## Package 'SCE'

July 2, 2025

Title Stepwise Clustered Ensemble

Version 1.1.0

Description Implementation of Stepwise Clustered Ensemble (SCE) and Stepwise Cluster Analysis (SCA) for multivariate data analysis. The package provides comprehensive tools for feature selection, model training, prediction, and evaluation in hydrological and environmental modeling applications. Key functionalities include recursive feature elimination (RFE), Wilks feature importance analysis, model validation through out-of-bag (OOB) validation, and ensemble prediction capabilities. The package supports both single and multivariate response variables, making it suitable for complex environmental modeling scenarios. For more details see Li et al. (2021) <doi:10.5194/hess-25-4947-2021>.

URL https://doi.org/10.5194/hess-25-4947-2021

License GPL-3 Encoding UTF-8 RoxygenNote 7.2.3 Depends R (>= 3.5.0) Imports stats (>= 3.5.0), utils (>= 3.5.0) Suggests testthat (>= 3.0.0), knitr, rmarkdown NeedsCompilation no Author Kailong Li [aut, cre] Maintainer Kailong Li <1k198509509@gmail.com> Repository CRAN Date/Publication 2025-07-02 07:00:02 UTC

## Contents

Air_quality_training	. 2
evaluate	. 3
importance	. 5
predict.SCA	
print.SCA	. 9
RFE_SCE	. 10

	SCE																
Index																2	23

Air\_quality\_training Air Quality Datasets

#### Description

These datasets contain air quality measurements for training and testing purposes. They include various air pollutant concentrations and meteorological variables measured at different locations and times.

#### Usage

```
data("Air_quality_training")
data("Air_quality_testing")
```

#### Format

Both datasets are data frames with 8760 rows and 12 variables:

**Date** Date and time of measurement (POSIXct format)

PM2.5 Particulate matter with diameter less than 2.5 micrometers (\mu g/m^3)

PM10 Particulate matter with diameter less than 10 micrometers (\mu g/m^3)

**SO2** Sulfur dioxide concentration (\mu g/m^3)

NO2 Nitrogen dioxide concentration (\mu g/m^3)

CO Carbon monoxide concentration (\mu g/m^3)

O3 Ozone concentration (\mu g/m^3)

**TEMP** Temperature (\textdegree C)

**PRES** Atmospheric pressure (hPa)

**DEWP** Dew point temperature (\textdegree C)

RAIN Precipitation amount (mm)

**WSPM** Wind speed (m/s)

## Details

#### **Dataset Differences:**

- Air\_quality\_training: Used for training SCA and SCE models
- Air\_quality\_testing: Used for testing trained models

#### Variable Descriptions:

- PM2.5, PM10: Particulate matter concentrations, important indicators of air quality
- SO2, NO2, CO, O3: Major air pollutants regulated by environmental agencies
- TEMP, PRES, DEWP: Meteorological variables affecting air quality
- RAIN, WSPM: Weather conditions that influence pollutant dispersion

## evaluate

#### Source

Air quality monitoring stations

Model Evaluation	luate	evaluate
------------------	-------	----------

#### Description

Functions for evaluating model performance using comprehensive metrics. The package provides both generic S3 methods and direct function calls for model evaluation.

## Usage

```
evaluate(object, ...)
## S3 method for class 'SCA'
evaluate(object, Testing_data, Predictant, digits = 3, ...)
## S3 method for class 'SCE'
evaluate(object, Testing_data, Training_data, Predictant, digits = 3, ...)
SCA_Model_evaluation(Testing_data, Simulations, Predictant, digits = 3)
```

```
SCE_Model_evaluation(Testing_data, Training_data, Simulations, Predictant, digits = 3)
```

#### Arguments

object	An object for which performance should be evaluated.
Testing_data	A data.frame containing the observations used during model testing. Must include all specified predictants.
Training_data	A data.frame containing the observations used during model training. Required only for SCE objects and SCE_Model_evaluation.
Simulations	A list containing model predictions:
	<ul><li>For SCE: must contain 'Training', 'Validation', and 'Testing' components</li><li>For SCA: must contain 'Testing_sim' component</li></ul>
	The structure should align with the output generated by the respective model training function.
Predictant	A character vector specifying the name(s) of the dependent variable(s) to be evaluated (e.g., c("swvl3", "swvl4")). The specified names must exactly match those used in model training.
digits	An integer specifying the number of decimal places to retain when reporting evaluation metrics. Default value is 3.
	Additional arguments passed to methods.

### Details

#### **Evaluation Metrics:**

The functions evaluate model performance using six distinct metrics:

- 1. MAE (Mean Absolute Error): Average absolute difference between observed and predicted values
- 2. RMSE (Root Mean Square Error): Square root of the average squared differences
- NSE (Nash-Sutcliffe Efficiency): Measures the relative magnitude of residual variance compared to observed variance
- 4. Log.NSE: NSE calculated on log-transformed values for better handling of skewed distributions
- 5. R2 (R-squared): Coefficient of determination from linear regression
- 6. KGE (Kling-Gupta Efficiency): Combines correlation, bias, and variability ratio

#### **Function Differences:**

- evaluate.SCA(): S3 method for single SCA trees (calls SCA\_Model\_evaluation)
- evaluate.SCE(): S3 method for SCE ensembles (calls SCE\_Model\_evaluation)
- SCA\_Model\_evaluation(): Direct function for SCA model evaluation
- SCE\_Model\_evaluation(): Direct function for SCE model evaluation

Input Validation: The functions perform comprehensive input validation:

- 1. Data frame structure validation
- 2. Presence of required components in Simulations list
- 3. Existence of predictants in both data and simulations
- 4. Matching row counts between data and simulations
- 5. Proper handling of NaN values and zero/negative values

#### **Data Processing:**

- 1. Removes NaN values from both observed and simulated data
- 2. Handles zero or negative values by replacing them with 0.0001
- 3. Calculates all six metrics for each predictant
- 4. Formats the results with specified number of decimal places

#### Value

For SCA models and SCA\_Model\_evaluation:

- If single predictant: Returns a data.frame with column "Testing"
- If multiple predictants: Returns a list of data.frames, one for each predictant

For SCE models and SCE\_Model\_evaluation:

 If single predictant: Returns a data.frame with columns "Training", "Validation", and "Testing"

#### importance

• If multiple predictants: Returns a list of data.frames, one for each predictant

Each data.frame contains the following metrics:

- MAE: Mean Absolute Error (mean(abs(obs sim)))
- RMSE: Root Mean Square Error (sqrt(mean((obs sim)^2)))
- NSE: Nash-Sutcliffe Efficiency (1 (sum((obs sim)^2) / sum((obs mean(obs))^2)))
- Log.NSE: NSE calculated on log-transformed values
- R2: R-squared calculated using linear regression
- kge: Kling-Gupta Efficiency  $(1 \operatorname{sqrt}((r-1)^2 + (\operatorname{alpha-1})^2 + (\operatorname{beta-1})^2))$

#### Author(s)

Kailong Li <lkl98509509@gmail.com>

## See Also

SCA, SCE

importance Variable Importance Analysis

## Description

Functions for calculating variable importance scores using Wilks' Lambda method. The package provides both generic S3 methods and direct function calls for importance analysis.

#### Usage

```
importance(object, ...)
## S3 method for class 'SCA'
importance(object, ...)
## S3 method for class 'SCE'
importance(object, OOB_weight = TRUE, ...)
Wilks_importance(model, OOB_weight = TRUE)
SCA_importance(model)
```

#### Arguments

object	An object for which importance scores should be calculated.
model	A trained model object:
	• For Wilks_importance: SCE model object (S3 class "SCE") containing a list of SCA trees
	• For SCA_importance: Single SCA tree object (S3 class "SCA")
OOB_weight	Logical indicating whether to use out-of-bag weighting for importance calcula- tion. Default is TRUE. Only used for SCE objects and Wilks_importance.
	Additional arguments passed to methods.

#### Details

#### **Importance Calculation Method:**

All functions use the Wilks' Lambda statistic to calculate variable importance:

- 1. Extract Wilks' Lambda values and split information from tree(s)
- 2. Replace negative Wilks' Lambda values with zero
- 3. Calculate raw importance for each split:
  - Importance = (left\_samples + right\_samples) / total\_samples \* (1 Wilks' Lambda)
- 4. Aggregate importance scores by predictor
- 5. Normalize importance scores to sum to 1

#### **Function Differences:**

- importance.SCA(): S3 method for single SCA trees
- importance.SCE(): S3 method for SCE ensembles (calls Wilks\_importance)
- Wilks\_importance(): Direct function for SCE ensembles with OOB weighting options
- SCA\_importance(): Direct function for single SCA trees

## **OOB** Weighting:

- If OOB\_weight = TRUE: Importance scores are weighted by each tree's OOB performance
- If OOB\_weight = FALSE: Importance scores are calculated using the median across trees

#### Value

A data.frame containing:

- Predictor: Names of the predictors
- Relative\_Importance: Normalized importance scores (sum to 1)

## Author(s)

Kailong Li <1k198509509@gmail.com>

## predict.SCA

#### References

Li, Kailong, Guohe Huang, and Brian Baetz. "Development of a Wilks feature importance method with improved variable rankings for supporting hydrological inference and modelling." Hydrology and Earth System Sciences 25.9 (2021): 4947-4966.

#### See Also

SCA, SCE

predict.SCA Model Prediction and Simulation

## Description

Functions for making predictions and performing simulations using trained SCA and SCE models. The package provides both S3 methods and direct function calls for various prediction scenarios.

#### Usage

## S3 method for class 'SCA'
predict(object, newdata, ...)
## S3 method for class 'SCE'
predict(object, newdata, ...)
Model\_simulation(model, Testing\_data)
SCA\_tree\_predict(model, Testing\_data)
SCE\_Prediction(X\_sample, model)

OOB\_validation(model)

#### Arguments

object	An object for which predictions should be made.
newdata	A data.frame or matrix containing new data for prediction. Must contain the same predictor variables as used in training.
model	A trained model object:
	• For Model_simulation: SCE model object (S3 class "SCE")
	<ul> <li>For SCA_tree_predict: SCA model object (S3 class "SCA")</li> </ul>
	<ul> <li>For SCE_Prediction: SCE model object (S3 class "SCE")</li> </ul>
	<ul> <li>For OOB_validation: SCE model object (S3 class "SCE")</li> </ul>
Testing_data	A data.frame or matrix comprising the data that will be used to test the model. Must contain all the predictors used in the model. Must not contain missing values.

X_sample	A data.frame or matrix containing the predictor variables for which predictions
	are to be made. Must contain all predictors used in model training.
	Additional arguments passed to methods.

## Details

## **Prediction Methods:**

- predict.SCA(): S3 method for single SCA trees (calls SCA\_tree\_predict)
- predict.SCE(): S3 method for SCE ensembles (calls Model\_simulation)
- Model\_simulation(): Comprehensive simulation for SCE models with training, validation, and testing predictions
- SCA\_tree\_predict(): Direct function for single SCA tree predictions
- SCE\_Prediction(): Direct function for SCE ensemble predictions
- OOB\_validation(): Internal function for calculating out-of-bag predictions

#### **Prediction Process:**

For SCA models:

- 1. Input validation (data types, missing values, predictor matching)
- 2. Data preparation (conversion to matrix format)
- 3. Tree traversal and prediction using leaf node mappings

#### For SCE models:

- 1. Input validation (data types, missing values, predictor matching)
- 2. Data preparation (conversion to matrix format)
- 3. Training predictions using all trees
- 4. Out-of-bag predictions using trees not trained on each sample
- 5. Testing predictions using all trees
- 6. Weighting predictions based on tree weights

#### **Out-of-Bag (OOB) Validation:**

- OOB predictions are made using only trees that did not use a particular observation during training
- Provides unbiased estimate of model performance
- Used internally by Model\_simulation for validation predictions

Input Validation: All functions perform comprehensive validation:

- 1. Data type and structure checks (data.frame or matrix)
- 2. Missing value checks
- 3. Predictor matching with training data
- 4. Numeric data validation

#### print.SCA

#### Value

## For S3 methods:

- predict.SCA(): A matrix of predicted values for the predictant variables
- predict.SCE(): A list containing Training, Validation, and Testing predictions

#### For direct functions:

- Model\_simulation(): A list containing three components:
  - Training: Predictions for the training dataset
  - Validation: Out-of-bag (OOB) predictions
  - Testing: Predictions for the testing dataset
- SCA\_tree\_predict(): A list containing predictions for the test data
- SCE\_Prediction(): A matrix containing ensemble predictions for each predictant
- OOB\_validation(): A data.frame containing OOB predictions for each predictant

#### Author(s)

Kailong Li <lkl98509509@gmail.com>

## References

Li, Kailong, Guohe Huang, and Brian Baetz. "Development of a Wilks feature importance method with improved variable rankings for supporting hydrological inference and modelling." Hydrology and Earth System Sciences 25.9 (2021): 4947-4966.

#### See Also

SCA, SCE

print.SCA

Print and Summary Methods for SCA and SCE Objects

#### Description

Methods for printing and summarizing SCA (Stepwise Cluster Analysis) and SCE (Stepwise Clustered Ensemble) objects.

### Usage

```
## S3 method for class 'SCA'
print(x, ...)
## S3 method for class 'SCA'
summary(object, ...)
## S3 method for class 'SCE'
print(x, ...)
## S3 method for class 'SCE'
summary(object, ...)
```

## Arguments

x,object	An SCA or SCE object returned by the SCA() or SCE() function.
	Additional arguments passed to methods.

#### Value

print.SCA and print.SCE return the object invisibly. summary.SCA returns a summary of the SCA model including tree statistics. summary.SCE returns a summary of the SCE model including ensemble statistics.

#### See Also

SCA, SCE

RFE\_SCE

**Recursive Feature Elimination for SCE Models** 

#### Description

This function implements Recursive Feature Elimination (RFE) to identify the most important predictors for SCE models. It iteratively removes the least important predictors based on Wilks' feature importance scores and evaluates model performance. The function supports both single and multiple predictants, with comprehensive input validation and performance tracking across iterations.

The package also provides a Plot\_RFE function for visualizing RFE results, showing validation and testing R2 values as a function of the number of predictors.

#### Usage

```
RFE_SCE(
   Training_data,
   Testing_data,
   Predictors,
```

10

```
Predictant,
 Nmin,
 Ntree,
 alpha = 0.05,
 resolution = 1000,
 step = 1,
 verbose = TRUE,
 parallel = TRUE
)
Plot_RFE(
  rfe_result,
 main = "Validation and Testing R2 vs Number of Predictors",
 col_validation = "blue",
  col_testing = "red",
  pch = 16,
  1wd = 2,
 cex = 1.2,
 legend_pos = "bottomleft",
  . . .
)
```

## Arguments

Training_data	A data frame containing the training data. Must include all specified predictors and predictants.
Testing_data	A data.frame containing the testing data. Must include all specified predictors and predictants.
Predictors	A character vector specifying the names of independent variables to be evaluated (e.g., c("Prcp", "SRad", "Tmax")). Must contain at least 2 elements.
Predictant	A character vector specifying the name(s) of dependent variable(s) (e.g., c("swvl3", "swvl4")). Must be non-empty.
Nmin	Integer specifying the minimal number of samples in a leaf node for cutting.
Ntree	Integer specifying the number of trees in the ensemble.
alpha	Numeric significance level for clustering, between 0 and 1. Default value is 0.05.
resolution	Numeric value specifying the resolution for splitting. Default value is 1000.
step	Integer specifying the number of predictors to remove at each iteration. Must be
	between 1 and (number of predictors - number of predictants). Default value is 1.
verbose	A logical value indicating whether to print progress information during RFE iterations. Default value is TRUE.
parallel	A logical value indicating whether to use parallel processing for SCE model construction. When TRUE, uses multiple CPU cores for faster computation. When FALSE, processes trees sequentially. Default value is TRUE.
Diot DEE Angun	

## **Plot\_RFE** Arguments:

rfe_result	The result object from RFE_SCE function containing summary and performances components.
main	Title for the plot. Default is "Validation and Testing R2 vs Number of Predictors".
col_validation	Color for validation line. Default is "blue".
col_testing	Color for testing line. Default is "red".
pch	Point character for markers. Default is 16 (filled circle).
lwd	Line width. Default is 2.
cex	Point size. Default is 1.2.
legend_pos	Position of legend. Default is "bottomleft".
	Additional arguments passed to plot function.

#### Details

RFE\_SCE Process: The RFE process involves the following steps:

- 1. Input validation:
  - Data frame structure validation
  - Predictor and predictant validation
  - Step size validation
- 2. Initialization:
  - Set up history tracking structures
  - Initialize current predictor set
- 3. Main RFE loop (continues while predictors > predictants + 2):
  - Train SCE model with current predictors
  - Generate predictions using Model\_simulation
  - Evaluate model using SCE\_Model\_evaluation
  - Store performance metrics and importance scores
  - Remove least important predictors based on Wilks' scores

The function handles:

- Single and multiple predictants
- Performance tracking across iterations
- Importance score calculation
- Step-wise predictor removal

**Plot\_RFE Function:** Creates a base R plot showing validation and testing R2 values as a function of the number of predictors during the RFE process. The function:

- Extracts R2 values from RFE results
- · Converts formatted strings to numeric values
- · Creates a line plot with points and lines
- · Includes a legend distinguishing validation and testing performance
- Supports customization of colors, line styles, and plot appearance
- Uses only base R graphics (no external dependencies)

## RFE\_SCE

#### Value

**RFE\_SCE:** A list containing:

- summary: Data.frame with columns:
  - n\_predictors: Number of predictors at each iteration
  - predictors: Comma-separated list of predictors used
- · performances: List of performance evaluations for each iteration
  - For single predictant: Direct performance data.frame
  - For multiple predictants: Named list of performance data.frames
- importance\_scores: List of Wilks' importance scores for each iteration

**Plot\_RFE:** Invisibly returns a list containing:

- n\_predictors: Vector of predictor counts
- validation\_r2: Vector of validation R2 values
- testing\_r2: Vector of testing R2 values

#### Author(s)

Kailong Li <lk198509509@gmail.com>

#### See Also

See the generic functions importance and evaluate for SCE objects. For visualization of RFE results, see Plot\_RFE.

#### Examples

```
#
    # This example is computationally intensive and may take a long time to run.
    # It is recommended to run this example on a machine with a high-performance CPU.
#
#
    ## Load SCE package and the supporting packages
#
#
    library(SCE)
#
    library(parallel)
#
#
   data(Streamflow_training_22var)
#
    data(Streamflow_testing_22var)
#
    # Define predictors and predictants
#
    Predictors <- c(</pre>
#
      "Precipitation", "Radiation", "Tmax", "Tmin", "VP",
#
      "Precipitation_2Mon", "Radiation_2Mon", "Tmax_2Mon", "Tmin_2Mon", "VP_2Mon",
#
      "PNA", "Nino3.4", "IPO", "PDO",
#
      "PNA_lag1", "Nino3.4_lag1", "IPO_lag1", "PDO_lag1",
"PNA_lag2", "Nino3.4_lag2", "IPO_lag2", "PDO_lag2"
#
#
#
    )
#
    Predictants <- c("Flow")</pre>
#
    # Perform RFE
#
```

```
set.seed(123)
#
    result <- RFE_SCE(</pre>
#
#
      Training_data = Streamflow_training_22var,
      Testing_data = Streamflow_testing_22var,
#
      Predictors = Predictors,
#
#
      Predictant = Predictants,
#
      Nmin = 5,
      Ntree = 48,
#
      alpha = 0.05,
#
      resolution = 1000,
#
      step = 3, # Number of predictors to remove at each iteration
#
      verbose = TRUE,
#
#
      parallel = TRUE
   )
#
#
#
   ## Access results
#
    summary <- result$summary</pre>
#
    performances <- result$performances</pre>
#
    importance_scores <- result$importance_scores</pre>
#
    ## Plot RFE results
#
#
   Plot_RFE(result)
#
    ## Customized plot
#
   Plot_RFE(result,
#
             main = "My RFE Results",
#
#
             col_validation = "darkblue",
             col_testing = "darkred",
#
#
             1wd = 3,
#
             cex = 1.5)
#
#
    ## Note: The RFE_SCE function internally uses S3 methods for SCE models
#
    ## including importance() and evaluate() for model analysis
#
#
```

SCE

Stepwise Clustered Ensemble (SCE) and Stepwise Cluster Analysis (SCA) Models

#### Description

This package provides two main modeling approaches:

**SCA (Stepwise Cluster Analysis):** A single tree model that recursively partitions the data space based on Wilks' Lambda statistic, creating a tree structure for prediction.

**SCE (Stepwise Clustered Ensemble):** An ensemble of SCA trees built using bootstrap samples and random feature selection, providing improved prediction accuracy and robustness.

Both functions include comprehensive input validation for data types, missing values, and sample size requirements, and support both single and multiple predictants.

14

## Usage

```
SCA(Training_data, X, Y, Nmin, alpha = 0.05, resolution = 1000, verbose = FALSE)
```

```
SCE(Training_data, X, Y, mfeature, Nmin, Ntree,
alpha = 0.05, resolution = 1000, verbose = FALSE, parallel = TRUE)
```

## Arguments

Training_data	A data.frame or matrix containing the training data. Must include all specified predictors and predictants. Must not contain missing values.
Х	A character vector specifying the names of independent variables (e.g., c("Prcp", "SRad", "Tmax")). Must be present in Training_data. All variables must be numeric.
Υ	A character vector specifying the name(s) of dependent variable(s) (e.g., c("swvl3","swvl4")). Must be present in Training_data. All variables must be numeric.
Nmin	Integer specifying the minimal number of samples in a leaf node for cutting. Must be a positive number and less than the sample size.
mfeature	An integer specifying how many features will be randomly selected for each tree. Recommended value is $round(0.5 * length(X))$ . Only used for SCE.
Ntree	An integer specifying how many trees (ensemble members) will be built. Rec- ommended values range from 50 to 500 depending on data complexity. Only used for SCE.
alpha	Numeric significance level for clustering, between 0 and 1. Default value is 0.05.
resolution	Numeric value specifying the resolution for splitting. Controls the granularity of the search for optimal split points. Default value is 1000.
verbose	A logical value indicating whether to print progress information during model building. Default value is FALSE.
parallel	A logical value indicating whether to use parallel processing for tree construc- tion. When TRUE, uses multiple CPU cores for faster computation. When FALSE, processes trees sequentially. Default value is TRUE. Only used for SCE.

## Details

## **Model Building Process:**

SCA (Single Tree):

- 1. Input validation (data types, missing values, sample size requirements)
- 2. Data preparation (conversion to matrix format, parameter initialization)
- 3. Tree construction (recursive partitioning based on Wilks' Lambda)

#### SCE (Ensemble):

- 1. Input validation (data types, missing values, sample size requirements)
- 2. Data preparation (conversion to matrix format, parameter initialization)

- 3. Tree construction (bootstrap samples, random feature selection, parallel SCA tree building)
- 4. Model evaluation (OOB error calculation, tree weighting)

#### **Key Differences:**

- SCA: Single tree, deterministic, faster training, potentially less robust
- SCE: Multiple trees, ensemble approach, improved accuracy, OOB validation, parallel processing

## When to Use:

- SCA: Quick exploration, simple relationships, limited computational resources
- SCE: Production models, complex relationships, when accuracy is critical

#### Value

For SCA: An S3 object of class "SCA" containing:

- Tree: The SCA tree structure
- Map: Mapping information for predictions
- XName: Names of predictors used
- YName: Names of predictants
- type: Mapping type (currently "mean")
- totalNodes: Total number of nodes in the tree
- leafNodes: Number of leaf nodes
- cuttingActions: Number of cutting actions performed
- mergingActions: Number of merging actions performed
- call: Function call

For SCE: An S3 object of class "SCE" containing the ensemble model with the following components:

- trees: A list of SCA tree models, each containing:
  - Tree: The SCA tree structure
  - Map: Mapping information
  - XName: Names of predictors used
  - YName: Names of predictants
  - type: Mapping type
  - totalNodes: Total number of nodes
  - leafNodes: Number of leaf nodes
  - cuttingActions: Number of cutting actions
  - mergingActions: Number of merging actions
  - 00B\_error: Out-of-bag R-squared error
  - 00B\_sim: Out-of-bag predictions
  - Sample: Bootstrap sample indices

- Tree\_Info: Tree-specific information
- Training\_data: Training data used for the tree
- weight: Tree weight based on OOB performance
- predictors: Names of predictor variables
- predictants: Names of predictant variables
- parameters: Model parameters
- call: Function call

Both objects support S3 methods: print(), summary(), predict(), importance(), and evaluate().

#### Author(s)

Xiuquan Wang <xxwang@upei.ca> (original SCA) Kailong Li <lkl98509509@gmail.com> (Resolution-search-based SCA and SCE ensemble)

#### References

Li, Kailong, Guohe Huang, and Brian Baetz. Development of a Wilks feature importance method with improved variable rankings for supporting hydrological inference and modelling. Hydrology and Earth System Sciences 25.9 (2021): 4947-4966.

Wang, X., G. Huang, Q. Lin, X. Nie, G. Cheng, Y. Fan, Z. Li, Y. Yao, and M. Suo (2013), A stepwise cluster analysis approach for downscaled climate projection - A Canadian case study. Environmental Modelling & Software, 49, 141-151.

Huang, G. (1992). A stepwise cluster analysis method for predicting air quality in an urban environment. Atmospheric Environment (Part B. Urban Atmosphere), 26(3): 349-357.

Liu, Y. Y. and Y. L. Wang (1979). Application of stepwise cluster analysis in medical research. Scientia Sinica, 22(9): 1082-1094.

#### See Also

predict, importance, evaluate for S3 methods, RFE\_SCE for recursive feature elimination

#### Examples

```
## Load SCE package
library(SCE)
```

## Load training and testing data
data("Streamflow\_training\_10var")
data("Streamflow\_testing\_10var")

```
## Define independent (x) and dependent (y) variables
Predictors <- c("Prcp","SRad","Tmax","Tmin","VP","smlt","swvl1","swvl2","swvl3","swvl4")
Predictants <- c("Flow")</pre>
```

```
## Example 1: Build SCA model (single tree)
sca_model <- SCA(
Training_data = Streamflow_training_10var,</pre>
```

```
X = Predictors,
Y = Predictants,
Nmin = 5,
alpha = 0.05,
resolution = 1000
)
## Use S3 methods for SCA model inspection
print(sca_model)
summary(sca_model)
## Make predictions using S3 method
sca_predictions <- predict(sca_model, Streamflow_testing_10var)</pre>
## Calculate variable importance using S3 method
sca_importance <- importance(sca_model)</pre>
## Evaluate SCA model performance using S3 method
sca_evaluation <- evaluate(</pre>
object = sca_model,
Testing_data = Streamflow_testing_10var,
Predictant = Predictants
)
## Example 2: Build SCE model (ensemble)
sce_model <- SCE(</pre>
Training_data = Streamflow_training_10var,
X = Predictors,
Y = Predictants,
mfeature = round(0.5 * length(Predictors)),
Nmin = 5,
Ntree = 48,
alpha = 0.05,
resolution = 1000,
parallel = FALSE
)
## Use S3 methods for SCE model inspection
print(sce_model)
summary(sce_model)
## Generate predictions using S3 method
sce_predictions <- predict(sce_model, Streamflow_testing_10var)</pre>
## Access different prediction components
training_predictions <- sce_predictions$Training</pre>
validation_predictions <- sce_predictions$Validation</pre>
testing_predictions <- sce_predictions$Testing</pre>
## Calculate variable importance using S3 method
sce_importance <- importance(sce_model)</pre>
## Evaluate SCE model performance using S3 method
```

18

#### Streamflow\_training\_10var

```
sce_evaluation <- evaluate(
object = sce_model,
Testing_data = Streamflow_testing_10var,
Training_data = Streamflow_training_10var,
Predictant = Predictants
)</pre>
```

Streamflow\_training\_10var

Streamflow Datasets

#### Description

These datasets contain streamflow and related environmental variables for training and testing purposes. They are used in examples to demonstrate the SCE package functionality with different levels of complexity.

#### Usage

```
data("Streamflow_training_10var")
data("Streamflow_training_22var")
data("Streamflow_testing_10var")
data("Streamflow_testing_22var")
```

#### Format

Streamflow\_training\_10var: A data frame with basic environmental variables:

Date The date and time of the data point

- Prcp The monthly mean daily precipitation measured in millimeters (mm), derived from the Daymet dataset
- **SRad** The monthly mean daily short-wave solar radiation measured in Watts per square meter (W/m^2), sourced from the Daymet dataset
- **Tmax** The monthly mean daily maximal temperature recorded in degrees Celsius, taken from the Daymet dataset
- Tmin The monthly mean daily minimal temperature recorded in degrees Celsius, also derived from the Daymet dataset
- **VP** The monthly mean daily vapor pressure measured in Pascals (Pa), obtained from the Daymet dataset
- smlt The sum of monthly snowmelt measurements in meters (m), taken from the ERA5 land dataset
- **swvl1** The volumetric soil water content in layer 1 measured in cubic meters per cubic meter (m^3/m^3), sourced from the ERA5 land dataset
- swvl2 The volumetric soil water content in layer 2, measured similarly to swvl1, sourced from the ERA5 land dataset

- **swvl3** The volumetric soil water content in layer 3, measured similarly to swvl1, sourced from the ERA5 land dataset
- swvl4 The volumetric soil water content in layer 4, measured similarly to swvl1, sourced from the ERA5 land dataset
- **Flow** The monthly mean daily streamflow rate measured in cubic feet per second (cfs), provided by the United States Geological Survey (USGS)

Streamflow\_training\_22var: A data frame with extended variables including climate indices:

Flow Streamflow measurements

IPO Interdecadal Pacific Oscillation

**IPO\_lag1** IPO with 1-month lag

**IPO\_lag2** IPO with 2-month lag

Nino3.4 Nino 3.4 index

Nino3.4\_lag1 Nino 3.4 with 1-month lag

Nino3.4\_lag2 Nino 3.4 with 2-month lag

PDO Pacific Decadal Oscillation

PDO\_lag1 PDO with 1-month lag

PDO\_lag2 PDO with 2-month lag

**PNA** Pacific North American pattern

**PNA\_lag1** PNA with 1-month lag

**PNA\_lag2** PNA with 2-month lag

Precipitation Monthly precipitation

Precipitation\_2Mon 2-month precipitation

Radiation Solar radiation

Radiation\_2Mon 2-month solar radiation

Tmax Maximum temperature

Tmax\_2Mon 2-month maximum temperature

Tmin Minimum temperature

Tmin\_2Mon 2-month minimum temperature

**VP** Vapor pressure

VP\_2Mon 2-month vapor pressure

**Streamflow\_testing\_10var:** A data frame with basic environmental variables (same structure as training):

Flow Streamflow measurements

Prcp Precipitation

SRad Solar radiation

Tmax Maximum temperature

Tmin Minimum temperature

VP Vapor pressure
X Index variable
smlt Snow melt
swvl1 Soil water volume layer 1
swvl2 Soil water volume layer 2
swvl3 Soil water volume layer 3
swvl4 Soil water volume layer 4

**Streamflow\_testing\_22var:** A data frame with extended variables including climate indices (same structure as training):

Flow Streamflow measurements

- IPO Interdecadal Pacific Oscillation
- IPO\_lag1 IPO with 1-month lag

IPO\_lag2 IPO with 2-month lag

Nino3.4 Nino 3.4 index

Nino3.4\_lag1 Nino 3.4 with 1-month lag

Nino3.4\_lag2 Nino 3.4 with 2-month lag

PDO Pacific Decadal Oscillation

PDO\_lag1 PDO with 1-month lag

**PDO\_lag2** PDO with 2-month lag

PNA Pacific North American pattern

PNA\_lag1 PNA with 1-month lag

PNA\_lag2 PNA with 2-month lag

Precipitation Monthly precipitation

Precipitation\_2Mon 2-month precipitation

Radiation Solar radiation

Radiation\_2Mon 2-month solar radiation

Tmax Maximum temperature

Tmax\_2Mon 2-month maximum temperature

Tmin Minimum temperature

Tmin\_2Mon 2-month minimum temperature

**VP** Vapor pressure

VP\_2Mon 2-month vapor pressure

#### Details

#### **Dataset Categories:**

- Training Datasets: Used for building SCA and SCE models
  - Streamflow\_training\_10var: Basic dataset with 12 variables, suitable for introductory examples
  - Streamflow\_training\_22var: Extended dataset with 24 variables, includes climate indices and lagged values
- Testing Datasets: Used for evaluating trained models
  - Streamflow\_testing\_10var: Basic dataset with 12 variables, matches training structure
  - Streamflow\_testing\_22var: Extended dataset with 24 variables, matches training structure

## Variable Categories:

- Hydrological: Flow, Precipitation, Snow melt, Soil water volumes
- Meteorological: Temperature (max/min), Solar radiation, Vapor pressure
- Climate Indices: IPO, Nino3.4, PDO, PNA (with lagged versions)
- Time Aggregations: 2-month averages for key variables

#### **Climate Indices:**

- IPO: Interdecadal Pacific Oscillation long-term climate pattern
- Nino3.4: El Niño-Southern Oscillation index
- PDO: Pacific Decadal Oscillation long-term ocean temperature pattern
- PNA: Pacific North American pattern atmospheric circulation pattern

Data Sources: The data is compiled from various recognized sources including:

- ERA5 Land: A global land-surface dataset at 9km resolution, available from the Copernicus Climate Change Service
- Daymet Version 4: Daily Surface Weather and Climatological Summaries
- United States Geological Survey (USGS): A scientific agency of the United States government that studies natural resources, natural hazards, and the landscape of the United States
- Climate indices databases for the extended datasets

#### Source

Environmental monitoring stations, climate indices databases, ERA5 Land, Daymet, and USGS

22

# Index

Air\_quality\_testing (Air\_quality\_training), 2 Air\_quality\_training, 2

evaluate, 3, 17

importance, 5, 17

Model\_simulation (predict.SCA), 7

OOB\_validation (predict.SCA), 7

Plot\_RFE (RFE\_SCE), 10
predict. I7
predict.SCA, 7
predict.SCE (predict.SCA), 7
print.SCA, 9
print.SCE (print.SCA), 9

RFE\_SCE, 10, 17

```
SCA, 5, 7, 9, 10
SCA (SCE), 14
SCA_importance (importance), 5
SCA_Model_evaluation (evaluate), 3
SCA_tree_predict (predict.SCA), 7
SCE, 5, 7, 9, 10, 14
SCE_Model_evaluation (evaluate), 3
SCE_Prediction (predict.SCA), 7
Streamflow_testing_10var
        (Streamflow_training_10var), 19
Streamflow_testing_22var
        (Streamflow_training_10var), 19
Streamflow_training_10var, 19
Streamflow_training_22var
        (Streamflow_training_10var), 19
summary.SCA(print.SCA),9
summary.SCE (print.SCA), 9
```

Wilks\_importance (importance), 5