

Supervised Multiblock analyses

CODE ▼

Florence Mehl

March 17, 2023

- Nutrimouse dataset
- Discriminant analysis of genotypes
 - Question 1: based on lipids and genes data, can we discriminate wt vs ppar samples ?
 - Question 2: Choose optimal number of latent variables?
 - Question 3: Is the model statistically significant?
 - Question 4: what is the variance explained for each block by each latent variable and globally?
 - Question 5: observe the samples distributions in the space of the latent variables.
 - Question 6: which genes and lipids are discriminant for genotype?

Nutrimouse dataset

The data sets come from a nutrigenomic study in the mouse (Martin et al., 2007) in which the effects of five regimens with contrasted fatty acid compositions on liver lipids and hepatic gene expression in mice were considered.

Two sets of variables were acquired on forty mice: - genes: expressions of 120 genes measured in liver cells, selected (among about 30,000) as potentially relevant in the context of the nutrition study. These expressions come from a nylon macroarray with radioactive labelling - lipids: concentrations (in percentages) of 21 hepatic fatty acids measured by gas chromatography

Biological units (mice) were cross-classified according to two factors experimental design (4 replicates): - genotype: 2-levels factor, wild-type (WT) and PPAR α -/- (PPAR) - diet: 5-levels factor. Oils used for experimental diets preparation were corn and colza oils (50/50) for a reference diet (REF), hydrogenated coconut oil for a saturated fatty acid diet (COC), sunflower oil for an Omega6 fatty acid-rich diet (SUN), linseed oil for an Omega3-rich diet (LIN) and corn/colza/enriched fish oils for the FISH diet (43/43/14)

HIDE

```
data("nutrimouse")
genes <- nutrimouse$gene
lipids <- nutrimouse$lipid
metadata <- data.frame(genotype = nutrimouse$genotype, diet = nutrimouse$diet)
metadata$sample_name <- paste0(rownames(metadata), "_", metadata$genotype, "_", metadata$diet)
rownames(genes) <- metadata$sample_name
rownames(lipids) <- metadata$sample_name
```

Discriminant analysis of genotypes

Question 1: based on lipids and genes data, can we discriminate wt vs ppar samples ?

Run block.plsda analysis with block.plsda() from mixomics package

HIDE

```
# prepare data
blockPLS_data <- list(genes=genes, lipids=lipids)
genotype <- as.factor(metadata$genotype)

# run analysis
blockPLS_res <- block.plsda(X = blockPLS_data, Y = genotype, design = "full", all.outputs =
T, ncomp = 10)
```

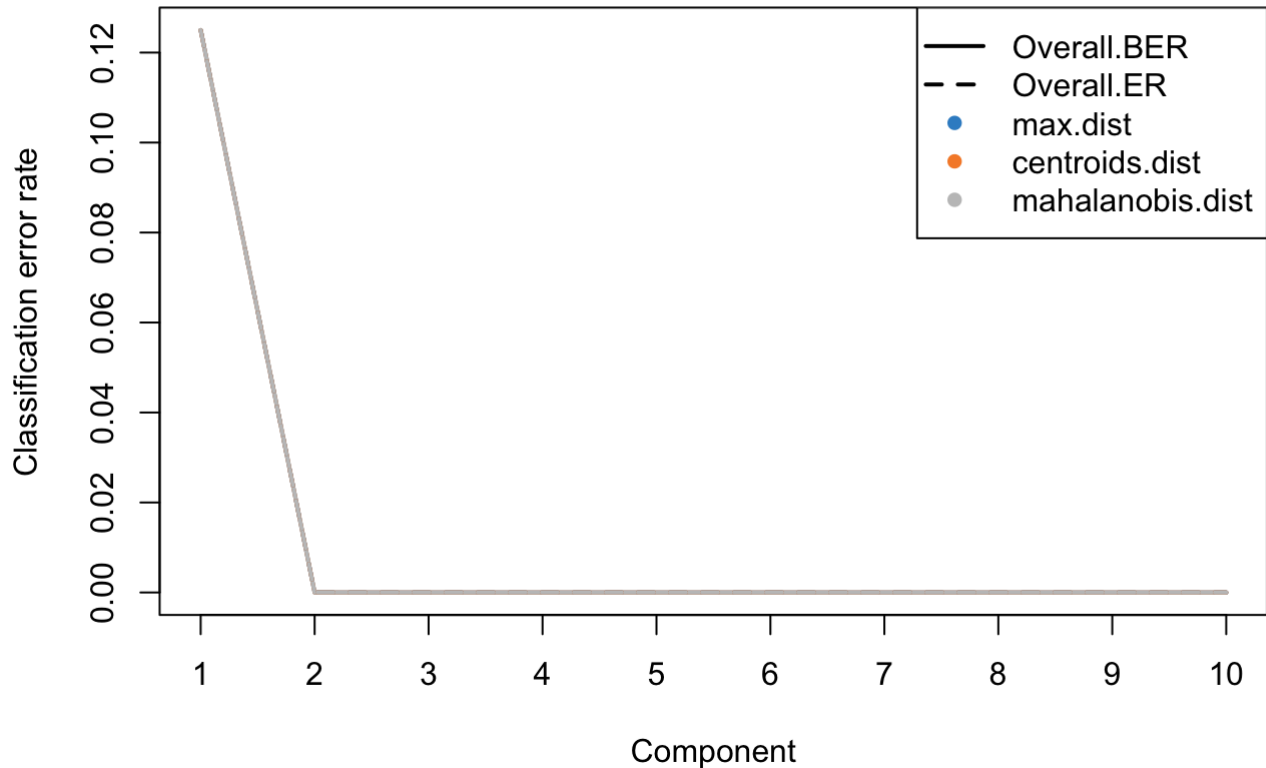
Question 2: Choose optimal number of latent variables?

Run perf() plot the results with plot() Run the analysis with optimal number of latent variables

HIDE

```
blockPLS_perf <- perf(blockPLS_res, validation = 'Mfold', folds = 7, nrepeat = 1, auc = TRUE,
cpus=2, progressBar = FALSE)

plot(blockPLS_perf)
```



HIDE

```
blockPLS_res <- block.plsda(X = blockPLS_data, Y = genotype, design = "full", all.outputs =
T, ncomp = 2)
```

Question 3: Is the model statistically significant?

Run a permutation test with `DIABLO.test()` from `RVAideMemoire` package

HIDE

```
blockPLS_permtest <- DIABLO.test(blockPLS_res, progress = FALSE)
```

Question 4: what is the variance explained for each block by each latent variable and globally?

- for each block: AVE_X
- global: AVE[["AVE_outer"]]

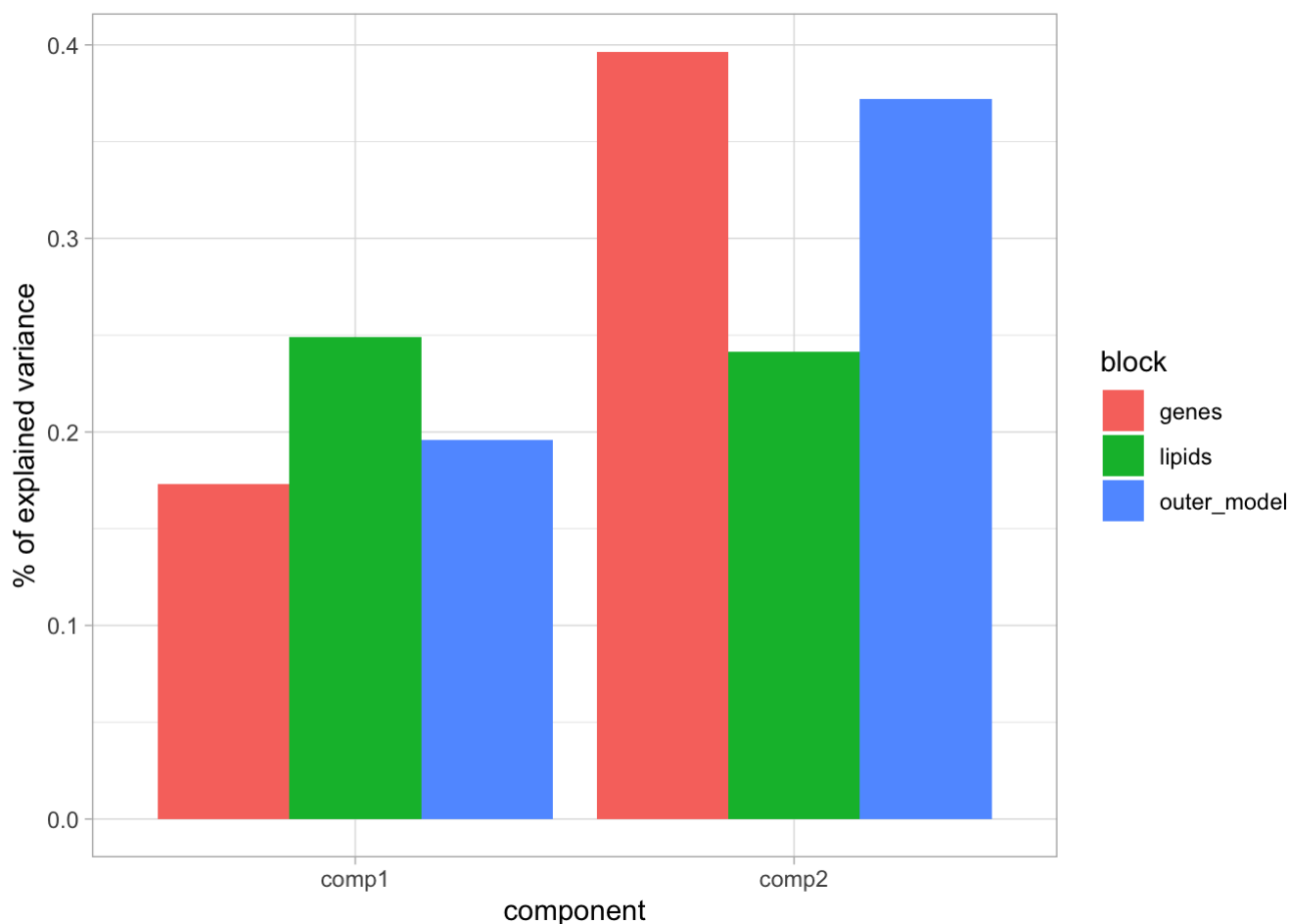
HIDE

```

blockPLS_expl <- do.call("rbind",blockPLS_res$AVE$AVE_X[1:2])
blockPLS_expl <- rbind(blockPLS_expl, blockPLS_res$AVE[["AVE_outer"]])
rownames(blockPLS_expl)[3] <- "outer_model"
blockPLS_expl <- melt(blockPLS_expl)
colnames(blockPLS_expl) <- c("block", "comp", "value")

ggplot(blockPLS_expl, aes(x=comp, y=value, fill=block)) +
  geom_bar(stat="identity", position=position_dodge()) +
  labs(x="component",
       y="% of explained variance") +
  theme_light()

```

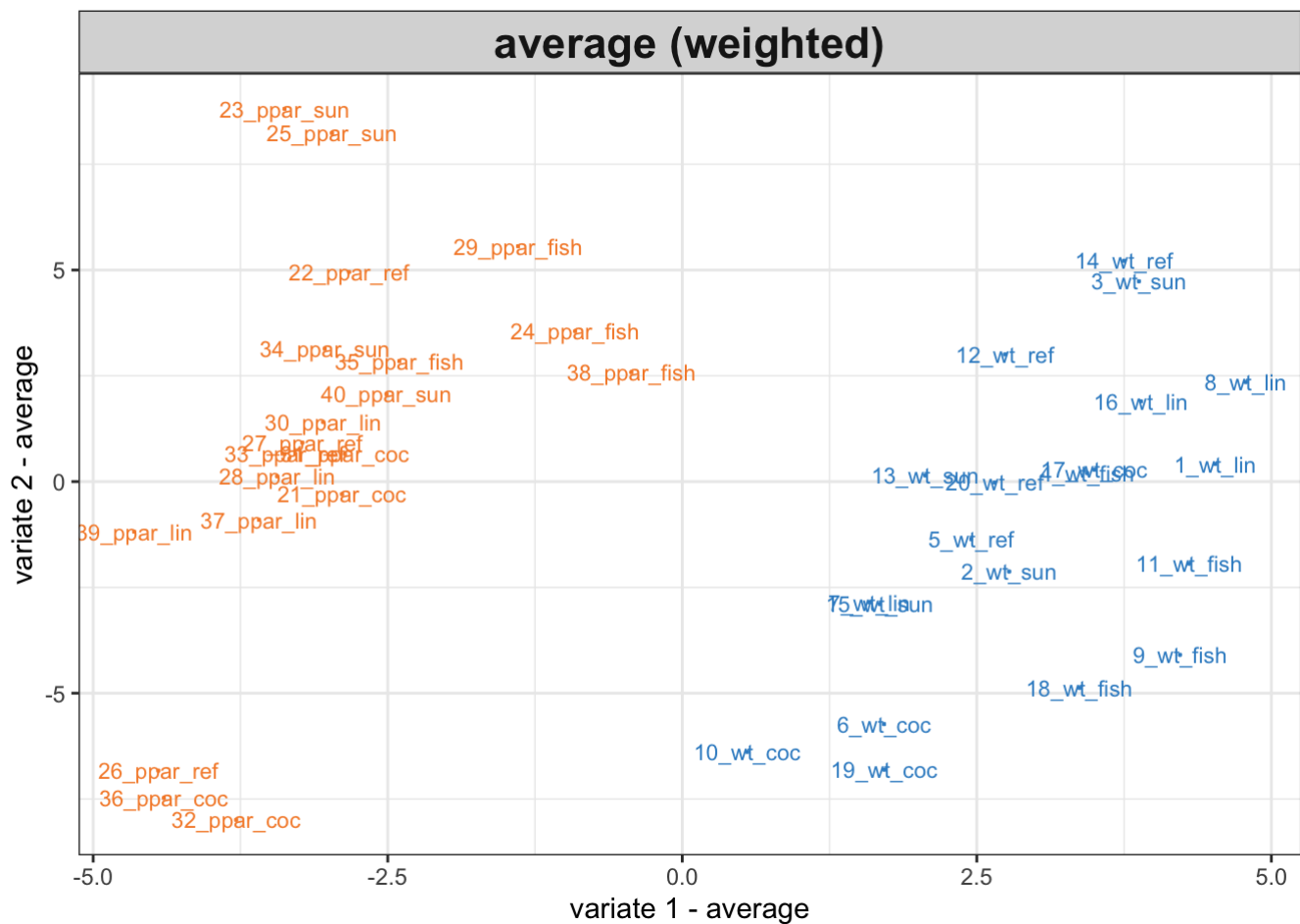


Question 5: observe the samples distributions in the space of the latent variables.

- plot scores with plotIndiv()

HIDE

```
plotIndiv(blockPLS_res, block = "weighted.average")
```



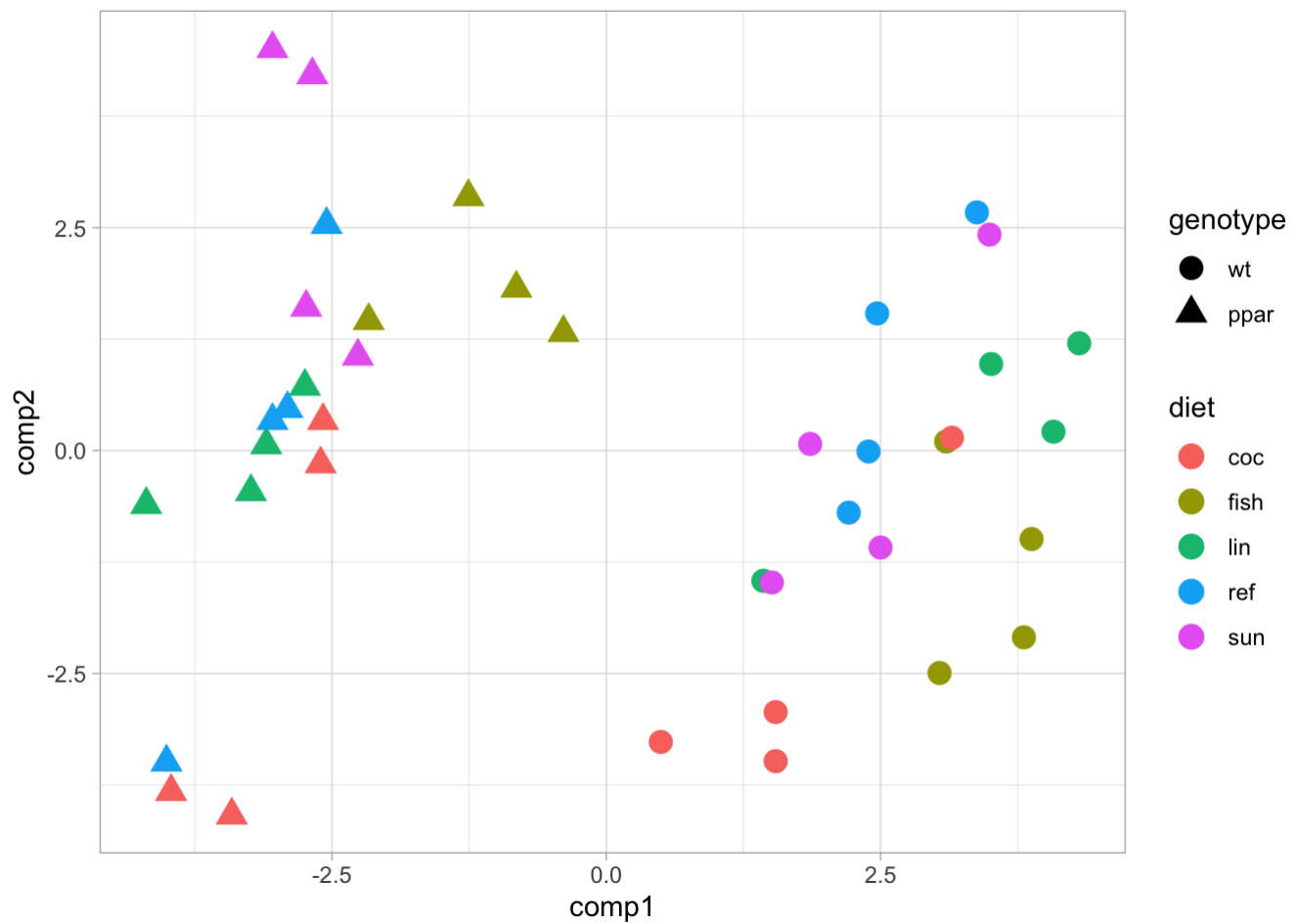
HIDE

ou:

```
blockPLS_variates.weighted <- blockPLS_res$variates[c("genes", "lipids")]
for(omic in c("genes", "lipids")){
  for(comp in c("comp1", "comp2")){
    blockPLS_variates.weighted[[omic]][,comp] <- blockPLS_variates.weighted[[omic]][,comp]
    p] * blockPLS_res$weights[omic, comp]
  }
}
blockPLS_scores.weighted <- abind(blockPLS_variates.weighted[c("genes", "lipids")], along =
3)
blockPLS_scores.weighted <- apply(blockPLS_scores.weighted, c(1,2), mean)

blockPLS_scores.weighted <- data.frame(metadata, blockPLS_scores.weighted)

ggplot(blockPLS_scores.weighted, aes(x=comp1, y=comp2, col=diet, shape = genotype)) +
  geom_point(size=4) +
  theme_light()
```



Question 6: which genes and lipids are discriminant for genotype?

- plot loadings with plotVar()

HIDE

```
plotVar(blockPLS_res)
```