# Multiway Classification with Real Data

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We apply R package **cpfa** (Asisgress, 2025) to three real datasets. First, we apply the package to the MNIST dataset (LeCun, Cortes, and Burges, 1998; LeCun et al., 2002)—showing how to use the package to distinguish between digits of 2 and 3, a binary classification problem. We also apply it to the Fashion MNIST dataset (Xiao, Rasul, and Vollgraf, 2017)—distinguishing among images of tops, trousers, and sandals, a multiclass classification problem. Finally, we apply it to the VesselMNIST3D dataset (Yang et al., 2020) from the MedMNIST database (Yang et al., 2023; Yang, Shi, Ni, 2021), which contains three-dimensional representations of blood vessels. Specifically, we distinguish healthy blood vessels from aneurysm blood vessels, a binary classification problem.

## A.) MNIST

MNIST consists of 70,000 grayscale images of handwritten digits from 0 to 9. We use R package **dslabs** (Irizarry and Gill, 2025) to download the dataset. We subset to only 2000 images from the original training set. The images include 980 images of the digit 2 and 1020 images of the digit 3.

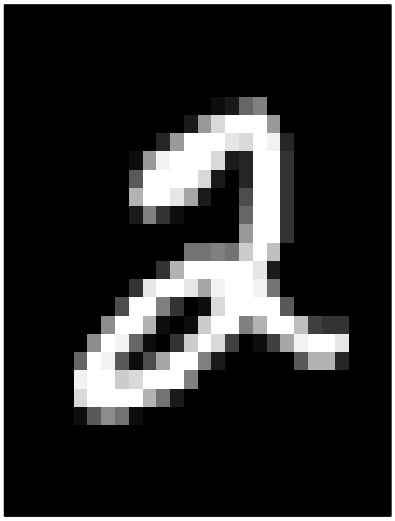
### Download

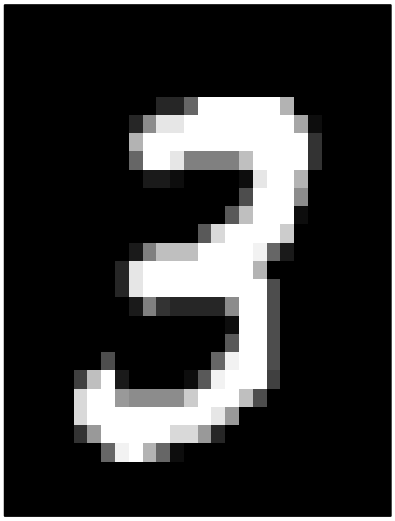
```
# load library
library(dslabs)

# download MNIST data and subset training set to digits of 2 or 3
mnist <- read_mnist()
inde <- which(mnist$train$labels %in% c(2, 3))
images <- mnist$train$images[inde, ]
labels <- mnist$train$labels[inde]

# restructure data into three-way array and prepare labels
X0 <- array(images, c(nrow(images), 28, 28))
y0 <- as.factor(as.numeric(as.factor(labels)) - 1)

# subset to first 2000 images
ind <- 1:2e3
X <- X0[ind, , ]
y <- y0[ind]
```

We plot an example of digit 2 and digit 3.

```
# plot example of 2 and 3
par(mfrow = c(1, 2))
pdigit <- function(imat) {
  m <- t(apply(imat, 2, rev))
  image(m, col = gray(seq(0, 1, 0.05)), xaxt = "n", yaxt = "n")
```

```
}
for (i in 0:1) {pdigit(t(X[which(y == i)[1], , ]))}
```





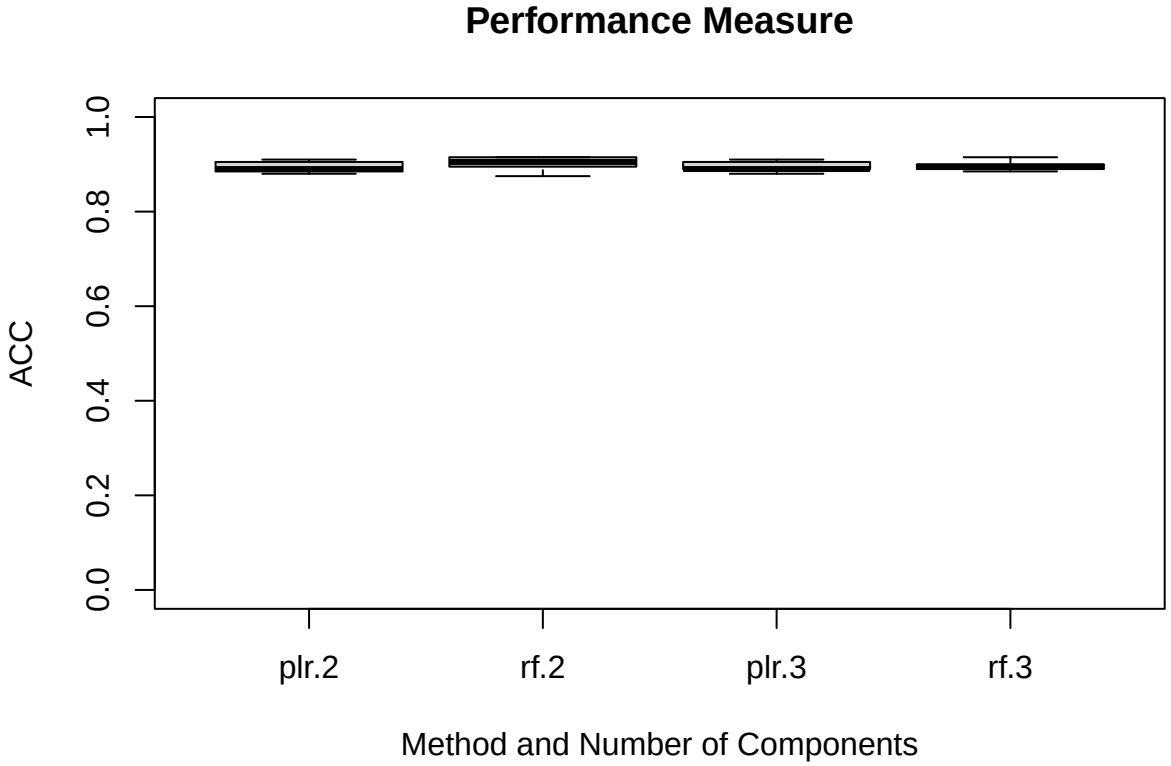
## Analysis

We load R package **cpfa** and initialize the tensor model. First, the data array is a regular three-way array; so we set `model <- "parafac"` to use a Parafac model (Harshman, 1970). Second, we initialize the number of components to fit for the model by setting `nfac <- c(2, 3)` in order to fit both a two-component Parafac model and a three-component Parafac model. We set `nstart <- 10` to allow for 10 random starts in the Parafac alternating least squares algorithm fit by R package **multiway** (Helwig, 2025), upon which R package **cpfa** depends. Third, we specify the constraint desired for each array mode using `const`. Fourth, we use `cmode <- 1` to specify that the classification mode is the first mode of the input array (i.e., the mode connected to the class labels). Note that numerous constraint options are available; after loading **cpfa**, type `const()` in the R console to access a constraint options list provided by R package **CMLS** (Helwig, 2025).

Next, we initialize classification methods. First, we use `method = c("PLR", "RF")` to employ penalized logistic regression (PLR) and random forest (RF) classifiers for this problem. See `help(cpfa)` for information on additional classification methods. Second, we specify that the problem is a binary classification problem by setting `family <- "binomial"`. Third, we use 10-fold cross-validation (CV) in our inner training, setting `nfolds <- 10`; and fourth, we set `nrep <- 5` to perform five outer train-test splits of our data. Fifth, we set `ratio <- 0.9` to specify that each outer training set contains a proportion of 0.9 of the full input data while the outer testing set contains a proportion of 0.1. Finally, we specify ranges for tuning parameters alpha (PLR), the number of trees (RF), and node size (RF), wrapping them into the list called `parameters`.

```
# load library
library(cpfa)

# set seed
set.seed(500)

# initialize model
model <- "parafac"
nfac <- c(2, 3)
nstart <- 10
const <- c("uncons", "uncons", "uncons")
cmode <- 1

# initialize classification
```

```
method <- c("PLR", "RF")
family <- "binomial"
nfolds <- 10
nrep <- 5
ratio <- 0.9

# initialize tuning parameters
alpha <- seq(0, 1, length = 8)
ntree <- c(400, 600, 800, 1000)
nodesize <- c(4, 8, 16, 32)
parameters <- list(alpha = alpha, ntree = ntree, nodesize = nodesize)

# implement train-test splits with inner k-fold CV to optimize classification
outputR <- cpfa(x = X, y = y, model = model, nfac = nfac, nstart = nstart,
                const = const, cmode = cmode, method = method, family = family,
                nfolds = nfolds, nrep = nrep, ratio = ratio,
                parameters = parameters, type.out = "descriptives",
                seeds = NULL, plot.out = TRUE, parallel = FALSE,
                verbose = FALSE)
```




## Results

We examine classification performance metrics error (`err`) and accuracy (`acc`) for each model and for each classifier, looking at median metrics across outer train-test splits. We also examine, averaged across train-test splits, optimal tuning parameters chosen for each classifier.

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

```
##            err   acc
```

```
## fac.2plr 0.110 0.890
## fac.2rf  0.095 0.905
## fac.3plr 0.110 0.890
## fac.3rf  0.105 0.895
```

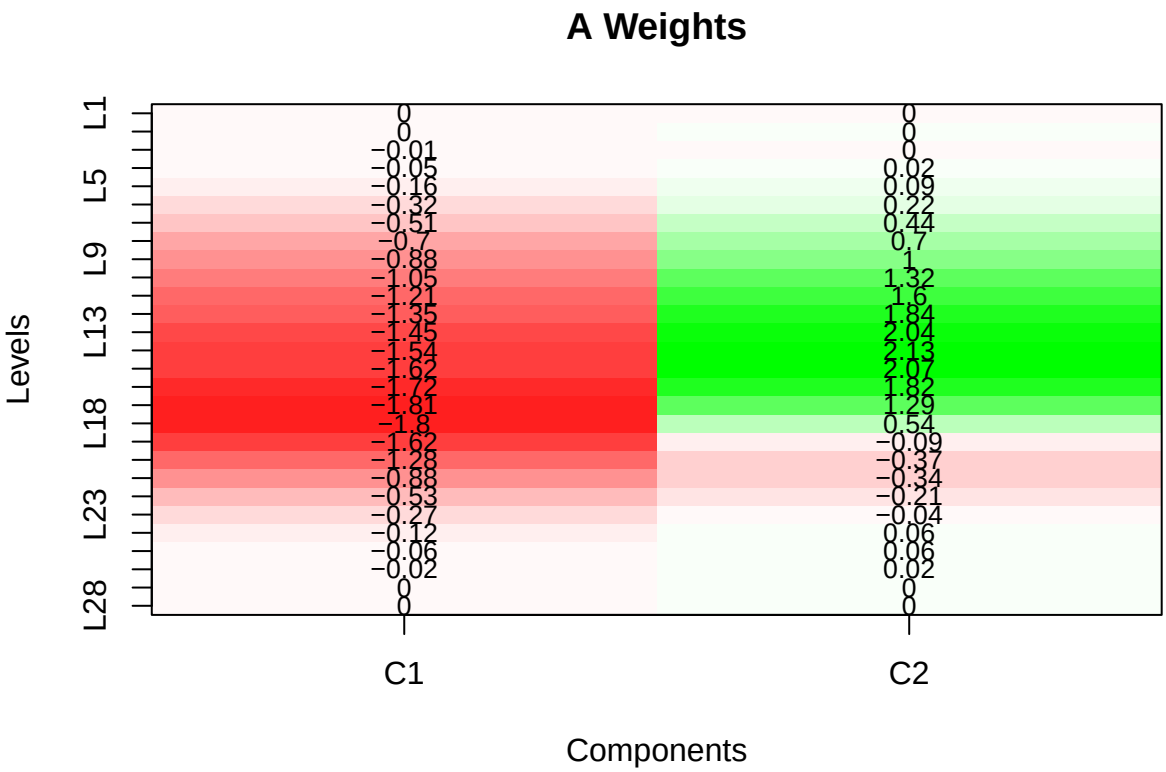
```
# examine optimal tuning parameters - mean across train-test splits
outputR$mean.opt.tune
```

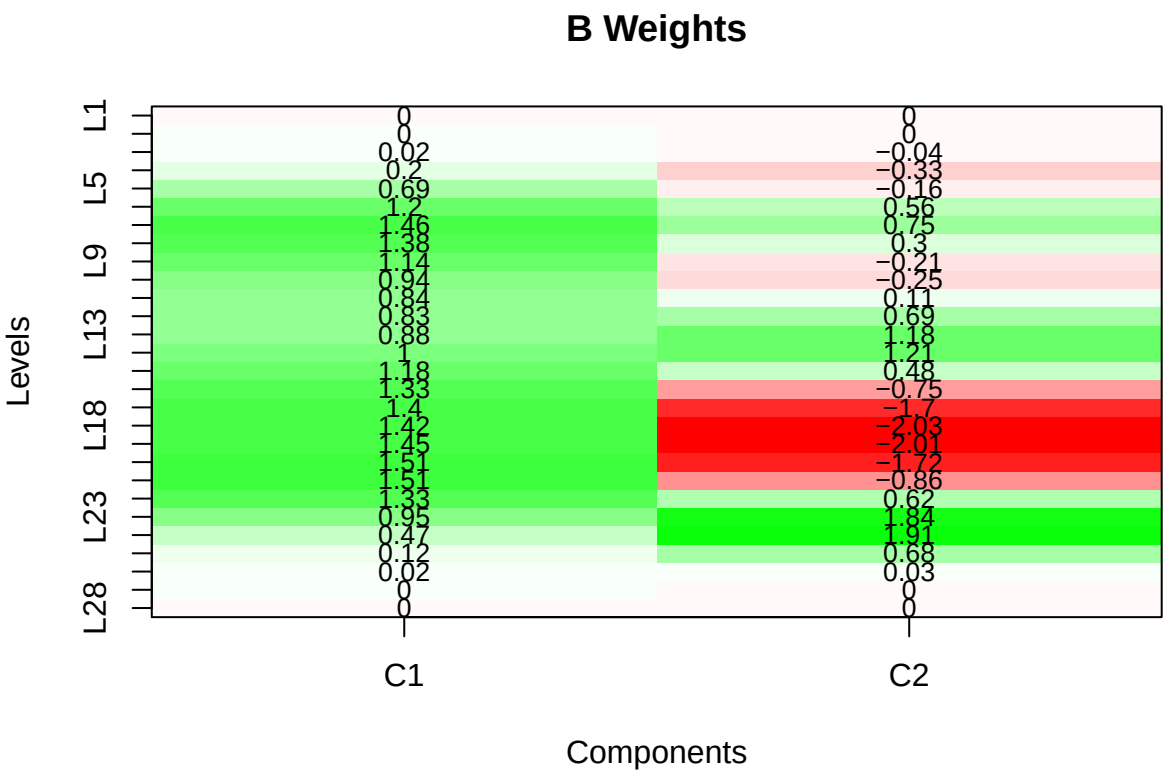
```
##   nfac      alpha   lambda gamma cost ntree nodesize size decay rda.alpha delta
## 1    2 0.11428571 2.350755    NA   NA   600     32.0   NA    NA         NA    NA
## 2    3 0.02857143 6.256281    NA   NA   680     10.4   NA    NA         NA    NA
##   eta max.depth subsample nrounds
## 1  NA        NA        NA      NA
## 2  NA        NA        NA      NA
```

We see that accuracy values are close to 0.9 for both two-component and three-component models. The two-component Parafac model with the RF classifier performed best. In addition, we can see average optimal tuning parameters for each classifier. Note that PLR optimized lambda internally.

Next, we use function `plotcpfa`. This function performs two tasks: (1) it fits the optimal model among those fit using function `cpfa`; and (2) it plots estimated component weights from that model for non-classification modes. Looking at such plots, we can search for relationships between model components and levels of mode A or B. In this case, mode A corresponds to the horizontal axis of MNIST images while mode B corresponds to the vertical axis.

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

# plot heatmaps of component weights for optimal model
results <- plotcpfa(outputR, nstart = 10, ctol = 1e-6, verbose = FALSE)
```






For the A mode, component weights are stronger between levels 5 and 24 for the first component. Looking at the B mode, weights are stronger between levels 4 and 25. Whether viewed from mode A or B the first component appears to be a general component identifying the presence of non-zero values, distinguishing empty outer parts of images from non-zero inner parts. The digits 2 and 3 have systematic differences in the presence of non-zero values in these areas.

Examining the second component for the A mode, weights are stronger around level 14 where there appears to be a greater presence of zero values in digit 3, compared to digit 2. A similar pattern exists in mode B around levels 18 and 19 with more non-zero values for 2, compared to 3. Taken together between the two modes, this component might be identifying the closed circle present in the digit 2, which differs from the open or half circle seen in digit 3.

# B.) Fashion MNIST

Fashion MNIST consists of 70,000 grayscale images of fashion objects within 10 different categories, indexed by class labels of 0 through 9 (Xiao, Rasul, and Vollgraf, 2017). We use R package **keras3** (Kalinowski, Allaire, and Chollet, 2025) to download the dataset. We subset to 1000 images from the training set. We only use images within the categories of top (with a label of 0), trouser (1), or sandal (5). Images include 308 tops, 357 trousers, and 335 sandals.

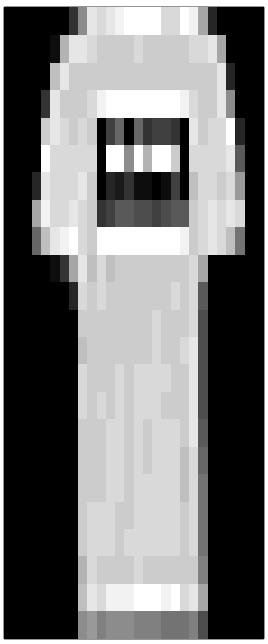
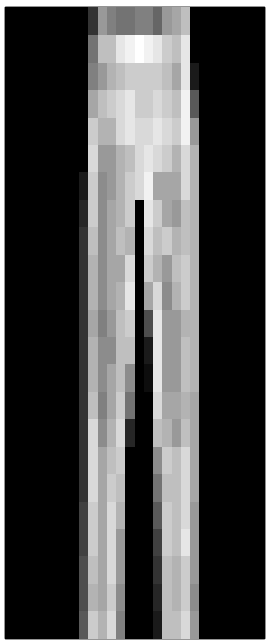
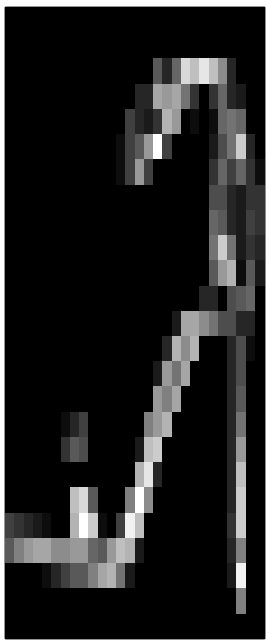
We remove a different number of horizontal levels from each image, randomly selecting a number of levels between three and six (inclusive) to remove for each image. The resulting array is ragged: mode A (the horizontal mode) contains a different number of rows for each image while mode B (the vertical mode) contains exactly 28 levels for all images. This removal is meant to simulate data corruption or sensor malfunction that could lead to incomplete images. To continue forward, we use a Parafac2 model (Harshman, 1972), which can be fit to a ragged array (i.e., one mode has a different number of levels, conditional on another mode). Parafac2 maintains properties similar to the Parafac model, including the intrinsic axis property (for details, see Harshman and Lundy, 1994, 1996).

## Download

```
# load library
library(keras3)

# download Fashion MNIST and subset training set to categories of 0, 1, 5
fmnist <- dataset_fashion_mnist()
inde <- which(fmnist$train$y %in% c(0, 1, 5))
X0 <- fmnist$train$x[inde, ,]
labels <- fmnist$train$y[inde]

# prepare labels by converting to class factor with levels of 0, 1, and 2
y0 <- as.factor(as.numeric(as.factor(labels)) - 1)

# subset to first 1000 images
ind <- 1:1e3
nimage <- length(ind)
Xp <- X0[ind, , ]
y <- y0[ind]

# permute array to make third mode classification mode
X <- aperm(Xp, c(2, 3, 1))

# set seed
set.seed(500)

# remove rows from each image and restructure array into list of images
nremove <- sample(3:6, nimage, replace = TRUE)
Xrag <- vector(mode = "list", length = nimage)
for (i in 1:nimage) {
   ranremove <- c(sample(1:28, nremove[i]))
   image0 <- X[-ranremove, , i]
   Xrag[[i]] <- image0
}
```

We plot an example of a top, trouser, and sandal.

```
# plot example of top, trouser, and sandal
par(mfrow = c(1, 3))
pdigit <- function(imat) {
  m <- t(apply(imat, 2, rev))
  image(m, col = gray(seq(0, 1, 0.05)), xaxt = "n", yaxt = "n")
}
for (i in 0:2) {pdigit(Xrag[[which(y == i)[1]]])}
```

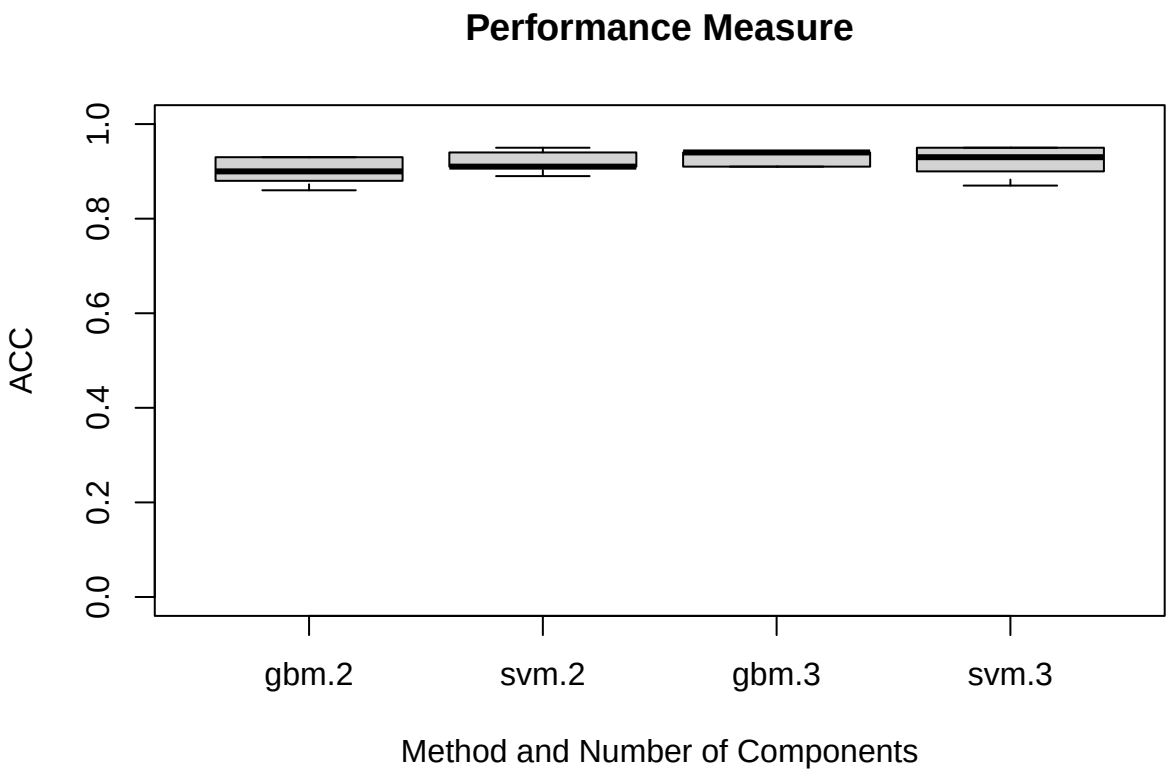
## Analysis

We load R package **cpfa** and initialize the tensor model. First, the data array is a ragged, irregular three-way array; so we set `model <- "parafac2"` to use a Parafac2 model. Second, we initialize the number of components to fit by setting `nfac <- c(2, 3)`. Third, we set `nstart <- 10` for 10 random starts. Fourth, we specify the constraint for each mode using `const`. For Parafac2, we set the third mode to have non-negative weights.

Next, we initialize classification methods. First, we use `method = c("SVM", "GBM")` to use support vector machine (SVM) and gradient boosting machine (GBM). Second, we specify that the problem is a multiclass classification problem by setting `family <- "multinomial"`. Third, we use 10-fold CV in our inner training, setting `nfolds <- 10`; and fourth, we set `nrep <- 5`. Fifth, we set `ratio <- 0.9`. Finally, we specify ranges for tuning parameters gamma (SVM), cost (SVM), eta (GBM), maximum depth (GBM), subsample (GBM), and number of rounds (GBM), wrapping them into `parameters`.

```
# load library
library(cpfa)

# set seed
set.seed(500)

# initialize model
model <- "parafac2"
nfac <- c(2, 3)
nstart <- 10
const <- c("uncons", "uncons", "nonneg")

# initialize classification
method <- c("SVM", "GBM")
family <- "multinomial"
nfolds <- 10
nrep <- 5
ratio <- 0.9
```

```
# initialize tuning parameters
gamma <- c(0, 0.1, 1, 10); cost <- c(0.1, 1, 10, 100)
eta <- c(0.3, 0.7); max.depth <- c(1, 2)
subsample <- c(0.75, 0.9); nrounds <- c(100, 400)
parameters <- list(gamma = gamma, cost = cost, eta = eta, max.depth = max.depth,
                   subsample = subsample, nrounds = nrounds)

# implement train-test splits with inner k-fold CV to optimize classification
outputR2 <- cpfa(x = Xrag, y = y, model = model, nfac = nfac, nstart = nstart,
                 const = const, method = method, family = family,
                 nfolds = nfolds, nrep = nrep, ratio = ratio,
                 parameters = parameters, type.out = "descriptives",
                 seeds = NULL, plot.out = TRUE, parallel = FALSE,
                 verbose = FALSE)
```




## Results

We examine classification performance metrics for each model and for each classifier, this time averaged across train-test splits. We also examine, averaged across train-test splits, the optimal tuning parameters chosen for each classifier.

```
# examine classification performance measures - mean across train-test splits
outputR2$descriptive$mean[, 1:2]
```

```
##            err   acc
## fac.2svm 0.080 0.920
## fac.2gbm 0.100 0.900
## fac.3svm 0.080 0.920
## fac.3gbm 0.072 0.928
```

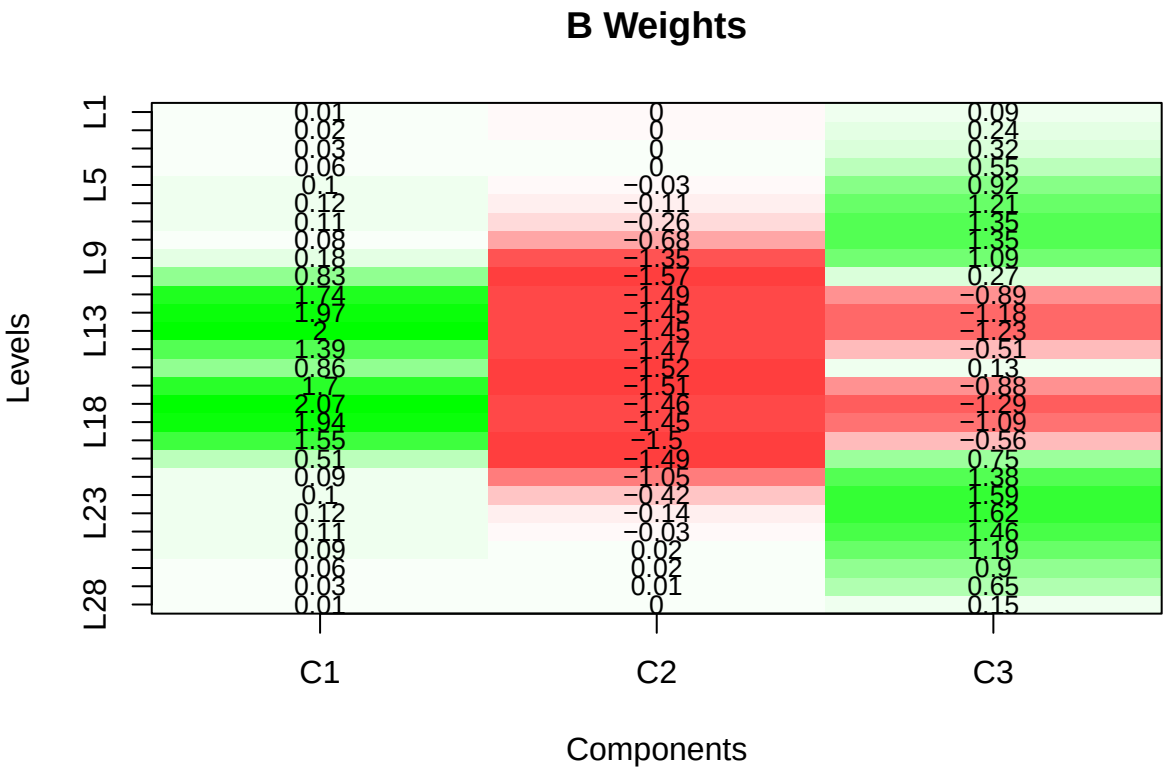
```
# examine optimal tuning parameters - mean across train-test splits
outputR2$mean.opt.tune
```

```
##   nfac alpha lambda gamma cost ntree nodesize size decay rda.alpha delta  eta
## 1    2    NA     NA  6.40 26.2    NA       NA   NA    NA        NA    NA 0.54
## 2    3    NA     NA  0.64 40.6    NA       NA   NA    NA        NA    NA 0.46
##   max.depth subsample nrounds
## 1       1.6      0.84     100
## 2       1.6      0.81     100
```

Accuracy values are between 0.9 and 0.928. The three-component Parafac2 model with the GBM classifier performed best. In addition, average optimal tuning parameters span a range for each classifier.

Next, we use function `plotcpfa`. Because the number of levels differs among images for mode A, we cannot inspect mode A weights easily. Function `plotcpfa` automatically excludes mode A weights from plots based on the Parafac2 model. Instead, we inspect only the component weights for mode B to search for relationships between the levels of B and the Parafac2 model components.

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

# plot heatmaps of component weights for optimal model
results2 <- plotcpfa(outputR2, nstart = 10, ctol = 1e-6, verbose = FALSE)
```




For the B mode (i.e., vertical axis), for the first component, weights are stronger between levels 11 to 14 and between 16 and 19. This first component might be capturing non-zero changes displayed at the center of the top images. The first component might help distinguish tops from trousers and sandals.

For the second component, weights are stronger between levels 6 to 23. This component could be a general component distinguishing non-zero values in the middle columns of images from zero values at the far left and far right columns. While the sandal has some non-zero values in the far left and far right columns, the top and trouser generally do not; so this second component might help distinguish the top and the trouser

from the sandal.

For the third component, weights are stronger between levels 6 and 9 and between 22 and 25. This third component might be capturing zero values to the left and right of images, contrasting them with non-zero values in the middle. Interestingly, we see two negative bands between levels 11 and 14 and between 16 and 19; however, level 15 is positive. Level 15 might correspond to the empty space between the trouser legs while the negative bands might represent non-zero values in the legs. If so, this component might help distinguish trousers from tops or sandals.

These interpretations are limited. For all components, more work would need to be done to explore the estimated A mode weights (or C mode weights) to understand the components from other perspectives. Such work could clarify the components further and change the current interpretations.

# C.) VesselMNIST3D from MedMNIST

VesselMNIST3D consists of 1,908 three-dimensional models of brain blood vessels based on reconstructed magnetic resonance imaging data. Vessels exist in two categories: healthy vessels (indexed by 0) or aneurysm vessels (1). We download the dataset manually from https://medmnist.com/, which gives us a .npz file. We use the Python script `convert_npz_to_h5.py` to convert VesselMNIST3D from a file format of .npz to .h5. This script can be found on the project's repository. Next, we use R package **rhdf5** (Fischer, Smith, and Pau, 2025) to read the data (as a .h5) into R. We subset to only 300 objects from the training set, including 150 healthy vessels and 150 aneurysm vessels.

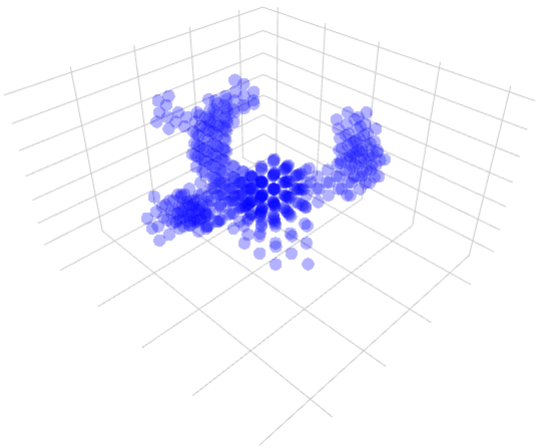
## Download

```r
# load library
library(rhdf5)

# import VesselMNIST3D data
h5file <- "vesselmnist3d.h5"
imag4d <- h5read(h5file, name = "train_images")
labels <- h5read(h5file, name = "train_labels")

# subset to first 300 objects
ind <- 1:300
Xp <- imag4d[ , , , ind]
y <- as.factor(as.numeric(labels))[ind]

# convert array to double
storage.mode(Xp) <- "double"

# remove full dataset
rm(imag4d)
```

We use R package **plotly** (Sievert, 2020) to generate a point cloud representation of a healthy blood vessel.

```r
# load library
library(plotly)

# prepare data from vessel 205 for plotting
voxel_df <- as.data.frame(which(Xp[, , , 205] > 0, arr.ind = TRUE))
colnames(voxel_df) <- c("x", "y", "z")

# generate 3D plot
scene1 <- list(title = "", showticklabels = FALSE, showgrid = TRUE,
```

```
               showline = FALSE, zeroline = FALSE)
plot_ly(voxel_df, x = ~x, y = ~y, z = ~z, type = "scatter3d", mode = "markers",
        marker = list(size = 3.5, color = "blue", opacity = 0.3)) %>%
          layout(title = "3D Blood Vessel Example - Point Cloud Representation",
                 scene = list(xaxis = scene1, yaxis = scene1, zaxis = scene1))
```



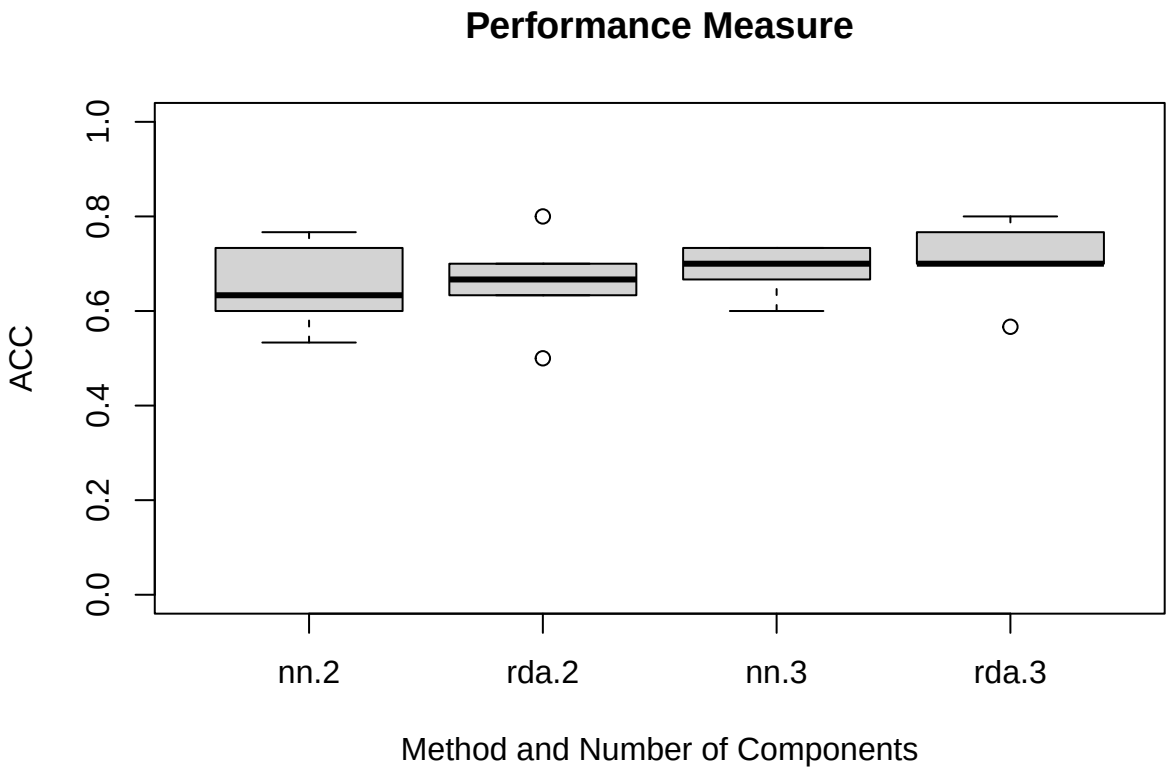

## Analysis

We load **cpfa** and initialize the tensor model. First, the data array is a regular four-way array; so we set `model <- "parafac"`. Second, we initialize the number of components to fit by setting `nfac <- c(2, 3)`. Third, we set `nstart <- 10`. Fourth, we specify the constraint for each mode using `const`. For Parafac, we set the fourth mode to have non-negative weights.

Next, we initialize classification methods. First, we use `method = c("NN", "RDA")` to use feed-forward neural networks (NN) and regularized discriminant analysis (RDA). Second, we specify that the problem is a binary classification problem, setting `family <- "binomial"`. Third, we use 10-fold CV in our inner training, setting `nfolds <- 10`; and fourth, we set `nrep <- 5` to perform five outer train-test splits. Fifth, we set `ratio <- 0.9`. Finally, we specify ranges for tuning parameters alpha (RDA), delta (RDA), size (NN), and decay (NN), wrapping them into `parameters`.

```
# load library
library(cpfa)

# set seed
set.seed(500)

# initialize model
model <- "parafac"
nfac <- c(2, 3)
nstart <- 10
const <- c("uncons", "uncons", "uncons", "nonneg")

# initialize classification
method <- c("NN", "RDA")
family <- "binomial"
nfolds <- 10
```

```
nrep <- 5
ratio <- 0.9

# initialize tuning parameters
rda.alpha <- seq(0, 0.999, length = 4); delta <- c(0, 0.1, 1, 2)
size <- c(1, 2, 4, 8); decay <- c(0.001, 0.01, 0.1, 1)
parameters <- list(rda.alpha = rda.alpha, delta = delta, size = size,
                   decay = decay)

# implement train-test splits with inner k-fold CV to optimize classification
outputR3 <- cpfa(x = Xp, y = y, model = model, nfac = nfac, nstart = nstart,
                 const = const, method = method, family = family,
                 nfolds = nfolds, nrep = nrep, ratio = ratio,
                 parameters = parameters, type.out = "descriptives",
                 seeds = NULL, plot.out = TRUE, parallel = FALSE,
                 verbose = FALSE)
```




## Results

We examine classification performance metrics of error and accuracy for each model and for each classifier, averaged across train-test splits. We also examine, averaged across train-test splits, the optimal tuning parameters chosen for each classifier.

```
# examine classification performance measures - mean across train-test splits
outputR3$descriptive$mean[, 1:2]
```

```
##                err       acc
## fac.2nn  0.3466667 0.6533333
## fac.2rda 0.3400000 0.6600000
## fac.3nn  0.3133333 0.6866667
```

```
## fac.3rda 0.2933333 0.7066667
```

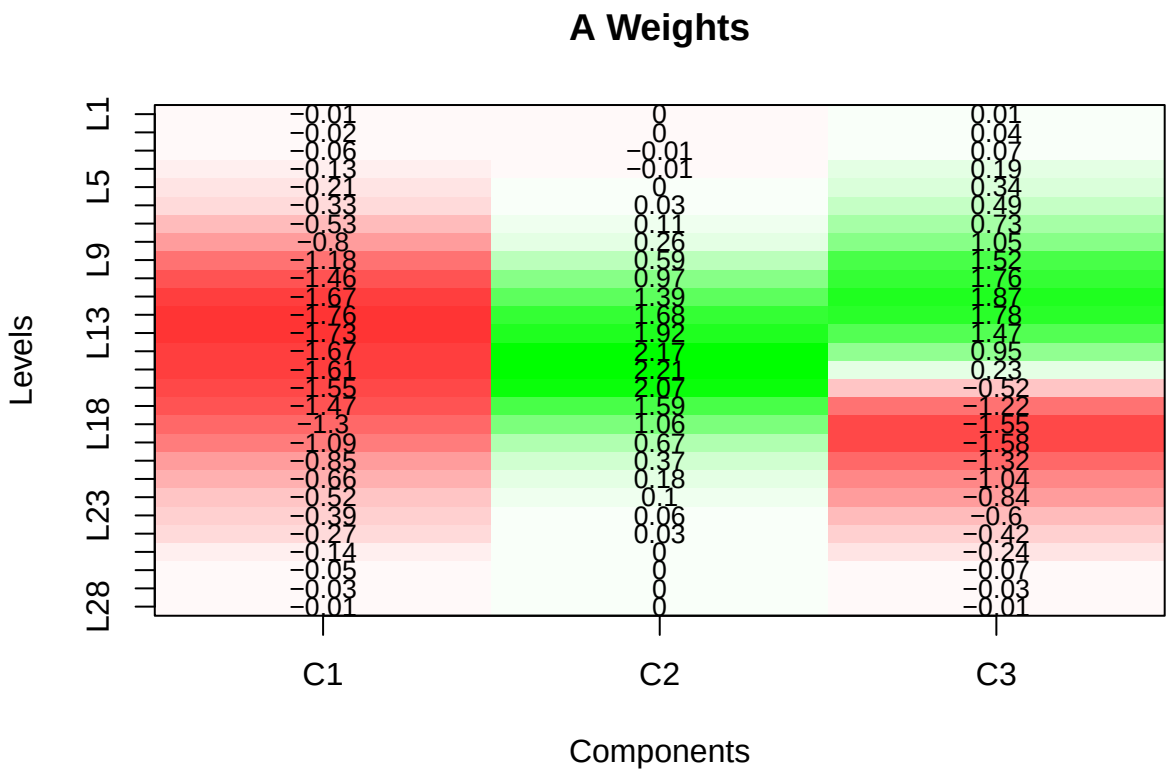
```
# examine optimal tuning parameters - mean across train-test splits
outputR3$mean.opt.tune
```

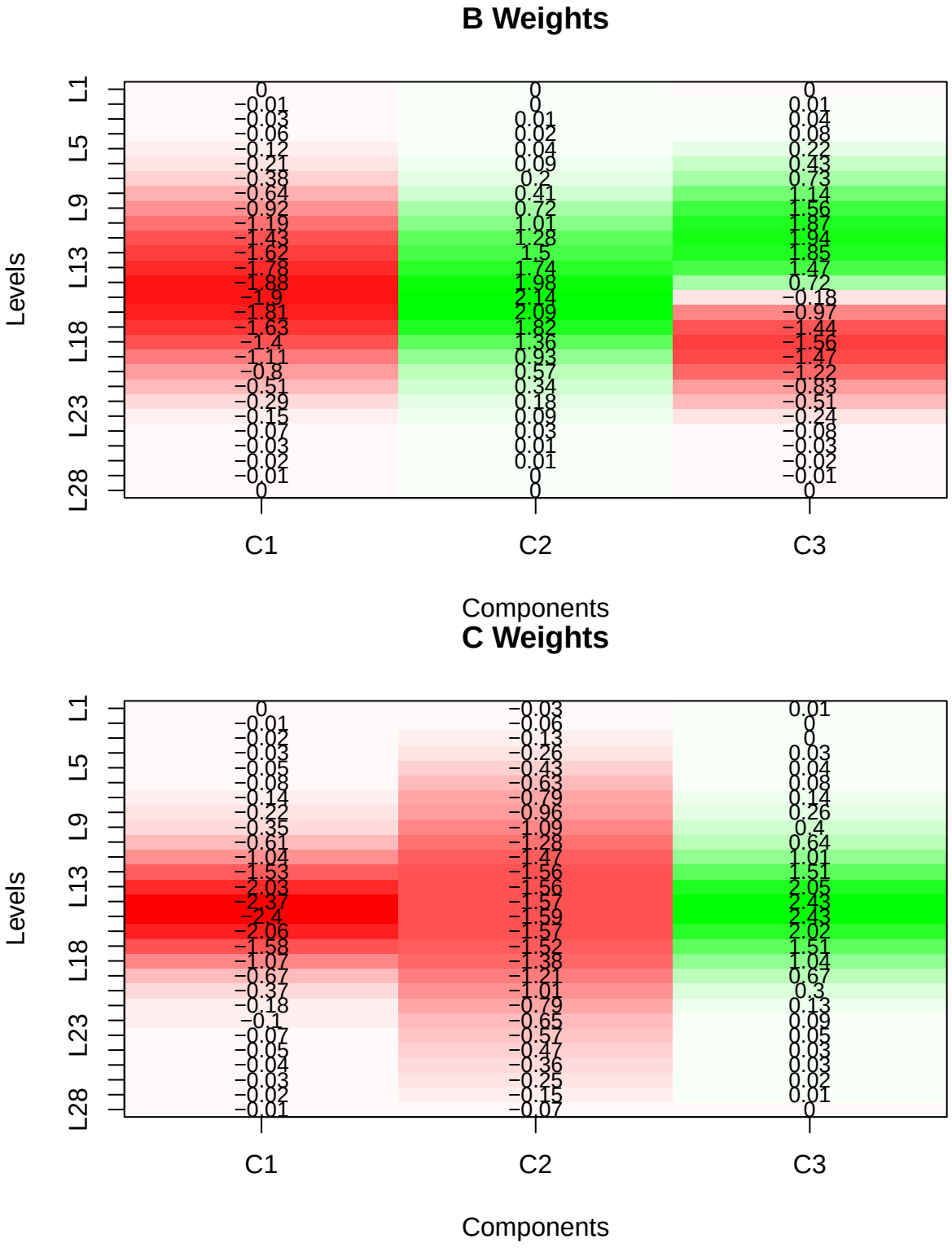
```
##   nfac alpha lambda gamma cost ntree nodesize size  decay rda.alpha delta eta
## 1    2    NA     NA    NA   NA    NA       NA  3.6 0.0082    0.5328  0.02  NA
## 2    3    NA     NA    NA   NA    NA       NA  5.6 0.0226    0.5328  0.04  NA
##   max.depth subsample nrounds
## 1        NA        NA      NA
## 2        NA        NA      NA
```

Accuracy values are between 0.65 and 0.71. The three-component Parafac model with the RDA classifier performed best. In addition, average optimal tuning parameters are available for each classifier.

Next, we use `plotcpfa`. Looking at plots, we can search for relationships between the levels of mode A, B, or C and model components. In this case, the three modes correspond to the three dimensions of the vessels.

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

# plot heatmaps of component weights for optimal model
results3 <- plotcpfa(outputR3, nstart = 10, ctol = 1e-6, verbose = FALSE)
```






We omit interpretations of the three components, given the difficulty of visualizing each blood vessel object. For more information about this dataset and classification work using it, consider exploring Yang, Xia, Kin, and Igarashi (2020); Yang et al. (2023); and Yang, Shi, and Ni (2021).

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