

Errata for “Chemometrics with R: Multivariate Data Analysis in the Natural Sciences and Life Sciences” by Ron Wehrens

Changes in the R code of the book, described below, are already included in the latest version of the `ChemometricsWithR` package.

p. 20: “This leads to the right plot in Figure 3.6.” should read: “This leads to the smooth line in the left plot of Figure 3.6.”

p. 25: Argument “`global`” in the construction of object `lcms.warpglobal` should be “`multiple`”.

p. 29: The lines

```
> plot(mz, x[,1], type = "l", xlab = "m/z", ylab = "I")
> points(mz, x[w2,2], col = "gray")
```

should be replaced by

```
> plot(time, lcms[1,,2], type = "l", xlab = "Time", ylab = "I",
+       xlim = c(time[600], time[1300]))
> lines(time, lcms[1,,3] + 1e6, lty = 2, col = "blue")
> lines(time, lcms[1, w2, 3] + 2e6, col = "green")
> legend("topleft", col = c("black", "blue", "green"), lty = c(1,2,1),
+       legend = c("Reference", "Sample", "Warped sample"))
```

to get Figure 3.12.

p. 32: Before the first `plot` command, the following code should be inserted:

```
> prostate.mz <- Prostate2000Raw$mz
```

p. 36: Before the first `boxplot` command, issue `wines.mc <- scale(wines, scale = FALSE)`

p. 49: the second `barplot` should use `wines.vars` rather than `wines.variances`.

p. 55: three lines from the bottom: the line containing the `abline` command should be removed.

p. 58: the `plot` command for classical MDS should use `wines.cmdscale`, without the `points` list element.

p. 114: the three lines

```
> x <- seq(.4, 5.4, length = 251)
> y <- seq(250, 1750, length = 251)
> gridXY <- cbind(rep(x, each = length(y)), rep(y, length(x)))
```

should appear before the last chunk of R code on page 113.

p. 127: Variable `X.rpart` should be `wines.rpart` in the second piece of R code, creating Figure 7.6.

p. 131: Variable `vint` should be `vintages[odd]` in the for-loop of the R code creating Figure 7.9; in the beginning of that bit of code the following command is missing:

```
X <- wines[odd,c(7, 13)]
```

- p. 136:** Variable `prost.rpart` should be `prost.rprt` in the plotting command for Figure 7.10.
- p. 143:** the second line in the second chunk of R code should read: `predict(wines.nnet, w.df[even,], type = "class")`
- p. 152:** the `rms` line should read `rms(Ytr, fitted(Blm))`
- p. 169:** the code `gas.nnet.pred <- predict(gas.nnet, Xeven.scores)` should be added before the call to the `rms` function
- p. 203:** function `addtest` needs `prost.df[even, -1]` rather than `prost[even,]` in order to have corresponding variable names.
- p. 209:** the RMSEP values reported in the book are calculated using the odd samples only: `subset = odd` should be added to the `pcr` function call to obtain the same numbers.
- p. 213:** `Tii <- solve(TSS)` should be added before the call to the `mahalanobis` function.
- p. 213:** in the function definition of `pls.cvfun` one should use the number of components rather than the number of variables – the last line of the function should read
- ```
-MSEP(pls.obj, estimate = "CV")$val[pls.obj$ncomp + 1]
```
- p. 214:** `xlim` is `c(0, .2)` rather than `c(0, .1)`.
- p. 246:** Nine lines from the bottom of the page, one should plot `prost.trn.err` rather than `1 - prost.trn.err`. In addition, there is a comma missing before `ylab`, 8 lines from the bottom.
- p. 248:** The last lines of the page should read:
- ```
> prostate.pls <- pls(class ~ msdata, ncomp = 16,
+                   data = prostate.df, subset = odd,
+                   validation = "CV", scale = TRUE)
```
- p. 271:** The `signal` package was mistakenly omitted from the list of R packages in the appendix.