

Chapter 2

Mathematical Modeling of Biosystems

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Abstract Mathematics is an important tool for system modeling allows us to describe the behavior of a phenomenon or system in the real world, in particular biological systems. This chapter gives an overview of mathematical models, their construction, types of models, and examples of possible applications in biosystems models. Essential for building a model is determining its scope. In addition, the mechanistic and phenomenological mathematical models are described. Applications on fish biomass estimation, quality of fruits and crops are presented.

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2.1 Introduction

When we meet with the problem of describing the behavior of a real-world phenomenon or system, there is a need to resort to models. These models allow us to answer the question about important features and the behavior of the system studied under different conditions. There are different types of models such as verbal, mental, physical, and mathematical (Ljung and Gland 1994). In mathematical modeling, a number of assumptions translate into the language of mathematics. This has many advantages

1. Mathematics is a very precise language. This helps us to formulate ideas.
2. Mathematics is concise language, with well-defined rules for manipulations.
3. The mathematical results that have been proven over years are available to us.
4. Computers can be used to perform numerical calculations.

There are different mathematical models related to biochemical, physiological, and physical variables related to biosystems. Biosystems consist in any system of living creatures, however this term has been widely used for either plant or animal groups. Systems as constructed wetlands (CWs) have been recognized as effective means of “green technology” for wastewater treatment because their use of biological processes (assimilation by the plant tissue and microbial transformations); thus they may be also considered as biosystems (Kumar and Zhao 2011). Biosystem’s technology uses mathematical models applications in biomass and productivity forecasting. This can be accomplished by using the instrumentation systems for measuring variables related to plant production (Espinosa-Calderon et al. 2011; Gómez et al. 2005; Guzmán-Cruz et al. 2009; Guzmán-Cruz 2010; Millan-Almaraz et al. 2009).

Mathematical models can be based on several methods and principles such as steady-state mechanistic, temperature functions, Gaussian integration, stomatal conductance, nitrogen analysis, dynamic biological systems models, PAR, 3-D gradients of climatologic parameters, linear regression, nonlinear regression, and

diffusion-reaction (Bernacchi et al. 2009; Boonen et al. 2002; Farquhar et al. 2001; Gómez et al. 2005; Hoffman et al. 2004; Lombardozzi and Sparks 2012; Müller et al. 2009; Murray 2002).

2.2 Building a Mathematical Model

Essential for building a model is determining its scope. The process by which a mathematical model can be used to solve real world situations is usually called the mathematical modeling process (Miwa 1986a). Typically the process consists of the following four steps: (1) mathematical formulation, (2) programming, (3) parameter estimation, and (4) model evaluation (Soltani and Sinclair 2012). Sometimes, the developers of crop models do not always explicitly proceed through each step; it is valuable to be clear about these steps. If each step is not fully developed, the resultant model may be seriously compromised if its use is attempted outside the context in which the developer visualized it. It is likely a more robust model will result from the modeling process that recognizes each of these stages (Haefner 2005; Sinclair and Seligman 2000). The most important stage in this process is the formulation stage, assumptions based on deliberate suppression or neglect of irrelevant details are set up. If these assumptions are not appropriately setup, the nature of the situation is distorted, and the problem cannot be solved correctly. The setting up of adequate assumptions can be considered as the most important decision in performing mathematical modeling. Therefore, it is necessary to consider the role of assumptions in mathematical modeling process (Miwa 1986b).

2.2.1 Definition of Objectives

Before starting a modeling project, it is important to be clear about the model objectives. This step determines the future direction of the project in two ways. At the beginning of the modeling process, the objectives of the modeling effort should be explicitly and fully defined. A clear statement of specific objectives is essential to define needs and nature of a crop model (Sinclair and Seligman 1996).

It is more likely that success will be achieved when the objectives are clear, modest, and tractable (Sinclair and Seligman 1996). Criteria for judging the acceptability of a model should be defined in relation to the model's objectives. It is possible to quantitatively define stopping rules, in terms of statistical criteria concerning model predictions relative to a sample of observations.

Based on the objective, a list of specific hypotheses to be included in the model is prepared. Initially, it may be useful to list the hypotheses in the form of words and sentences. Some of the following points need to be considered in identifying hypotheses to be used to construct the model: (1) Models need to have generality, (2) Hypotheses will require input data either as parameters or driving variables,

- (3) The most useful models will be those that include parameters and state variables that can be readily determined by simple measurements or observations, (4) Existing hypotheses/models are a useful resource, but they need to be evaluated in view of objectives of the current model construction (Sinclair and Seligman 1996).

2.2.2 Quantitative Description of Hypotheses

Qualitative hypotheses need to be expressed as mathematical functions. Equations need to be developed to express how each hypothesis can be expressed in the model system. The interaction of hypotheses also needs to be taken into account, which often introduces a whole new layer of assumptions. Commonly, it is assumed that there is no interaction among hypotheses other than what has been explicitly defined.

The quantification of the model can be the most challenging because it requires a thorough knowledge of the system being modeled, and an understanding of the most relevant relationships. Additional functions can always be added to the model, but do these functions enhance the performance of the model for the stated objective? Often, the most critical phase of the model construction will be selection of the quantitative functions that sufficiently and efficiently describe the model component being modeled. Assembling equations without understanding and evaluating their relevance to the objectives overlooks a critical aspect of the modeling (Soltani and Sinclair 2012).

2.2.3 Programming

Once the hypotheses have been defined and quantified, the model is finally constructed into computer code. That is, the knowledge and insight about the system should have been captured and it should be a straightforward, even a trivial task, to translate the hypotheses into computer code. However, considerable care is required to accurately express the model in computer code. It is necessary to verify the computer algorithms and the codes are correct from mathematical relationships defined. Preparing computer programs usually requires debugging to eliminate the errors that arise during programming.

The program code can usually be organized in individual sections as represented in a flow diagram. In more expensive models, it is often useful to structure the code so that each section is placed into its own submodel. Placing parameter values for the various functions in their own separate, initialization section can facilitate the use of the model in simulations using different parameters. That is, code the functions in the model using parameter names, and then define all parameters at the beginning of the program. In this way, simulations of other

conditions such as a different cultivar are facilitated by adjusting the relevant parameters in the initialization (Haefner 2005).

2.2.4 Estimating Parameters

There are two acceptable general methods for parameter estimation:

1. *Literature* If the value of a parameter has been defined in research previously published, then these data are a strong starting point. This source of parameters is desirable because the research has been subjected to the rigors of peer review and the results are available to everyone.
2. *Measurement* Experiments or observations need to be done by the person constructing the model. Special research protocols need to be established and executed to obtain information about the desired parameters. Careful statistical analysis of the results is needed to obtain parameters. This method is time-consuming, laborious, and expensive. Soltani et al. (2004, 2006) presented examples of parameter estimation procedures related to different aspects of crop growth and development.

Another method that is too frequently used for parameter estimation is “calibration” of parameters so that the final output of the overall models matches the expected results. That is, the model is tested using different values for a specific parameter, then values are chosen that provide the closest match to the observations of the major outputs. Adjustments in parameters to achieve closer matches with observations by the complete model are difficult because it is not clear what parameters need adjusting. A major problem is that parameter adjustments can compensate each other and the parameters diverge from how the plant system operates.

The major limitation of the “calibration” approach is that reduces the model to an exercise in empirically fitting the model to the observations under a particular set of circumstances. Parameters are adjusted to achieve end results rather than relying on understanding about how the plants are performing and defining specific functions for the individual processes.

Sometimes “calibration” is done by reserving a separate data set for the calibration procedure. This approach does not overcome the basic empirical problem in this approach. Success of “calibrated” parameters in matching a second set of data only indicates success in splitting the two datasets, so that they represent the same population of data. That is, success with a calibrated model only assures that the calibration dataset were adequate to empirically match the second set of data (Soltani and Sinclair 2012).

2.2.5 Model Evaluation

Every model should be evaluated with respect to transparency and robustness. Transparency refers to how easy it is to understand a model and robustness refers to how closely the predictions of the model match with observed outputs from the system. However, after the above-mentioned steps in constructing a model, the model can be run and its output can be compared with measurements from the system. A test of the model output against observations is especially necessary when a model is to be used in an application mode. The users of the model need to be given some notion of situations in which the model has proven useful, with a disclaimer for reliability in any other situations (Sinclair and Seligman 1996). Model evaluation should be done based on predefined criteria established in the objective-definition stage. If the predictions are reasonably matched with the measurements from the system, based on predefined criteria, the modeling process is complete and the model is ready to use. If the results of the model evaluation stage are not satisfactory, it is necessary to reconsider the hypotheses, equations, and the quantitative methods used to construct the model. If alternative methods and equations are identified, then the model evaluation should be repeated. If predictions and the output are not still satisfactory, it is likely that there is some basic problem with the hypotheses. More experimental investigation is required and the modeling process should be set aside until observations allow improved hypotheses (Soltani and Sinclair 2012).

There are two critical criteria in evaluating the suitability of a model: transparency and robustness. Transparency means that the model parameters, flow diagrams, and code can be readily understood by those that were not involved in its development. As much as possible, the functions are stand-alone descriptions of processes in the plant and crop. Transparency is facilitated by a minimum number of empirical coefficients, and these coefficients can be independently observed and measured. Robustness means that the model produces simulation results that compare favorably with observation. The judgment of “favorable” will depend directly on the original objectives for the model (Teh 2006).

2.3 Types of Models

Mathematical modeling can be divided in two principal groups: mechanistic (white box) and phenomenological (black box) models. The white box models are deterministic and use physical modeling, thus they are explicative about the modeled system. Black box models, also called identification models, are direct descriptions of the data. Black box models have the disadvantage of not giving an explanation of the subjacent mechanisms. A combination of these two models results in gray box models.

2.3.1 Mechanistic Models

The development of a mechanistic mathematical model requires sufficient understanding of the physical, chemical, and biological processes that occur in a system and its use demands a proper validation. These kind of models are explanatory models, and they can be static or dynamic (Kita 2011). In addition, the study and description of a system involves two processes construction of mathematical models and numerical solution of the set of equations that describe the behavior of the system, through the use of a digital computer.

Mechanistic models are based on the assumption that the state of a system can be quantified and that changes in the state can be described by mathematical equations, equations of rate of change or differential equations. These models include several components: state variables, differential equations, parameters, and inputs. Normally, a state variable is a variable that appears in the accumulation term of adynamic balance of mass or energy. A state variable is a variable that can be quantified (at least conceptually) and it allows knowing the behavior of the system at all future instant in time (Kita 2011).

2.3.1.1 Modeling Phases

There are three phases in the process of the mathematical modeling (Ljung and Glad 1994):

1. The problem is structured.
2. The basic equations are formulated.
3. The state-space model is formed.

If the model is not too complex in terms of state variables, it can be used to design control systems for example optimal control strategies (Seginer and Ioslovich 1998; Van Henten 1994; Tap 2000) for the best growth, production, and crop quality.

The problem is structured

It is important to understand the general structure of the system (Ljung and Glad 1994). Thus, we need to answer the following questions:

- What signals are outputs and inputs?
- What happen in the system?
- What quantities are constants?
- What signals are internal variables?

When we have decided what variables in the systems are of interest and how they interact, then we attempt to divide the system into subsystems. This phase puts the great demands on the modeler because it requires the understanding of the

intuition for the physical system. In addition, in this phase, the level of complexity and degree of approximation are determined (Ljung and Glad 1994).

The basic equations are formulated

We have to formulate quantitative relationships between the inputs and outputs of the system (Ljung and Glad 1994). We must use knowledge about the mechanics, physics, chemists, and biological processes occurred in the system.

The relationships between the system variables can be of different kinds: conservation laws and constitutive relationships. Conservation laws are well-established laws like physics, chemises, or mechanics laws can be used. On the other hand, constitutive relationships might be given by experimental data or can be simple formulas that describe the general character of the relationship (Ljung and Glad 1994).

A good way of formulating the basic equation of a subsystem is the following:

1. Write down the conservation laws that are relevant for the subsystem.
2. Use suitable constitutive relationship to express the conservation laws in the model variables. Calculate the dimensions of the different quantities as a check (Ljung and Glad 1994).

The state-space model is formed

In this phase, we need to choose which internal variables will be considered state variables. Express the derivative of each state variable as function of state variables $x(t)$ and inputs $u(t)$. Express the outputs $y(t)$ as functions of the state and input variables (Ljung and Glad 1994). This is,

$$\begin{aligned}\frac{d}{dt}x(t) &= f(x(t), u(t)) \\ y(t) &= h(x(t), u(t))\end{aligned}\tag{2.1}$$

2.3.2 Phenomenological Models

2.3.2.1 Linear Regression

Measurement accuracy depends on the model used and on the knowledge of the studied process. The specificity of the studied system to particular applications simplifies the equations of the model (André 2013).

One example of a linear black box model is the measurement of photorespiration at the biochemical whole plant and atmosphere levels. It solves the fitting of oxygen (O_2) and carbon dioxide (CO_2) gas exchanges, avoiding complex equations and revealing the main factors of regulation of photosynthesis with its inseparable association with photorespiration (André 2013). Models as this one might be simple, but they represent a useful tool with a good approximation to understand the global relationships between plants and biosphere.

By observing the fitting of different variable curves related to the process, it can be deduced if such variable plays, or not, a crucial role in the regulation of the studied process.

2.3.2.2 Multiple Linear Regression

In many cases, y will depend on several independent variables such as $x_1, x_2, x_3, \dots, x_n$. This case can be treated by the multiple linear regression (MLR) method.

For example, Sousa et al. (2010) used MLR to model the pollen and fungal spores, considering nonbiological pollutant concentrations, the daily mean of ozone (O_3) and PM_{10} concentrations and meteorological parameters temperature (T), relative humidity (RH), precipitation (PP), and wind velocity (WV) as predictors. As results the models for each pollen and fungal spore were different depending on the analyzed period, which means that the correlations identified as statistically significant cannot be, even so, consistent enough.

2.3.2.3 Nonlinear Regression

In many applications, the regression functions will depend in a nonlinear way on the regression coefficients.

Nonlinear regression models are important tools as many crop and soil processes are better represented by nonlinear than by linear models, depending on the objective and the application domain, different priorities are set when fitting nonlinear models and these include obtaining acceptable parameter estimates, and a good model fit while meeting standard assumptions of statistical models.

A nonlinear regression model was used for Aufhammer et al. (2006), in order to model the role of brown clouds using a panel of yields and weather outcomes in India.

2.3.2.4 Logistic Type

There are indeed many phenomena in nature exhibiting a fast (virtually exponential) initial growth that then slow down after a certain point (where the curve reaches an inflection point) until a point of equilibrium or saturation of the system (carrying capacity). The logistic curve was introduced by Verhulst in the nineteenth century. The objective of Verhulst was to study population growth. In the 1920s, the interest in such method revived because of its excellence for modeling the development and evolution of many other growth phenomena (Román-Román and Torres Ruiz 2012). This type of models has been used in Ecology, Demography, and in Biology and Medicine, for the analysis of the growth of bacteria, tumors, and several species of animals and plants.

The deterministic logistic model is defined in terms of a differential equation where the linear constant defines the growth rate, whereas the quadratic term serves to inhibit or retard this rate. In this sense, the quadratic term is usually smaller than the linear one. When the population is small, the quadratic term, or inhibiting term, has little effect on the rising, so the population starts off with almost exponential growth. However, as the population increases, the inhibiting term eventually slows the rate of growth dramatically. Environmental fluctuations and lack of precision measurements represent ubiquitous noises that contribute with randomness to the logistic model (Li et al. 2011).

For processes whose mean function will be a logistic curve, it is possible to explicitly determine the transition density function, which allows to answer questions like the estimation of parameters through discrete sampling of paths after finding the likelihood from the transition density functions and the initial distribution. Such improvement enables the researcher to calculate the first passage time density, which requires an explicit form of such densities (Román-Román and Torres Ruiz 2012).

Logistic models offer the possibility of finding explicitly transition densities. This characteristic allows analyzing inference from the discrete sampling of trajectories. They also permit the estimation of functions, which allow predictive uses of the model. Finally, by studying first passage times, these models help in the determination of time variables used to locate when a preset condition is verified.

2.3.2.5 Statistical Approaches

The statistical approaching methods for modeling systems and processes consist, mainly, in the evaluation through, and application of, statistical techniques to datasets. Their only limitation is large number of datasets with different experimental conditions required for the application of any statistical packages. This limitation maybe seems to be small, but it usually is a challenging task.

Some examples of statistical techniques are: Levenberge-Marquardt (LeM) method, Nonlinear mixed effects (NLME), and first-order kinetics (Stein et al. 2007).

Since these models use a large number of datasets, it is commonly found that the magnitude of the generated coefficients varies strongly by species.

2.3.2.6 Time-Dependent Retardation Model

Time-dependent retardation models assume that there is a continuous variation in the studied process, which is common for every biosystem process, where time is a common degradation variable. However, it is important to note that the performance of this kind of models is often limited by a residual outlet concentration of certain variables in the studied system.

This kind of modeling has been considered to be one of the most efficient methods for designing CWs, because it allows a steady-state decrease in chemical

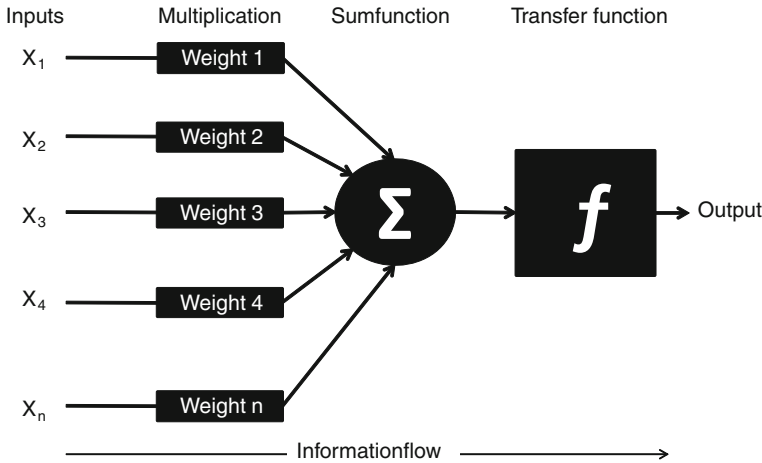


Fig. 2.1 Basic architecture of an artificial neuron

oxygen demand, or any other component. In such applications, it has been assumed that removal rates decrease during the course of time, because easily biodegradable substances are removed first and fast, thus leaving a solution with less biodegradable constituents and hence with slower removal kinetics. This continuous change in solution composition can be represented by a continuously varying volumetric first-order rate constant (Kumar and Zhao 2011).

2.3.2.7 Neuronal Networks

Artificial neural networks (ANNs) are parallel computational models, comprised of densely interconnected adaptive processing units. These networks are fine-grained parallel implementations of nonlinear static or dynamic systems. A very important feature of these networks is their adaptive nature where “learning by example” replaces “programming” in solving problems. This feature makes such computational models very appealing in application domains where one has little or incomplete understanding of the problem to be solved, but where training data is available (Hassoun 1995).

An ANN is a mathematical model that tries to simulate the structure and functionalities of biological neural networks. Basic building block of every ANN is artificial neuron, that is, a simple mathematical model (function). Such a model has three simple sets of rules: multiplication, summation, and activation. At the entrance of artificial neuron the inputs are weighted what means that every input value is multiplied with individual weight. In the middle section of artificial neuron is sum function that sums all weighted inputs and bias. At the exit of artificial neuron is sum of previously weighted inputs and bias is passing through activation function that is also called transfer function (Krenker et al. 2011) (Fig. 2.1).

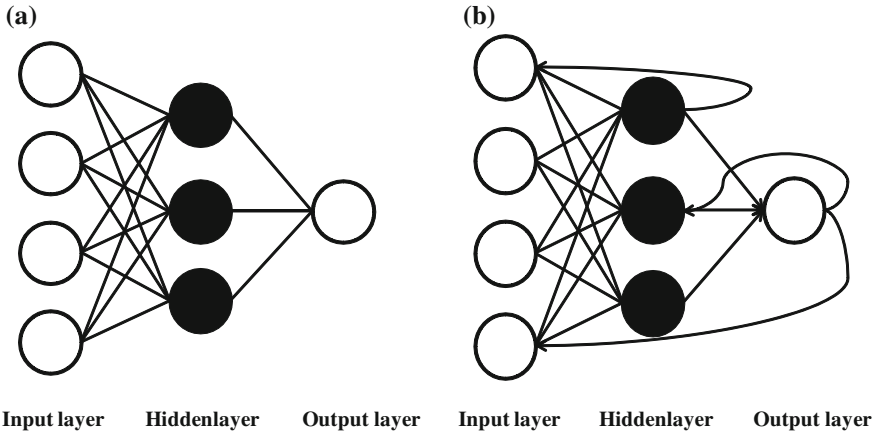


Fig. 2.2 Architecture of simple artificial neural networks: **a** Feed-forward (FNN) and **b** recurrent (RNN) topology of an artificial neural network

ANNs consist of two elements (i) formal neurons and (ii) connections between the neurons. The way that individual artificial neurons are interconnected is called topology, architecture or graph of an ANN. The full potential and calculation capabilities become clear when we start to interconnect neurons into ANNs. Neurons are arranged in layers, where at least two layers of neurons (an input layer and an output layer) are required for construction of a neural network. In any architecture every neuron of a layer is connected to every neuron of the following layer, and no intra-layer connections exist. This property allows referred to them as “multilayer perceptrons” although the classical perception contains only a single neuron (Minsky and Papert 1969). The fact that interconnection can be done in numerous ways results in different possible topologies that are divided into two basic types (Fig. 2.2). In the feed-forward topology (a) the information flows from inputs to outputs in only one direction and in the recurrent topology (b) some information flows not in only one direction from input to output but also in opposite direction. Fully connected feed-forward networks are by far the most frequently used neural networks for nonlinear modeling, pattern recognition, classification, signal filtering, and forecasting (Sumpter et al. 1994).

Formal neurons transform a numerical input to an output value, and the neuron connections represent numerical weight values. The weights and neurons’ internal variables (termed bias or threshold values) are free variables of the system which must be determined in the so-called “training stage” of the network development. This training set the proper response of an ANN according to the characteristics of the problem to be solved.

2.4 Validation

Model verification and validation are the primary processes for quantifying and building credibility in numerical models. Verification is the process of determining that a model implementation accurately represents the developer's conceptual description of the model and its solution. Validation is the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model. Both verification and validation are processes that accumulative evidence of a model's correctness or accuracy for a real situation; thus verification and validation cannot prove that a model is correct and accurate for all possible scenarios, but, rather, it can provide evidence that the model is sufficiently accurate for its intended use. It is important to perform a proper validation and verification to the model to extrapolate the results to other similar situations and predict new events.

The data used for model validation have not been used to build the model. There is a strong reason for not using data as we used in parameter estimation, it will make us think that the model gives better predictions than it is really capable. In linear regression, we correct for the effect of estimating two parameters by dividing the residual sum of squares by $(n-2)$ instead of (n) . Since data often contain errors, it is sometimes sufficient to prove that there is a not statistically significant difference between experimental data and model predictions (Bender 1978).

The differences between data and model predictions can be measured by graphical comparison, confidence intervals, and statistical tests. Hypothesis tests are particularly useful in comparing distributions, variances, or time series of model outputs to determine whether the model predictions are within an acceptable range of precision.

2.4.1 Validation Criteria

Some consist of comparisons with results available, others require the generation of new results for comparison, while others are based on responses from experts. Some of these criteria are used for verification to model validation. According to Godoy and Dardati (2001), the validation types can be classified as follows:

Comparison with other numerical solutions: the results of the model are associated with another solution identifying the proximity between them, that is, approximate results validate other approximate also obtained by other authors or other methods.

This technique does not involve a check of the representation of reality model. This type of comparison is also used to verify the model that can be verified when it is otherwise (Freedman and Ibaraki 2003).

Comparison with other analytical solutions: In this case, it is assumed that the researcher agrees with the theory behind the analytical formulation and with the same mathematical approach, as it also can be used for model verification. If this numeric code fails at playing an analytical solution, there must be a problem with the model formulation (Freedman and Ibaraki 2003).

Comparison with experimental results: This type of validation is the best, because it shows the consistency of the model with reality. However, obtained results of experiments are usually very complex and can be errors if not taken into account a correct consideration of environmental conditions. There is a risk that the model only works for a particular case and is not able to predict for another similar situation, or that the results do not accurately represent reality.

2.4.2 Statistical Tools

There are many statistical tools for model validation, but the primary tool for most process modeling applications is graphical residual analysis. These statistics can be classified in two categories:

- (a) Differences between the predictions and the measurements.
- (b) Correlation between the model outputs and the measurements from the system.

Deviation-based statistics has often used with correlation-based statistics. Although these different statistics may represent different aspects of the model measurement discrepancy, the deviation-based statistics (e.g., root mean square of deviation) and the correlation-based statistics (e.g., correlation coefficient) are not really with each other in their assumptions.

The residuals from a fitted model are the differences between the responses observed at each combination values of the explanatory variables and the corresponding predictions of the response computed using the model. Respectively, these values can be standardized by subtracting the mean and dividing by the standard deviation. Mathematically, the definition of the residual for the i th observation in the dataset is written.

$$e_i = y_i - x_i \quad (2.2)$$

The residuals plot can also be used to test the homogeneity of variance assumption. A residual score serves for determining the accuracy of your model (how much variability is explained by the model) and being used to test the assumptions inherent in the regression analysis (Shier and Wallenius 1999).

Mechanistic models provide a degree of understanding or explanation of the phenomena being modeled. To achieve this, the model must be constructed on (at least) two levels of description. A mechanistic model is based on our ideas of how the system works, what the important elements are and how they relate to each other (Thornley and France 2007).

A regression line between simulated and measured output is commonly included in the graph of simulated versus measured variable. This regression model will help to identify any bias in model prediction and determine correlation between model predictions and systems measurements.

Perhaps the most important statistic is the root mean square of deviation (RMSD), which is calculated from the following equation:

$$\text{RMSD} = \left(\frac{\sum (x_i - y_i)}{n - 1} \right)^{0.5} \quad (2.3)$$

With y_i the predicted variable with respect to the variable x_i and n the number of pairs of measured and simulated values. RMSD is usually reported and discussed as a percentage of average measured performance of the system.

In the second approach, the correlation coefficient between measured and simulated values are calculated. Correlation coefficient (r) can be obtained as follows:

$$r = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^n (y_i - \bar{y})^2}} \quad (2.4)$$

where x_i and y_i are the measured data and estimated given respectively in time i , and $\bar{x}$ and $\bar{y}$ are the means of the measured and estimated data, respectively, verifying that $-1 \leq r \leq 1$.

With a high r one might conclude that the model is robust with a finite number of variable records y_i to predict with respect to the variable x_i , then the following criteria are used to determine the relationship between the model and the quantized data.

$$\text{Bias } (B) = \frac{1}{n} \sum_{i=1}^n (y_i - x_i) \quad (2.5)$$

$$\text{Standard deviation (SD)} = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - x_i - B)^2} \quad (2.6)$$

$$\text{Prediction mean square (MSE)} = \frac{1}{n} \sum_{i=1}^n (y_i - x_i)^2 = \text{SD}^2 + B^2 \quad (2.7)$$

Each of these could be plotted against a chosen variable to test for homogeneity in performance. It is often a good idea to scale these summary statistics by the mean observation (Bender 1978).

For dynamics models that predict how quantities vary with time, so a dynamical model is generally presented as a set of ordinary differential equations with time to carry out the analyses of the obtained results some techniques of general statistics are used (Benes and Feireisl 2008).

Some measures of variance is the standard error of prediction percentage (%SEP); which establishes the degree of dispersion between the observed variable and the estimated variable. The coefficient of efficiency (E) and the average relative variance (ARV) are used to determine how the model can explain the total variation of the data (Rios Moreno et al. 2006). The percentage standard error of prediction is defined as:

$$\%SEP = \frac{100}{\bar{x}} \sqrt{\frac{\sum_{i=1}^n (x_i - y_i)^2}{n}} \quad (2.8)$$

Efficiency (E) is a sum of squares that provide a relative index of model behavior. Values can be obtained less or equal to 1, values of 1 indicates a perfect fit. A value of zero indicates that the model predictions are no better than taking the average values of the observed data and a negative value can be interpreted as a bad approach is that the results are worse than using the mean values of the observed data. The coefficient of efficiency (E) and the ARV are defined as $E = \frac{S_{obs} - S}{S_{obs}}$ and $ARV = \frac{S}{S_{obs}}$ where $S_{obs} = \sum_{i=1}^n (x_i - \bar{x})^2$ and $S = \sum_{i=1}^n (x_i - y_i)^2$ to have a perfect match, r and E should be close to 1 and the values %SEP and ARV close to 0.

If the results of the model validation stage are not satisfactory, it is necessary to reconsider the hypotheses, equations, and the quantitative methods and the data used to construct the model. If alternative methods and equations are identified, the model validation should be repeated. If the predictions and the output are not still satisfactory, it is likely that there is some basic problem with the hypotheses (Soltani and Sinclair 2012). More experimental investigation is required and the modeling process should be set aside until observations allow improved hypotheses.

2.5 Applications

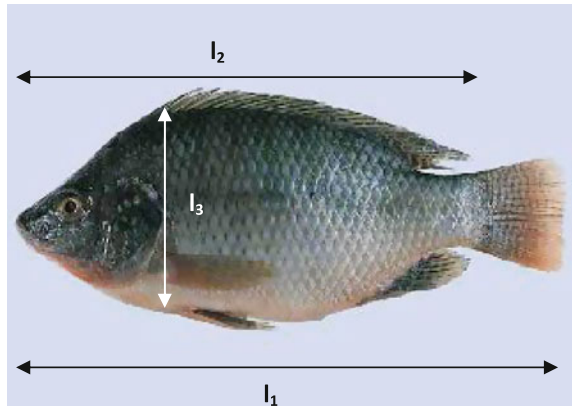
2.5.1 Estimating the Biomass of Fish

In crops of different aquacultural species it is important to determine the growth to know the development with respect to environmental conditions. In the literature, there are several studies which characterized the growth of various species of fish, but the authors recommend using the equations and statistical models obtained cautiously since the coefficients and constants involved in these equations depend mainly on the data analyzed.

The following is a study to determine the biomass of tilapia fish grown in ponds in greenhouses during the months of July and December of 2008, Fig. 2.4. Data were obtained from a random sample of fish to measure manually. Three measures and the weight were considered for the study of which are shown in Fig. 2.3.

One way to estimate the biomass of fish is using the lengths, for example, Hockaday et al. (2000) built two types of mathematical models for estimating fish

Fig. 2.3 Lengths measured during the growth cycle of the fish



biomass tilapia, first using least squares regression and through ANNs, these models are based on data on different lengths of fish. Another example is the research of Lines et al. (2001), which a system based on image analysis to estimate the mass of the salmon is proposed. The system was developed and tested under certain conditions. As well, Martínez et al. (2002) proposed a relation length–weight. In this case, a multiple regression was applied to relate the measured lengths with the weight of the fish. Thus, the mathematical model can be represented as follows:

$$p(l_1, l_2, l_3) = 0.155l_1l_2l_3 - 0.7209l_2l_3 + 5.0869l_1 - 7.6005l_2 + 3.7588l_3 \quad (2.9)$$

Figure 2.5 shows a comparison between the measurement data and estimated results by means of the Eq. (2.9). Some general statistics are used to analyze the obtained, such as: the correlation coefficient $r = 0.99$, bias $B = -0.05$, standard deviation $SD = 2.28$. According to these results, a good fit of the estimated data to the measured data was obtained.

2.5.2 Fruit Quality Changes

What constitutes quality largely depends on the consumer and the final destination of the product (Sloof et al. 1996). Quality can be seen as the concerted action of several quality attributes each based on their own physiological or physical product property. To predict keeping quality of a product, monitoring of a single attribute suffices but not necessarily gives a complete picture of the quality. For this, a compound quality index is required (Hertog et al. 2004). Quality is not a static parameter in general it decreases with time. Depending on the position of the product in the postharvest chain, this might be interpreted as a gain or loss (Hertog and Tijskens 1998).

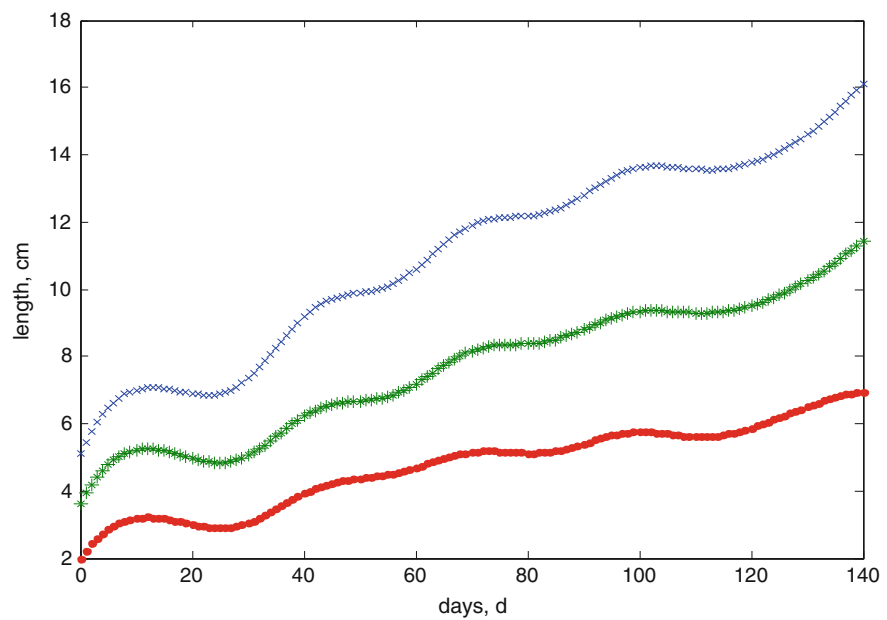


Fig. 2.4 Measurements obtained during the growth cycle of the fish: l_1 (xxx), l_2 (***) and l_3 (…)

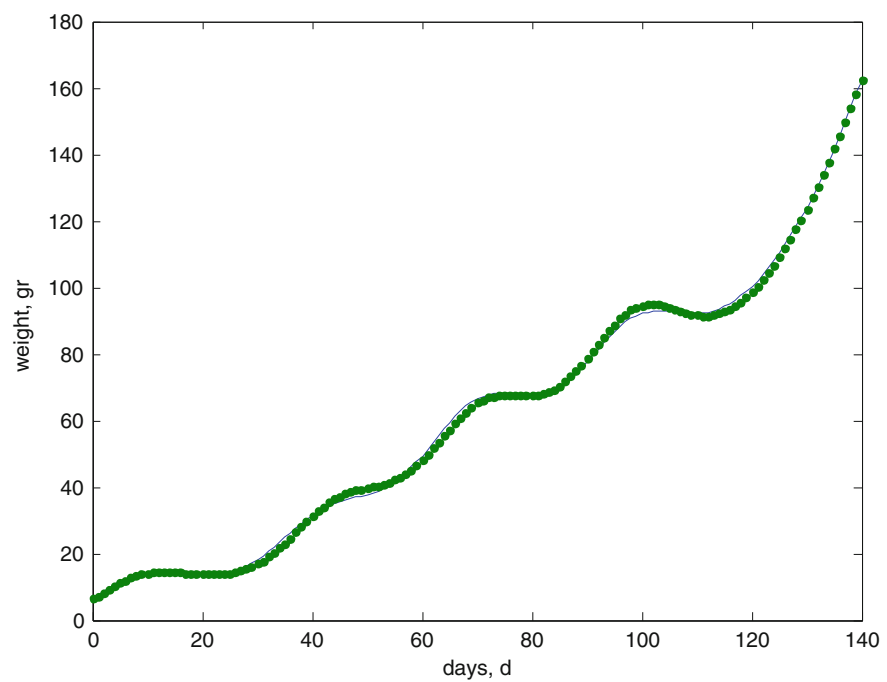


Fig. 2.5 Measurement data (- - -) and estimate data (…)

2.5.3 Modeling of Fruit Quality

A wide range of mathematical models has found their application in the wider food area (Tijskens et al. 2001). Important quality traits are manifested at the fruit scale. This is especially true for fruit size, dry matter content, and percentage of edible tissues. Fruit size and dry matter content result from the exchange of resources with the plant and the atmosphere. The carbohydrate supply has often been modeled according to the source/sink concepts (Léchaudel et al. 2005). An important variable of these models is the fruit demand for carbohydrates which is positively correlated to the seed number (Lescourret et al. 1998). In some models, a more mechanistic approach has considered that processes involved in sugar unloading from the phloem to the fruit tissues. For example, Fishman and Génard (1998) and Bruchou and Génard (1999) modeled sugar phloem unloading through mass flow, diffusion, and active transport.

In a postharvest context, the gas (O_2 , CO_2 , ethylene, and water vapor) fluxes through the skin have been related to the concentrations gradients, according to physical laws of gas diffusion. A model of fruit surface conductance to water vapor has been proposed recently (Gibert et al. 2005), which could improve the prediction of fruit transpiration as a function of fruit growth. More generally, fruit surface conductance to gas needs to be modeled in the future because it has a strong implication for fruit quality through its effect on fruit physiology, ripening, and quality (Paul and Srivastava 2006). Biomass allocation to the fruit tissues (which determines the percentage of edible tissues) also needs to be considered at the fruit scale. However, to our knowledge, there is no mechanistic model of biomass allocation into fruit tissues. Establishing empirical laws relating the size of any given tissue to that of another one or to that of the whole fruit may be a solution. Such laws are common in biology, mainly in the framework of allometric growth (West et al. 1997). For example, the dry masses of each fruit tissue and the dry mass of the fruit have been linked by allometric relationships (Lescourret and Génard 2005).

In order to assess the key processes underlying sugar concentration, an approach combining ecophysiological modeling and quality trait loci (QTL) analysis was proposed by Prudent et al. (2010). For this purpose, a first model predicting tomato fruit sugar concentration was adapted from a previous model built on peach fruit (Quilot et al. 2004), allowing the dissection of three interrelated elementary processes: the assimilate supply provided to the fruit, the metabolic transformation of sugars into other compounds, and the dilution of sugars by water uptake. In this work, two sources of variation were used to modulate the sugar concentration: a genetic method and a physiological method. This approach allowed observation of the inter-genotypic relationships first among elementary processes and then between elementary processes and sugar concentration; estimation of whether two different sources of variation for sugar concentration lead to similar changes in the underlying processes; and identification at each QTL for sugar concentration those processes which were supposedly involved.

In recent years, fruit quality has become an increasingly important aspect of fruit production. For example, in Europe, the new market organization enjoins farmers to form producer organizations whose goal is to improve fruit quality. Research efforts directed toward understanding the effects of climate and management techniques on fruit quality are needed, and mathematical models are useful frameworks for these research efforts (Lescourret and Génard 2005). Fruit quality, even when reduced to organoleptic qualities (such as sweetness or acidity) that meet consumer's demand, is a multicriterion concept. Each quality trait is the result of a complex chain of biological processes that depend on environmental conditions. These processes are interrelated (sugar metabolism depends on the carbon fluxes) and their effects on quality traits may be opposite (enhancing water fluxes into fruit increases sugar concentration; Génard and Lescourret 2004). Clearly, a useful fruit quality model must take into account several quality traits, the underlying processes, and their interactions.

However, following the researches of C.T. de Wit (van Ittersum and Donatelli 2003), most process-based fruit models have focused on carbon relationships leading to predictions of fruit growth in dry mass. Such photosynthesis-driven models have been developed for apples (Baumgaertner et al. 1984), grapes (Gutierrez et al. 1985), kiwifruit (Buwalda 1991), olives (Abdel-Razik 1989), peaches (Grossman and DeJong 1994), and tomatoes (Heuvelink and Bertin 1994). Some models have dealt with nitrogen content, representing nitrogen and carbon dynamics on a similar conceptual basis. Researchers have modeled water accumulation in fruit, considering water uptake and transpiration per unit fruit area as constant or variable (Génard and Huguet 1996). In a more mechanistic work applied to tomatoes, the difference between water potentials in the stem and the fruit was assumed to be the driving force of water import rate (Bussi eres 1994). Another tomato water model focused on the role of pedicel resistance and calyx transpiration (Bussi eres 2002). A few models of fruit metabolism describing synthesis and degradation processes have been designed for sugar (G enard and Souty 1996) and citric acid accumulation (Lobit et al. 2003). However, few models consider several processes together. Nevertheless, the virtual peach fruit model proposed by Lescourret and G enard (2005) is the first model to integrate in systemic framework knowledge of many interrelated processes, resulting in a complex quality profile and emergent properties that are typical of complex systems. The model offers various possibilities as a research tool, both for performing theoretical experiments and for helping to understand experimental results when studying the effects of technical scenarios for which there is no literature. Lescourret and G enard (2005) examined relationships between quality traits, physiological variables, and between both and found patterns that did not derive just from the aggregation of modeled basic functions. Moreover, the virtual peach fruit model may help in assessing the relative importance of processes for a given complex function or trait.

Virtual plants are being viewed as a novel means to simulate the genetic variability of plant responses to environmental conditions (Tardieu 2003). Combining either gene regulatory networks or quantitative trait loci (QTL) and models (Reymond et al. 2003) are two possible avenues, assuming that a genotype is

presented by ne parameter set (Tardieu 2003). Analyzing genotypic variation by means of models is a first step, and has been done with the carbon submodel on a contrasting population of peach genotypes (Quilot et al. 2004). In addition, incorporating the virtual peach fruit model in a crop model will be of value in simulating the combined effects of changes in climate, pest events changing leaf area or photosynthesis, genotype, and technical operations on profiles of quality traits, and will thereby help to improve breeding and crop management processes (Lescourret and Génard 2005).

2.5.3.1 Modeling Crop Quality: A Case of Study in Tomato

Fruit quality at harvest is a complex trait, including size, overall flavor (taste and texture), and visual attractiveness (color, shape), which depend on both genotype and environment. The improvement of fresh product quality is slowed down by its complexity. It is expected that the development of process-based models and their integrations in ecophysiological models should facilitate quality management, provided that integration properly accounts for interactions among biological processes (Bertin et al. 2006).

2.5.4 Applications of Neural Networks in Agriculture and Biosystems

Agricultural systems, such as environment–plant system, are quite complex and uncertain and they can be considered as ill-defined systems. They are characterized by nonlinearities, time-varying properties, climatic interactions, and many other factors. It is, therefore, difficult to quantify complex relationships between the input and the output of a system based on analytical methods. Recently, intelligent system control based on artificial intelligence has been one of the most prosperous technologies in the complex system science (Hashimoto 1997). ANN is also a promising tool for predicting crop yield and offers insight into the casual relationships through the use of sensitivity analyses, but the complex parameterization and optimum model structure require special attention (Park et al. 2005). The machine learning tools used to model the effects of environmental conditions on apparent photosynthesis provided a very powerful modeling alternative to ordinary curve fitting methods. Their major advantages are the flexibility to select between accuracy and generality and their robustness against outliers and mixtures of differentia responses (Dalaka et al. 2000). Resources capture and plant responses to energetic stimuli (solar radiation, temperature, CO₂ concentration, and humidity) present complex ecophysiological mechanisms, which conduct to dynamic modifications of the canopy development and architecture (Vazquez-Cruz et al. 2010).

In agronomic research, ANNs have been presented as alternative methodology to modeling and simulating crop biophysical properties. ANN models are specially

designed for dynamic nonlinear systems (Rahimikhoob 2010). ANNs are now used in many computer-based applications where there is a need to identify patterns or “learn” relationships between a set of input variables and a set of output variables (Danson and Rowland 2003). During the last decade, there has been a significant increase in agronomic ANN applications (Huang et al. 2010) including crop development modeling, crop yield prediction, evapotranspiration estimations, soil water, and salt content assessments (Dai et al. 2011; Fortin et al. 2010; Liu et al. 2009). Another important variable, which is commonly used in modeling crop, is leaf area. There have been a few attempts to produce leaf area estimation models predicting leaf area by means of using simple linear measurements like length and width (Beyhan et al. 2008). Vazquez-Cruz et al. (2012) developed an ANN model to determine the response of tomato leaf area to different climate conditions such as CO₂ concentration, PAR, and temperature along with different salicylic acid treatments. The results showed that ANN model was a useful tool in research and understanding the complex relationships between greenhouse conditions and leaf area development.

More research is needed in order to increase performance of training algorithms to improve the ability of neural systems to learn from climatic and physiological data patterns for crop growth prediction, and the forecasting performance to provide a useful guidance or reference for yield estimation.

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