An Introduction to cpfa

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Outline

Overview

Package **cpfa** implements a k-fold cross-validation procedure to predict class labels using component weights from a single mode of a Parallel Factor Analysis model-1 (Parafac; Harshman, 1970) or a Parallel Factor Analysis model-2 (Parafac2; Harshman, 1972), which is fit to a three-way or four-way data array. After fitting a Parafac or Parafac2 model with package **multiway** via an alternating least squares algorithm (Helwig, 2025), estimated component weights from one mode of this model are passed to one or more classification methods. For each method, a k-fold cross-validation is conducted to tune classification parameters using estimated Parafac component weights, optimizing class label prediction. This process is repeated over multiple train-test splits in order to improve the generalizability of results. Multiple constraint options are available to impose on any mode of the Parafac model during the estimation step (see Helwig, 2017). Multiple numbers of components can be considered in the primary package function `cpfa`. This vignette describes how to use the **cpfa** package.

Installation

cpfa can be installed directly from CRAN. Type the following command in an R console: `install.packages("cpfa", repos = "https://cran.r-project.org/")`. The argument `repos` can be modified according to user preferences. For more options and details, see `help(install.packages)`. In this case, the package **cpfa** has been downloaded and installed to the default directories. Users can download the package source at https://cran.r-project.org/package=cpfa and use Unix commands for installation.

Example: Four-way Array with Multiclass Response

We start by using the simulation function `simcpfa` and examining basic operations and outputs related to this function.

First, we load the **cpfa** package:

```
library(cpfa)
```

We simulate a four-way array where the fourth mode (i.e., the classification mode) of the simulated array is related to a response vector, which is also simulated. To generate data, we specify the data-generating model as a Parafac2 model via the `model` argument and specify three components for this model with the nfac argument. We specify the number of dimensions for the simulated array using the arraydim argument. However, because a Parafac2 model is used, the function ignores the first element of arraydim and looks for input provided through the argument pf2num instead. Argument pf2num specifies the number of rows in each three-way array that exists within each level of the fourth mode of the four-way ragged array being simulated. As a demonstration, we set pf2num <- rep(c(7, 8, 9), length.out = 100), which specifies that the number of rows alternates from 7, to 8, to 9, and back to 7, across all 100 levels of the fourth mode of the simulated array. Note that a useful feature of Parafac2 is that it can be fit to ragged arrays directly, while maintaining the intrinsic axis property of Parafac (see Harshman and Lundy, 1994).

For these simulated data, we specify that the response vector should have three classes using nclass. Moreover, we set a target correlation matrix, corrpred, specifying correlations among the columns of the classification mode's weight matrix (i.e., the fourth mode, in this case). We also specify correlations, contained in corresp, between columns of the classification mode's weight matrix and the response vector. Input modes sets the number of modes in the array; and we use meanpred to specify the target means for the columns of the classification mode weight matrix. Finally, onreps specifies the number of classification mode weight matrices to generate while nreps specifies, for any one classification mode weight matrix, the number of response vectors to generate (see help(simcpfa) for additional details of the simulation procedure). Then, in R we have the following:

```
# set seed for reproducibility
set.seed(500)

# specify correlation
cp <- 0.1

# define target correlation matrix for columns of fourth mode weight matrix
corrpred <- matrix(c(1, cp, cp, cp, 1, cp, cp, cp, 1), nrow = 3, ncol = 3)

# define correlations between fourth mode weight matrix and response vector
corresp <- rep(.85, 3)

# specify number of rows in the three-way array for each level of fourth mode
pf2num <- rep(c(7, 8, 9), length.out = 100)

# simulate a four-way ragged array connected to a response
data <- simcpfa(arraydim = c(10, 11, 12, 100), model = "parafac2", nfac = 3,
                nclass = 3, nreps = 10, onreps = 10, corresp = corresp,
                pf2num = pf2num, modes = 4, corrpred = corrpred,
                meanpred = c(10, 20, 30))

# define simulated array 'X' and response vector 'y' from the output
X <- data$X
y <- data$y
```

The above creates a four-way array X with Parafac2 structure that is connected through its fourth mode to response vector y. We confirm the dimensions of X and y, confirm their classes, and inspect the possible values of y:

```
# examine data object X
class(X)
```

```
## [1] "list"
```

```
length(X)
```

```
## [1] 100
```

```r
dim(X[[1]])
```

```
## [1]  7 11 12
```

```r
dim(X[[2]])
```

```
## [1]  8 11 12
```

```r
# examine data object y
class(y)
```

```
## [1] "matrix" "array"
```

```r
length(y)
```

```
## [1] 100
```

```r
table(y)
```

```
## y
##  0  1  2
## 36 24 40
```

As shown, X is a list where each element is a three-way array. The dimensions of X match those specified in input arguments arraydim and pf2num. Likewise, y is a vector with length equal to the number of levels of the fourth mode of X. As desired, we can see that y contains three classes. However, note that no control currently exists to specify the proportions of output classes in y, which is a limitation of simcpfa. Future enhancements are planned to address this limitation.

We confirm that the columns of the fourth mode's weights are linearly associated with y:

```r
# examine correlations between columns of fourth mode weights 'Dmat' and
# simulated response vector 'y'
cor(data$Dmat, data$y)
```

```
##           [,1]
## [1,] 0.3955246
## [2,] 0.3557359
## [3,] 0.4321371
```

As shown, the classification mode weight matrix Dmat contains columns that have a positive correlation with the response vector y. The target correlations (i.e., 0.85) were not achieved, especially given that nreps = 10 and onreps = 10 were small values. Nevertheless, achieved positive correlations indicate that building a classifier between X and y through the fourth mode of a three-component Parafac2 model could prove useful.

We initialize values for tuning parameter α from penalized logistic regression (PLR) implemented through package **glmnet** (Friedman, Hastie, and Tibshirani, 2010; Zou and Hastie, 2005). We specify the classification method as PLR through method, the model of interest as Parafac2 through model, the number of folds in the k-fold cross-validation step as three through nfolds, and the number of random starts for fitting the Parafac2 model as three through nstart. Further, we specify nfac to be two or three because we wish to explore classification performance for a two-component model and for a three-component model. The classification problem is multiclass, which is specified by setting multinomial for input family. In this demonstration, we allow for three train-test splits by setting nrep <- 3 with a split ratio of ratio <- 0.9. We also specify pre-determined fold IDs for k-fold cross-validation using foldid. Finally, when fitting Parafac2 models, we set a constraint: the fourth mode must have non-negative weights. We use const to set this constraint. In R:

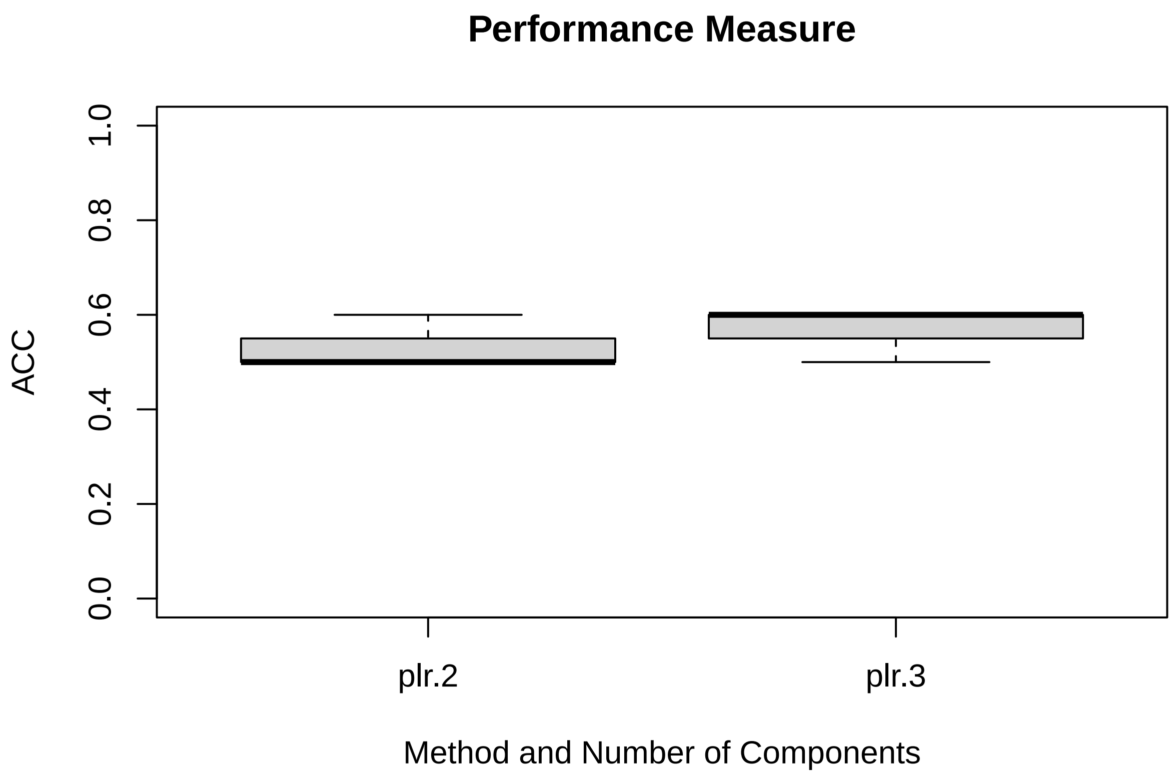
```r
# set seed
set.seed(500)

# initialize alpha and store within a list called 'parameters'
```

```r
alpha <- seq(0, 1, length.out = 11)
parameters <- list(alpha = alpha)

# initialize inputs
method <- "PLR"
model <- "parafac2"
nfolds <- 3
nstart <- 3
nfac <- c(2, 3)
family <- "multinomial"
nrep <- 3
ratio <- 0.9
plot.out <- TRUE
const <- c("uncons", "uncons", "uncons", "nonneg")
foldid <- rep(1:nfolds, length.out = ratio * length(y))

# implement train-test splits with inner k-fold CV to optimize classification
output <- cpfa(x = X, y = as.factor(y), model = model, nfac = nfac,
               nrep = nrep, ratio = ratio, nfolds = nfolds, method = method,
               family = family, parameters = parameters, plot.out = plot.out,
               parallel = FALSE, const = const, foldid = foldid,
               nstart = nstart, verbose = FALSE)
```



The function generates box plots of classification accuracy for each number of components and for each classification method. In greater detail, we examine classification performance in the output object:

```r
# examine classification performance measures - median across train-test splits
output$descriptive$median[, 1:2]
```

```
##         err acc
```

```
## fac.2plr 0.5 0.5
## fac.3plr 0.4 0.6
```

As shown, classification accuracy (i.e., 'acc') is relatively good and certainly above baseline (for more details on classification performance measures, see help file for package function `cpm` via `help(cpm)`). In this case, the data-generating model with three components worked for classification purposes. We also examine, averaged across train-test splits, optimal tuning parameters. Note that **glmnet** optimized tuning parameter λ internally.

```
# examine optimal tuning parameters averaged across train-test splits
output$mean.opt.tune
```

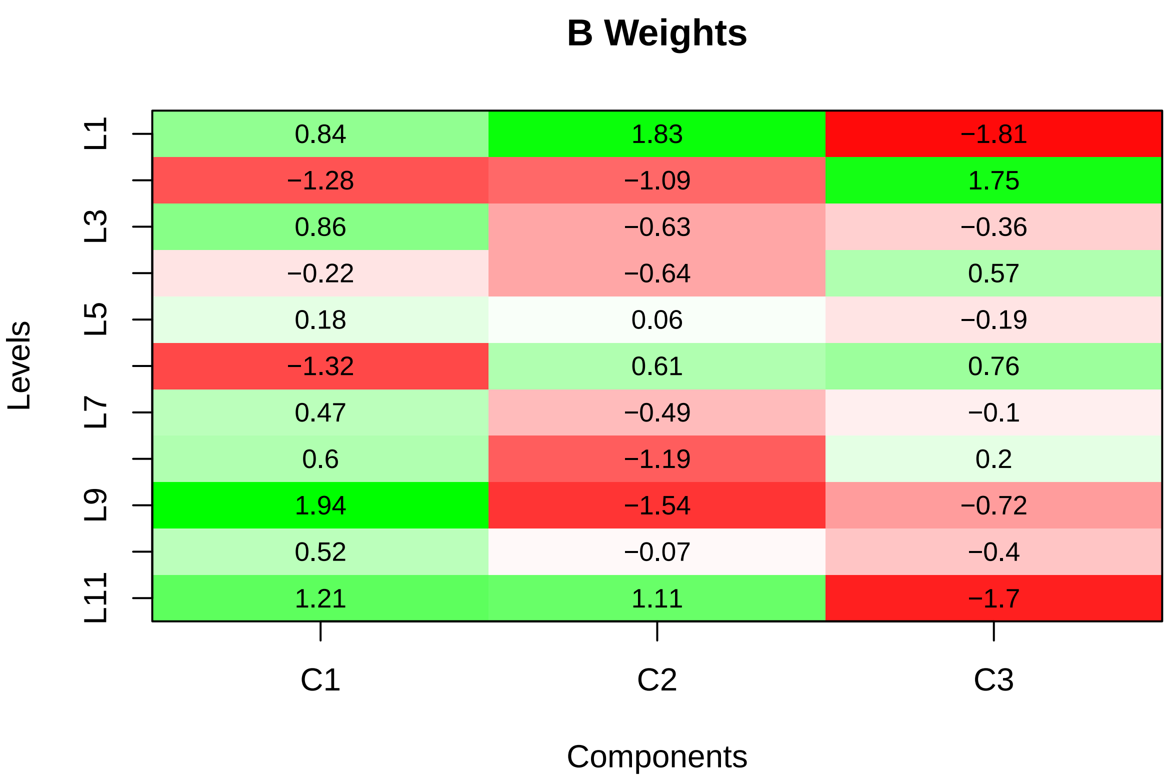
```
##   nfac      alpha     lambda gamma cost ntree nodesize size decay rda.alpha
## 1    2 0.03333333 974.374043    NA   NA    NA       NA   NA    NA        NA
## 2    3 0.06666667   9.291151    NA   NA    NA       NA   NA    NA        NA
##   delta eta max.depth subsample nrounds
## 1    NA  NA        NA        NA      NA
## 2    NA  NA        NA        NA      NA
```

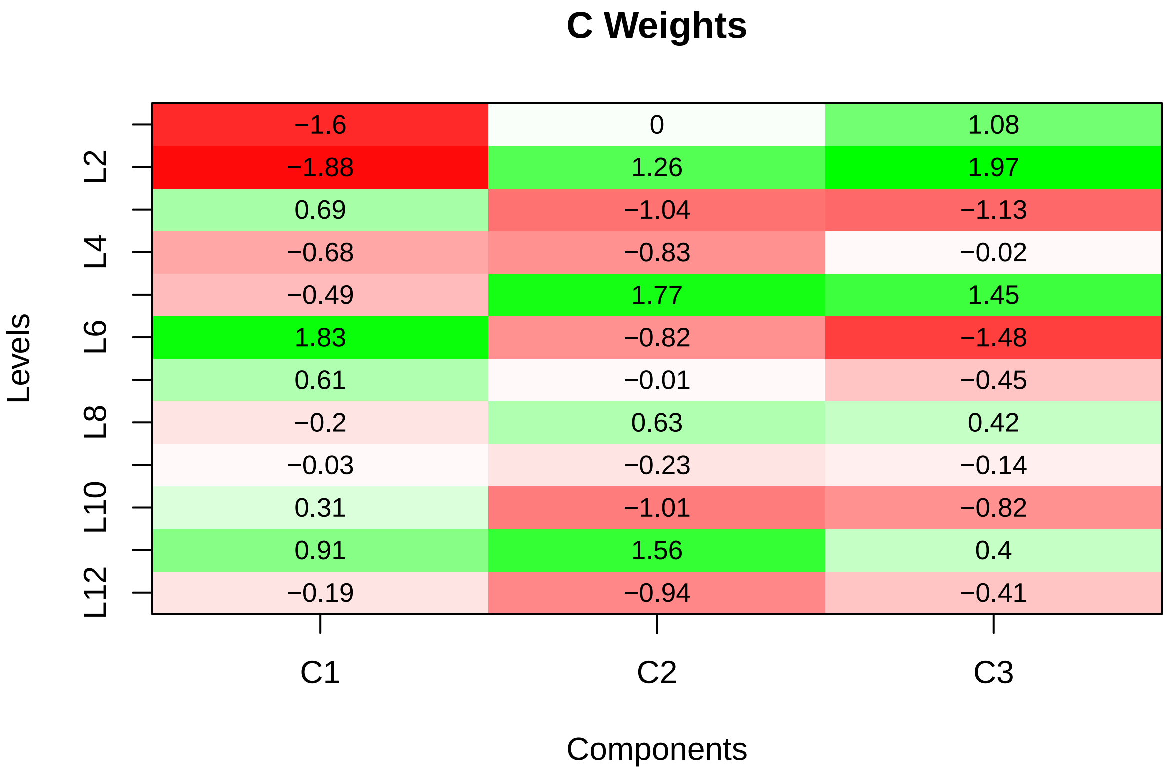
We can see average values for α that worked best. In addition, the best average λ values are also displayed. Note that other classifiers were not used in this demonstration, but their tuning parameters are indicated in the output with placeholders of NA.

We next use package function `plotcpfa` to fit the best (in terms of mean accuracy) Parafac2 model and to plot the results:

```
# set seed
set.seed(500)

# plot heatmaps of component weights for optimal model
results <- plotcpfa(output, nstart = 3, ctol = 1e-1, verbose = FALSE)
```





Generated plots are heatmaps displaying the size of estimated component weights for the second (B) and third (C) modes. Because the input array was simulated, these plots do not display meaningful results but serve only to demonstrate the utility of function `plotcpfa` for visualizing the component weights of the optimal classification model (i.e., the model with the best classification performance, based on output from function `cpfa`). Thus, where function `cpfa` can serve as a guide to identify a meaningful number of components and a meaningful set of constraints for different modes, function `plotcpfa` can be used to visualize component weights of the best model to better understand how different levels of each mode map onto the set of components.

Concluding Thoughts

Package **cpfa** implements a k-fold cross-validation procedure, connecting Parafac models fit by **multiway** to classification methods implemented through six popular packages used for classification: **glmnet**; **e1071** (Meyer et al., 2024; Cortes and Vapnik, 1995); **randomForest** (Liaw and Wiener, 2002; Breiman, 2001); **nnet** (Ripley, 1994; Venables and Ripley, 2002); **rda** (Guo, Hastie, and Tibshirani, 2007, 2023; Friedman, 1989), and **xgboost** (Chen et al., 2025; Friedman, 2001). Parallel computing is implemented through packages **parallel** (R Core Team, 2025) and **doParallel** (Microsoft Corporation and Weston, 2022). The example above highlights the use of **cpfa** and three of its functions. For more information about the package, see https://CRAN.R-project.org/package=cpfa or examine package help files with `help(simcpfa)`, `help(cpfa)`, or `help(plotcpfa)`.

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