values, i.e. concentrations or read numbers) corresponding to the maximum a posteriori parameter estimate param_map. It has length equal to river\$AG\$nNodes. Vector of best-fit detection probabilities corresponding to the maximum a posprobDet_map teriori parameter estimate param_map. It has length equal to river\$AG\$nNodes. If a custom likelihood is provided, this is a vector of null length (in which case the user should calculate the probability of detection independently, based on the chosen likelihood). Output of the call to getCredibleIntervals. сI Output of the call to gelmanDiagnostics. gD covariates Data frame containing input covariate values (possibly Z-normalized). Vector of source area values. source.area outMCMC Object of class mcmcSampler returned by the call to runMCMC.

Moreover, arguments 11. type (possibly changed to "custom" if a custom likelihood is specified), no.det and data are added to the list.

Examples

```
data(wigger)
data(dataCD)
# reduce number of iterations for illustrative purposes
# (use default mcmc.settings to ensure convergence)
settings.short <- list(iterations = 1e3, thin = 10)</pre>
set.seed(1)
out <- run_eDITH_BT_joint(dataCD, wigger, mcmc.settings = settings.short)</pre>
library(rivnet)
# best-fit (maximum a posteriori) map of eDNA production rates
plot(wigger, out$p_map)
# best-fit map (maximum a posteriori) of detection probability
plot(wigger, out$probDet_map)
# compare best-fit vs observed values
data.e <- which(dataCD$type=="e")</pre>
data.d <- which(dataCD$type=="d")</pre>
plot(out$C_map[dataCD$ID[data.e]], dataCD$values[data.e],
xlab="Modelled (MAP) eDNA concentrations", ylab="Observed eDNA concentrations")
abline(a=0, b=1)
plot(out$p_map[dataCD$ID[data.d]], dataCD$values[data.d],
xlab="Modelled (MAP) eDNA production rate", ylab="Observed density data")
```

run_eDITH_optim

Optimize eDITH

Description

Function that performs search of optimal parameters of an eDITH model

Usage

```
log_p0.prior = list(spec="unif",min=-20, max=0),
    beta.prior = list(spec="norm",sd=1),
    sigma.prior = list(spec="unif",min=0, max=1*max(data$values, na.rm = TRUE)),
    omega.prior = list(spec="unif",min=1, max=10*max(data$values, na.rm = TRUE)),
    Cstar.prior = list(spec="unif",min=0, max=1*max(data$values, na.rm = TRUE)),
    verbose = FALSE)
```

Arguments

data eDNA data. Data frame containing columns ID (index of the AG node/reach

where the eDNA sample was taken) and values (value of the eDNA measure-

ment, expressed as concentration or number of reads).

river A river object generated via aggregate_river.

covariates Data frame containing covariate values for all river reaches. If NULL (default

option), production rates are estimated via AEMs.

Z.normalize Logical. Should covariates be Z-normalized?

use.AEM Logical. Should eigenvectors based on AEMs be used as covariates? If covariates

= NULL, it is set to TRUE. If TRUE and covariates are provided, AEM eigenvec-

tors are appended to the covariates data frame.

n.AEM Number of AEM eigenvectors (sorted by the decreasing respective eigenvalue)

to be used as covariates. If par.AEM\$moranI = TRUE, this parameter is not used. Instead, the eigenvectors with significantly positive spatial autocorrelation are

used as AEM covariates.

par.AEM List of additional parameters that are passed to river_to_AEM for calculation

of AEMs. In particular, par.AEM\$moranI = TRUE imposes the use of AEM covariates with significantly positive spatial autocorrelation based on Moran's I

statistic.

no.det Logical. Should a probability of non-detection be included in the model?

11. type Character. String defining the error distribution used in the log-likelihood for-

mulation. Allowed values are norm (for normal distribution), 1norm (for lognormal distribution), nbinom (for negative binomial distribution) and geom (for geometric distribution). The two latter choices are suited when eDNA data are expressed as read numbers, while norm and 1norm are better suited to eDNA

concentrations.

source area Defines the extent of the source area of a node. Possible values are "AG" (if the

source area is the reach surface, i.e. length*width), "SC" (if the source area is the subcatchment area), or, alternatively, a vector with length river\$AG\$nodes.

likelihood Likelihood function. If not specified, it is generated based on arguments no. det

and 11. type.

sampler Function generating sets of initial parameter values for the optimization algo-

rithm. If NULL, initial parameter values are drawn from the default prior distri-

butions of run_eDITH_BT. See details.

n.attempts Number of times the optimizing function optim is executed. Every time a

"restart" happens (see n.restarts), sampler is used to draw an initial parameter set. If a "restart" does not happen, the optimal parameter set from the previ-

ous attempt is used as initial parameter set.

n.restarts Number of times a random parameter set is drawn as initial condition for optim.

par.optim List of parameters to be passed to optim. By default, the likelihood is maxi-

mized (i.e., $control\finscale = -1$), and the maximum number of iterations is set to 1e6. The default optimization method is "Nelder-Mead" (same default as

in optim).

tau.prior, log_p0.prior,beta.prior,sigma.prior,omega.prior,Cstar.prior

Prior distribution for the relevant parameters of the eDITH model.

verbose Logical. Should console output be displayed?

Details

This function attempts to maximize the log-posterior (sum of log-likelihood and log-prior) via the non-linear optimization function optim.

If specified by the user, sampler must be a function that produces as output a "named num" vector of parameters. Parameter names must be same as in the likelihood. See example.

By default, AEMs are computed without attributing weights to the edges of the river network. Use e.g. par.AEM = list(weight = "gravity") to attribute weights.

Value

A list with objects:

p Vector of best-fit eDNA production rates corresponding to the optimum param-

eter estimates param. It has length equal to river\$AG\$nNodes.

C Vector of best-fit eDNA values (in the same unit as data\$values, i.e. concen-

trations or read numbers) corresponding to the optimum parameter estimates

param. It has length equal to river\$AG\$nNodes.

probDet Vector of best-fit detection probabilities corresponding to the optimum parame-

ter estimate param_map. It has length equal to river\$AG\$nNodes. If a custom likelihood is provided, this is a vector of null length (in which case the user should calculate the probability of detection independently, based on the chosen

likelihood).

param Vector of named parameters corresponding to the best-fit estimate.

covariates Data frame containing input covariate values (possibly Z-normalized).

source.area Vector of source area values.

out_optim List as provided by optim. Only the result of the call to optim (out of n.attempts)

yielding the highest likelihood is exported.

attempts.stats List containing relevant output for the different optimization attempts. It con-

tains 1p (vector of maximized log-posterior values for each single attempt), counts (total function evaluations), conv (convergence flags as produced by

optim), and tau (best-fit decay time values in h).

Moreover, arguments 11.type (possibly changed to "custom" if a custom likelihood is specified), no.det and data are added to the list.

Examples

```
data(wigger)
data(dataC)
data(dataRead)
## fit eDNA concentration data - use AEMs as covariates
set.seed(9)
out <- run_eDITH_optim(dataC, wigger, n.AEM = 10,
n.attempts = 1) # reduced n.AEM, n.attempts for illustrative purposes
# it is recommended to attempt optimization several times to ensure convergence
library(rivnet)
# best-fit map of eDNA production rates
plot(wigger, out$p)
# best-fit map of detection probability
plot(wigger, out$probDet)
# compare best-fit vs observed eDNA concentrations
plot(out$C[dataC$ID], dataC$values,
xlab = "Modelled concentrations", ylab = "Observed concentrations")
abline(a=0, b=1)
## fit eDNA read number data - use AEMs as covariates
set.seed(5)
out <- run_eDITH_optim(dataRead, wigger, ll.type = "nbinom",
par.AEM = list(weight = "gravity"),
n.attempts = 1) # reduced n.attempts for illustrative purposes
## use user-defined covariates
covariates <- data.frame(urban = wigger$SC$locCov$landcover_1,</pre>
                         agriculture = wigger$SC$locCov$landcover_2,
                         forest = wigger$SC$locCov$landcover_3,
                         elev = wigger$AG$Z,
                         log_drainageArea = log(wigger$AG$A))
set.seed(2)
out.cov <- run_eDITH_optim(dataC, wigger, covariates, n.attempts = 1)</pre>
# reduced n.attempts for illustrative purposes
# use user-defined covariates and AEMs
set.seed(1)
out.covAEM <- run_eDITH_optim(dataC, wigger, covariates, use.AEM = TRUE,</pre>
par.AEM = list(weight = "gravity"),
n.attempts = 1) # reduced n.attempts for illustrative purposes
# use AEMs with significantly positive spatial autocorrelation
set.seed(1)
out.AEM.moran <- run_eDITH_optim(dataC, wigger, use.AEM = TRUE,
par.AEM = list(weight = "gravity", moranI = TRUE),
n.attempts = 1) # reduced n.attempts for illustrative purposes
```

```
# define sampler function when the first 10 AEMs are used as covariates
samp_fun <- function(n){ # input argument needed but not used
    mins = c(0, -20, rep(-5,10), 0)
    maxs = c(10, 0, rep(5,10), 5e-12)
    nams = c("tau", "log_p0", paste0("beta_AEM",1:10), "sigma")
    vec <- runif(numeric(13), min=mins, max=maxs)
    names(vec) <- nams
    return(vec)}
set.seed(1)
out.samp <- run_eDITH_optim(dataC, wigger, n.AEM = 10,
    sampler = samp_fun,
n.attempts = 1) # reduced n.attempts for illustrative purposes</pre>
```

run_eDITH_optim_joint Optimize eDITH based on joint eDNA and direct sampling data

Description

Function that performs search of optimal parameters of an eDITH model fitted on both eDNA and direct sampling data.

Usage

```
run_eDITH_optim_joint(data, river, covariates = NULL, Z.normalize = TRUE,
           use.AEM = FALSE, n.AEM = NULL, par.AEM = NULL,
           no.det = FALSE, 11.type = "norm", source.area = "AG",
           likelihood = NULL, sampler = NULL, n.attempts = 100,
           n.restarts = round(n.attempts/10), par.optim = NULL,
           tau.prior = list(spec="lnorm",a=0,b=Inf, meanlog=log(5),
                    sd=sqrt(log(5)-log(4))),
           log_p0.prior = list(spec="unif",min=-20, max=0),
           beta.prior = list(spec="norm",sd=1),
           sigma.prior = list(spec="unif",min=0,
                              max=1*max(c(1e-6, data$values[data$type=="e"]),
          omega.prior = list(spec="unif",min=1,
                              max=10*max(c(0.11, data$values[data$type=="e"]),
 na.rm = TRUE)),
          Cstar.prior = list(spec="unif", min=0,
                              max=1*max(c(1e-6, data$values[data$type=="e"]),
 na.rm = TRUE)),
           omega_d.prior = list(spec="unif", min=1,
                               max=10*max(c(0.11, data$values[data$type=="d"]),
na.rm = TRUE)),
           alpha.prior = list(spec="unif", min=0, max=1e6),
           verbose = FALSE)
```

Arguments

data eDNA and direct observation data. Data frame containing columns ID (index of

the AG node/reach where the sample was taken), values (value of the eDNA or direct measurement) and type (equal to "e" for eDNA data and to "d" for direct observation data). eDNA values are expressed as concentration or number

of reads; direct observations are expressed as numbers of individuals.

river A river object generated via aggregate_river.

covariates Data frame containing covariate values for all river reaches. If NULL (default

option), production rates are estimated via AEMs.

Z.normalize Logical. Should covariates be Z-normalized?

use.AEM Logical. Should eigenvectors based on AEMs be used as covariates? If covariates

= NULL, it is set to TRUE. If TRUE and covariates are provided, AEM eigenvec-

tors are appended to the covariates data frame.

n.AEM Number of AEM eigenvectors (sorted by the decreasing respective eigenvalue)

to be used as covariates. If par.AEM\$moranI = TRUE, this parameter is not used. Instead, the eigenvectors with significantly positive spatial autocorrelation are

used as AEM covariates.

par.AEM List of additional parameters that are passed to river_to_AEM for calculation

of AEMs. In particular, par.AEM\$moranI = TRUE imposes the use of AEM covariates with significantly positive spatial autocorrelation based on Moran's I

statistic.

no.det Logical. Should a probability of non-detection be included in the model?

11. type Character. String defining the error distribution used in the log-likelihood for-

mulation. Allowed values are norm (for normal distribution), 1norm (for log-normal distribution), nbinom (for negative binomial distribution) and geom (for geometric distribution). The two latter choices are suited when eDNA data are expressed as read numbers, while norm and 1norm are better suited to eDNA

concentrations.

source.area Defines the extent of the source area of a node. Possible values are "AG" (if the

source area is the reach surface, i.e. length*width), "SC" (if the source area is the subcatchment area), or, alternatively, a vector with length river\$AG\$nodes.

likelihood Likelihood function. If not specified, it is generated based on arguments no. det

and 11. type.

sampler Function generating sets of initial parameter values for the optimization algo-

rithm. If NULL, initial parameter values are drawn from the default prior distri-

butions of run_eDITH_BT. See details.

"restart" happens (see n.restarts), sampler is used to draw an initial parameter set. If a "restart" does not happen, the optimal parameter set from the previ-

ous attempt is used as initial parameter set.

n.restarts Number of times a random parameter set is drawn as initial condition for optim.

par.optim List of parameters to be passed to optim. By default, the likelihood is maximized (i.e., control\$fnscale = -1), and the maximum number of iterations is

set to 1e6. The default optimization method is "Nelder-Mead" (same default as

in optim).

tau.prior, log_p0.prior,beta.prior,sigma.prior,omega.prior,Cstar.prior

Prior distribution for the relevant parameters of the eDITH model.

omega_d.prior Prior distribution for the overdispersion parameter for direct sampling density

observations.

alpha.prior Prior distribution for the inverse DNA shedding rate (i.e., the organismal density

that sheds a unit eDNA value per unit time).

verbose Logical. Should console output be displayed?

Details

This function attempts to maximize the log-posterior (sum of log-likelihood and log-prior) via the non-linear optimization function optim.

If specified by the user, sampler must be a function that produces as output a "named num" vector of parameters. Parameter names must be same as in the likelihood. See example.

By default, AEMs are computed without attributing weights to the edges of the river network. Use e.g. par.AEM = list(weight = "gravity") to attribute weights.

Value

A list with objects:

p Vector of best-fit eDNA production rates corresponding to the optimum param-

eter estimates param. It has length equal to river\$AG\$nNodes.

C Vector of best-fit eDNA values (in the same unit as data\$values, i.e. concen-

trations or read numbers) corresponding to the optimum parameter estimates

param. It has length equal to river\$AG\$nNodes.

probDet Vector of best-fit detection probabilities corresponding to the optimum parame-

ter estimate param_map. It has length equal to river\$AG\$nNodes. If a custom likelihood is provided, this is a vector of null length (in which case the user should calculate the probability of detection independently, based on the chosen

likelihood).

param Vector of named parameters corresponding to the best-fit estimate.

covariates Data frame containing input covariate values (possibly Z-normalized).

source.area Vector of source area values.

out_optim List as provided by optim. Only the result of the call to optim (out of n.attempts)

yielding the highest likelihood is exported.

attempts.stats List containing relevant output for the different optimization attempts. It con-

tains 1p (vector of maximized log-posterior values for each single attempt), counts (total function evaluations), conv (convergence flags as produced by

optim), and tau (best-fit decay time values in h).

Moreover, arguments 11.type (possibly changed to "custom" if a custom likelihood is specified), no.det and data are added to the list.

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Examples

```
data(wigger)
data(dataCD)
## fit eDNA concentration and direct observation data - use AEMs as covariates
set.seed(9)
out <- run_eDITH_optim_joint(dataCD, wigger, n.AEM = 10,
n.attempts = 1) # reduced n.AEM, n.attempts for illustrative purposes
# it is recommended to attempt optimization several times to ensure convergence
library(rivnet)
# best-fit map of eDNA production rates
plot(wigger, out$p)
# best-fit map of detection probability
plot(wigger, out$probDet)
# compare best-fit vs observed values
data.e <- which(dataCD$type=="e")</pre>
data.d <- which(dataCD$type=="d")</pre>
plot(out$C[dataCD$ID[data.e]], dataCD$values[data.e],
xlab="Modelled (MAP) eDNA concentrations", ylab="Observed eDNA concentrations")
abline(a=0, b=1)
plot(out$p[dataCD$ID[data.d]], dataCD$values[data.d],
xlab="Modelled (MAP) eDNA production rate", ylab="Observed density data")
```

run_eDITH_single

Run eDITH for a single parameter set

Description

Function that runs the eDITH model for a given parameter set

Usage

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Arguments

Parameter set. It has to be a named vector, with names:

tau Decay time (expressed in h).

log_p0 Natural logarithm of the baseline production rate.

beta_X Effect size of covariate X. There must be as many beta_X as columns in covariates. X must be the name of the corresponding column in covariates.

omega, sigma, Cstar Parameters for estimation of the log-likelihood and detec-

tion probability. Only required if 11. type is provided.

river A river object generated via aggregate_river.

covariates Data frame containing covariate values for all river reaches.

Z.normalize Logical. Should covariates be Z-normalized?

no.det Logical. Should a probability of non-detection be included in the model?

11. type Character. String defining the error distribution used in the log-likelihood for-

mulation. Allowed values are norm (for normal distribution), 1norm (for lognormal distribution), nbinom (for negative binomial distribution) and geom (for geometric distribution). The two latter choices are suited when eDNA data are expressed as read numbers, while norm and 1norm are better suited to eDNA

concentrations.

data eDNA data. Data frame containing columns ID (index of the AG node/reach

where the eDNA sample was taken) and values (value of the eDNA measure-

ment, expressed as concentration or number of reads).

source.area Defines the extent of the source area of a node. Possible values are "AG" (if the

source area is the reach surface, i.e. length*width), "SC" (if the source area is the subcatchment area), or, alternatively, a vector with length river\$AG\$nodes.

tau.prior, log_p0.prior,beta.prior,sigma.prior,omega.prior,Cstar.prior

Prior distribution for the relevant parameters of the eDITH model. Only used if

both 11. type and data are provided.

Value

A list with objects:

p Vector of eDNA production rates corresponding to the parameter set param. It

has length equal to river\$AG\$nNodes.

C Vector of eDNA values (concentrations or read numbers) corresponding to the

parameter set param. It has length equal to river\$AG\$nNodes.

probDet Vector of detection probabilities corresponding to the parameter set param. It is

only computed if 11. type is provided. It has length equal to river\$AG\$nNodes.

logprior Value of the log-prior distribution (computed only if 11. type and data are pro-

vided).

loglik Value of the log-likelihood distribution (computed only if 11. type and data are

provided).

logpost Value of the log-posterior distribution (computed only if 11. type and data are

provided).

See Also

See run_eDITH_BT, run_eDITH_optim for details on parameters names and log-likelihood specification.

Examples

```
library(rivnet)
data(wigger)
# calculate AEMs and use the first 10 as covariates
ae <- river_to_AEM(wigger)
covariates <- data.frame(ae$vectors[,1:10])</pre>
names(covariates) <- paste0("AEM",1:10)</pre>
# covariates names must correspond to param names
set.seed(1); param <- c(3,-15, runif(10,-1,1))
names(param) <- c("tau", "log_p0", paste0("beta_AEM",1:10))</pre>
# param names must correspond to covariates names
out <- run_eDITH_single(param, wigger, covariates)</pre>
# add parameter sigma and compute detection probability
param <- c(param, 5e-12)
names(param)[length(param)] <- "sigma"</pre>
# note that the value of sigma has to be within the range indicated by sigma.prior
out2 <- run_eDITH_single(param, wigger, covariates, ll.type="norm")</pre>
# include data and compute logprior, loglikelihood, logposterior
data(dataC)
out3 <- run_eDITH_single(param, wigger, covariates,</pre>
11.type="norm", data=dataC)
```

sampling_strategy_direct

Determine optimal spatial arrangement for direct sampling

Description

Function that determines the optimal spatial arrangement for direct sampling sites

Usage

```
sampling_strategy_direct(river, nSites)
```

Arguments

river A river object generated via aggregate_river.

nSites Number of sites to be deployed. Cannot be higher than river\$AG\$nNodes.

Value

A vector containing the ID of the nSites selected sites according to this strategy. Sites are sorted according to their rank (i.e., the first site in the vector is the first one that has been selected).

Examples

```
library(rivnet)
data(wigger)
wigger <- paths_river(wigger)
sites <- sampling_strategy_direct(wigger, 20)
plot(wigger)
points_colorscale(wigger$AG$X[sites], wigger$AG$Y[sites], 1:20)
title("Rank of selected sites")</pre>
```

```
sampling_strategy_eDNA
```

Determine optimal spatial arrangement for eDNA sampling

Description

Function that determines the optimal spatial arrangement for eDNA sampling sites

Usage

```
sampling_strategy_eDNA(river, nSites)
```

Arguments

river A river object generated via paths_river.

nSites Number of sites to be deployed. Cannot be higher than river\$AG\$nNodes.

Value

A vector containing the ID of the nSites selected sites according to this strategy. Sites are sorted according to their rank (i.e., the first site in the vector is the first one that has been selected).

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Examples

```
library(rivnet)
data(wigger)
wigger <- paths_river(wigger)
sites <- sampling_strategy_eDNA(wigger, 20)
plot(wigger)
points_colorscale(wigger$AG$X[sites], wigger$AG$Y[sites], 1:20)
title("Rank of selected sites")</pre>
```

wigger

River Wigger

Description

```
It is built via
wigger <- extract_river(outlet=c(637478,237413), EPSG=21781, ext=c(6.2e5,6.6e5,2e5,2.5e5),
z=9)
wigger <- aggregate_river(wigger, maxReachLength = 2500)
hydrodata <- data.frame(data=c(8, 15), type=c("w","Q"), node=wigger$AG$outlet*c(1,1))
wigger <- hydro_river(hydrodata, wigger)
r1 <- rast(system.file("extdata/landcover.tif", package="rivnet"))
wigger <- covariate_river(r1, wigger)</pre>
```

Usage

data(wigger)

Format

A river object. See extract_river documentation for details.

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