

Package ‘dycdtools’

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Title Tools for DYRESM-CAEDYM Model Development: Auto-Calibration and Post-Processing

Version 0.1.0

Description Tools for DYRESM-CAEDYM model development, including auto-calibrate selected model parameters and visualise model output through time series plot, profile plot, contour plot, and scatter plot.

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Suggests testthat

NeedsCompilation no

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autoCalibration	<i>Automatically calibrate DYRESM-CAEDYM model.</i>
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Description

This function tries different combinations of selected parameter values and outputs corresponding values of fit-of-goodness by calculating some objective functions. Then users can choose the optimal set of parameter values to calibrate the model.

Usage

```
autoCalibration(
  cal.para = "Data/Calibration parameters.csv",
  combination = "random",
  n = 1,
  model.var = c("TEMP", "DO", "TN", "TP", "NO3", "PO4", "NH4", "SALINITY"),
  phyto.group = NA,
  obs.data = "Data/Obs LHM.csv",
  objective.function = c("nse", "rmse"),
  start.date = "2017-06-06",
  end.date = "2020-02-29",
  dycd.wd = "Data/200318-lhm-ref",
  dycd.output = "Data/200318-lhm-ref/DYsim.nc",
  file_name = "Data/auto-calibration.csv",
  verbose = TRUE,
  write.out = FALSE
)
```

Arguments

cal.para	a character string naming a file where parameters to be calibrated and their value ranges. this file need to have fixed colnames.
combination	a vector of string character of how to pick up combinations of parameter values."random" or "all".
n	the number of randomly selections. Must be provided if combination = random.
model.var	a vector of string character of modelled variables for calibration. When multiple phytoplankton groups will be combined for calibration, use "CHLA" and the following argument of "phyto.group" to specify them. When phytoplankton groups

	will be calibrated separately, put their abbrev. in this argument. Currently, five abbrevs are supported: CHLOR, FDIAT, NODUL, CYANO and CRYPT.
phyto.group	a vector of simulated phytoplankton groups, including CHLOR, FDIAT, NODUL, CYANO and CRYPT.
obs.data	a character string naming a file of observed lake data. This file need to have fixed column names and orders.
objective.function	a vector of string character claiming what objective function(s) to be used for calibration. either Nash-Sutcliffe Efficiency coefficient ("nse") or Root Mean Square Error ("rmse")
start.date, end.date	the beginning and ending simulation dates for the intended DYRESM-CAEDYM model run. The date format must be "%Y-%m-%d".
dycd.wd	working directory where input files (including the bat file) to DYRESM-CAEDYM are stored.
dycd.output	a character string naming the output file from the model run.
file_name	a character string naming a png file for writing out the auto-calibration results.
verbose	if TRUE, the auto-calibration information is printed.
write.out	if TRUE, the auto-calibration results are saved a file with a file name set by the "file_name" argument.

Value

a dataframe of trialed values of parameters and corresponding values of objective function(s).

Note

No executable examples are provided to illustrate the use of this function, as this function relies on the DYRESM-CAEDYM executables to work.

change_input_file	<i>change parameter value of input files to DYRESM_CAEDYM model.</i>
-------------------	--

Description

change parameter value of input files to DYRESM_CAEDYM model.

Usage

```
change_input_file(input_file = "par", row_no = 12, new_value)
```

Arguments

input_file	vector of input format, such as "par","cfg".
row_no	the number of row where the variable of interest is in the input file
new_value	the new value that will be assigned to the variable of interest.

cont.plot	<i>Contour plot of a variable simulation, with observed data shown as dots in the generated contour plot.</i>
-----------	---

Description

Contour plot a matrix of a bio-geochemical variable values, which can be generated through "interpol" function.

Usage

```
cont.plot(
  sim = temp.interpolated,
  start.date = "2017-06-06",
  end.date = "2017-06-15",
  legend.title = "T °C",
  min.depth = 0,
  max.depth = 13,
  by.value = 0.5,
  nlevels = 20,
  plot.save = TRUE,
  file_name = "Contour_temp.png",
  height = 5,
  width = 8,
  ppi = 150
)
```

Arguments

sim	a matrix of simulated variables that have been interpolated
start.date, end.date	the beginning and ending simulation dates for the intended DYRESM-CAEDYM model run. The date format must be "%Y-%m-%d".
legend.title	the legend title of the contour figure.
min.depth, max.depth, by.value	minimum and maximum depth used to be the start of y axis of the contour plot, at the increment of by.value.
nlevels	a set of levels which are used to partition the range of simulation variable.
plot.save	if TRUE, the plot is saved with the "height", "width", and "ppi" parameters.
file_name	the file path to save the generated contour figure.
height, width	the relative height/width of the figure.
ppi	the ppi value of the figure.

Value

a graph file of contour plot saved in the Figure folder.

Examples

```
# extract simulated temperature values from DYRESM-CAEDYM simulation file
library(dycdtools)
var.values<-ext.output(dycd.output=system.file("extdata", "dysim.nc", package = "dycdtools"),
  var.extract=c("TEMP"))

for(i in 1:length(var.values)){
  expres<-paste0(names(var.values)[i],"<-data.frame(var.values[[",i,"]])")
  eval(parse(text=expres))
}

# interpolate temperature for depths from 0 to 13 m at increment of 0.5 m
temp.interpolated<-interpol(layerHeights = dyresmLAYER_HTS_Var,
  var = dyresmTEMPTURE_Var,
  min.dept = 0,max.dept = 13,by.value = 0.5)

# contour plot of temperature simulations
cont.plot(sim=temp.interpolated,
  start.date="2017-06-06",end.date="2017-06-15",
  legend.title="T \u00B0C",
  min.depth=0,max.depth=13,by.value=0.5,
  nlevels=20,
  plot.save=FALSE,
  file_name="Contour_temp.png",
  height=5,width=8,ppi=150)
```

cont.plot.comp	<i>Contour plot of a variable simulation, with observed data shown as dots in the generated contour plot.</i>
----------------	---

Description

Contour plot a matrix of a bio-geochemical variable values, which can be generated through "interpol" function.

Usage

```
cont.plot.comp(
  sim = temp.interpolated,
  obs = obs_temp,
  file_name = "Contour_temp.png",
  start.date = "2017-06-06",
  end.date = "2017-06-15",
  date = NULL,
  legend.title = "T °C",
  min.depth = 0,
  max.depth = 13,
```

```

    by.value = 0.5,
    nlevels = 20,
    plot.save = TRUE,
    height = 5,
    width = 8,
    ppi = 150
  )

```

Arguments

<code>sim</code>	a matrix of simulated variables that have been interpolated
<code>obs</code>	observed values of variable.
<code>file_name</code>	the file path to save the generated contour figure.
<code>start.date, end.date</code>	the beginning and ending simulation dates for the intended DYRESM-CAEDYM model run. The date format must be "%Y-%m-%d".
<code>date</code>	all dates within the simulation period.
<code>legend.title</code>	the legend title of the contour figure.
<code>min.depth, max.depth, by.value</code>	minimum and maximum depth used to be the start of y axis of the contour plot, at the increment of <code>by.value</code> .
<code>nlevels</code>	a set of levels which are used to partition the range of simulation variable.
<code>plot.save</code>	if TRUE, the plot is saved with the "height", "width", and "ppi" parameters.
<code>height, width</code>	the relative height/width of the figure.
<code>ppi</code>	the ppi value of the figure.

Value

a graph file of contour plot saved in the Figure folder.

Examples

```

# extract simulated temperature values from DYRESM-CAEDYM simulation file
var.values<-ext.output(dycd.output=system.file("extdata", "dysim.nc", package = "dycdtools"),
  var.extract=c("TEMP"))

for(i in 1:length(var.values)){
  expres<-paste0(names(var.values)[i],"<-data.frame(var.values[,i,""])"")
  eval(parse(text=expres))
}

# interpolate temperature for depths from 0 to 13 m at increment of 0.5 m
temp.interpolated<-interpol(layerHeights = dyresmLAYER_HTS_Var,
  var = dyresmTEMPTURE_Var,
  min.dept = 0,max.dept = 13,by.value = 0.5)

data(obs_temp)
# contour plot of temperature simulations with observed data shown as colour-coded dots

```

```
cont.plot.comp(sim=temp.interpolated,
               obs=obs_temp,
               start.date="2017-06-06",end.date="2017-06-15",
               date=NULL,
               legend.title="T \u00B0C",
               min.depth=0,max.depth=13,by.value=0.5,
               nlevels=20,
               plot.save=FALSE,
               file_name="Contour_temp.png",
               height=5,width=8,ppi=150)
```

delete.space	Delete all whitespace until a non-whitespace character.
--------------	---

Description

Delete all whitespace until a non-whitespace character.

Usage

```
delete.space(extract_val)
```

Arguments

extract_val a vector.

ext.output	Extract simulations from DYRESM-CAEDYM output.
------------	--

Description

Extract simulations from DYRESM-CAEDYM output. It is recommended to use the following example code to assign values of each simulated variable to a corresponding matrix.

Usage

```
ext.output(
  dycd.output = "data/dysim.nc",
  var.extract = c("TEMP", "DO", "TP", "TN", "N03", "NH4", "CHLA")
)
```

Arguments

dycd.output	a string of characters of the output netcdf file names of DYRESM-CAEDYM model
var.extract	a vector of variables to be extracted from the output file. Options include TEMP, DO, TP, NO3, NH4, TN, CHLOR, FDIAT, SSOL1, SSOL2, and PO4. Apart from nominated variables, simulation period and layer height data are also extracted.

Value

a list of values of those variables of interest, as well as two compulsory variables (i.e. simulation period, water level)

Examples

```
# extract simulated temperature values from DYRESM-CAEDYM simulation file
var.values<-ext.output(dycd.output=system.file("extdata", "dysim.nc", package = "dycdtools"),
                       var.extract=c("TEMP"))

for(i in 1:length(var.values)){
  expres<-paste0(names(var.values)[i],"<-data.frame(var.values[["",i,"]])")
  eval(parse(text=expres))
}
```

hgt.to.dpt	<i>convert from height to depth</i>
------------	-------------------------------------

Description

convert from height to depth

Usage

```
hgt.to.dpt(height)
```

Arguments

height	a vector of height profile
--------	----------------------------

interpol	<i>Interpolation of simulation for a series of user-defined depths.</i>
----------	---

Description

Convert simulated variable at irregular layer heights to a dataframe of the same variable at sequenced layer heights.

Usage

```
interpol(layerHeights, var, min.depth, max.depth, by.value)
```

Arguments

layerHeights	layer heights, extracted from DYCD outputs
var	simulated variable values, extracted from DYCD outputs
min.depth, max.depth, by.value	minimum and maximum depth for interpolation at the depth increment of by.value.

Value

a matrix of interpolated values of such variable.

Examples

```
# extract simulated temperature values from DYRESM-CAEDYM simulation file
var.values<-ext.output(dycd.output=system.file("extdata", "dysim.nc", package = "dycdtools"),
  var.extract=c("TEMP"))

for(i in 1:length(var.values)){
  expres<-paste0(names(var.values)[i],"<-data.frame(var.values[[",i,"]])")
  eval(parse(text=expres))
}
# interpolate temperature for depths from 0 to 13 m at increment of 0.5 m
temp.interpolated<-interpol(layerHeights = dyresmLAYER_HTS_Var,
  var = dyresmTEMPTURE_Var,
  min.dept = 0,max.dept = 13,by.value = 0.5)
```

nse.rmse

Calculate fit of goodness of DYCD model simulations.

Description

Two objective functions can be calculated: 1) Nash-Sutcliffe efficiency coefficient (NSE), and 2) Root Mean Square Error (RMSE).

Usage

```
nse.rmse(
  sim,
  obs,
  start.date = "2017-06-06",
  end.date = "2020-02-29",
  min.depth = 0,
  max.depth = 33,
  by.value = 0.5
)
```

Arguments

sim	a matrix of bio-geochemical variable values with column of time and row of depth.
obs	a data frame of observed value, with three columns: Date, depth, value.
start.date, end.date	the beginning and ending simulation dates for the intended DYRESM-CAEDYM model run. The date format must be "%Y-%m-%d".
min.depth, max.depth	minimum and maximum depth to be compared between simulations and observations.
by.value	the value of increment for depth.

Value

a vector of objective function values. The first is NSE and the second is RMSE.

obs_temp	<i>Example observed profiling temperature data across different depths over the period of 6-11 June 2017.</i>
----------	---

Description

A table has three columns. The first column name is Date in the form of dd-mm-YY. The second column is Depth where the temperature data was monitored. The third column is monitored temperature value.

Usage

```
data(obs_temp)
```

Format

A data frame with 77 rows and 3 variables:

Date date when the monitoring happened

Depth depth of monitoring

TEMP temperature value

Source

self-made.

output_name	<i>Default DYCD simulation variable names with their variable name</i>
-------------	--

Description

A table has two columns. The first column name is var.name, meaning variable names that are used in the extract.output function. The second column is the default DYCD simulation variable names, such as "dyresmLAYER_HTS_Var".

Usage

```
data(output_name)
```

Format

A data frame with 65 rows and 2 variables:

var.name variable name

output.name default DYCD simulation variable name

Source

self-made.

prof.plot

Profile plot of simulated variable values vs. depth

Description

A post-processing function used to visualise model output in a profile graph.

Usage

```
prof.plot(
    sim = temp.interpolated,
    obs = obs.temp,
    sim.start = "2017-06-06",
    sim.end = "2020-02-29",
    plot.start = "2017-06-06",
    plot.end = "2020-02-29",
    xlabel = "Temperature °C",
    min.depth = 0,
    max.depth,
    by.value,
    plot.save = FALSE,
    file_name,
    height = 11,
    width = 18
)
```

Arguments

sim	interpolated values of variable.
obs	observed values of variable.
sim.start, sim.end	the beginning and ending simulation dates for the intended DYRESM-CAEDYM model run. The date format must be "%Y-%m-%d".
plot.start, plot.end	the beginning and ending dates for the plotting purpose. The date format must be "%Y-%m-%d".
xlabel	the x axis label of the profile figure
min.depth, max.depth, by.value	minimum and maximum depth for the profile plot at the depth increment of by.value.
plot.save	if TRUE, the plot is saved with the "height", "width", and "ppi" parameters.
file_name	the file path to save the generated profile figure
height, width	the height and width of the profile figure.

Value

a profile plot of sim~depth

Examples

```
var.values<-ext.output(dycd.output=system.file("extdata", "dysim.nc", package = "dycdtools"),
  var.extract=c("TEMP"))

for(i in 1:length(var.values)){
  expres<-paste0(names(var.values)[i],"<-data.frame(var.values[[",i,"]])")
  eval(parse(text=expres))
}

# interpolate temperature for depths from 0 to 13 m at increment of 0.5 m
temp.interpolated<-interpol(layerHeights = dyresmLAYER_HTS_Var,
  var = dyresmTEMPTURE_Var,
  min.dept = 0,max.dept = 13,by.value = 0.5)

data(obs_temp)
# profile plot of temperature sim and obs
prof.plot(sim=temp.interpolated,
  obs = obs_temp,
  sim.start="2017-06-06",
  sim.end="2017-06-15",
  plot.start="2017-06-06",
  plot.end="2017-06-15",
  xlabel = "Temperature \u00B0C",
  min.depth = 0,max.depth = 13,by.value = 0.5)
```

scatter.plot

Scatter plot of sim and obs var values

Description

Scatter plot of sim and obs var values

Usage

```
scatter.plot(
  sim = temp.interpolated,
  obs = obs.temp,
  sim.start = "2017-06-06",
  sim.end = "2020-02-29",
  plot.start = "2017-06-06",
  plot.end = "2020-02-29",
  min.depth = 0,
  max.depth,
```

```

    by.value,
    plot.save = TRUE,
    file_name,
    height = 4,
    width = 7
  )

```

Arguments

<code>sim</code>	interpolated values of variable.
<code>obs</code>	observed values of variable. This data need to have fixed types of colnames and orders.
<code>sim.start, sim.end</code>	the beginning and ending simulation dates for the intended DYRESM-CAEDYM model run. The date format must be "%Y-%m-%d".
<code>plot.start, plot.end</code>	the beginning and ending dates for the plotting purpose. The date format must be "%Y-%m-%d".
<code>min.depth, max.depth, by.value</code>	minimum and maximum depth for the profile plot at the depth increment of <code>by.value</code> .
<code>plot.save</code>	if TRUE, the plot is saved with the "height", "width", and "ppi" parameters.
<code>file_name</code>	the file path to save the generated scatter plot.
<code>height, width</code>	the height and width of the scatter figure.

Value

a scatter plot of `sim` vs. `obs`

Examples

```

var.values<-ext.output(dycd.output=system.file("extdata", "dysim.nc", package = "dycdtools"),
  var.extract=c("TEMP"))

for(i in 1:length(var.values)){
  expres<-paste0(names(var.values)[i], "<-data.frame(var.values[[", i, "]])" )
  eval(parse(text=expres))
}

# interpolate temperature for depths from 0 to 13 m at increment of 0.5 m
temp.interpolated<-interpol(layerHeights = dyresmLAYER_HTS_Var,
  var = dyresmTEMPTURE_Var,
  min.dept = 0,max.dept = 13,by.value = 0.5)

data(obs_temp)

# scatter plot of sim and obs temperature
scatter.plot(sim=temp.interpolated,
  obs=obs_temp,

```

```

sim.start="2017-06-06",
sim.end="2017-06-15",
plot.start="2017-06-06",
plot.end="2017-06-15",
plot.save=FALSE,
min.depth = 0,max.depth = 13,by.value = 0.5)

```

ts.plot

*Time series plot of simulated and observed values***Description**

Time series plot of simulated and observed values

Usage

```

ts.plot(
  sim = temp.interpolated,
  obs = obs.temp,
  target.depth = c(1, 6, 12, 30),
  sim.start = "2017-06-06",
  sim.end = "2020-02-29",
  plot.start = "2017-06-06",
  plot.end = "2020-02-29",
  min.depth = 0,
  max.depth = 33,
  by.value = 0.5,
  ylabel = "Temperature °C",
  plot.save = FALSE,
  file_name,
  height = 7,
  width = 11
)

```

Arguments

sim	interpolated values of variable
obs	observed values of variable
target.depth	a vector of depth (unit:m) to be used to extract and plot variable values.
sim.start, sim.end	the beginning and ending simulation dates for the intended DYRESM-CAEDYM model run. The date format must be "%Y-%m-%d".
plot.start, plot.end	the beginning and ending dates for the plotting purpose. The date format must be "%Y-%m-%d".

min.depth, max.depth, by.value
 minimum and maximum depth for the profile plot at the depth increment of by.value.

ylabel the y axis title.

plot.save if TRUE, the plot is saved with the "height", "width", and "ppi" parameters.

file_name the file path to save the generated ts plot.

height, width the height and width of the time series figure.

Value

a plot of sim and obs time series.

Examples

```
var.values<-ext.output(dycd.output=system.file("extdata", "dysim.nc", package = "dycdtools"),
                       var.extract=c("TEMP"))

for(i in 1:length(var.values)){
  expres<-paste0(names(var.values)[i], "<-data.frame(var.values[[", i, "]])" )
  eval(parse(text=expres))
}

# interpolate temperature for depths from 0 to 13 m at increment of 0.5 m
temp.interpolated<-interpol(layerHeights = dyresmLAYER_HTS_Var,
                             var = dyresmTEMPTURE_Var,
                             min.dept = 0,max.dept = 13,by.value = 0.5)

data(obs_temp)
# time series plot of temperature sim and obs
ts.plot(sim = temp.interpolated,
        obs = obs_temp,
        target.depth=c(1,6),
        sim.start="2017-06-06",
        sim.end="2017-06-15",
        plot.start="2017-06-06",
        plot.end="2017-06-15",
        ylabel="Temperature \u00B0C",
        min.depth=0,
        max.depth=13,
        by.value=0.5)
```


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