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Chapter

Modeling Accumulated Evapotranspiration Over Time

Omar Cléo Neves Pereira and Altair Bertonha

Abstract

The knowledge of accumulated evapotranspiration by seasonal vegetation crops throughout their life cycle can be an important tool in decision-making when considering the economic viability of the crop. This knowledge can help understand how much the plants, subject to specific management, can evapotranspirate at the end of their cycle. This information assists in estimating the quantity of a production variable, for example, the mass of shoot fresh matter, besides indicating a more interesting period for its harvest. The objective of this chapter is, from the daily evapotranspiration estimative throughout the cycle, to model the accumulated evapotranspiration over the entire growth period of the crop. In order to do so, we must understand that the behavior of the response variable, i.e., the accumulated evapotranspiration, over time is not linear and keep in mind that the several observations performed in the same experimental unit have correlations and these correlations are more intense the closer temporally the measurements are. This understanding leads us to the analysis of longitudinal data from the nonlinear mixed effect models perspective.

Keywords: longitudinal data, nonlinear mixed effect model, growth curve, correlation structure, irrigation

1. Introduction

With available water in the soil, the water flow through the plants depends only on atmospheric demand. Therefore, physical variables as temperature, relative air humidity, and wind and solar radiation affect directly the evapotranspiration (*ET*) of a vegetated surface [1]. Besides that, the plants development state may also affect the *ET*.

Seasonal vegetation crops present a small demand for water, while their root system is small, reaching maximum rates in full growths and decreasing in the final stages of development. For these species, the accumulated *ET* over the plant cycle is directly related to its productivity. In other words, the greater the accumulated amount of evapotranspirated water, the greater the quantity of the production variables as shoot fresh and dry matter masses, number of leaves, and leaf area [2, 3].

The objective of this chapter is to illustrate the use of nonlinear mixed effect models to fit accumulated *ET* over time in seasonal vegetation crops.

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2. Response profile

Figure 1 presents the accumulated *ET* from a single lettuce plant over 23 consecutive days, being the first day equivalent to the 35^{th} day after seeding. Throughout this period, the plant's daily *ET* was measured. Hence, the first day in the graph presents the *ET* value from the last 24 h, the second day refers to the last 48 h, and so on. The daily *ET* must be understood as the rate at which the accumulated *ET* occurs over time. In mathematical terms, the daily *ET* can be understood as an approximation of the derivative (rate) of the accumulated *ET* with respect to time.

We wish to describe the behavior of our variable of interest or *response variable*, the accumulated *ET* over time for seasonal vegetation crops. As the amount of evapotranspirated water in 1 day is added to the accumulated *ET* from previous days, its values over time are equal (in case *ET* from a whole day is null) or greater than the immediately preceding value.

Observations from the response variable in more than one moment in the same experimental unity constitute what we call as *response profile*. Therefore, **Figure 1** presents the response profile of a lettuce plant over time. This profile, apparently, presents an *S*-shaped format.

At the first days of observations (**Figure 1**), the accumulated *ET* is small because the plant is at the beginning of its growth. As the days go by, the daily *ET* values increase successively approximately until the 20^{th} day. After the 20^{th} day, the daily *ET*, i.e., the rate of change of the accumulated *ET*, begins to decrease. This causes the accumulated *ET*, which has been growing exponentially, to have a less vigorous growth and, therefore, tending slowly to a maximum value.

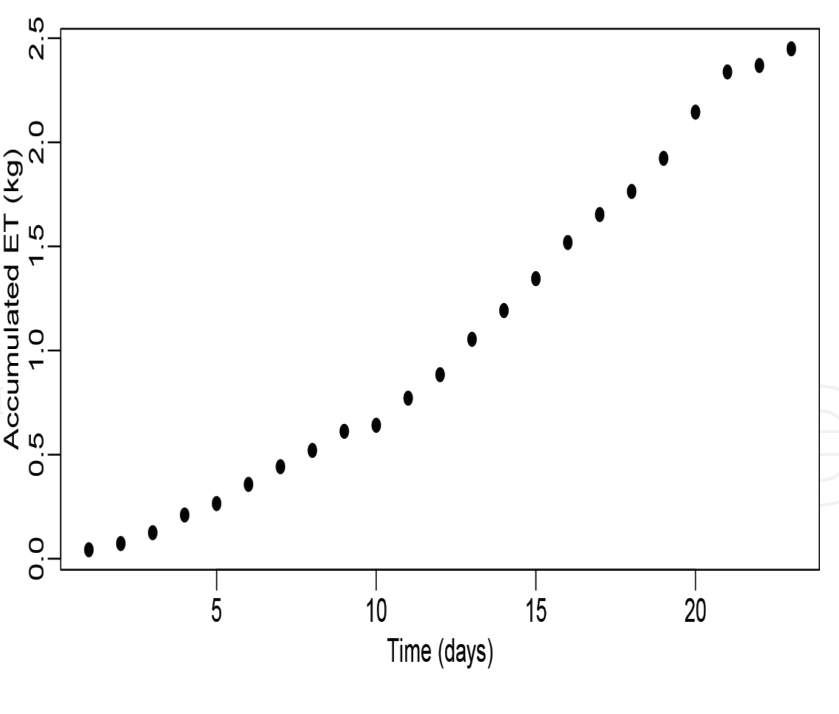

Figure 1.
Response profile of the accumulated ET for a single lettuce plant over 23 consecutive days.

3. A model for growth data

In order to describe the behavior of the accumulated *ET* over time, we also need an *S*-shaped function. In addition, it is expected that the chosen model will be interpretable and parsimonious in the parameters. An empirical option is the polynomial model, which has linear parameters. This type of model can promote good statistical adjustments and be computationally simpler but does not add any theoretical consideration to the physical and/or biological mechanisms that generated the data. On the other hand, a nonlinear model is associated with some theoretical knowledge regarding the studied phenomenon. Besides the interpretability, these models use few parameters when compared to linear models, thus configuring a more parsimonious description of the data [4].

Regarding the accumulated ET over time, we have some physical and biological aspects that we can use to choose a proper model. A function that describes this response variable needs parameters that delimit it between a minimum and a maximum value. In other words, the minimum value should be really close to zero and indicate the beginning of the plant's growth, and the maximum should be a value to which the accumulated ET tends asymptotically as the end of the life cycle approaches. Another aspect to highlight is that the model should present an inflection point, which indicates the day that the accumulated ET rate (daily ET) reaches its maximum value.

There are several functions capable of characterizing the accumulated ET over time in the sense we just described. For example, we will use the four-parameter logistic function ($4PL$) to describe our response variable. This function is widely used to fit growth or decay data. There are some parametrizations for this function in the literature, but we are using the one given by [4]

$$ET(t) = \phi_1 + \frac{\phi_2 - \phi_1}{1 + \exp\left[(\phi_3 - t)/\phi_4\right]} \tag{1}$$

with $ET(t)$ being the accumulated ET over time and ϕ_{1-4} the model parameters (**Figure 2**). ϕ_1 is the inferior horizontal asymptote which gives the accumulated ET value when $t \to -\infty$. Biologically, this parameter does not have a consistent interpretation, but it is important in the fitting because it ensures the accumulated ET, in times close to zero, to be very small [2, 3]. ϕ_2 is the superior horizontal asymptote and gives the accumulated ET value when $t \to \infty$. This parameter can be

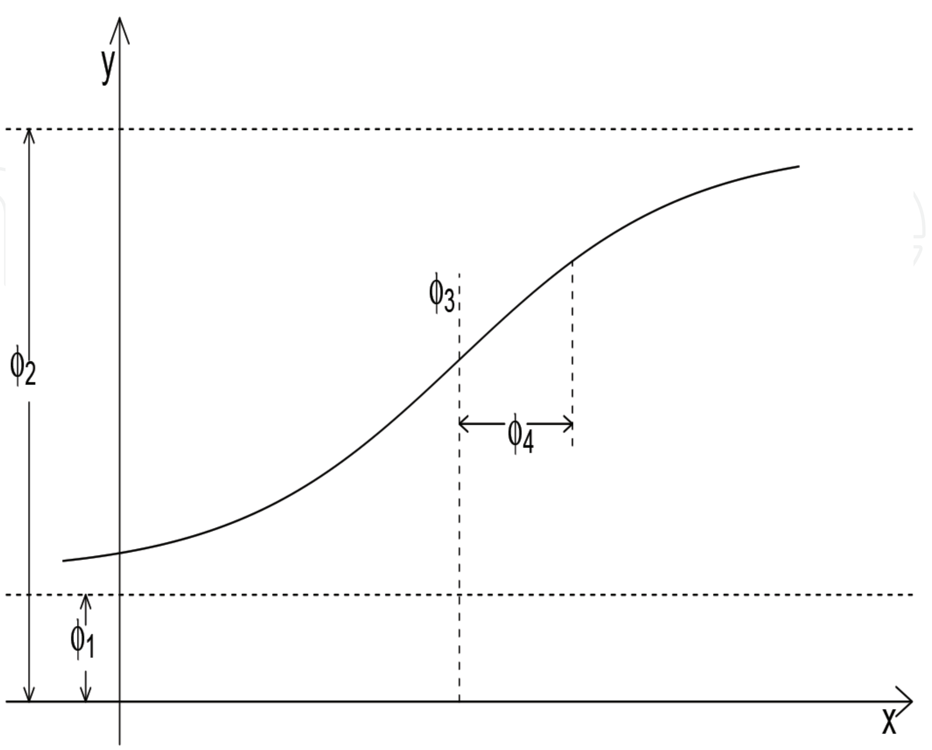

Figure 2.
Graphical representation of the 4PL parameters (Eq. (1)). Figure adapted from [4].

interpreted as the maximum accumulated ET estimative that the plant can reach in its final life cycle. ϕ_3 is the curve's inflection point and indicates the day (time) in which the daily ET reaches a maximum value. The corresponding time to ϕ_3 results in an accumulated ET between ϕ_1 and ϕ_2. More precisely, the accumulated ET until time ϕ_3 is the mean value of both asymptotes, i.e., $(\phi_1 + \phi_2)/2$. ϕ_4 is the scale parameter. The day (time) corresponding to $\phi_3 + \phi_4$ gives $\sim 0.75(\phi_2 - \phi_1)$ of the accumulated ET. Therefore, ϕ_4 indicates how quickly the accumulated ET leaves the proximity of ϕ_1 until it reaches values close to ϕ_2. The greater the ϕ_4, the slower this occurs.

To better understand what we have said, let's observe **Figure 3**. It brings the observed data shown in **Figure 1** represented by the black dots and two other curves representing two different fits made from this data. The first is a fifth-degree polynomial model, and the second is given by Eq. (1). The graph in this figure was extended until the 40^{th} day in order to present the behavior of these fittings over time.

Both the fifth-degree polynomial and the nonlinear $4PL$ models have fitted well with the data. However, the polynomial model goes to zero after the 30^{th} day, which physically is impossible. Besides that, this model presents five parameters without any physical and/or biological explanation for the phenomenon in this study. The $4PL$ nonlinear model is a strictly increasing function, being compatible with a variable which is accumulated over time. Nevertheless, this fitting does not allow the infinite growth of the accumulated ET as time grows larger and larger. It limits the accumulated ET to a value which can be understood as a maximum amount in which this plant can evapotranspirate throughout its life cycle.

We also see that, from approximately the 20^{th} day, the accumulation of evapotranspiration water is decreasing. This indicates that this day is the inflection point of the nonlinear $4PL$ model. For a practical example of the model's inflection point regarding seasonal vegetation crops, suppose that the commercial product of a given crop plant is its leaves. It is known that the production variables present a positive correlation with the amount of total evapotranspired water throughout the

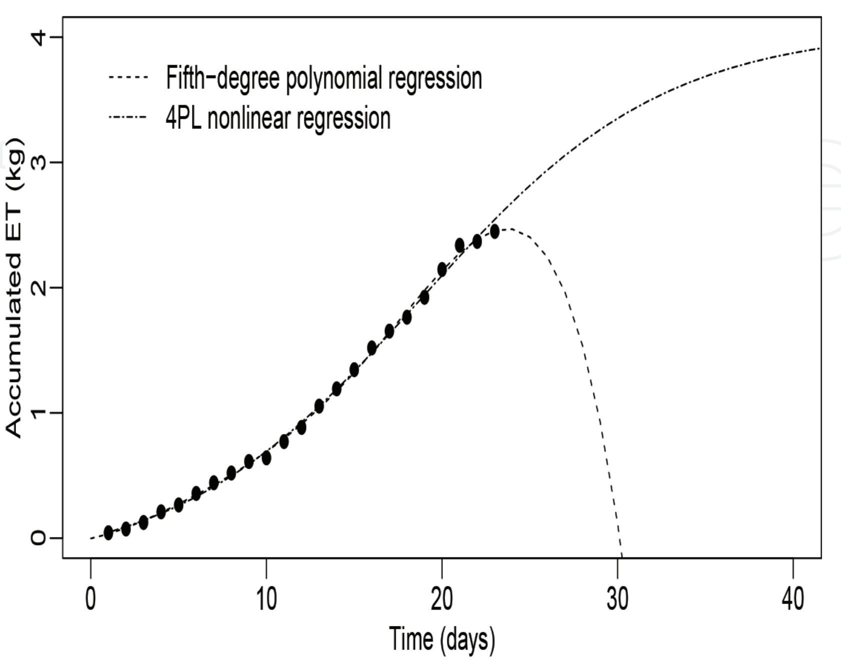

Figure 3.
Accumulated ET response profile for a single lettuce plant over 23 consecutive days. The graph was extended until the 40^{th} day to present the behavior of two fittings made for this data, a fifth-degree polynomial and a nonlinear model given by Eq. (1).

plants' life cycle. That is, the larger the total evapotranspiration water, the higher the values of the production variables [2, 3]. Hence, the inflection point can indicate the proximity of the harvest day. From this point, the *ET* rates decrease, and therefore, the plants start to accumulate less quantities of shoot fresh matter over time. Thus, this point can be considered when thinking in terms of the economic viability of the crop.

Another important aspect, besides the parameter interpretability, is that the nonlinear 4*PL* model is more parsimonious than the linear model. In general, nonlinear models use a small number of parameters than the linear ones, which grant them more parsimony. Besides that, as can be observed in **Figure 3**, in regions outside the data interval, the nonlinear model gives a more trustworthy prediction for the response variable [4].

4. Longitudinal data

Clearly, in order to make sense, an experiment must provide data from more than one experimental unit. In our case, more than one plant should be observed over time, i.e., we must obtain more than one response profile. Studies in which the response variable is observed repeatedly throughout time in the experimental units are called *longitudinal studies*. This kind of work is common in agriculture when analyzing the increase or decrease of the response variable over time [2, 3, 5–8].

Measurements performed in the same experimental unit are most likely to be correlated. Suppose two plants which its *ET* is registered daily. If all covariables (fertilization, cultivate, planting season, soil water, and so on) were kept constant over time, plants with high rates of *ET* in a given day will most likely also have high rates of *ET* in the next day, the same for plants with smaller *ET* rates. If in a day the rate is small, probably in the next day it will also be small. In other words, measurements performed in the same experimental unit tend to be similar over time. It's the individual expression of each plant.

Besides the correlation between the observations within the same experimental unit, we must consider that, most likely, these correlations are greater for observations performed between neighboring times than those performed between more distant times.

5. Mixed effect model

In a longitudinal study, the monitoring of the experimental units over time generates correlated dataset. As mentioned, these correlations within the same experimental unit are stronger among neighboring observations. The greater the time distance between two measures, the weaker the correlation between them. Besides that, when we observe experimental units which received the same conditions regarding growth over time and are part of the same treatment, we have a variability among them that we attribute to chance. The treatment effects, the correlations, and the variabilities in a longitudinal study indicate that we need a tool that, in addition to being flexible in specifying a mathematical model, also emphasizes each experimental unit.

In mixed effect models, we select an ordinary function to describe the response variable regarding the studied covariables, that is, the responses of the experimental units in a population. Besides that, specific coefficients of this function can be unique for each experimental unit. In a mixed effect model, we assume that the experimental units of a population have the same functional form, but the function parameters may vary among the units.

The name *mixed model* comes from the fact that this model combines *fixed effects* and *random effects*. A mixed effect model is a parametric model which describes the relations between the response variable and the covariables (fixed effects) and takes into account the individual responses of each experimental unit (random effects). In other words, the fixed effects parameters describe the relations of the response variable and the covariables in an entire population, and the random effects specify the contribution of each individual within the population [4, 9–12].

To illustrate how to write a 4*PL* nonlinear model with mixed effect, let's assume that we are studying the accumulated *ET* regarding four levels of water in the soil, W_1, W_2, W_3, and W_4 (there could be more levels of water in the soil or less, but to exemplify, let's assume four treatments). We will consider that the response variable, the accumulated *ET*, has a normal probability distribution. Consider ET_{ij} as the accumulated *ET* at the j situation, for plant i, with $j = 1, 2, \cdots, n_i$ e $i = 1, 2, \cdots, N$, where n_i is the number of observations for the i-th plant and N is the total number of plants. The nonlinear 4*PL* mixed effect model can be expressed by [2, 3]

$$ET_{ij} = \phi_{1i} + \frac{\phi_{2i} - \phi_{1i}}{1 + \exp\left[(\phi_{3i} - t_j)/\phi_{4i}\right]} + \varepsilon_{ij} \tag{2}$$

being

$$\boldsymbol{\phi}_i = \begin{bmatrix} \phi_{1i} \\ \phi_{2i} \\ \phi_{3i} \\ \phi_{4i} \end{bmatrix} = \begin{bmatrix} \beta_1 + \gamma_1 x_{1i} + \delta_1 x_{2i} + \zeta_1 x_{3i} \\ \beta_2 + \gamma_2 x_{1i} + \delta_2 x_{2i} + \zeta_2 x_{3i} \\ \beta_3 + \gamma_3 x_{1i} + \delta_3 x_{2i} + \zeta_3 x_{3i} \\ \beta_4 + \gamma_4 x_{1i} + \delta_4 x_{2i} + \zeta_4 x_{3i} \end{bmatrix} + \begin{bmatrix} b_{1i} \\ b_{2i} \\ b_{3i} \\ b_{4i} \end{bmatrix} \tag{3}$$

$$= \boldsymbol{\beta} + \boldsymbol{\gamma} x_{1i} + \boldsymbol{\delta} x_{2i} + \boldsymbol{\zeta} x_{3i} + \boldsymbol{b}_i, \tag{4}$$

with the parameters $\boldsymbol{\beta}$, $\boldsymbol{\gamma}$, $\boldsymbol{\delta}$, $\boldsymbol{\zeta}$ representing the fixed effects and $\boldsymbol{b}_i$ the random effects in the model. x_{ki} with $k = 1, 2, 3$ are indicative covariables of treatments or groups and may have values zero or one. The parameter $\boldsymbol{\beta}$ is the reference level in the study. When $x_{1i} = x_{2i} = x_{3i} = 0$, thus, $\boldsymbol{\phi}_i = \boldsymbol{\beta} + \boldsymbol{b}_\mathbf{i}$ and the i-th plant belongs to the treatment W_1. When $x_{1i} = 1$ and $x_{2i} = x_3 i = 0$, $\boldsymbol{\phi}_i = \boldsymbol{\beta} + \boldsymbol{\gamma} + \boldsymbol{b}_\mathbf{i}$ and the i-th plant belongs to the treatment W_2. If $x_{2i} = 1$ and $x_{1i} = x_3 i = 0$, $\boldsymbol{\phi}_i = \boldsymbol{\beta} + \boldsymbol{\delta} + \boldsymbol{b}_\mathbf{i}$ and the i-th plant belongs to the treatment W_3. And lastly, if $x_{3i} = 1$ and $x_{1i} = x_{2i} = 0$, $\boldsymbol{\phi}_i = \boldsymbol{\beta} + \boldsymbol{\zeta} + \boldsymbol{b}_\mathbf{i}$ and the i-th plant belong to the treatment W_4. The random effects $\boldsymbol{b}_\mathbf{i}$ are considered independent among the plants and are normally distributed with mean zero and covariance matrix $\boldsymbol{\Psi}$ ($\boldsymbol{b}_\mathbf{i} \sim N(\mathbf{0}, \boldsymbol{\Psi})$). In this case, the covariance matrix is given by

$$\boldsymbol{\Psi} = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \sigma_{13} & \sigma_{14} \\ \sigma_{12} & \sigma_2^2 & \sigma_{23} & \sigma_{24} \\ \sigma_{13} & \sigma_{23} & \sigma_3^2 & \sigma_{34} \\ \sigma_{14} & \sigma_{24} & \sigma_{34} & \sigma_4^2 \end{bmatrix} \tag{5}$$

with σ_1^2, σ_2^2, σ_3^2, and σ_4^2 being the variances of random effects b_{1i}, b_{2i}, b_{3i}, and b_{4i}, respectively, and σ_{12}, σ_{13}, σ_{14}, σ_{23}, σ_{24}, and σ_{34} are the covariances between them. The variances of the random effects indicate how a model parameter varies between the experimental units. Frequently, we suppose that the errors within the groups ε_{ij} are independent between the observations of the same experimental unit and that they are distributed the same way among the experimental units. For a given sample unit i, we can describe the error ε_{ij} as the time j indexed vector, i.e.,

$$\boldsymbol{\varepsilon}_\mathbf{i} = \begin{bmatrix} \varepsilon_{1i} \\ \varepsilon_{2i} \\ \vdots \\ \varepsilon_{n_i i} \end{bmatrix},$$

where each vector $\boldsymbol{\varepsilon}_\mathbf{i}$ has n_i observations throughout time and we assume that they follow a normal multivariate distribution with mean zero and covariance matrix $\boldsymbol{\Lambda}_\mathbf{i}$, i.e.,

$$\boldsymbol{\varepsilon}_\mathbf{i} \sim N(\mathbf{0}, \boldsymbol{\Lambda}_\mathbf{i}). \tag{6}$$

Most of the times, we consider $\boldsymbol{\Lambda}_\mathbf{i} = \sigma^2 \boldsymbol{I}$, being σ^2 a constant variance for all j times.

By using nonlinear mixed effect models, we must consider the technical difficulty in the parameter estimation. In a mixed effects linear model, the derivative of the logarithmic of the likelihood function allows, in a simple way, the algorithm implementation, like Newton-Raphson, to obtain the estimative of the models parameters. Nonlinear models can, however, present nonlinear random coefficients which make it impossible to directly explain the parameters from the likelihood function. Methods that depend on linear approximations such as the first-order Taylor approximation can be used to estimate the model.

Nonlinear mixed effect model analysis can be, preferably, made by the R software [13] with the package name [14], also, at the SAS software using PROC NLMIXED. An excellent text to learn how to use these skills is given in [4].

6. Covariance structure of $\boldsymbol{\Lambda}_\mathbf{i}$

Mixed effect model allows the dependence between the observations to be specified in the model parameters through random effects. In other words, the experimental unit responses from a population tend to follow a nonlinear growth path; however, each experimental unit has its own growth path, and the mixed effect model allows the inclusion of specific coefficients to obtain fitted growth curves that align better with the individual responses of these experimental units.

Thus, mixed models allow relevant flexibility for the specification of the random effects correlation structure. However, the dependence structure of the observations within the experimental units $\boldsymbol{\Lambda}_\mathbf{i}$ until now has been considered independent, identically distributed with mean zero and constant variance. Depending on the chosen model, the growth responses can be explained just by including specific coefficients for the experimental units. However, this may not be enough, and, in this case, modeling the residual dependence of the data becomes important.

There are cases where dependence on observations not accommodated by the growth function is not well understood or, sometimes, additional covariables that could explain this dependences are absent from the model. Thus, an important resource to model this dependence is to identify the covariance structure that allows correlation between the residuals in different occasions. Then, let us relax on the assumption that the errors are independent and allow them to have heteroscedasticity and/or are correlated within the experimental units.

There are several covariance structures for the residues available in the software to help model longitudinal data. However, in our text, we will highlight only two that we consider more important for these studies, the covariance structure with heterogeneous variance and the first-order auto-regressive.

6.1 Heterogeneous variance

The first covariance structure we will consider for $\mathbf{\Lambda_i}$ is the one that admits heterogeneity of the n_i residual variances. In this structure, which has n_i parameters, we assume that the residuals associated with the observed values at the n_i occasions for the i-th experimental unit are independent:

$$\mathbf{\Lambda_i} = \begin{bmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_{n_i}^2 \end{bmatrix}. \quad (7)$$

Other variables, besides time, can also be considered with heterogeneous variance in the model. For example, there are cases in which it is important to model the heterogeneity of the treatments, and we can do it by using mixed models.

6.2 First-order auto-regressive

Another covariance structure for $\mathbf{\Lambda_i}$ which is widely used for longitudinal data is the first-order auto-regressive, also called $AR(1)$:

$$\mathbf{\Lambda_i} = \sigma^2 \begin{bmatrix} 1 & \rho & \cdots & \rho^{n_i-1} \\ \rho & 1 & \cdots & \rho^{n_i-2} \\ \vdots & \vdots & \ddots & \vdots \\ \rho^{n_i-1} & \rho^{n_i-2} & \cdots & 1 \end{bmatrix}. \quad (8)$$

This structure has only two parameters, the variance parameter σ^2, always positive, and the covariance parameter ρ, which may vary between -1 and 1. This kind of structure allows the residues associated with the observations in neighboring occasions to be more correlated than those whose observations are further apart. The $AR(1)$ is preferred for datasets in which the longitudinal observations are equally spaced.

7. Real data example

To exemplify what we have done so far, let's work with some real data of the ET from lettuce plants grown in pots. A total of $N = 12$ were completely randomized into three levels of water in the soil. At the first treatment, W_1, the water level for the plant were kept between 50.0 and 75.0% of the substrate's retention capacity. In the other two treatments, W_2 and W_3, the water level in the substrate was kept between 50.0 and 87.5% and between 50.0 and 100.0%, respectively. When the retention capacity of the substrate reached 50.0%, the pots were irrigated until their maximum level regarding each treatment.

The profile graphs from the accumulated ET for all pots in each treatment are shown in **Figure 4**. Note that the inferior asymptote, when $t \to -\infty$, is apparently

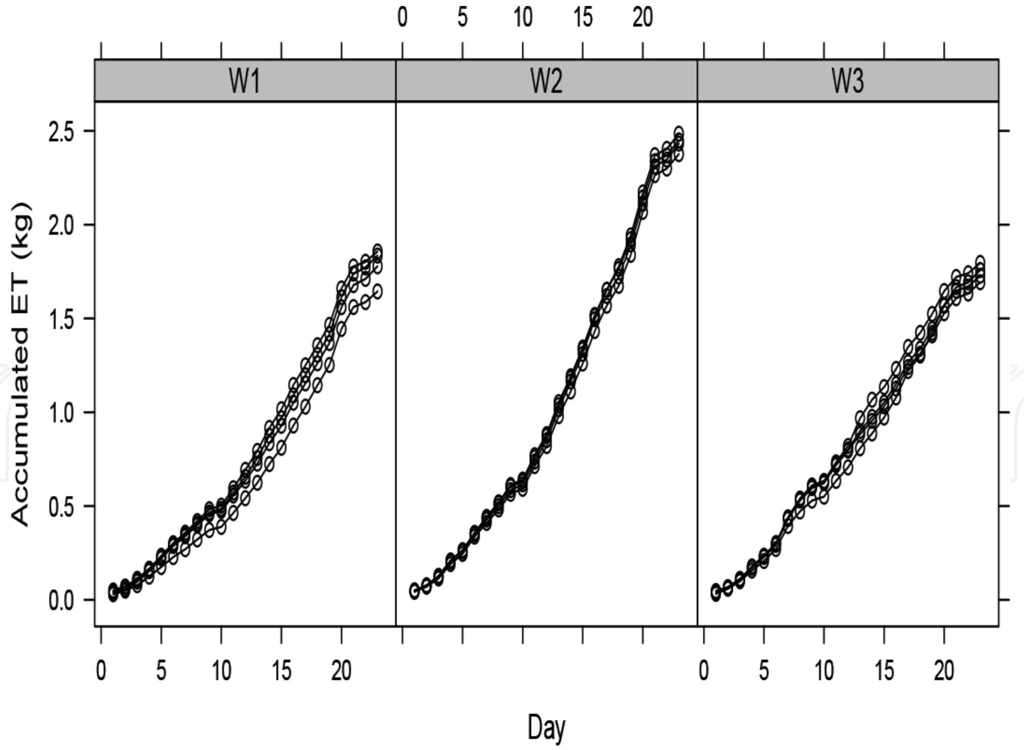

Figure 4.
Response profile for the accumulated ET of the lettuce plants over 23 consecutive days for the soil water levels W_1, W_2, and W_3.

Parameters	$\hat{\beta}$ (W_1)	$\hat{\gamma}$ (W_2)	$\hat{\delta}$ (W_3)
ϕ_1	-0.133363	—	—
ϕ_2	2.439746	0.935210	-0.272847
ϕ_3	16.648272	0.405882^{NS}	-2.302124
ϕ_4	5.765065	—	—

The only nonsignificant parameter (^{NS}) was ϕ_{3i} for the treatment W_2 with p-value >0.34. *The other parameters presented p-value* < 0.001.

Table 1.
Estimative for the models fixed effects parameters.

the same for all plants, i.e., the individual and treatment effects do not seem to be important for this parameter.

We model this data using Eq. (2) and considering treatment W_1 as baseline. The random effects were added to the parameters ϕ_{2i}, ϕ_{3i}, and ϕ_{4i}, and the treatments were important to explain the parameters ϕ_{2i} e ϕ_{3i}. Besides that, we consider the heterogeneity in the treatments and an AR(1) correlation structure for $\mathbf{\Lambda_i}$. The parameter estimative of the model is presented in **Table 1**.

The parameter ϕ_{2i} seems to be influenced by the other treatments, and its value was estimated in ~ 2.44 kg for W_1, $\sim 2.44 + 0.94 = 3.38$ kg for W_2, and $\sim 2.44 + (-0.27) = 2.17$ kg for W_3. The inflection point, i.e., the day the accumulated ET rate was maximum, also seems to be influenced by the treatments. W_1 and W_2 were not statistically different for the parameter ϕ_{3i}, but W_3, with estimative of ~ 14 days, appears to be statistically different from W_1 (~ 17 days).

The first graph presented in **Figure 5** brings the accumulated ET mean in each day of the four plants in each treatment. The solid lines are fitting for the treatments

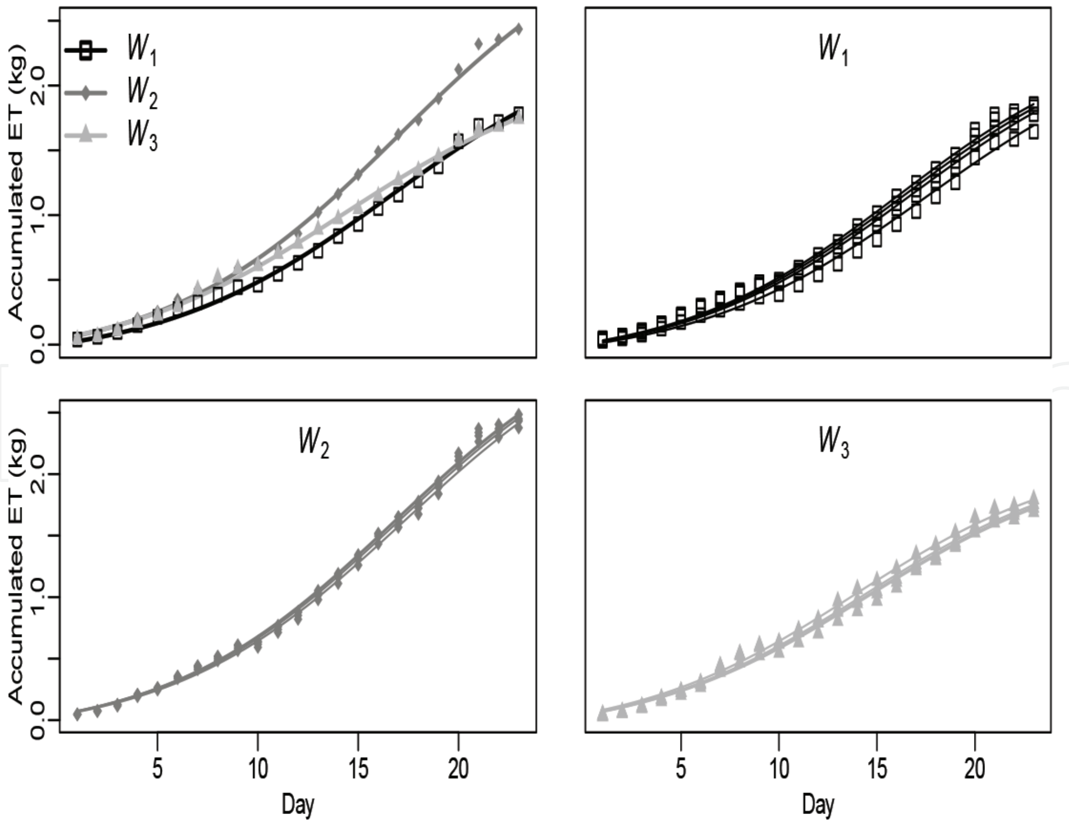

Figure 5.
Response profile of the accumulated ET by the lettuce plants over 23 consecutive days for the water soil levels W_1, W_2, and W_3.

made by Eq. (2). The other graphs present all values observed for the four plants in each treatment, and the solid lines indicate the individual model for each plant.

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