Orthogonal Nonlinear Least-Squares Regression in R

Andrej-Nikolai Spiess
Department of Andrology
University Hospital Hamburg-Eppendorf
a.spiess@uke.de

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Abstract

Orthogonal nonlinear least squares (ONLS) regression is a scarcely applied and largely over-looked regression technique that comes into question when one encounters an "error in variables" problem. While classical nonlinear least squares (NLS) aims to minimize the sum of squared vertical residuals, ONLS minimizes the sum of squared orthogonal residuals. The method is based on finding points on the fitted line that are orthogonal to the data by minimizing for each (x_i, y_i) the Euclidean distance $\|D_i\|$ to some point (x_{0i}, y_{0i}) on the fitted curve. There is a 25 year old FORTRAN implementation for ONLS available (ODRPACK, http://www.netlib.org/toms/869.zip), which has been included in the 'scipy' package for Python (http://docs.scipy.org/doc/scipy-0.14.0/reference/odr.html). Here, `onls` has been developed for easy future algorithm tweaking in R. The results obtained from `onls` are exactly similar to those found in [1, 4]. The implementation is based on an inner loop using `optimize` for each (x_i, y_i) to find $\min \|D_i\|$ within some border $[x_{i-w}, x_{i+w}]$ and an outer loop for the fit parameters using `nls.lm` of the 'minpack' package.

Overview

The `onls` package offers orthogonal nonlinear least-squares regression in R. In a standard nonlinear regression setup, we estimate parameters $\boldsymbol{\beta}$ in a nonlinear model $y_i = f(x_i, \boldsymbol{\beta}) + \varepsilon_i$, with $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$, by minimizing the residual sum-of-squares of the vertical distances

$$\min_{\beta} \sum_{i=1}^{n} (y_i - f(x_i, \boldsymbol{\beta}))^2 \tag{1}$$

In contrast, orthogonal nonlinear regression aims to estimate parameters $\boldsymbol{\beta}$ in a nonlinear model $y_i = f(x_i + \delta_i, \boldsymbol{\beta}) + \varepsilon_i$, with $\varepsilon_i, \delta_i \sim \mathcal{N}(0, \sigma^2)$, by minimizing the sum-of-squares of the orthogonal distances

$$\min_{\boldsymbol{\beta}, \delta} \sum_{i=1}^{n} ([y_i - f(x_i + \delta_i, \boldsymbol{\beta})]^2 + \delta_i^2) \tag{2}$$

We do this by using the orthogonal distance D_i from the point (x_i, y_i) to some point (x_{0i}, y_{0i}) on the curve $f(x_i, \hat{\boldsymbol{\beta}})$ that minimizes the Euclidean distance

$$\min \|D_i\| \equiv \min \sqrt{(x_i - x_{0i})^2 + (y_i - y_{0i})^2} \tag{3}$$

The minimization of the Euclidean distance is conducted by using an inner loop on each (x_i, y_i) with the `optimize` function that finds the corresponding (x_{0i}, y_{0i}) in some window $[a, b]$:

$$\operatorname*{argmin}_{x_{0i} \in [a,b]} \sqrt{(x_i - x_{0i})^2 + (y_i - f(x_{0i}, \hat{\boldsymbol{\beta}}))^2} \tag{4}$$

Algorithm and Implementation

In detail, `onls` conducts the following steps:

1) A normal (non-orthogonal) nonlinear model is fit by `nls.lm` to the data. This approach has been implemented because parameters of the orthogonal model are usually within a small window of the standard NLS model. The obtained parameters are passed to the ONLS routine, which is:

2) Outer loop: Levenberg-Marquardt minimization of the orthogonal distance sum-of-squares $\sum_{i=1}^{N} \|D_i\|^2$ using `nls.lm`, optimization of $\boldsymbol{\beta}$.

3) Inner loop: For each (x_i, y_i), find $(x_{0i}, f(x_{0i}, \hat{\boldsymbol{\beta}}))$, $x_{0i} \in [a, b]$, that minimizes $\|D_i\|$ using `optimize`. Return vector of orthogonal distances $\|\vec{D}\|$.

The outer loop (`nls.lm`) scales with the number of parameters p in the model, probably with $\mathcal{O}(p)$ for evaluating the 1-dimensional Jacobian and $\mathcal{O}(p^2)$ for the two-dimensional Hessian. The inner loop has $\mathcal{O}(n)$ for finding $\min \|D_i\|$, summing up to $\mathcal{O}(n(p + p^2))$. Simulations with different number of n by fixed p showed that the processor times scale exactly linearly.

How to use

1. Building the model

As in the 'Examples' section of `nls` (here with 10% added error), we supply a formula, data environment and starting parameters to the model:

```
> library(onls)
> DNase1 <- subset(DNase, Run == 1)
> DNase1$density <- sapply(DNase1$density, function(x) rnorm(1, x, 0.1 * x))
> mod1 <- onls(density ~ Asym/(1 + exp((xmid - log(conc))/scal)),
+              data = DNase1, start = list(Asym = 3, xmid = 0, scal = 1))

Obtaining starting parameters from ordinary NLS...
  Passed...
 Relative error in the sum of squares is at most `ftol'.
Optimizing orthogonal NLS...
  Passed... Relative error in the sum of squares is at most `ftol'.
```

2. Looking at the model and checking orthogonality

`print`ing the model will give us the estimated coefficients, the (classical) vertical residual sum-of-squares, the orthogonal residual sum-of-squares, and **most importantly** information on how many points (x_i, y_i) are orthogonal to (x_{0i}, y_{0i}) on the fitted curve $f(x_i + \delta_i, \boldsymbol{\beta}) + \varepsilon_i$. This is accomplished using the independent checking routine `check_o` which calculates the angle between the slope m_i of the tangent obtained from the first derivative at (x_{0i}, y_{0i}) and the slope n_i of the `onls`-minimized Euclidean distance between (x_{0i}, y_{0i}) and (x_i, y_i):

$$\tan(\alpha_i) = \left| \frac{m_i - n_i}{1 + m_i \cdot n_i} \right|, \ m_i = \frac{df(x, \beta)}{dx_{0i}}, \ n_i = \frac{y_i - y_{0i}}{x_i - x_{0i}}$$

$$=> \alpha_i[°] = \tan^{-1}\left(\left| \frac{m_i - n_i}{1 + m_i \cdot n_i} \right| \right) \cdot \frac{360}{2\pi}$$

(5)

which should be 90°, if the Euclidean distance has been minimized.

```
> mod1

Nonlinear orthogonal regression model
  model: density ~ Asym/(1 + exp((xmid - log(conc))/scal))
   data: DNase1
  Asym   xmid   scal
2.0807 1.2000 0.9195
 vertical residual sum-of-squares: 0.08725
 orthogonal residual sum-of-squares: 0.08509
 PASSED: 16 out of 16 fitted points are orthogonal.

Number of iterations to convergence: 3
Achieved convergence tolerance: 1.49e-08
```

In this case, all points have been fitted orthogonal, giving the `PASSED` message and all is well. If a `FAILED` message is given, not all of the points are orthogonal and some tweaking is necessary, see next chapter.

3. Tweaking the model in case of non-orthogonality

Two arguments to the `onls` function mainly influence the success of overall orthogonal fitting:

extend: By default, it is set to `c(0.2, 0.2)`, which means that (x_{0i}, y_{0i}) in the inner loop

are also optimized in an extended predictor value x range of $[\min(x) - 0.2 \cdot \text{range}(x), \max(x) + 0.2 \cdot \text{range}(x)]$. This is important for the values at the beginning and end of the data, because the resulting model can display significantly different curvature if (x_{0i}, y_{0i}) are forced to be within the predictor range, often resulting in a loss of orthogonality at the end points.

In the following, we will take an example from the ODRPACK implementation [1].

```
> x <- c(0, 10, 20, 30, 40, 50, 60, 70, 80, 85, 90, 95, 100, 105)
> y <- c(4.14, 8.52, 16.31, 32.18, 64.62, 98.76, 151.13, 224.74, 341.35,
+         423.36, 522.78, 674.32, 782.04, 920.01)
> DAT <- data.frame(x, y)
> mod4 <- onls(y ~ b1 * 10^(b2 * x/(b3 + x)), data = DAT,
+              start = list(b1 = 1, b2 = 5, b3 = 100))

Obtaining starting parameters from ordinary NLS...
  Passed...
 Relative error in the sum of squares is at most `ftol'.
Optimizing orthogonal NLS...
  Passed... Relative error in the sum of squares is at most `ftol'.
```

With

```
> coef(mod4)

       b1         b2         b3
 4.487871   7.188155 221.837807
```

we get the same coefficients as in the ODRPACK implementation (4.4879/7.1882/221.8383) and with

```
> deviance_o(mod4)

[1] 15.26281
attr(,"label")
[1] "Deviance (RSS) of orthogonal residuals from orthogonal model"
```

the same orthogonal residual sum-of-squares (15.263), as both given on page 363.

However, if we **do not use** the (default) extended predictor range and set `extend = c(0, 0)`, x_1 and x_{14} are non-orthogonal, as analyzed by the `check_o` function. See α_1 and α_{14}:

```
> mod5 <- onls(y ~ b1 * 10^(b2 * x/(b3 + x)), data = DAT,
+              start = list(b1 = 1, b2 = 5, b3 = 100), extend = c(0, 0))

Obtaining starting parameters from ordinary NLS...
  Passed...
 Relative error in the sum of squares is at most `ftol'.
Optimizing orthogonal NLS...
  Passed... Relative error in the sum of squares is at most `ftol'.

> check_o(mod5)

    x           x0      y          y0      alpha       df/dx Ortho
1    0 6.268415e-09   4.14    4.519317 71.480996  0.3349642 FALSE
2   10 9.701772e+00   8.52    9.005909 89.999996  0.6137531  TRUE
3   20 1.934099e+01  16.31   16.928822 89.999997  1.0649360  TRUE
4   30 2.999583e+01  32.18   32.182244 89.998082  1.8596599  TRUE
5   40 4.244013e+01  64.62   63.893359 89.999994  3.3580964  TRUE
6   50 5.094935e+01  98.76   98.564953 89.999995  4.8672676  TRUE
7   60 5.988618e+01 151.13  151.146249 89.999556  7.0049505  TRUE
8   70 6.872289e+01 224.74  224.870231 89.999820  9.8067846  TRUE
9   80 7.862153e+01 341.35  341.448888 89.999995 13.9398003  TRUE
10  85 8.398467e+01 423.36  423.420823 89.999851 16.6939640  TRUE
```

```
11   90 8.942638e+01 522.78 522.808813 89.999961 19.9081116   TRUE
12   95 9.625199e+01 674.32 674.269107 89.999989 24.6004639   TRUE
13  100 1.003675e+02 782.04 782.026781 89.998525 27.8176079   TRUE
14  105 1.050000e+02 920.01 919.996237  1.793663 31.8165855  FALSE
```

window: is the window $[x_{i-w}, x_{i+w}]$ in which `optimize` searches for (x_{0i}, y_{0i}) to minimize $\|D_i\|$. The default of `window = 12` works quite well with sample sizes $n > 25$, but may be tweaked, as in the following example when the x values are very close in a region:

```
> x <- 1:100
> y <- x^2
> set.seed(123)
> y <- sapply(y, function(a) rnorm(1, a, 0.1 * a))
> DAT <- data.frame(x, y)
> mod6 <- onls(y ~ x^a, data = DAT, start = list(a = 1))

Obtaining starting parameters from ordinary NLS...
  Passed...
 Relative error in the sum of squares is at most `ftol'.
Optimizing orthogonal NLS...
  Passed... Relative error in the sum of squares is at most `ftol'.

> mod6

Nonlinear orthogonal regression model
  model: y ~ x^a
   data: DAT
     a
2.005
 vertical residual sum-of-squares: 17496215
 orthogonal residual sum-of-squares: 675.3
 FAILED: Only 98 out of 100 fitted points are orthogonal.

Number of iterations to convergence: 2
Achieved convergence tolerance: 1.49e-08
```

Here fitting fails, while it passes when using a larger window size:

```
> mod7 <- onls(y ~ x^a, data = DAT, start = list(a = 10), window = 17)

Obtaining starting parameters from ordinary NLS...
  Passed...
 Conditions for `info = 1' and `info = 2' both hold.
Optimizing orthogonal NLS...
  Passed... Conditions for `info = 1' and `info = 2' both hold.

> mod7

Nonlinear orthogonal regression model
  model: y ~ x^a
   data: DAT
     a
2.005
 vertical residual sum-of-squares: 17496215
 orthogonal residual sum-of-squares: 675.3
 PASSED: 100 out of 100 fitted points are orthogonal.

Number of iterations to convergence: 2
Achieved convergence tolerance: 1.49e-08
```

4. Analysing the orthogonal model with classical `nls` functions

Plotting.

```
> plot(mod1)
```

Due to different scaling of x- and y-axes, orthogonality is often not evident (Figure 1). Scaling both axes equally resolves this issue (Figure 2):

```
> plot(mod1, xlim = c(0, 1), ylim = c(0, 1))
```

Fit features and summaries.

The usual **summary** as in `summary.nls` but with information for *vertical* and *orthogonal* residual standard errors:

```
> summary(mod1)

Formula: density ~ Asym/(1 + exp((xmid - log(conc))/scal))

Parameters:
     Estimate Std. Error t value Pr(>|t|)
Asym   2.0807     0.2171   9.586 2.93e-07 ***
xmid   1.2000     0.2445   4.909 0.000286 ***
scal   0.9195     0.1172   7.843 2.78e-06 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error of vertical distances: 0.08192 on 13 degrees of freedom
Residual standard error of orthogonal distances: 0.0809 on 13 degrees of freedom

Number of iterations to convergence: 3
Achieved convergence tolerance: 1.49e-08
```

Coefficients:

```
> coef(mod1)

    Asym     xmid     scal
2.080736 1.200037 0.919463
```

Variance-Covariance matrix:

```
> vcov(mod1)

           Asym       xmid       scal
Asym 0.04711612 0.05163555 0.02229276
xmid 0.05163555 0.05976263 0.02481897
scal 0.02229276 0.02481897 0.01374315
```

Response value prediction:

```
> predict(mod1, newdata = data.frame(conc = 6))

[1] 1.364039
```

Profiling confidence intervals:

```
> confint(mod1)

           2.5%     97.5%
Asym 1.7474653 2.892930
xmid 0.8038644 2.014958
scal 0.7000968 1.242400
```

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5. Extracting information based on vertical residuals

Models fitted with `onls` incorporate information in respect to the vertical residuals using the classical `S3` functions.

Vertical residuals:

```
> residuals(mod1)

 [1] -0.005079619 -0.002908738  0.041400836  0.047593751 -0.004648065
 [6] -0.002479954 -0.049468760 -0.019612386  0.093471549 -0.031320708
[11] -0.048832182 -0.016833558  0.030648943  0.026080247  0.171009622
[16] -0.192688306
attr(,"label")
[1] "Vertical residuals from orthogonal model"
```

Fitted values corresponding to x:

```
> fitted(mod1)

 [1] 0.02093222 0.02093222 0.09130883 0.09130883 0.18491793 0.18491793
 [7] 0.35726058 0.35726058 0.63631424 0.63631424 1.00609455 1.00609455
[13] 1.38475201 1.38475201 1.68276364 1.68276364
attr(,"label")
[1] "Fitted values from orthogonal model"
```

Vertical residual sum-of-squares:

```
> deviance(mod1)

[1] 0.08725149
attr(,"label")
[1] "Deviance (RSS) of vertical residuals from orthogonal model"
```

Log-likelihood of model using vertical residuals:

```
> logLik(mod1)

'log Lik.' 18.98938 (df=4)
"Log-likelihood using vertical residuals from orthogonal model"
```

6. Extracting information based on orthogonal residuals

The following functions are meant to extract `S3`-type values based on orthogonal residuals. The naming convention is `function_o`.

Orthogonal residuals:

```
> residuals_o(mod1)

 [1] 0.004613135 0.002641351 0.037237239 0.042808006 0.004207884 0.002245143
 [7] 0.045718360 0.018130601 0.089380880 0.029933373 0.048050728 0.016564629
[13] 0.030549923 0.025995981 0.170942651 0.192612742
attr(,"label")
[1] "Orthogonal residuals from orthogonal model"
```

Orthogonal residual sum-of-squares:

```
> deviance_o(mod1)

[1] 0.08508738
attr(,"label")
[1] "Deviance (RSS) of orthogonal residuals from orthogonal model"
```

Log-likelihood of model using orthogonal residuals:

```
> logLik_o(mod1)
```

```
'log Lik.' 19.19031 (df=4)
"Log-likelihood using orthogonal residuals from orthogonal model"
```

7. Extracting information about x_{0i} and y_{0i}

Orthogonal fitting is based on finding some pair (x_{0i}, y_{0i}) on the fitted curve that is orthogonal to (x_i, y_i). Values for x_{0i} and y_{0i} can be extracted with x0 and y0:

Extracting x$_{0i}$:

```
> x0(mod1)
```

```
 [1]  0.04689915  0.04772259  0.21158050  0.21401133  0.38883723  0.38967130
 [7]  0.76374053  0.77432911  1.58853792  1.55367673  3.11642716  3.12204962
[13]  6.25245306  6.25208758 12.50478213 12.49460437
attr(,"label")
[1] "x0 values from orthogonal model"
```

Extracting y$_{0i}$:

```
> y0(mod1)
```

```
 [1] 0.02004308 0.02042235 0.09921394 0.10039442 0.18407909 0.18447050
 [7] 0.35002435 0.35440588 0.64428158 0.63359697 1.00454216 1.00556075
[13] 1.38494968 1.38492024 1.68289751 1.68261249
attr(,"label")
[1] "y0 values from orthogonal model"
```
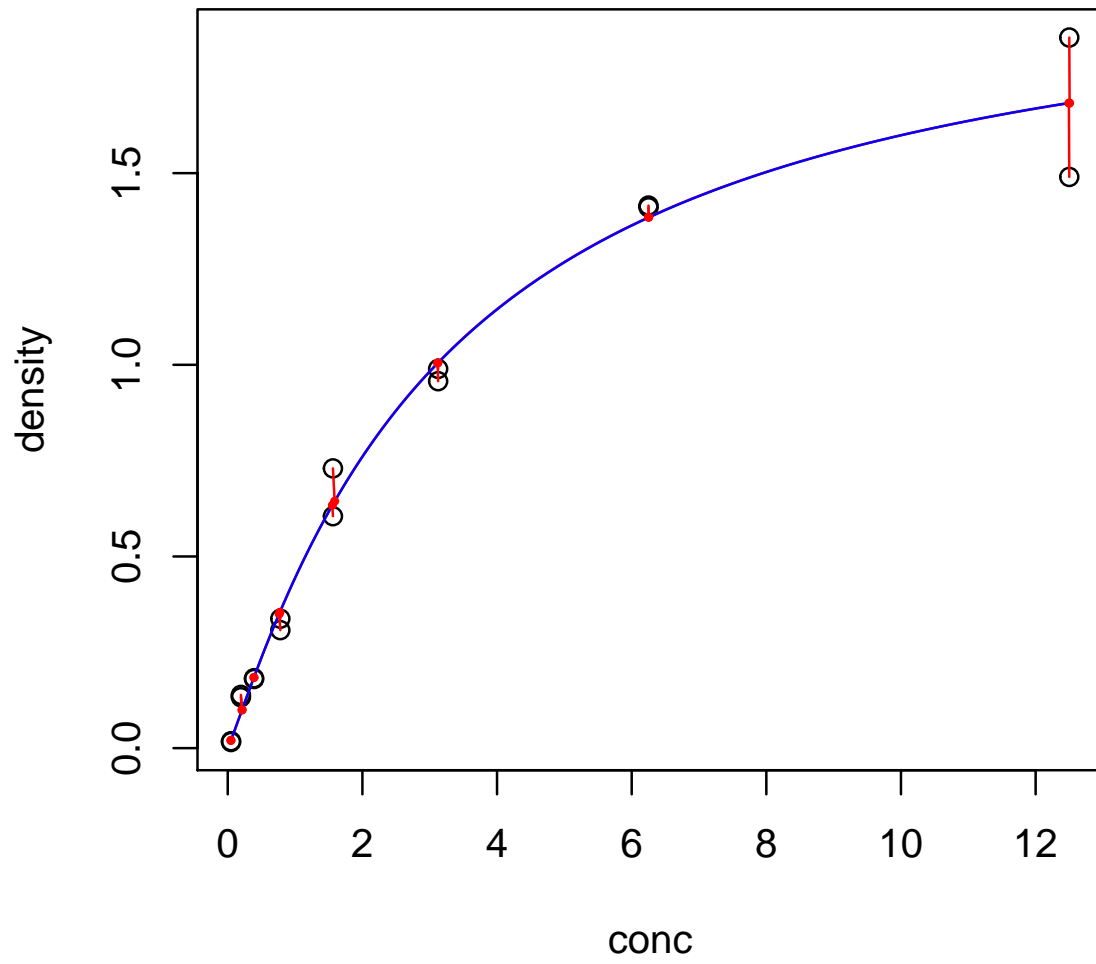
Figure 1: Plot of `mod1` showing the (x_i, y_i) values as black circles, (x_{0i}, y_{0i}) values as red circles and orthogonal lines in red.
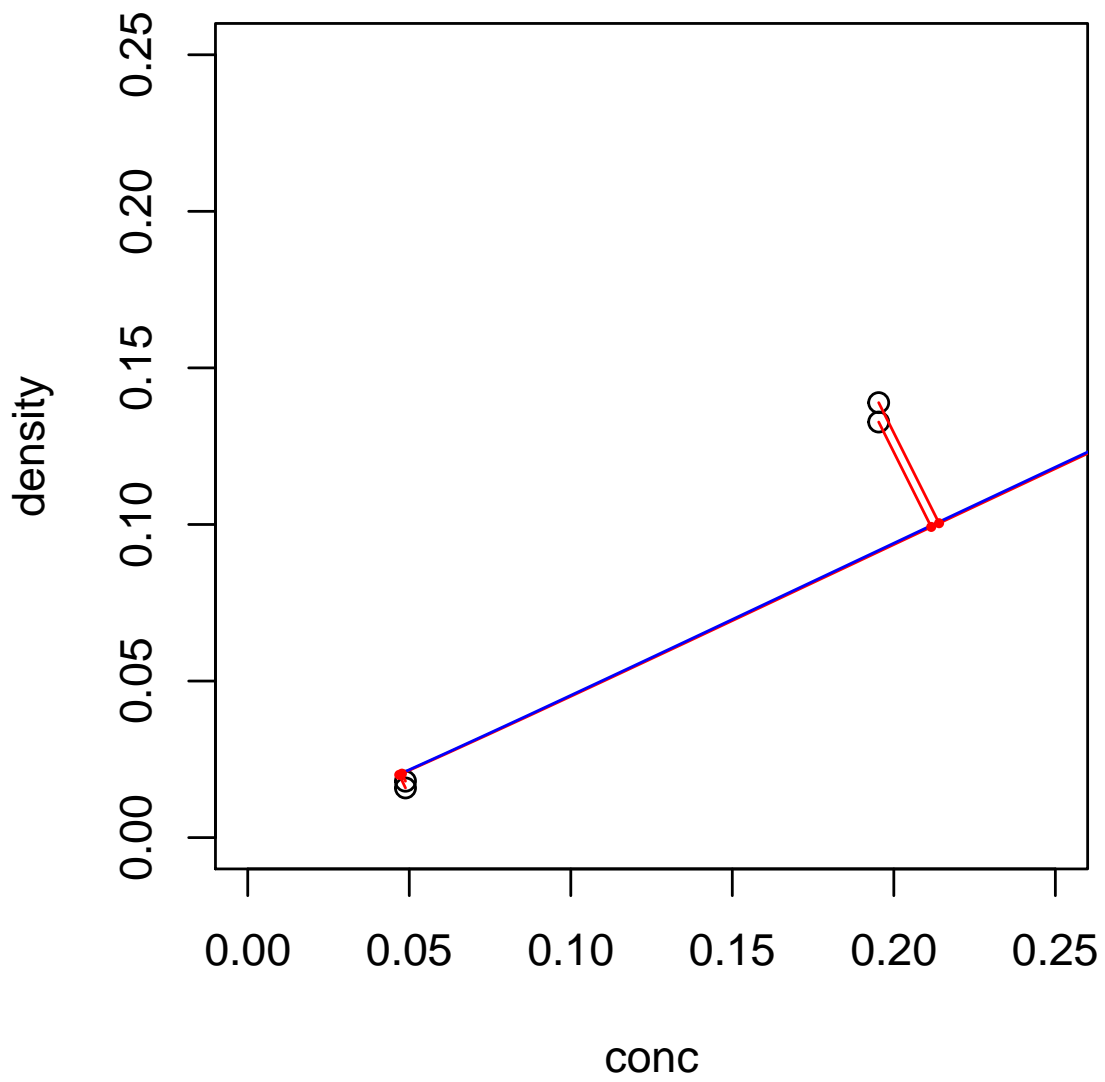
Figure 2: Plot of `mod1` as in Figure 1 with equal scaling for better visualization of orthogonality.

References

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