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[wx2,2], 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, 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:

> 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 \texttt{prost.rpart} should be \texttt{prost.rprt} in the plotting command for Figure 7.10.

p. 143: the second line in the second chunk of R code should read: \texttt{predict(wines.nnet, w.df[even,], type = "class")}

p. 152: the \texttt{rms} line should read \texttt{rms(Ytr, fitted(Blm))}

p. 169: the code \texttt{gas.nnet.pred <- predict(gas.nnet, Xeven.scores)} should be added before the call to the \texttt{rms} function

p. 203: function \texttt{addtest} needs \texttt{prost.df[even, -1]} rather than \texttt{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: \texttt{subset = odd} should be added to the \texttt{pcr} function call to obtain the same numbers.

p. 213: \texttt{Tii <- solve(TSS)} should be added before the call to the \texttt{mahalanobis} function.

p. 213: in the function definition of \texttt{pls.cvfun} one should use the number of components rather than the number of variables – the last line of the function should read

\[-\text{MSEP}(\texttt{pls.obj, estimate = "CV"})\texttt{val[pls.obj$ncomp + 1]}\]

p. 214: \texttt{xlim} is \texttt{c(0, .2)} rather than \texttt{c(0, .1)}.

p. 246: Nine lines from the bottom of the page, one should plot \texttt{prost.trn.err} rather than \texttt{1 - prost.trn.err}. In addition, there is a comma missing before \texttt{ylab}, 8 lines from the bottom.

p. 248: The last lines of the page should read:

\[ \texttt{> prostate.pls <- plsr(class ~ msdata, ncomp = 16,} \]
\[ \texttt{+ \hspace{1cm} data = prostate.df, subset = odd,} \]
\[ \texttt{+ \hspace{1cm} validation = "CV", scale = TRUE)} \]

p. 271: The \texttt{signal} package was mistakenly omitted from the list of R packages in the appendix.
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