detlimitr

Peter Watkins

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An introduction to the detlimitr package

The *detlimitr* (estimating **det**ection **limit**s using **R**) package contains functions for use with calibration data in analytical chemistry,

The detection limit is an important figure of merit in chemical analysis. It is also known as the lower limit of detection, or LOD (limit of detection), and can be defined as the lowest quantity of a substance that can be distinguished from the absence of that substance (a blank value) with a stated confidence level (generally 99%).

If required, the *detlimiter* package can be downloaded using

```
#install.packages("devtools")
devtools::install_github("peterjwatkins/detlimitr", force=TRUE)
```

In this package, the detection limit is calculated using three approaches; i) Miller and Miller, ii) Vogelsang and Hädrich, iii) Hubert and Vos, and iv) the R chemCal package. Note that references are listed below, and that a linear relationship is assumed between the measured response and standard concentration.

The function *reportDL* returns the calculated detection limits according to the three approaches while *plotDL* shows a segment of the calibration curve, indicating where each point lies on the curve. The function *tabulateDL* summarises the data in a tabular format.

Some example code:

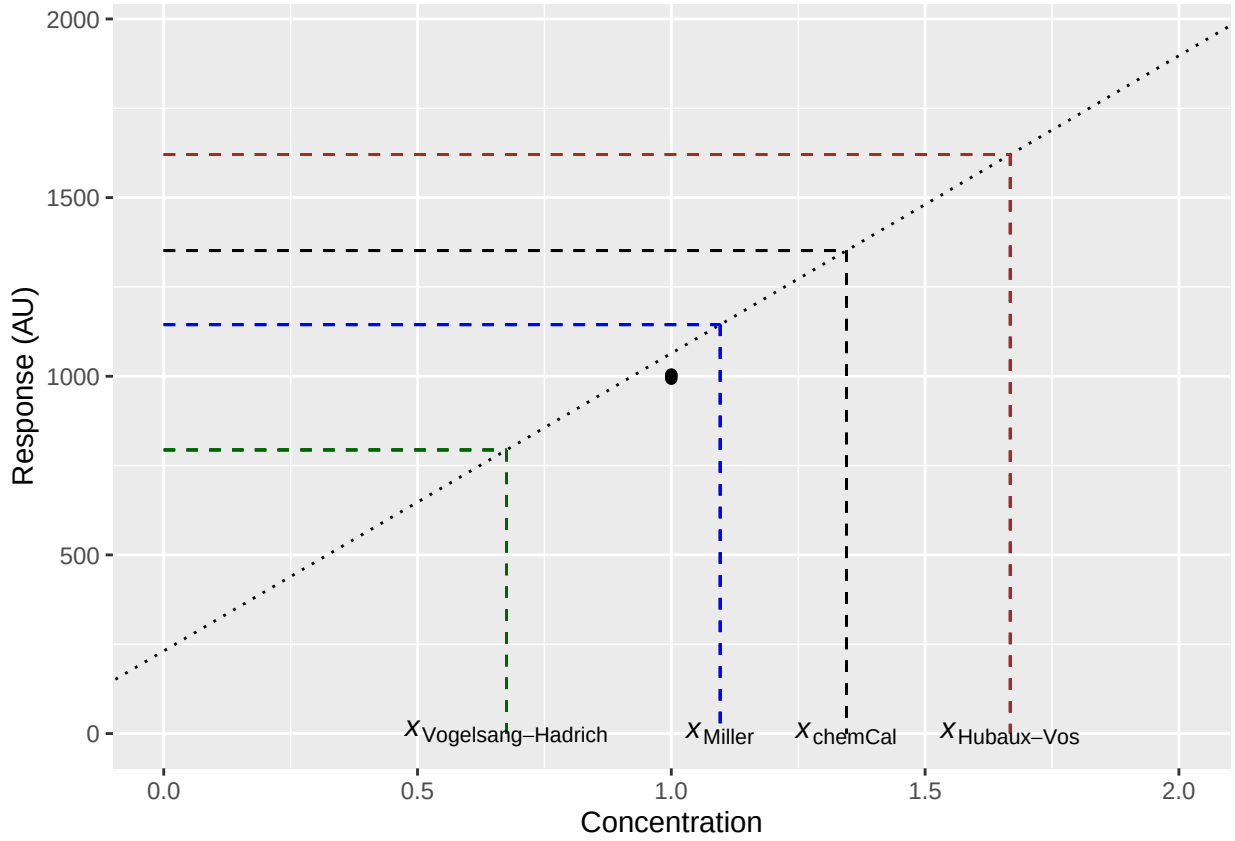
```
library(detlimitr)
data(mtbe)
head(mtbe)
```

```
## # A tibble: 6 x 2
##       x     y
##   <dbl> <dbl>
## 1   1    1005
## 2   1    1003
## 3   1     998
## 4   1     993
## 5   2.9  2551
## 6   2.9  2548
```

```
summaryDL(mtbe)
```

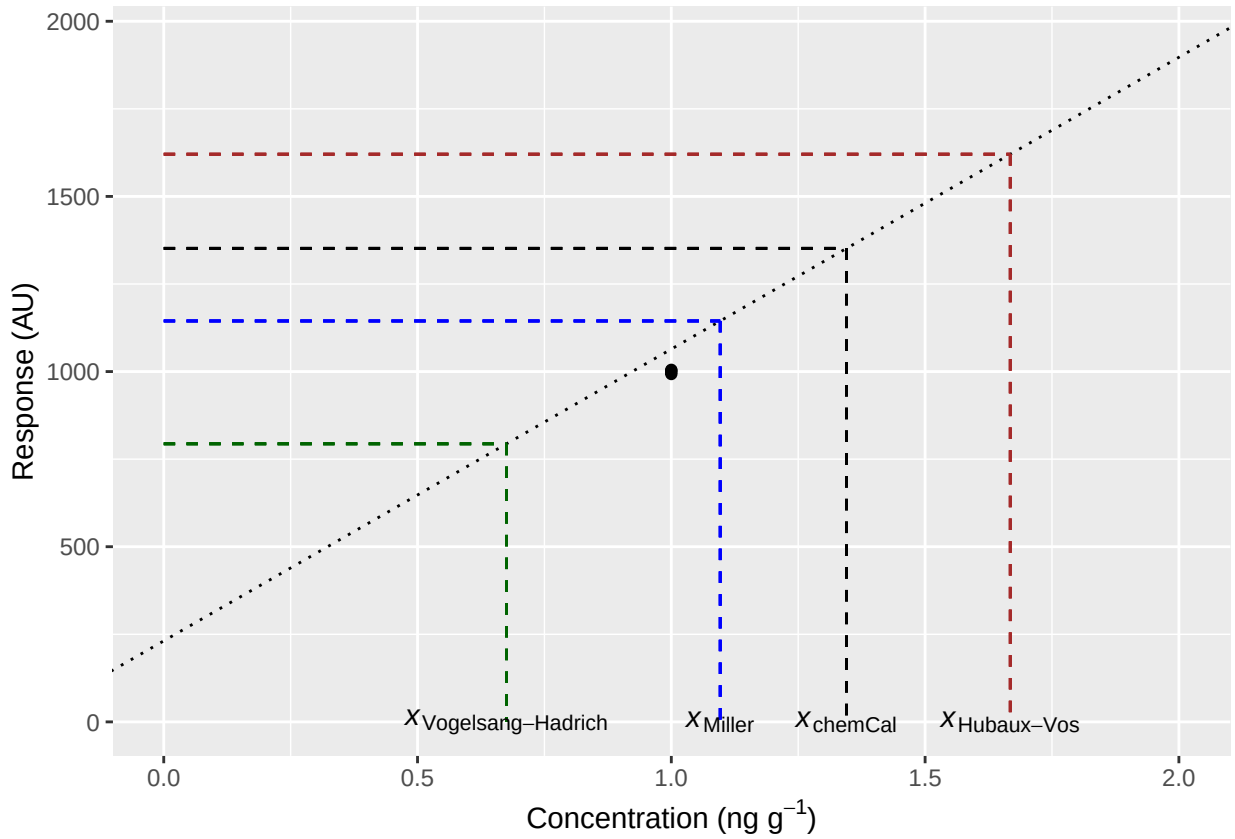
```
## Miller 1.1
## Vogelsang-Hadrich 0.7
## chemCal 1.3
## Hubaux-Vos 1.7
```

```
#tabulateDL(mtbe)
plotDL(mtbe)
```



The graph resulting from *plotDL* has generic labels on the plot. This can be changed using appropriate *ggplot2* commands. For example,

```
p <- plotDL(mtbe)
p +
  ggplot2::xlab(expression(paste("Concentration (ng", " ", "g" ^ {-1}, ")")))
```



References

i) J.C. Miller and J.N. Miller (1993), "Statistics for Analytical Chemistry", 3rd ed., Prentice-Hall.

ii) J. Vogelgesang and J. Hädrich (1998), Accred. Qual. Assur., 3:242-255.

iii) A. Hubaux and G. Vos (1970), Anal. Chem., 42:849-855 & D.T. O'Neill, E.A. Rochette and P.J. Ramsay, (2002), Anal. Chem., 74:5907-5911

iv) J. Ranke (2018), chemCal: Calibration Functions for Analytical Chemistry, https://CRAN.R-project.org/package=chemCal