



RESEARCH ARTICLE

DETERMINATION OF MAXIMUM CURVATURE POINT WITH THE R PACKAGE *SOILPHYSICS*

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ABSTRACT

The problem of determining the maximum curvature point in fitted curves is introduced and the implementation and use of the function `maxcurv()` of the R package *soilphysics* are presented and exemplified using two usual models in experimental design and soil physics. The function `maxcurv()` can be used for numerically determining the maximum curvature point through four methods: the method of general curvature function, perpendicular distances, linear response plateau and linear piecewise spline. Using the first method does not require knowing the first or second derivatives of the underlying function and allows one to analyse the corresponding curvature function. The latter three methods can be used to determine *local* points of maximum curvature. The package *soilphysics* is distribution free (under GLP-2/3) and currently available from the CRAN website: <http://CRAN.R-project.org/package=soilphysics>.

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INTRODUCTION

In agriculture, the solution of many problems requires fitting a curve and subsequent determination of the maximum curvature point (MCP). Studies (Lima *et al.*, 2007; Cargnelutti Filho *et al.*, 2011; Lorentz *et al.*, 2012; Leonardo *et al.*, 2014; Souza *et al.*, 2015) about optimum plot size for field experiments are usually based on the model proposed by Lessman and Atkins (1963) for modelling the coefficient of variation as a function of plot size. Afterwards, the MCP is taken as the optimum plot size. Faria *et al.* (2012) used this model and calculated the MCP for determining the optimum number of pepper clusters. After fitting nonlinear growth models, Souza *et al.* (2013) calculated MCP in order to determine the age at which sheep had lower weight gain. In soil physics, the most usual method (the method of Casagrande, 1936) for determining preconsolidation stress is based on MCP. The Gompertz equation, as presented by Gregory *et al.* (2006), is often used for modelling the soil void ratio as a function of the applied stress. Afterwards, according to the methodology proposed, MCP is visually determined. However, the value of MCP could roughly change the value of preconsolidation stress, such as observed by Silva and Lima (2016) and Rucknagel *et al.* (2010), which quantified the variance of subjectivity implied

by the person executing the graphic method and compared with mathematical models. The authors stated that the mean error reaches about 15% on the value of preconsolidation stress when using graphic ("eye") method. Silva and Lima (2015) stated that the calculation of MCP is necessary for avoiding the subjectivity of the method, especially when the user has little experience. In other areas, MCP is also a remarkable issue. To quantify the uncertainty estimation for plate dimensions and surface quality, Ali and Buajarern (2013) used MCP. According to Li-pi *et al.* (2010), features commonly used in image registration contain a maximum curvature point. Cecon *et al.* (2008) and Faria *et al.* (2012) present a method described by Larson *et al.* (1998) for determining MCP geometrically, based on vertical distances from the function to an imaginary secant line. Likewise, Lorentz *et al.* (2012) propose a similar method, but their approach is based on perpendicular distances. Both are iterative methods. There is also the method based on linear response *plateau*, as suggested by Cargnelutti Filho *et al.* (2011) to estimate optimum experimental plot size.

The R (www.R-project.org) package *soilphysics* (Silva and Lima, 2015; Lima *et al.*, 2016) contains a function that can be used for numerically determining the maximum curvature point. Therefore, the aim of this work is to present the implementation and use of the function `maxcurv()`, from *soilphysics*.

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MATERIALS AND METHODS

Implementation

In this section we present the four methods available in `maxcurv()`. All of them are numerical-based. Thus, `maxcurv()` simulates a numeric step vector of size 5,000 covering the support interval of x , $\mathbf{x} = [x_1 \ x_2 \ \dots \ x_{5,000}]^T$, where $x_1 = \min(x)$ and $x_{5,000} = \max(x)$, as defined by the user through the argument `x.range`.

The method of the general curvature function

Consider a bidimensional space defined by the coordinates $x \in \mathfrak{R}$ and $f(x)$, being the later any function with non null first and second derivatives, $\frac{d}{dx} f(x) = f'(x)$ and $\frac{d^2}{dx^2} f(x) = f''(x)$, respectively. The general curvature function is given by

$$\kappa(x) = \frac{|f''(x)|}{\left(1 + [f'(x)]^2\right)^{3/2}} \quad (1)$$

The value of MCP is then the points at the x -axis that maximizes $\kappa(x)$, which calculated upon evaluating $\frac{d}{dx} \kappa(x) = 0$. For this last purpose, a numerical algorithm can be used, such as Newton-Raphson. A comprehensive mathematical explanation and geometric interpretation of $\kappa(x)$ is given by Dineen (2014). It is noteworthy that the methodology presented depends on finding the first and second derivative of $f(x)$. Although it may be a difficult task, especially when dealing with complex functions, the implementation in `maxcurv()` was automatically set to calculate them through the function `deriv3()`. For this purpose, `maxcurv()` calls another function, `fun2form()`, that transforms an object of class "function" in a formula or expression to be evaluated by `deriv3()`. Two vector are computed by `maxcurv()` in order to evaluate $\kappa(\cdot)$ numerically, the gradient and the hessian functions evaluated at \mathbf{x} . Then, MCP is the point at x -axis corresponding to $\max[\kappa(\mathbf{x})]$.

The method of the perpendicular distances

This method consists of an adaptation of the method presented by Lorentz *et al.* (2012). In the present approach, a tangent line, say $h(x) = b_0 \pm b_1 x$, is drawn along the underlying function $f(x)$, connecting its (x, y) limits, as shown in Fig. 1. Observe that the sign of the coefficient b_1 depends on the general behaviour of $f(x)$. Afterwards, perpendicular lines for each simulated point x_i ($i = 1, 2, \dots, 5,000$) are determined by $g_i(x) = a_{0,i} + a_1 x$. Note that $a_1 = -b_1^{-1}$ is constant, whereas $a_{0,i} = f(x_i) - a_1 x_i$ is not. Take for example the point x_i . There is a corresponding perpendicular point x_j at which $g_i(x) = h(x)$ so that

$x_j = (b_0 - a_{0,i}) / (a_1 - b_1)$. Thus, the method consists of taking MCP as the value x_i whose distance $d_i = \left\{ (x_i - x_j)^2 + [f(x_i) - h(x_j)]^2 \right\}^{1/2}$ is the greatest. An empirical curvature function consists of assuming $\kappa(x_i) = d_i$.

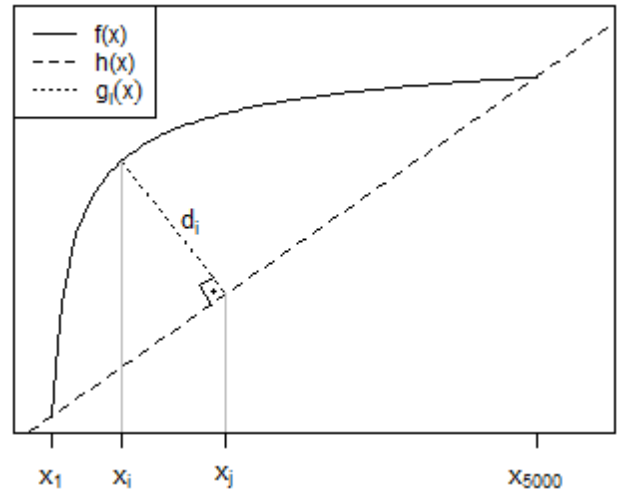


Fig. 1. Illustrating the method of perpendicular distances

The Linear Response Plateau method

The MCP is taken as the breaking point (x_0) of the regression model of *linear response plateau*, $y = h(x) + \varepsilon$, where

$$h(x) = \begin{cases} a_0 + a_1 x, & x \leq x_0 \\ a_0 + a_1 x_0, & x > x_0 \end{cases} \quad (2)$$

where a_0 and a_1 are parameters of the linear regression model fitted for the first part of the simulated data, i.e., when $x \leq x_0$, as illustrated in Fig. 2.

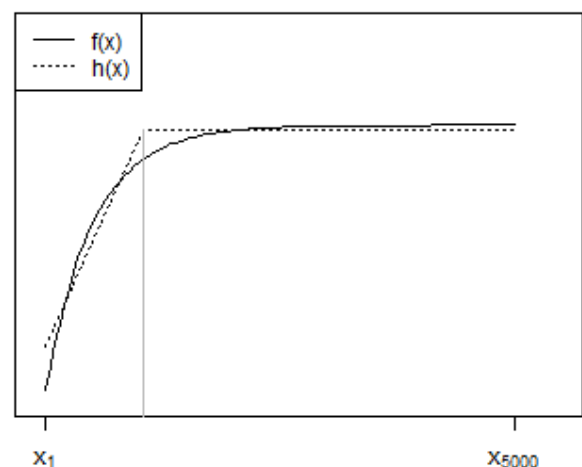


Fig. 2. Illustrating the Linear Response Plateau method

`maxcurv()` determines nonlinear least-squares estimates of the parameters (a_0 , a_1 and x_0) using the Gauss-Newton algorithm. Note that the method LRP in `maxcurv()` allows one

to fit a LRP model where the plateau is located at the first part of the data, i.e., where $x \leq x_0$. Initial values for a_0 and a_1 are obtained fitting a linear regression for the corresponding part of the simulated data, defined by the starting estimate of x_0 with the argument x_0 .

The spline method

This is a generalization of the LRP method. The MCP is here taken as the breaking point (x_0) of the regression model of *linear piecewise spline*, $y = h(x) + \varepsilon$, where

$$h(x) = \begin{cases} a_0 + a_1x, & x \leq x_0 \\ b_0 + b_1x, & x > x_0 \end{cases} \quad (3)$$

where a_0 and a_1 are parameters of the linear regression model fitted for the first part of the simulated data, i.e., when $x \leq x_0$. Likewise, b_0 and b_1 are parameters of the linear regression model fitted when $x > x_0$, as illustrated in Fig. 3.

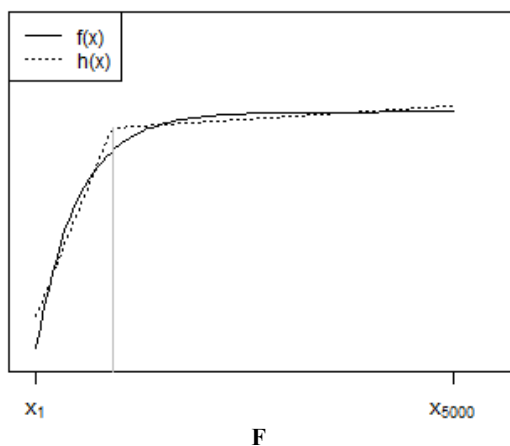


fig. 3. Illustrating the spline method

In this case, the breaking point such that $a_0 + a_1x_0 = b_0 + b_1x_0$. Then, `maxcurv()` considers $b_0 = a_0 + x_0(a_1 - b_1)$ as an off-set parameter in the nonlinear least-squares estimation. Initial values for a_0 , a_1 and b_0 are obtained fitting linear regressions for each part of the simulated data, defined by the initial value of x_0 with the argument x_0 .

Illustrations

Two usual models are used here to exemplify the use of the function `maxcurv()`. The first is the equation proposed by Lessman and Atkins (1963) for modelling the coefficient of variation (CV) as a function of plot size (x):

$$CV = ax^{-b} \quad (4)$$

where a and b are fitting parameters. The corresponding curvature function is given in Appendix in Eq. A1. Consider

that the range of x is $[1, 50]$. Let us then assume the following values of the parameters: $a = 40.1$ and $b = 0.72$. In R, we first should define a “function” object, as follows:

```
R>f1 <- function(x) 40.1 * x^-0.72
```

Then, before calling the function `maxcurv()`, we need to load the package `soilphysics`.

```
R> library(soilphysics)
```

Finally, using the function `maxcurv()` requires one to pass the following arguments: `x.range` – the minimum and maximum value of x and `fun` – the function at which to determine MCP. By default the method of the general curvature function is used.

```
R>maxcurv(x.range = c(1, 50), fun = f1)
```

The following output is printed out:

Maximum curvature point

```
f(x) = 40.1 * x^-0.72
critical x: 6.841968
critical y: 10.04186
method: general curvature
```

And a graphical solution (Figure 4) can be shown if the argument `graph` is set to be `TRUE`, as default.

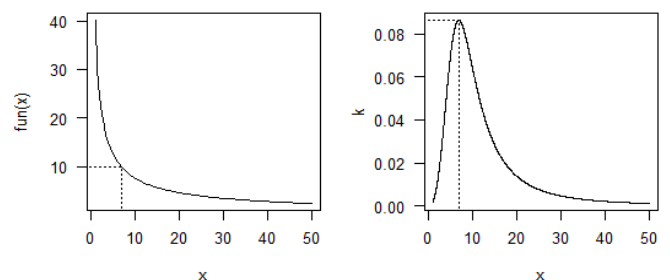


Fig.4. Graphical solution of the function `maxcurv()`, package `soilphysics`. On the left, a fitting curve of CV as a function of plot size; on the right, the curvature function

Thus, $MCP = 6.84$, which corresponds to a CV of 10.04%. This result is in agreement with the method proposed by Meier and Lessman (1971) for determining the optimum plot size. In their approach (Eq. 5),

$$x_0 = \frac{a^2 b^2 (2b + 1)}{(b + 2)^{\frac{1}{2b+2}}} \quad (5)$$

which corresponds to the optimum plot size. In the example, $x_0 = 6.84$. Our second example is based on the Gompertz equation (Eq. 6), as presented by Gregory *et al.* (2006), for modelling the void ratio (e) as a function of the applied stress (x).

$$e = a + c \exp\{-\exp[b(x - m)]\} \quad (6)$$

where a , b , c and m are fitting parameters. The corresponding curvature function is given in Appendix in Eq. A2. Here we will assume that the range of x is $[0, 4]$ and the value of the parameters presented by Keller *et al.* (2011), where $a = 0.539$ and $b = 2.215$, $c = 1.284$ and $m = 1.748$. Now we define a function in R:

```
R>f2<- function(x) 0.539 + 1.284*exp(-exp( 2.215*(x - 1.748)))
```

Calling `maxcurv()`,

```
R> maxcurv(x.range = c(0, 4), fun = f2)
```

will produce the output:

Maximum curvature point

```
f(x) = 0.539 + 1.284 * exp(-exp(2.215 * (x - 1.748)))
critical x: 2.277255
critical y: 0.5898216
method: general curvature
```

And the Figure 5 is displayed.

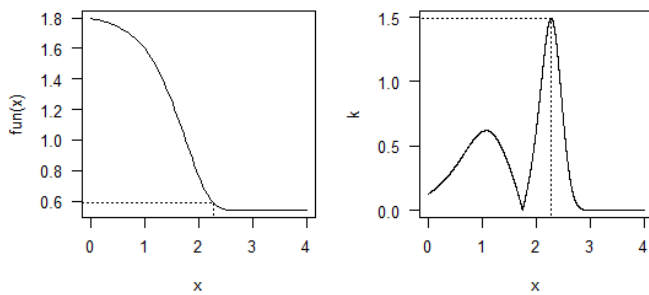


Fig.5. Graphical solution of the function `maxcurv()`, package *soilphysics*. On the left, a fitting curve of the Gompertz model for a compression curve; on the right, the curvature function

Note, the method implemented in `maxcurv()` allows one to identify two peaks at the curvature function, whose height correspond to the curve degree. But the point here is that, when fitting compression curves for determination of preconsolidation stress through Casagrande method, the second root is the one being sought out ($x \approx 1.1$), although its lower peak. In this case, the methods the three other methods can be used to determine *local* MCPs, i.e., according to the x limits informed by the user in `x.range` instead of finding the global MCP as does the general method. For example, we could determine the second root mentioned using the methods of perpendicular distances and linear piecewise spline as follows:

```
R> maxcurv(x.range = c(0, 2), fun = f2, method = "pd")
R> maxcurv(x.range = c(0, 2), fun = f2, method = "spline", x0 = 1)
```

Producing the outputs:

Maximum curvature point

```
f(x) = 0.539 + 1.284 * exp(-exp(2.215 * (x - 1.748)))
critical x: 1.081416
critical y: 1.560774
```

method: perpendicular distances

Maximum curvature point

```
f(x) = 0.539 + 1.284 * exp(-exp(2.215 * (x - 1.748)))
critical x: 1.101699
critical y: 1.550105
method: piecewise linear spline
```

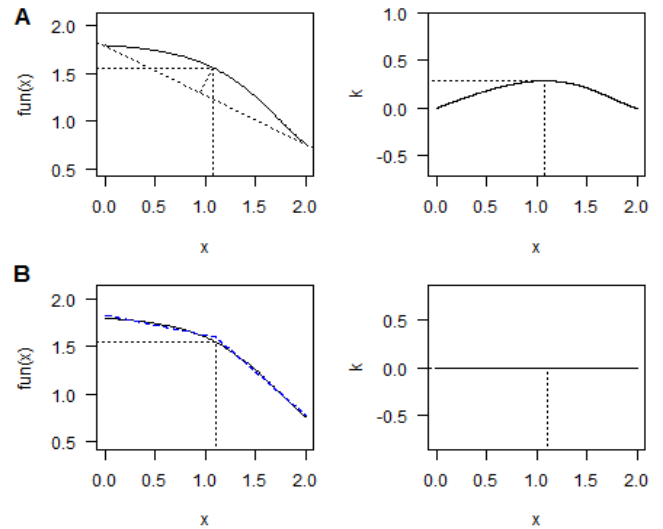


Fig.6. Graphical solution of the function `maxcurv()` with the methods (A) perpendicular distances and (B) linear piecewise spline for the Gompertz model

Closing remarks

The function `maxcurv()` can be used for numerically determining the maximum curvature point through four methods: the method of general curvature function, perpendicular distances, linear response plateau and linear piecewise spline. Using the first method does not require knowing the first or second derivatives of the underlying function and allows one to analyse the corresponding curvature function. The latter three methods can be used to determine *local* points of maximum curvature. The package *soilphysics* is distribution free (under GPL-2/3) and currently available at the CRAN website: <http://CRAN.R-project.org/package=soilphysics>.

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Appendix

Curvature function of the experimental plot size equation (Eq. 4):

$$\kappa(x) = \frac{|ab(b+1)x^{-b-2}|}{[1 + a^2 b^2 x^{-b+1}]^{3/2}} \quad (\text{A1})$$

Curvature function of the Gompertz equation (Eq. 6):

$$\kappa(x) = \frac{b^2 c \exp(b(x-m) - \exp[b(x-m)]) \{ \exp[b(x-m)] - 1 \}}{\{1 + [-bc \exp(b(x-m) - \exp[b(x-m)])]^2\}^{3/2}} \quad (\text{A2})$$

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