

Ejemplo: modelos transformables a lineales

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Descripción del conjunto de datos

El conjunto de datos L.minor contiene ocho observaciones de dos variables: tasa (`rate`) y concentración (`conc`). Las observaciones corresponden a las tasas de absorción de nitrógeno de una especie de planta acuática (*Lemna minor*) que puede llegar a causar problemas en cuerpos de agua debido a su rápido y eficiente crecimiento.

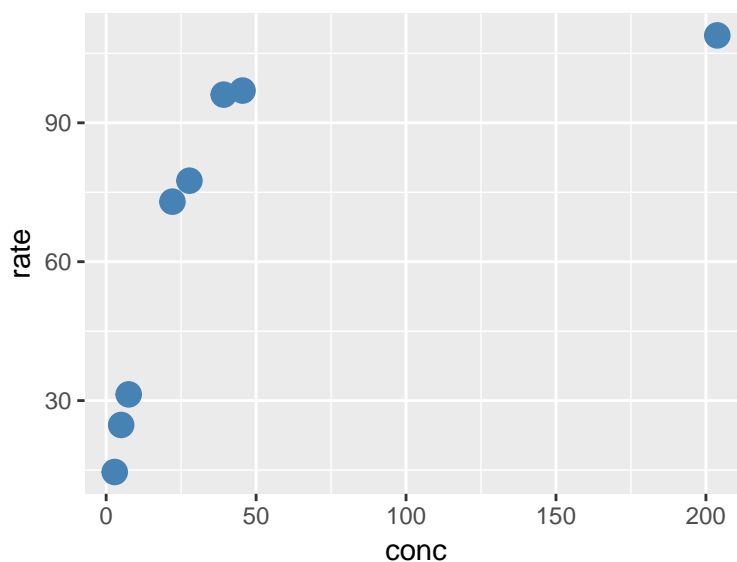
El conjunto de datos fue publicado en:

Cedergreen, N. and Madsen, T. V. (2002) Nitrogen uptake by the floating macrophyte *Lemna minor*, *New Phytologist*, 155, 285–292.

DOI: <https://doi.org/10.1046/j.1469-8137.2002.00463.x>

L.minor

##	conc	rate
## 1	2.856829	14.58342
## 2	5.005303	24.74123
## 3	7.519473	31.34551
## 4	22.101664	72.96985
## 5	27.769976	77.50099
## 6	39.198025	96.08794
## 7	45.483269	96.96624
## 8	203.784238	108.88374



Modelo de Michaelis-Menten

$$V_i = \frac{V_m S}{K_m + S} + \epsilon_i, \quad \epsilon_i \sim (0, \sigma^2)$$

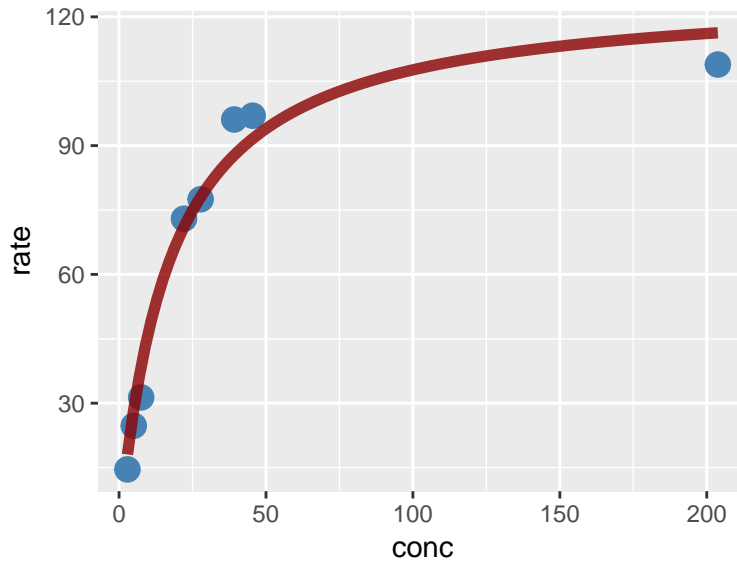


Figure 1: Ajuste del modelo MM con los datos originales

Ajuste del modelo MM

```
nl.fit <- nls(rate ~ Vm * conc/(K + conc), data = L.minor,
             start = list(K = 20, Vm = 120))
summary(nl.fit)
```

```
##
## Formula: rate ~ Vm * conc/(K + conc)
##
## Parameters:
##   Estimate Std. Error t value Pr(>|t|)
## K      17.079     2.953   5.784 0.00117
## Vm    126.033     7.173  17.570 2.18e-06
##
## Residual standard error: 6.25 on 6 degrees of freedom
##
## Number of iterations to convergence: 7
## Achieved convergence tolerance: 8.141e-06
```

Intervalos de confianza del ajuste no lineal (aproximación lineal)

```
confint2(nl.fit)

##           2.5 %    97.5 %
## K      9.853828  24.30416
## Vm    108.480813 143.58470
```

Modelo de Lineweaver-Burk

$$V_i^{-1} = \frac{1}{V_m} + \frac{K_m}{V_m} S_i^{-1} + \epsilon_i, \quad \epsilon_i \sim (0, \sigma^2)$$

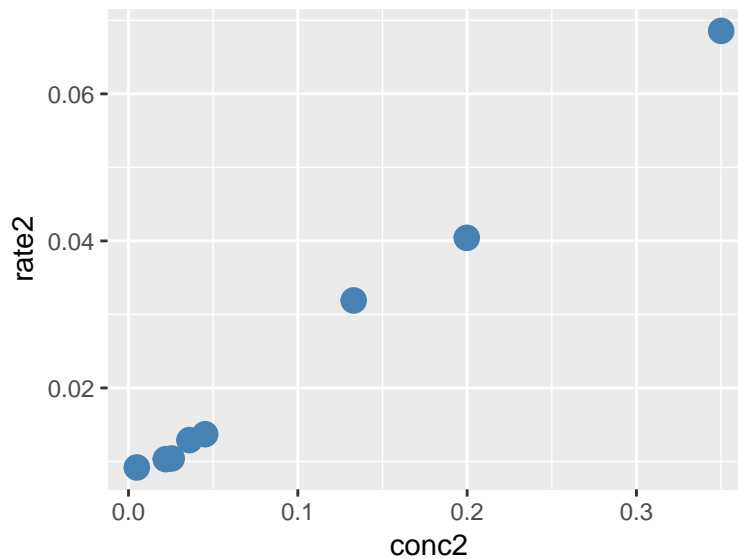
Datos transformados

```
L.minor2 <- transmute(L.minor, rate2 = 1/rate, conc2 = 1/conc)
```

```
## Warning: package 'bindrcpp' was built under R version 3.4.4
```

```
L.minor2
```

```
##      rate2      conc2
## 1 0.068571026 0.350038402
## 2 0.040418371 0.199788120
## 3 0.031902500 0.132988036
## 4 0.013704289 0.045245462
## 5 0.012903061 0.036010114
## 6 0.010407133 0.025511489
## 7 0.010312868 0.021986106
## 8 0.009184108 0.004907151
```



Ajuste del modelo LB

```
lm.fit <- lm(rate2 ~ conc2, data = L.minor2)
summary(lm.fit)
```

```
##
## Call:
## lm(formula = rate2 ~ conc2, data = L.minor2)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.0014249 -0.0008636 -0.0002329  0.0006440  0.0017939
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  0.0067468  0.0006042   11.17 3.08e-05
## conc2        0.1756681  0.0039770   44.17 9.02e-09
##
```

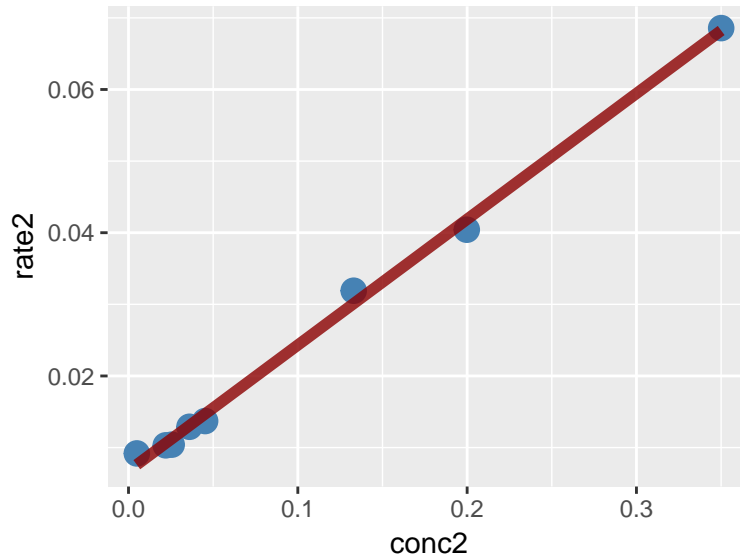


Figure 2: Ajuste del modelo LB con los datos transformados

```
## Residual standard error: 0.001266 on 6 degrees of freedom
## Multiple R-squared:  0.9969, Adjusted R-squared:  0.9964
## F-statistic: 1951 on 1 and 6 DF,  p-value: 9.016e-09
```

Intervalos de confianza con el método delta

```
deltaMethod(lm.fit, '1/Vm', parameterNames = c('Vm', 'K'))
```

```
##      Estimate      SE   2.5 %   97.5 %
## 1/Vm 148.2174 13.27283 122.2031 174.2316
```

```
deltaMethod(lm.fit, 'K/Vm', parameterNames = c('Vm', 'K'))
```

```
##      Estimate      SE   2.5 %   97.5 %
## K/Vm  26.03706  2.762347 20.62296 31.45116
```

Intervalos de confianza con *bootstrap*

```
confint(Boot(lm.fit, f = function(obj) 1/coef(obj)[1], method = 'residual'))
```

```
## Loading required namespace: boot
## Bootstrap quantiles, type = bca
##
##              2.5 %   97.5 %
## (Intercept) 124.3726 174.1931
```

```
confint(Boot(lm.fit, f = function(obj) coef(obj)[2]/coef(obj)[1], method = 'residual'))
```

```
## Bootstrap quantiles, type = bca
##
##              2.5 %   97.5 %
## conc2      21.35141 31.1819
```

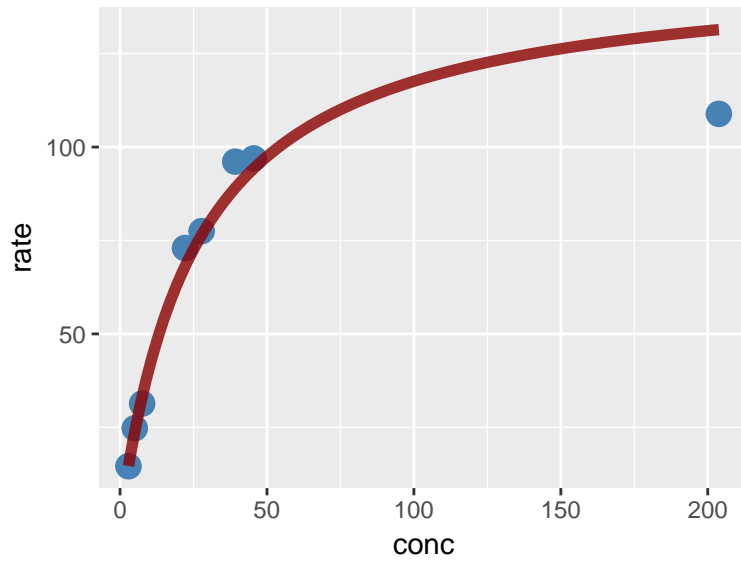


Figure 3: Ajuste del modelo LB con los datos originales