

Package: ClustAll (via r-universe)

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Type Package

Title ClustAll: Data driven strategy to find groups of patients within complex diseases

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Description Data driven strategy to find hidden groups of patients with complex diseases using clinical data. ClustAll facilitates the unsupervised identification of multiple robust stratifications. ClustAll, is able to overcome the most common limitations found when dealing with clinical data (missing values, correlated data, mixed data types).

Depends R (>= 4.2.0)

License GPL-2

Encoding UTF-8

biocViews Software, StatisticalMethod, Clustering, DimensionReduction, PrincipalComponent

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VignetteBuilder knitr

git_url <https://github.com/TranslationalBioinformaticsUnit/ClustAll>

Repository <https://bioc.r-universe.dev>

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| | |
|-------------------|--|
| addValidationData | <i>Add the validation data into the ClustAllObject</i> |
|-------------------|--|

Description

Generic function to add validation data to the [ClustAllObject-class](#) object

Usage

```
addValidationData(Object, dataValidation)
```

Arguments

Object [ClustAllObject-class](#) object
 dataValidation numericOrCharacter

Details

addValidationData

Value

[ClustAllObject-class](#) object

See Also

[ClustAllObject-class](#)

Examples

```
data("BreastCancerWisconsin", package = "ClustAll")
label <- as.numeric(as.factor(wdbc$Diagnosis))
wdbc <- wdbc[,-c(1, 2)] # delete patients IDs & label
obj_noNA <- createClustAll(data = wdbc)
obj_noNA <- addValidationData(Object = obj_noNA,
                             dataValidation = label)
```

characterOrNA

characterOrNA Class union of character, null or missing

Description

Contains either character, NULL or missing object

Value

characterOrNA class object

| | |
|----------------------|-----------------------|
| ClustAllObject-class | <i>ClustAllObject</i> |
|----------------------|-----------------------|

Description

Stores the original data used, the imputed datasets and the results of the ClustAll pipeline.

Value

ClustAllObject class object

Slots

data Data Frame of the data used. Maybe modified from the input data.
dataOriginal Data Frame of the original data introduced.
dataImputed Mids object derived from the mice package that stores the imputed data, in case imputation was applied. Otherwise NULL.
dataValidation labelling numericOrNA. Original data labelling.
nImputation Number of multiple imputations to be applied.
processed Logical if the ClustAll pipeline has been executed previously
summary_clusters listOrNULL. List with the resulting stratifications for each combination of clustering methods (distance + clustering algorithm) and depth, in case ClustAll pipeline has been executed previously. Otherwise NULL.
JACCARD_DISTANCE_F matrixOrNULL. Matrix containing the Jaccard distances derived from the robust populations stratifications if ClustAll pipeline has been executed previously. Otherwise NULL.

| | |
|--------------|---------------------|
| cluster2data | <i>cluster2data</i> |
|--------------|---------------------|

Description

Returns the original data in a dataframe, including the selected robust stratification(s) as variables. The representative stratification names can be obtained using the method. [resStratification](#)

Usage

```
cluster2data(Object,
              stratificationName)
```

Arguments

| | |
|--------------------|--|
| Object | ClustAllObject-class object |
| stratificationName | Character vector with one or more stratification names |

Value

data.frame

See Also[resStratification](#), [plotJACCARD](#), [ClustAllObject-class](#)**Examples**

```
data("BreastCancerWisconsin", package = "ClustAll")
wdbc <- subset(wdbc, select=c(-ID, -Diagnosis))
wdbc <- wdbc[1:15, 1:8]
obj_noNA <- createClustAll(data = wdbc)

obj_noNA1 <- runClustAll(Object = obj_noNA, threads = 1, simplify = TRUE)
resStratification(Object = obj_noNA1, population = 0.05,
                  stratification_similarity = 0.88, all = FALSE)
df <- cluster2data(Object = obj_noNA1,
                  stratificationName = c("cuts_a_1", "cuts_b_5", "cuts_a_5"))
```

| | |
|----------------|---|
| createClustAll | <i>Creates ClustAllObject and perform imputations to deal with missing values</i> |
|----------------|---|

Description

This pipeline creates the `ClustAllObject` and computes the imputations if the dataset contains missing values. The next step would be [runClustAll](#)

Usage

```
createClustAll(data=data,
               nImputation=NULL,
               dataImputed=NULL,
               colValidation=NULL)
```

Arguments

| | |
|---------------|--|
| data | Data Frame of the using data. It may contain missing (NA) values. |
| nImputation | Numeric value with the number of imputations to be computed in case the data contains NAs. |
| dataImputed | mids object created with mice package. The introduced data for the imputation and the data using must be the same. |
| colValidation | Character value with the original labelling of the input data. |

Value

An object of class `ClustAllObject-class`

See Also

`runClustAll`, `ClustAllObject-class`

Examples

```
# Scenario 1: data does not contain missing values
data("BreastCancerWisconsin", package = "ClustAll")
wdbc <- wdbc[, -c(1,2)]
obj_noNA <- createClustAll(data = wdbc)

# Scenario 2: data contains NAs and imputed data is provided automatically
data("BreastCancerWisconsinMISSING", package = "ClustAll") # load example data
obj_NA <- createClustAll(wdbcNA, nImputation = 5)

# Scenario 3: data contains NAs and imputed data is provided manually
data("BreastCancerWisconsinMISSING", package = "ClustAll") # load the example data
ini <- mice::mice(wdbcNA, maxit = 0, print = FALSE)
pred <- ini$pred # predictor matrix
pred["radius1", c("perimeter1", "area1", "smoothness1")] <- 0 # example of how to remove predictors
imp <- mice::mice(wdbcNA, m=5, pred=pred, maxit=5, seed=1234, print=FALSE)
obj_imp <- createClustAll(data=wdbcNA, dataImputed = imp)
```

dataImputed

Retrieve the imputed data from ClustAllObject

Description

Generic function to retrieve the imputed data obtained in `createClustAll` from a `ClustAllObject-class` object

Usage

```
dataImputed(Object)
```

Arguments

Object `ClustAllObject-class` object

Value

Mids class object with the imputed data or NULL if imputation was not required

See Also

`createClustAll`, `ClustAllObject-class`, `runClustAll`

Examples

```
data("BreastCancerWisconsinMISSING", package = "ClustAll")
data("BreastCancerWisconsin", package = "ClustAll")
wdbc <- subset(wdbc,select=-ID)
obj_NA <- createClustAll(data = wdbcNA, colValidation = "Diagnosis",
                        dataImputed = wdbcMIDS)
dataImputed(obj_NA)
```

| | |
|--------------|--|
| dataOriginal | <i>Retrieve the initial dataOriginal from ClustAllObject</i> |
|--------------|--|

Description

Generic function to retrieve the initial data used for [createClustAll](#) from a [ClustAllObject-class](#) object

Usage

```
dataOriginal(Object)
```

Arguments

Object [ClustAllObject-class](#) object

Value

The Data Frame with the initial data

See Also

[createClustAll](#), [ClustAllObject-class](#), [runClustAll](#)

Examples

```
data("BreastCancerWisconsin", package = "ClustAll")
wdbc <- subset(wdbc,select=-ID)
obj_noNA <- createClustAll(data = wdbc, colValidation = "Diagnosis")
dataOriginal(obj_noNA)
```

| | |
|----------------|--|
| dataValidation | Retrieve the original data labelling from ClustAllObject |
|----------------|--|

Description

Generic function to retrieve numeric vector if it has been added with the true labels from a [ClustAllObject-class](#) object

Usage

dataValidation(Object)

Arguments

Object [ClustAllObject-class](#) object

Value

numeric vector if true labels have been added. Otherwise NULL

See Also

[ClustAllObject-class](#)

Examples

```
data("BreastCancerWisconsin", package = "ClustAll")
wdbc <- subset(wdbc,select=-ID)
obj_noNA <- createClustAll(data = wdbc, colValidation="Diagnosis")
dataValidation(obj_noNA)
```

| |
|----------------------------------|
| initialize,ClustAllObject-method |
| <i>initializeClustAllObject</i> |

Description

constuctor for [ClustAllObject-class](#)

Usage

```
## S4 method for signature 'ClustAllObject'
initialize(
  .Object,
  data,
  dataOriginal,
  dataImputed,
  dataValidation,
  nImputation,
  processed,
  summary_clusters,
  JACCARD_DISTANCE_F
)
```

Arguments

| | |
|---------------------------------|---|
| <code>.Object</code> | initializing object |
| <code>data</code> | Data Frame of the data used. Maybe modified from the input data. |
| <code>dataOriginal</code> | Data Frame of the original data introduced. |
| <code>dataImputed</code> | Mids object derived from the mice package that stores the imputed data, in case imputation was applied. Otherwise NULL. |
| <code>dataValidation</code> | labelling numericOrNA. Original data labelling. |
| <code>nImputation</code> | Number of multiple imputations to be applied. |
| <code>processed</code> | Logical if the ClustAll pipeline has been executed previously |
| <code>summary_clusters</code> | listOrNULL. List with the resulting stratifications for each combination of clustering methods (distance + clustering algorithm) and depth, in case ClustAll pipeline has been executed previously. Otherwise NULL. |
| <code>JACCARD_DISTANCE_F</code> | matrixOrNULL. Matrix containing the Jaccard distances derived from the robust populations stratifications if ClustAll pipeline has been executed previously. Otherwise NULL. |

Value

An object of class `ClustAllObject-class`

| | |
|---------------------------------|---|
| <code>JACCARD_DISTANCE_F</code> | <i>Retrieve the matrix with the Jaccard distances derived from the robust populations stratifications in ClustAllObject</i> |
|---------------------------------|---|

Description

Generic function to retrieve the matrix with the Jaccard distances derived from the robust populations stratifications in `runClustAll` from a `ClustAllObject-class` object

Usage

JACCARD_DISTANCE_F(Object)

Arguments

Object [ClustAllObject-class](#) object

Value

Matrix containing the Jaccard distances derived from the robust populations stratifications or NULL if runClustAll method has not been executed yet

See Also

[runClustAll](#), [ClustAllObject-class](#)

Examples

```
data("BreastCancerWisconsin", package = "ClustAll")
wdbc <- subset(wdbc,select=c(-ID, -Diagnosis))
wdbc <- wdbc[1:15,1:8]
obj_noNA <- createClustAll(data = wdbc)
obj_noNA1 <- runClustAll(Object = obj_noNA, threads = 1, simplify = FALSE)
JACCARD_DISTANCE_F(obj_noNA1)
```

| | |
|------------|-------------------------------|
| listOrNULL | <i>Class Union listOrNULL</i> |
|------------|-------------------------------|

Description

Contains either list, NULL or missing object

Details

Class union of list, null or missing

Value

listOrNULL class object

| | |
|-------------|--------------------|
| logicalOrNA | <i>logicalOrNA</i> |
|-------------|--------------------|

Description

Contains either logical, NULL or missing object

Details

Class union of logical, null or missing

Value

logicalOrNA class object

| | |
|--------------|---------------------|
| matrixOrNULL | <i>matrixOrNULL</i> |
|--------------|---------------------|

Description

Contains either matrix or NULL object

Details

Class union of matrix, null or missing

Value

matrixOrNULL class object

| | |
|-------------|--|
| nImputation | <i>Retrieve the number of imputations applied at the imputation step from ClustAllObject</i> |
|-------------|--|

Description

Generic function to retrieve the number of imputations in [createClustAll](#) from a [ClustAllObject-class](#) object

Usage

nImputation(Object)

Arguments

Object [ClustAllObject-class](#) object

Value

Numeric vector that contains the number of imputations. 0 in the case of no imputations were required

See Also

[createClustAll](#), [ClustAllObject-class](#), [runClustAll](#)

Examples

```
data("BreastCancerWisconsinMISSING", package = "ClustAll")
data("BreastCancerWisconsin", package = "ClustAll")
wdbc <- subset(wdbc, select=-ID)
obj_NA <- createClustAll(data = wdbcNA, colValidation = "Diagnosis",
                        dataImputed = wdbcMIDS)
nImputation(obj_NA)
```

numericOrCharacter *numericOrCharacter*

Description

Contains either numeric or character object

Details

Class union of numeric or character

Value

numericOrCharacter class object

| | |
|-------------|--------------------------------|
| numericOrNA | <i>Class Union numericOrNA</i> |
|-------------|--------------------------------|

Description

Contains either numeric, NULL or missing object

Details

Class union of numeric, null or missing

Value

numericOrNA class object

| | |
|-----------|---|
| obj_noNA1 | <i>obj_noNA1: Processed wdbc dataset for testing purposed</i> |
|-----------|---|

Description

Processed wdbc as appear in vignette

Usage

```
data("testData", package = "ClustAll")
```

Format

A processed ClustAllObject

Value

ClustAllObject Object

| | |
|-------------------|---|
| obj_noNA1simplify | <i>obj_noNA1simplify: Processed wdbc dataset for testing purposed</i> |
|-------------------|---|

Description

Processed wdbc as appear in vignette, with simplify TRUE parameter

Usage

```
data("testData", package = "ClustAll")
```

Format

A processed ClustAllObject

Value

ClustAllObject Object

| | |
|---------------------|---|
| obj_noNA1Validation | <i>obj_noNA1Validation: Processed wdbc dataset for testing purposed</i> |
|---------------------|---|

Description

Processed wdbc as appear in vignette, with no validation data

Usage

```
data("testData", package = "ClustAll")
```

Format

A processed ClustAllObject

Value

ClustAllObject Object

| | |
|-------------|---|
| plotJACCARD | <i>Correlation matrix heatmap showing the Jaccard distance between robust stratifications in the ClustAllObject</i> |
|-------------|---|

Description

This function plots the correlation matrix heatmap showing the Jaccard Distance between robust stratifications

Usage

```
plotJACCARD(Object,
             paint=TRUE,
             stratification_similarity=0.7)
```

Arguments

| | |
|---------------------------|---|
| Object | ClustAllObject-class object |
| paint | Logical vector with the annotation for the different stratifications |
| stratification_similarity | The minimum Jaccard Distance value to consider two stratifications similar. Default is 0.7. |

Value

plot

See Also

[resStratification](#), [cluster2data](#), [ClustAllObject-class](#)

Examples

```
data("BreastCancerWisconsin", package = "ClustAll")
wdbc <- subset(wdbc, select=c(-ID, -Diagnosis))
wdbc <- wdbc[1:15, 1:8]
obj_noNA <- createClustAll(data = wdbc)

obj_noNA1 <- runClustAll(Object = obj_noNA, threads = 1, simplify = TRUE)
plotJACCARD(obj_noNA1, paint = TRUE, stratification_similarity = 0.9)
```

| | |
|------------|---|
| plotSANKEY | <i>Plots Sankey Diagram showing the cluster distribution and shifts between a pair of stratifications derived from ClustAllObject</i> |
|------------|---|

Description

This function plots the Sankey Diagram with the cluster distribution and shifts between a pair of stratifications

Usage

```
plotSANKEY(Object,
            clusters,
            validationData=FALSE)
```

Arguments

| | |
|----------------|--|
| Object | ClustAllObject-class object |
| clusters | Character vector with the names of a pair of stratifications. Check <code>resStratification</code> to obtain the stratification names. |
| validationData | Logical value to use original labelling data to compare with the ClustALL selected stratification. |

Value

plot

See Also

[resStratification](#), [cluster2data](#), [ClustAllObject-class](#)

Examples

```
data("BreastCancerWisconsin", package = "ClustAll")
label <- as.numeric(as.factor(wdbc$Diagnosis))
wdbc <- subset(wdbc, select=c(-ID, -Diagnosis))
wdbc <- wdbc[1:15, 1:8]
label <- label[16:30]
obj_noNA <- createClustAll(data = wdbc)

obj_noNA1 <- runClustAll(Object = obj_noNA, threads = 1, simplify = TRUE)
resStratification(Object = obj_noNA1, population = 0.05,
                  stratification_similarity = 0.88, all = FALSE)
plotSANKEY(Object = obj_noNA1, clusters = c("cuts_a_1", "cuts_b_5"))

obj_noNA1 <- addValidationData(obj_noNA1, label)
plotSANKEY(Object = obj_noNA1, clusters = "cuts_a_1", validationData=TRUE)
```

| | |
|-----------|--|
| processed | <i>Retrieve logical if runClustAll has been executed considering ClustAllObject as input</i> |
|-----------|--|

Description

Generic function to retrieve the logical if `runClustAll` have been runned from a `ClustAllObject-class` object

Usage

```
processed(Object)
```

Arguments

Object `ClustAllObject-class` object

Value

TRUE if runClustAll has been already executed. Otherwise FALSE

See Also

`runClustAll`, `ClustAllObject-class`

Examples

```
data("BreastCancerWisconsin", package = "ClustAll")
wdbc <- subset(wdbc, select=c(-ID, -Diagnosis))
wdbc <- wdbc[1:15, 1:8]
obj_noNA <- createClustAll(data = wdbc)
processed(obj_noNA)
```

| | |
|-------------------|--|
| resStratification | <i>Show the stratification representatives from the ClustAllObject</i> |
|-------------------|--|

Description

This function returns the stratifications representatives by keeping those clusters with a minimum percentage of the population. Default is 0.05. It returns all the robust stratification (TRUE) or the representative for each group of stratifications (FALSE). Default is FALSE

Usage

```
resStratification(Object,
                   population=0.05,
                   all=FALSE,
                   stratification_similarity=0.7)
```

Arguments

| | |
|---------------------------|---|
| Object | ClustAllObject-class object |
| population | Numeric vector with the minimum percentage of the total population that a stratification must have to be considered as representative |
| all | Logical vector to return all the representative stratifications per group of clusters. If it is FALSE, only the centroid stratification of each group of clusters is returned |
| stratification_similarity | The minimum Jaccard distance value to consider two groups similar. Default is 0.7 |

Value

list

See Also

[plotJACCARD](#), [cluster2data](#), [ClustAllObject-class](#)

Examples

```
data("BreastCancerWisconsin", package = "ClustAll")
wdbc <- subset(wdbc, select=c(-ID, -Diagnosis))
wdbc <- wdbc[1:15, 1:8]
obj_noNA <- createClustAll(data = wdbc)

obj_noNA1 <- runClustAll(Object = obj_noNA, threads = 1, simplify = TRUE)
resStratification(Object = obj_noNA1, population = 0.05,
  stratification_similarity = 0.88, all = FALSE)
```

runClustAll

ClustAll: Data driven strategy to find hidden subgroups of patients within complex diseases using clinical data

Description

This method runs the ClustAll pipeline

Usage

```
runClustAll(Object,
  threads=1,
  simplify=FALSE)
```

Arguments

| | |
|----------|---|
| Object | ClustAllObject-class object |
| threads | Numeric vector that indicates the number of cores to use |
| simplify | if TRUE computes one out of four depths of the dendrogram |

Value

An object of class [ClustAllObject-class](#)

See Also

[resStratification](#), [plotJACCARD](#), [cluster2data](#), [ClustAllObject-class](#)

Examples

```
data("BreastCancerWisconsin", package = "ClustAll")
wdbc <- subset(wdbc, select=c(-ID, -Diagnosis))
wdbc <- wdbc[1:15, 1:8]

obj_noNA <- createClustAll(data = wdbc)
obj_noNA1 <- runClustAll(Object = obj_noNA, threads = 1, simplify = TRUE)
```

show,ClustAllObject-method

show method for ClustAllObject

Description

Show method for a [ClustAllObject-class](#) object

Usage

```
## S4 method for signature 'ClustAllObject'
show(object)
```

Arguments

| | |
|--------|---|
| object | ClustAllObject-class object |
|--------|---|

Value

summarize information about the object

| | |
|----------|--|
| showData | <i>Retrieve the initial data from ClustAllObject</i> |
|----------|--|

Description

Generic function to retrieve the initial data used for `createClustAll` from a `ClustAllObject-class` object

Usage

`showData(Object)`

Arguments

Object `ClustAllObject-class` object

Value

The Data Frame with the initial data

See Also

`createClustAll`, `ClustAllObject-class`, `runClustAll`

Examples

```
data("BreastCancerWisconsin", package = "ClustAll")
wdbc <- subset(wdbc,select=-ID)
obj_noNA <- createClustAll(data = wdbc, colValidation = "Diagnosis")
showData(obj_noNA)
```

| | |
|------------------|--|
| summary_clusters | <i>Retrieve the resulting stratifications for each combination of clusterings method (distance + clustering algorithm) and depth from ClustAllObject</i> |
|------------------|--|

Description

Generic function to retrieve the resulting stratifications for each combination of clusterings method (distance + clustering algorithm) and depth of `runClustAll` from a `ClustAllObject-class` object

Usage

`summary_clusters(Object)`

Arguments

Object [ClustAllObject-class](#) object

Value

List with the resulting stratifications for each combination of clusterings method (distance + clustering algorithm) and depth methods or NULL if runClustAll method has not been executed yet.

See Also

[runClustAll](#), [ClustAllObject-class](#)

Examples

```
data("BreastCancerWisconsin", package = "ClustAll")
wdbc <- subset(wdbc, select=c(-ID, -Diagnosis))
wdbc <- wdbc[1:15, 1:8]
obj_noNA <- createClustAll(data = wdbc)
obj_noNA1 <- runClustAll(Object = obj_noNA, threads = 1, simplify = FALSE)
summary_clusters(obj_noNA1)
```

validateStratification

validateStratification

Description

Returns the sensitivity and specificity of the selected stratification the original labelling. The representative stratification names can be obtained using the method [resStratification](#)

Usage

```
validateStratification(Object,
                       stratificationName)
```

Arguments

Object [ClustAllObject-class](#) object

stratificationName

Character vector with the name a stratification. Check resStratification to obtain stratification names.

Value

numeric

See Also

[resStratification](#), [plotJACCARD](#), [ClustAllObject-class](#)

Examples

```
data("BreastCancerWisconsin", package = "ClustAll")
label <- as.numeric(as.factor(wdbc$Diagnosis))
wdbc <- subset(wdbc, select=c(-ID, -Diagnosis))
wdbc <- wdbc[1:15, 1:8]
label <- label[16:30]
obj_noNA <- createClustAll(data = wdbc)

obj_noNA1 <- runClustAll(Object = obj_noNA, threads = 1, simplify = TRUE)
resStratification(Object = obj_noNA1, population = 0.05,
  stratification_similarity = 0.88, all = FALSE)
obj_noNA1 <- addValidationData(Object = obj_noNA1,
  dataValidation = label)
validateStratification(obj_noNA1, "cuts_a_1")
```

wdbc

wdbc: Diagnostic Wisconsin Breast Cancer Database.

Description

A dataset containing Features are computed from a digitized image of a fine needle aspirate (FNA) of a breast mass. They describe characteristics of the cell nuclei present in the image.

Usage

```
data("BreastCancerWisconsin", package = "ClustAll")
```

Format

A data frame with 660 rows and 31 variables

Details

The dataset comprises two types of features —categorical and numerical— derived from a digitized image of a fine needle aspirate (FNA) of a breast mass from 659 patients. Each patient is characterized by 31 features (10x3) and belongs to one of two target classes: ‘malignant’ or ‘benign’.

Value

wdbc dataset

Source

<<https://archive.ics.uci.edu/dataset/17/breast+cancer+wisconsin+diagnostic>>

- Diagnosis Label says tumor is malignant or benignant
- radius. Mean of distances from the center to points on the perimeter
- perimeter
- area
- smoothness. Local variation in radius lengths
- compactness. $(\text{Perimeter}^2 / \text{Area}) - 1.0$
- concavity. Severity of concave portions of the contour
- concave points. Number of concave portions of the contour
- symmetry.
- fractal dimension. "Coastline approximation" - 1.

wdbcMIDS

wdbcMIDS: Diagnostic Wisconsin Breast Cancer Database with imputed values

Description

We introduced imputed random values to the wdbcNA dataset. Using Mice. It is a mids object.
[wdbc](#)

Usage

```
data("BreastCancerWisconsinMISSING", package = "ClustAll")
```

Format

A data frame with 660 rows and 31 variables

Value

wdbcMIDS dataset

| | |
|--------|--|
| wdbcNA | <i>wdbcNA: Diagnostic Wisconsin Breast Cancer Database with missing values</i> |
|--------|--|

Description

We introduced random missing values to the wdbc dataset. [wdbc](#)

Usage

```
data("BreastCancerWisconsinMISSING", package = "ClustAll")
```

Format

A data frame with 660 rows and 31 variables

Value

wdbcNA dataset

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