# Package 'tempted'

January 11, 2024

	3411441 y 11, 2021
Туре	Package
	Temporal Tensor Decomposition, a Dimensionality Reduction Tool for Longitudinal Multivariate Data
Versio	on 0.1.0
Date	2024-1-9
Deper	<b>nds</b> R (>= 4.2.0), np (>= 0.60-17), ggplot2 (>= 3.4.0), methods (>= 4.2.1)
Autho	or Pixu Shi
Maint	tainer Pixu Shi <pixu.shi@duke.edu></pixu.shi@duke.edu>
	iption
	TEMPoral TEnsor Decomposition (TEMPTED), is a dimension reduction method for multivariate longitudinal data with varying temporal sampling. It formats the data into a temporal tensor and decomposes it into a summation of low-dimensional components, each consisting of a subject loading vector, a feature loading vector, and a continuous temporal loading function. These loadings provide a low-dimensional representation of subjects or samples and can be used to identify features associated with clusters of subjects or samples. TEMPTED provides the flexibility of allowing subjects to have different temporal sampling, so time points do not need to be binned, and missing time points do not need to be imputed
URL	https://github.com/pixushi/tempted
Licen	se GPL-3
Encod	ling UTF-8
LazyI	Data true
Roxve	genNote 7.2.3
	ppics documented:
	aggregate_feature
	bernoulli_kernel
	count_table
	est_test_subject
	meta_table
	plot_feature_summary
	plot_metafeature
	plot_time_loading
	processed table

2 aggregate\_feature

Index																		20
	tempted_all .				 					•	•							15
	tempted																	
	tdenoise				 				 									13
	svd_centralize																	
	ratio_feature .				 				 									10

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	$Output\ of\ {\tt format\_tempted}, the\ original\ temporal\ tensor\ that\ will\ be\ aggregated.$
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.

bernoulli\_kernel 3

**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.

#### References

Shi P, Martino C, Han R, Janssen S, Buck G, Serrano M, Owzar K, Knight R, Shenhav L, Zhang AR. (2023) *Time-Informed Dimensionality Reduction for Longitudinal Microbiome Studies*. bioRxiv. doi: 10.1101/550749. https://www.biorxiv.org/content/10.1101/550749.

### **Examples**

```
# Take a subset of the samples so the example runs faster
# Here we are taking samples from the odd months
sub_sample <- rownames(meta_table)[(meta_table$day_of_life%/%12)%%2==1]</pre>
count_table_sub <- count_table[sub_sample,]</pre>
processed_table_sub <- processed_table[sub_sample,]</pre>
meta_table_sub <- meta_table[sub_sample,]</pre>
datlist <- format_tempted(count_table_sub,</pre>
                            meta_table_sub$day_of_life,
                            meta_table_sub$studyid,
                            pseudo=0.5,
                            transform="clr")
mean_svd <- svd_centralize(datlist, r=1)</pre>
res_tempted <- tempted(mean_svd$datlist, r=2, smooth=1e-5)</pre>
contrast \leftarrow matrix(c(1/2,1), 2, 1)
res_aggregate <- aggregate_feature(res_tempted,</pre>
                                      mean_svd,
                                      datlist,
                                      pct=1,
                                      contrast=contrast)
# plot the aggregated features
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.

4 est\_test\_subject

#### **Usage**

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

#### **Arguments**

х, у

Two values between which the Bernoulli kernel is calculated.

#### Value

The calculated kernel between x and y.

#### References

Han, R., Shi, P. and Zhang, A.R. (2023) *Guaranteed functional tensor singular value decomposition*. Journal of the American Statistical Association, pp.1-13. doi: 10.1080/01621459.2022.2153689.

count\_table

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.

### References

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

est\_test\_subject

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)
```

est\_test\_subject 5

#### **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

#### References

Shi P, Martino C, Han R, Janssen S, Buck G, Serrano M, Owzar K, Knight R, Shenhav L, Zhang AR. (2023) *Time-Informed Dimensionality Reduction for Longitudinal Microbiome Studies*. bioRxiv. doi: 10.1101/550749. https://www.biorxiv.org/content/10.1101/550749.

```
# Take a subset of the samples so the example runs faster
# Here we are taking samples from the odd months
sub_sample <- rownames(meta_table)[(meta_table$day_of_life%/%12)%%2==1]</pre>
count_table_sub <- count_table[sub_sample,]</pre>
processed_table_sub <- processed_table[sub_sample,]</pre>
meta_table_sub <- meta_table[sub_sample,]</pre>
# split the example data into training and testing
id_test <- meta_table_sub$studyid=="2"</pre>
count_train <- count_table_sub[!id_test,]</pre>
meta_train <- meta_table_sub[!id_test,]</pre>
count_test <- count_table_sub[id_test,]</pre>
meta_test <- meta_table_sub[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=2, smooth=1e-5)
# get the overlapping features
count_test <- count_test[,rownames(datlist_train[[1]])[-1]]</pre>
datlist_test <- format_tempted(count_test,</pre>
```

6 format\_tempted

```
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>
# train logistic regression classifier on training subjects
metauni <- unique(meta_table_sub[,c("studyid", "delivery")])</pre>
rownames(metauni) <- metauni$studyid</pre>
Atrain <- as.data.frame(res_tempted_train$A_hat)</pre>
Atrain$delivery <- metauni[rownames(Atrain), "delivery"]=="Cesarean"</pre>
glm_train <- glm(delivery ~ PC1+PC2,</pre>
                  data=Atrain, family=binomial(link="logit"))
summary(glm_train)
# predict the label of testing subject, whose true label is "Cesarean"
predict(glm_train, newdata=as.data.frame(sub_test), type="response")
```

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,
  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.

meta\_table 7

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. "lfb" for log 2 fold change over baseline (first time point) 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

### **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.

#### References

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

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

#### **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.

plot\_metafeature 9

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

metafeature	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().

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

### Value

nrow

A ggplot2 object.

### See Also

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

### **Description**

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

### Usage

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

10 ratio\_feature

### **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.

### References

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

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.

ratio\_feature 11

#### 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.

#### References

Shi P, Martino C, Han R, Janssen S, Buck G, Serrano M, Owzar K, Knight R, Shenhav L, Zhang AR. (2023) *Time-Informed Dimensionality Reduction for Longitudinal Microbiome Studies*. bioRxiv. doi: 10.1101/550749. https://www.biorxiv.org/content/10.1101/550749.

```
# Take a subset of the samples so the example runs faster
# Here we are taking samples from the odd months
sub_sample <- rownames(meta_table)[(meta_table$day_of_life%/%12)%%2==1]</pre>
```

12 svd\_centralize

```
count_table_sub <- count_table[sub_sample,]</pre>
processed_table_sub <- processed_table[sub_sample,]</pre>
meta_table_sub <- meta_table[sub_sample,]</pre>
datlist <- format_tempted(count_table_sub,</pre>
                            meta_table_sub$day_of_life,
                            meta_table_sub$studyid,
                            pseudo=0.5,
                            transform="clr")
mean_svd <- svd_centralize(datlist, r=1)</pre>
res_tempted <- tempted(mean_svd$datlist, r=2, smooth=1e-5)</pre>
datalist_raw <- format_tempted(count_table_sub, meta_table_sub$day_of_life, meta_table_sub$studyid,</pre>
transform="none")
contrast <- cbind(c(1,1), c(1,-1))
res_ratio <- ratio_feature(res_tempted, datalist_raw, pct=0.1,</pre>
absolute=FALSE, contrast=contrast)
group <- unique(meta_table[, c("studyid", "delivery")])</pre>
# plot the log ratios
plot_metafeature(res_ratio$metafeature_ratio, group, bws=30)
```

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.

tdenoise 13

#### Value

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.

#### References

Shi P, Martino C, Han R, Janssen S, Buck G, Serrano M, Owzar K, Knight R, Shenhav L, Zhang AR. (2023) *Time-Informed Dimensionality Reduction for Longitudinal Microbiome Studies*. bioRxiv. doi: 10.1101/550749. https://www.biorxiv.org/content/10.1101/550749.

### 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

14 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
)
```

### **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**

```
# Take a subset of the samples so the example runs faster
# Here we are taking samples from the odd months
sub_sample <- rownames(meta_table)[(meta_table$day_of_life%/%12)%%2==1]</pre>
count_table_sub <- count_table[sub_sample,]</pre>
processed_table_sub <- processed_table[sub_sample,]</pre>
meta_table_sub <- meta_table[sub_sample,]</pre>
# for count data from longitudinal microbiome studies
datlist <- format_tempted(count_table_sub,</pre>
                           meta_table_sub$day_of_life,
                           meta_table_sub$studyid,
                            pseudo=0.5,
                            transform="clr")
mean_svd <- svd_centralize(datlist, r=1)</pre>
res_tempted <- tempted(mean_svd$datlist, r=2, smooth=1e-5)</pre>
# for preprocessed data that do not need to be transformed
datlist <- format_tempted(processed_table_sub,</pre>
                            meta_table_sub$day_of_life,
                            meta_table_sub$studyid,
                            pseudo=NULL,
                            transform="none")
mean_svd <- svd_centralize(datlist, r=1)</pre>
res_tempted <- tempted(mean_svd$datlist, r=2, smooth=1e-5)</pre>
# plot the temporal loading
plot_time_loading(res_tempted, r=2)
```

tempted\_all

Run all major functions of tempted

### Description

This function wraps functions 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. It is an input for format\_tempted.

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

an input for format\_tempted.

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

an 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. It is an 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"). It is an 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". It is an

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. It is an 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. It is an 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. It is an 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. It is an

input for tempted.

maxiter Maximum number of iteration. Default is 20. It is an input for tempted.

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

input for tempted.

r\_svd The number of ranks in the mean structure. Default is 1. It is an input for

svd\_centralize.

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

pct\_ratio The percent of features to sum up. Default is 0.05, i.e. 5%. It is an input for

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. It is an input for 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. It is an input for 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. It is an input for ratio\_feature and It is an 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.

#### References

Shi P, Martino C, Han R, Janssen S, Buck G, Serrano M, Owzar K, Knight R, Shenhav L, Zhang AR. (2023) *Time-Informed Dimensionality Reduction for Longitudinal Microbiome Studies*. bioRxiv. doi: 10.1101/550749. https://www.biorxiv.org/content/10.1101/550749.

```
# Take a subset of the samples so the example runs faster
# Here we are taking samples from the odd months
sub_sample <- rownames(meta_table)[(meta_table$day_of_life%/%12)%%2==1]</pre>
count_table_sub <- count_table[sub_sample,]</pre>
processed_table_sub <- processed_table[sub_sample,]</pre>
meta_table_sub <- meta_table[sub_sample,]</pre>
# for preprocessed data that do not need to be transformed
res.processed <- tempted_all(processed_table_sub,</pre>
                               meta_table_sub$day_of_life,
                              meta_table_sub$studyid,
                               threshold=1.
                               transform="none",
                               r=2,
                               smooth=1e-5,
                               do_ratio=FALSE)
# for count data that will have pseudo added and clr transformed
res.count <- tempted_all(count_table_sub,</pre>
                          meta_table_sub$day_of_life,
                          meta_table_sub$studyid,
                           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_sub/rowSums(count_table_sub),</pre>
                               meta_table_sub$day_of_life,
                               meta_table_sub$studyid,
                               threshold=0.95,
                               transform="clr",
                               pseudo=NULL,
                               r=2,
                               smooth=1e-5,
                               pct_ratio=0.1,
                               pct_aggregate=1)
\ensuremath{\mathtt{\#}} 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 the aggregated features
plot_metafeature(res.proportion$metafeature_aggregate, group, bws=30)
```

## **Index**

```
* datasets
    count_table, 4
    meta_table, 7
    processed_table, 10
aggregate_feature, 2, 9, 15, 17
bernoulli_kernel, 3
count_table, 4
\verb"est_test_subject", 4"
format_tempted, 2, 6, 15-17
meta_table, 7
plot_feature_summary, 8
plot_metafeature, 9
plot_time_loading, 9
processed_table, 10
ratio_feature, 9, 10, 15, 17
svd_centralize, 2, 5-7, 12, 13, 15, 17
tdenoise, 13
tempted, 2, 5-7, 9-11, 13, 14, 15-17
tempted_all, 9, 10, 15, 17
```