# Package 'tempted'

May 10, 2023

Type Package

<b>Title</b> Temporal Tensor Decomposition, a Dimensionality Reduction Tool for variate Data	or Longitudinal Multi-
Version 0.1.0	
<b>Depends</b> R (>= 4.2.0), np (>= 0.60-17), ggplot2 (>= 3.4.0), methods (>= 4	.2.1)
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<b>Description</b> A dimension reduction method for multivariate longitudinal damat the data into a temporal tensor, with three modes representing sultous time, respectively. The tensor is then decomposed into a summation ponents, each consisting of a subject loading vector, a feature loading ral loading function. These loadings provide low-dimensional representations ples, and can be used to identify features associated with clusters of supples. TEMPTED provides the flexibility of allowing subjects to have a pling, so time points do not need to be binned and missing time points	bject, feature, and continu- on of low-dimensional com- g vector, and a tempo- entation of subjects or sam- subjects or sam- different temporal sam-
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aggregate\_feature Aggregate features using feature loadings

# Description

This function aggregate the features into "meta features" by calculating a weighted summation of the features using feature loading of each component as weights. It can also aggregate features by using the combination of multiple components by ranking the features by a linear combination of feature loadings from multiple components.

## Usage

```
aggregate_feature(
  res_tempted,
  mean_svd = NULL,
  datlist,
  pct = 1,
  contrast = NULL
)
```

## **Arguments**

res\_tempted Output of tempted.

mean\_svd Output of svd\_centralize.

datlist Output of format\_tempted, the original temporal tensor that will be aggregated.

pct The percent of features to aggregate, features ranked by absolute value of the feature loading of each component. Default is 1, which means 100% of features are aggregated. Setting pct=0.01 means top 1% of features is aggregated, where features are ranked in absolute value of feature loading of each component.

contrast A matrix choosing how components are combined, each column is a contrast of length r and used to calculate the linear combination of the feature loadings of r components.

### Value

A list of results.

**metafeature\_aggregate** The meta feature obtained by aggregating the observed temporal tensor. It is a data.frame with four columns: "value" for the meta feature values, "subID" for the subject ID, "timepoint" for the time points, and "PC" indicating which component was used to construct the meta feature.

**metafeature\_aggregate\_est** The meta feature obtained by aggregating the denoised temporal tensor. It has the same structure as metafeature\_aggregate.

**contrast** The contrast used to linearly combine the components from input.

**toppct** A matrix of TRUE/FALSE indicating which features are aggregated in each component and contrast.

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#### **Examples**

```
datlist <- format_tempted(count_table,</pre>
                           meta_table$day_of_life,
                           meta_table$studyid,
                           pseudo=0.5,
                            transform="clr")
mean_svd <- svd_centralize(datlist, r=1)</pre>
res_tempted <- tempted(mean_svd$datlist, r=3, smooth=1e-5)</pre>
datalist_raw <- format_tempted(count_table,</pre>
                                meta_table$day_of_life,
                                meta_table$studyid,
                                transform="none")
contrast <- cbind(c(1/2,1,0), c(1/2,-1,0))
res_aggregate <- aggregate_feature(res_tempted,</pre>
                                     mean_svd,
                                     datlist,
                                     pct=1,
                                     contrast=contrast)
group <- unique(meta_table[, c("studyid", "delivery")])</pre>
plot_metafeature(res_aggregate$metafeature_aggregate, group, bws=30)
```

bernoulli\_kernel

Caculate the Bernoulli kernel

## **Description**

This function is used to calculate the kernel matrix for the RKHS regression that iteratively updates the temporal loading function.

## Usage

```
bernoulli_kernel(x, y)
```

#### **Arguments**

x, y

Two values between which the Bernoulli kernel is calculated.

## Value

The calculated kernel between x and y.

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OTU read count table from the ECAM data

## **Description**

OTU read count table from the ECAM data

## Usage

```
count_table
```

#### **Format**

A data.frame with rows representing samples and matching with data.frame meta\_table and columns representing microbial features (i.e. OTUs). Each entry is a read count.

#### **Source**

Bokulich, Nicholas A., et al. "Antibiotics, birth mode, and diet shape microbiome maturation during early life." Science translational medicine 8.343 (2016): 343ra82-343ra82.

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Estimate subject loading of testing data

## **Description**

This function estimates the subject loading of the testing data based on feature and temporal loading from training data, so that both the testing data and training data have the same dimensionality reduction.

### Usage

```
est_test_subject(datlist, res_tempted, mean_svd = NULL)
```

## **Arguments**

datlist Testing data formatted into datlist in the same fashion as the training data. The

same transformation needs to be used for both training and testing data.

res\_tempted Result from tempted ran on the training data.

mean\_svd Result from svd\_centralize ran on the training data.

## Value

estimated subject loading of testing data

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#### **Examples**

```
# split the example data into training and testing
id_test <- meta_table$studyid=="1"</pre>
count_train <- count_table[!id_test,]</pre>
meta_train <- meta_table[!id_test,]</pre>
count_test <- count_table[id_test,]</pre>
meta_test <- meta_table[id_test,]</pre>
# run tempted on training data
datlist_train <- format_tempted(count_train,</pre>
                                  meta_train$day_of_life,
                                  meta_train$studyid,
                                   threshold=0.95,
                                   pseudo=0.5,
                                   transform="clr")
mean_svd_train <- svd_centralize(datlist_train, r=1)</pre>
res_tempted_train <- tempted(mean_svd_train$datlist,</pre>
r=3, smooth=1e-5)
# get the overlapping features
count_test <- count_test[,rownames(datlist_train[[1]])[-1]]</pre>
datlist_test <- format_tempted(count_test,</pre>
                                 meta_test$day_of_life,
                                 meta_test$studyid,
                                 threshold=1,
                                 pseudo=0.5,
                                 transform="clr")
# estimate the subject loading of the testing subject
sub_test <- est_test_subject(datlist_test, res_tempted_train, mean_svd_train)</pre>
```

 ${\tt format\_tempted}$ 

Format data table into the input of tempted

#### **Description**

This function applies a variety of transformations to the read counts and format the sample by feature table and meta data into a data list that can be used as the input of tempted and svd\_centralize. For data that are not read counts, or data that are not microbiome data, the user can apply their desired transformation to the data before formatting into list.

# Usage

```
format_tempted(
  featuretable,
```

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```
timepoint,
subjectID,
threshold = 0.95,
pseudo = NULL,
transform = "clr"
)
```

#### **Arguments**

featuretable A sample by feature matrix.

timepoint The time stamp of each sample, matched with the rows of featuretable.

subjectID The subject ID of each sample, matched with the rows of featuretable.

threshold A threshold for feature filtering for microbiome data. Features with zero value

percentage > threshold will be excluded. Default is 0.95.

pseudo A small number to add to all the counts before normalizing into proportions and

log transformation. Default is 1/2 of the smallest non-zero value that is specific for each sample. This pseudo count is added for transform=c("logcomp",

"clr", "logit").

transform The transformation applied to the data. "logcomp" for log of compositions.

"comp" for compositions. "ast" for arcsine squared transformation. "clr" for central log ratio transformation. "logit" for logit transformation. "none" for no transformation. Default transform="clr" is recommended for microbiome

data. For data that are already transformed, use transform="none".

#### Value

A length n list of matrices as the input of tempted and svd\_centralize. Each matrix represents a subject, with columns representing samples from this subject, the first row representing the sampling time points, and the following rows representing the feature values.

#### See Also

Examples can be found in tempted.

meta\_table Meta data table from the ECAM data

#### **Description**

Meta data table from the ECAM data

## Usage

meta\_table

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#### **Format**

A data.frame with rows representing samples and matching with data.frame count\_table and processed\_table and three columns:

studyid character denoting the subject ID of the infants.

**delivery** character denoting the delivery mode of the infants.

day\_of\_life character denoting the age of infants measured in days when microbiome sample was taken.

#### **Source**

Bokulich, Nicholas A., et al. "Antibiotics, birth mode, and diet shape microbiome maturation during early life." Science translational medicine 8.343 (2016): 343ra82-343ra82.

 ${\it plot\_feature\_summary} \quad {\it Plot\ nonparametric\ smoothed\ mean\ and\ error\ bands\ of\ features\ versus} \\ time$ 

## **Description**

This is a handy function to plot the smoothed mean and error bands for multiple features.

#### Usage

```
plot_feature_summary(
  feature_mat,
  time_vec,
  group_vec,
  coverage = 0.95,
  bws = NULL,
  nrow = 1
)
```

## Arguments

feature_mat	A sample by feature matrix. Each feature will be plotted separately as a facet. The features can be original features, meta features, log ratios, or any variables of interest.
time_vec	A vector of time points matched to the rows of feature_mat.
group_vec	A vector of factor variable indicating the group membership of samples matched to the rows of feature_mat.
coverage	The coverage rate for the error band. Default is 0.95.
bws	The smoothness parameter for the smoothing lines and error bands. A larger value means a smoother line. Default is NULL and calculated by function np::npreg().
nrow	The number of rows to plot the features used in function ggplot2::facet_wrap().

#### Value

A ggplot2 object.

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#### **Examples**

plot\_metafeature

Plot nonparametric smoothed mesan and error bands of meta features versus time

## **Description**

This function plot the smoothed mean and error band of meta features grouped by a factor variable provided by the user.

### Usage

```
plot_metafeature(metafeature, group, coverage = 0.95, bws = NULL, nrow = 1)
```

## **Arguments**

 $\label{lem:metafeature} \textbf{It can be metafeature\_ratio from the output of ratio\_feature and tempted\_all},$ 

metafeature\_aggregate from the output of ratio\_feature and tempted\_all,

or metafeature\_aggregate\_est from the output of ratio\_feature.

group A subject by 2 data.frame with the first column for subject ID and second column

for group membership.

coverage The coverage rate for the error band. Default is 0.95.

bws The smoothness parameter for the smoothing lines and error bands. A larger

value means a smoother line. Default is NULL and calculated by function

np::npreg().

nrow The number of rows to plot the features used in function ggplot2::facet\_wrap().

## Value

A ggplot2 object.

#### See Also

Examples can be found in tempted\_all, ratio\_feature and aggregate\_feature.

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plot_time_loading	Plot the temporal loading functions

## **Description**

This function uses ggplot2::geom\_line() in ggplot2 to plot the temporal loading functions from tempted.

#### Usage

```
plot_time_loading(res, r = NULL, ...)
```

## **Arguments**

res Output of function tempted.

r The number of components to plot. By default all the components estimated by tempted will be plotted.

... Arguments to put in ggplot2::geom\_line(aes(...)).

#### Value

An ggplot2 object.

#### See Also

Examples can be found in tempted\_all and tempted.

processed\_table Central-log-ratio (clr) transformed OTU table from the ECAM data

#### **Description**

Central-log-ratio (clr) transformed OTU table from the ECAM data

## Usage

```
processed_table
```

#### **Format**

A data.frame with rows representing samples and matching with data.frame meta\_table and columns representing microbial features (i.e. OTUs). Entries do not need to be transformed, and will be directly used by tempted. This data.frame is used to illustrate how tempted can be used for general form of multivariate longitudinal data already preprocessed by user.

#### **Source**

Bokulich, Nicholas A., et al. "Antibiotics, birth mode, and diet shape microbiome maturation during early life." Science translational medicine 8.343 (2016): 343ra82-343ra82.

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ratio\_feature

Take log ratio of the abundance of top features over bottom features

#### **Description**

Top and bottom ranking features are picked based on feature loadings (and their contrasts). The log ratio abundance of the top ranking features over the bottom ranking features is produced as the main result. This function and its result is designed for longitudinal microbiome data, and may not be meaningful for other type of temporal data.

#### Usage

```
ratio_feature(
  res_tempted,
  datlist,
  pct = 0.05,
  absolute = FALSE,
  contrast = NULL
)
```

#### **Arguments**

res\_tempted Output of tempted.

datlist Output of format\_tempted(, transform="none"), the temporal tensor that in-

clude the raw read counts.

pct The percent of features to sum up. Default is 0.05, i.e. 5%.

absolute = TRUE means features are ranked by the absolute value of feature

loadings, and the top pct percent of features are picked. absolute = FALSE means features are ranked by the original value of feature loadings, and the top and bottom pct percent of features are picked. Then ratio is taken as the abundance of the features with positive loading over the abundance of the features

with negative loading.

contrast A matrix choosing how components are combined, each column is a contrast of

length r and used to calculate the linear combination of the feature loadings of r

components.

## Value

A list of results:

**metafeature\_ratio** The log ratio abundance of the top over bottom ranking features. It is a data.frame with five columns: "value" for the log ratio values, "subID" for the subject ID, and "timepoint" for the time points, and "PC" indicating which component was used to construct the meta feature.

**contrast** The contrast used to linearly combine the components from input.

**toppct** A matrix of TRUE/FALSE indicating which features are ranked top in each component (and contrast) and used as the numerator of the log ratio.

**bottompct** A matrix of TRUE/FALSE indicating which features are ranked bottom in each component (and contrast) and used as the denominator of the log ratio.

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#### **Examples**

svd\_centralize

Remove the mean structure of the temporal tensor

## **Description**

This function first average the feature value of all time points for each subject to form a subject by feature matrix. Next, it performs a singular value decomposition of this matrix and construct the matrix's rank-r approximation. Then, it subtracts this rank-r subject by feature matrix from the temporal tensor.

#### Usage

```
svd_centralize(datlist, r = 1)
```

#### **Arguments**

datlist

A length n list of matrices. Each matrix represents a subject, with columns representing samples from this subject, the first row representing the sampling time points, and the following rows representing the feature values.

The number of ranks in the mean structure. Default is 1.

Value

r

A list of results.

datlist The new temporal tensor after mean structure is removed.

**A\_tilde** The subject singular vector of the mean structure, a subject by r matrix.

**B\_tilde** The feature singular vector of the mean structure, a feature by r matrix.

lambda\_tilde The singular value of the mean structure, a length r vector.

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#### See Also

Examples can be found in tempted.

tdenoise

Calculate the de-noised temporal tensor

## Description

This function constructs a de-noised version of the temporal tensor using the low-rank components obtained by svd\_centralize tempted and uses the loadings to

## Usage

```
tdenoise(res_tempted, mean_svd = NULL)
```

## Arguments

```
res_tempted Output of tempted
mean_svd Output of svd_centralize
```

## Value

The de-noised functional tensor

tempted

Decomposition of temporal tensor

# Description

This is the main function of tempted.

## Usage

```
tempted(
  datlist,
  r = 3,
  smooth = 1e-06,
  interval = NULL,
  resolution = 101,
  maxiter = 20,
  epsilon = 1e-04
)
```

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## **Arguments**

datlist	A length n list of matrices. Each matrix represents a subject, with columns representing samples from this subject, the first row representing the sampling time points, and the following rows representing the feature values.
r	Number of components to decompose into, i.e. rank of the CP type decomposition. Default is set to 3.
smooth	Smoothing parameter for RKHS norm. Larger means smoother temporal loading functions. Default is set to be 1e-8. Value can be adjusted depending on the dataset by checking the smoothness of the estimated temporal loading function in plot.
interval	The range of time points to ran the decomposition for. Default is set to be the range of all observed time points. User can set it to be a shorter interval than the observed range.
resolution	Number of time points to evaluate the value of the temporal loading function. Default is set to 101. It does not affect the subject or feature loadings.
maxiter	Maximum number of iteration. Default is 20.
epsilon	Convergence criteria for difference between iterations. Default is 1e-4.

## Value

The estimations of the loadings.

**A\_hat** Subject loading, a subject by r matrix.

**B\_hat** Feature loading, a feature by r matrix.

**Phi\_hat** Temporal loading function, a resolution by r matrix.

**time\_Phi** The time points where the temporal loading function is evaluated.

**Lambda** Eigen value, a length r vector.

**r\_square** Variance explained by each component. This is the R-squared of the linear regression of the vectorized temporal tensor against the vectorized low-rank reconstruction using individual components.

**accum\_r\_square** Variance explained by the first few components accumulated. This is the R-squared of the linear regression of the vectorized temporal tensor against the vectorized low-rank reconstruction using the first few components.

## **Examples**

tempted\_all

Run all major functions of tempted

#### **Description**

This function wraps format\_tempted, svd\_centralize, tempted, ratio\_feature, and aggregate\_feature.

## Usage

```
tempted_all(
  featuretable,
  timepoint,
  subjectID,
  threshold = 0.95,
 pseudo = NULL,
  transform = "clr",
 r = 3,
 smooth = 1e-06,
  interval = NULL,
 resolution = 51,
 maxiter = 20,
 epsilon = 1e-04,
 r_svd = 1,
 do_ratio = TRUE,
 pct_ratio = 0.05,
 absolute = FALSE,
 pct_aggregate = 1,
  contrast = NULL
)
```

## **Arguments**

featuretable A sample by feature matrix. Input for format\_tempted.

timepoint The time stamp of each sample, matched with the rows of featuretable. Input for format\_tempted.

subjectID The subject ID of each sample, matched with the rows of featuretable. Input for format\_tempted.

threshold A threshold for feature filtering for microbiome data. Features with zero value

percentage >= threshold will be excluded. Default is 0.95. Input for format\_tempted.

pseudo A small number to add to all the counts before normalizing into proportions and

log transformation. Default is 1/2 of the smallest non-zero value that is specific for each sample. This pseudo count is added for transform=c("logcomp",

"clr", "logit"). Input for format\_tempted.

transform The transformation applied to the data. "logcomp" for log of compositions.

"comp" for compositions. "ast" for arcsine squared transformation. "clr" for central log ratio transformation. "logit" for logit transformation. "none" for no transformation. Default transform="clr" is recommended for microbiome data. For data that are already transformed, use transform="none". Input for

format\_tempted.

r Number of components to decompose into, i.e. rank of the CP type decomposi-

tion. Default is set to 3. Input for tempted.

smooth Smoothing parameter for RKHS norm. Larger means smoother temporal load-

ing functions. Default is set to be 1e-8. Value can be adjusted depending on the dataset by checking the smoothness of the estimated temporal loading function

in plot. Input for tempted.

interval The range of time points to ran the decomposition for. Default is set to be the

range of all observed time points. User can set it to be a shorter interval than the

observed range. Input for tempted.

resolution Number of time points to evaluate the value of the temporal loading function.

Default is set to 101. It does not affect the subject or feature loadings. Input for

tempted.

maxiter Maximum number of iteration. Default is 20. Input for tempted.

epsilon Convergence criteria for difference between iterations. Default is 1e-4. Input

 $for \ {\tt tempted}.$ 

 $r_svd$  The number of ranks in the mean structure. Default is 1. Input for \linke{svd\_centraliz}.

do\_ratio Whether to calculate the log ratio of features.

 $\label{eq:pct_ratio} \textbf{The percent of features to sum up. Default is 0.05, i.e. 5\%. Input for \textit{ratio\_feature}.}$ 

absolute absolute = TRUE means features are ranked by the absolute value of feature

loadings, and the top pct\_ratio percent of features are picked. absolute = FALSE means features are ranked by the original value of feature loadings, and the top and bottom pct\_ratio percent of features are picked. Then ratio is taken as the abundance of the features with positive loading over the abundance of the

 $features\ with\ negative\ loading.\ Input\ for\ {\tt ratio\_feature}.$ 

pct\_aggregate The percent of features to aggregate, features ranked by absolute value of the

feature loading of each component. Default is 1, which means 100% of features are aggregated. Setting pct\_aggregate=0.01 means top 1% of features is aggregated, where features are ranked in absolute value of feature loading of each

 $component. \ Input for \ {\tt aggregate\_feature}.$ 

contrast A matrix choosing how components are combined, each column is a contrast of

length r and used to calculate the linear combination of the feature loadings of r components. Input for ratio\_feature and Input for aggregate\_feature.

#### Value

A list including all the input and output of functions format\_tempted, svd\_centralize, tempted, ratio\_feature, and aggregate\_feature.

**input** All the input options of function tempted\_all.

datalist\_raw Output of format\_tempted with option transform="none".

datlist Output of format\_tempted.

mean svd Output of svd\_centralize.

**A\_hat** Subject loading, a subject by r matrix.

**B\_hat** Feature loading, a feature by r matrix.

**Phi\_hat** Temporal loading function, a resolution by r matrix.

time\_Phi The time points where the temporal loading function is evaluated.

Lambda Eigen value, a length r vector.

- **r\_square** Variance explained by each component. This is the R-squared of the linear regression of the vectorized temporal tensor against the vectorized low-rank reconstruction using individual components.
- **accum\_r\_square** Variance explained by the first few components accumulated. This is the R-squared of the linear regression of the vectorized temporal tensor against the vectorized low-rank reconstruction using the first few components.
- **metafeature\_ratio** The log ratio abundance of the top over bottom ranking features. It is a data.frame with five columns: "value" for the log ratio values, "subID" for the subject ID, and "timepoint" for the time points, and "PC" indicating which component was used to construct the meta feature.
- **toppct\_ratio** A matrix of TRUE/FALSE indicating which features are ranked top in each component (and contrast) and used as the numerator of the log ratio.
- **bottompct\_ratio** A matrix of TRUE/FALSE indicating which features are ranked bottom in each component (and contrast) and used as the denominator of the log ratio.
- **metafeature\_aggregate** The meta feature obtained by aggregating the observed temporal tensor. It is a data.frame with four columns: "value" for the meta feature values, "subID" for the subject ID, "timepoint" for the time points, and "PC" indicating which component was used to construct the meta feature.
- **toppct\_aggregate** A matrix of TRUE/FALSE indicating which features are aggregated in each component and contrast.

**contrast** The contrast used to linearly combine the components from input.

# Examples

```
threshold=0.95,
                         transform="clr",
                         pseudo=0.5,
                         r=2,
                         smooth=1e-5,
                         pct_ratio=0.1,
                         pct_aggregate=1)
\# for proportional data that will have pseudo added and clr transformed
res.proportion <- tempted_all(count_table/rowSums(count_table),</pre>
                              meta_table$day_of_life,
                              meta_table$studyid,
                              threshold=0.95,
                              transform="clr",
                              pseudo=NULL,
                              r=2,
                              smooth=1e-5,
                              pct_ratio=0.1,
                              pct_aggregate=1)
# plot the temporal loading and subject trajectories grouped by delivery mode
plot_time_loading(res.proportion, r=2)
group <- unique(meta_table[,c("studyid", "delivery")])</pre>
plot_metafeature(res.proportion$metafeature_aggregate, group, bws=30)
```

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