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

```r
> plot(mz, x[,1], type = "l", xlab = "m/z", ylab = "I")
> points(mz, x[wx2,2], col = "gray")
```

should be replaced by

```r
> 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[, wx2, 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:

```r
> 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

```r
> 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:

```r
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 <- plsr(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.
Chemometrics with R
Multivariate Data Analysis in the Natural Sciences and Life Sciences
Wehrens, R.
2011, XIV, 286 p. 99 illus., Softcover
ISBN: 978-3-642-17840-5