Working with Dynamic Crop Models

Evaluation, Analysis, Parameterization, and Applications

EDITED BY
D. Wallach, D. Makowski
and J.W. Jones

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Preface

This book focuses on the methods for working with crop models, in particular, on mathematical and statistical methods. Most crop modelers are painfully aware of the need for such methods. Parameter estimation, model evaluation, and sensitivity analysis are called for in essentially every modeling project. Other methods treated in this book, related to the use of in-season measurements for improving model predictions, to optimization of management decisions, to the use of models on a large spatial scale or to the use of models to aid in genetic improvement of crops, are also important but only in certain cases.

In crop modeling as in all fields, it is a challenge to keep up with progress, and this is particularly difficult when it comes to mathematical and statistical methods, which are developed outside the framework of crop models. The purpose of this book is to make these methods easily available to crop modelers. We felt that there is a gap in the literature in this respect. Many books treat the way to describe a crop system in terms of equations, but none seems to provide an in-depth presentation of a large range of methods for working with crop models.

This book is intended for use in a graduate level course in crop modeling (hence the exercises), and for researchers who wish to use crop models. It should be useful to biologists, agronomists, and plant physiologists who are comfortable with describing and quantifying the soil–plant–atmosphere system, but are not familiar with rigorous methods for dealing with complex dynamic models. Others who may benefit are students and researchers with more mathematical and statistical backgrounds who are interested in the applications of applied mathematics to crop models. The emphasis throughout is on crop models, but in fact, much of the material applies more generally to dynamic models of complex systems.

While preparing the contents of this book, we had three main goals. First, the book should reflect the latest knowledge about the different topics covered. Second, the material should be adapted to and applicable to complex dynamic models, in particular, crop models. This is achieved by discussing each method in the specific context of crop models, by using simple crop models to provide the illustrative examples in the text and by furnishing case studies involving crop models. Finally, the material should be accessible to someone who has had basic courses in statistics and linear algebra. To this end, we have tried to explain each method simply, but without sacrificing detail or accuracy. To help the reader, an appendix reviews the statistical notions that are used in the text.

The origins of this book go back to the year 2000, when a group of French researchers began to prepare an intensive week-long school for modelers. The book began as a syllabus for that course. The years since then have gone into testing the material in other courses, expanding the coverage and refining the contents.

Statistician G.E.P. Box once wrote, “All models are wrong, but some are useful”. Our hope is that this book, by improving access to important methods, will contribute to increasing the usefulness of crop models.

D. Wallach
D. Makowski
J. W. Jones

Overview

Herein is a brief overview of the contents of the book.

I. Methods

1. The two forms of crop models. This chapter is concerned with the mathematical form of crop models. Crop models consist of a set of dynamic equations (form 1), which one integrates to get predictions of responses *versus* inputs (form 2). The uses of the two forms are quite different.

2. Evaluation. This chapter first presents and discusses different measures of the distance between model predictions and observed values. It then discusses the notion of prediction error and insists on the difference between how well the model reproduces past data and predicts future values. There is also a discussion on how to evaluate a model when it is used to propose crop management decisions.

3. Uncertainty and sensitivity. Such analyses are aimed at describing how variations in input factors (variables or parameters) affect the output variables. The chapter begins by reviewing the uses of such analyses. The rest of the chapter discusses different sensitivity or uncertainty indices and how they are calculated, in particular, in the case where multiple input factors vary.

4. Parameter estimation. There is a very large statistical literature about parameter estimation, but most of it cannot be directly applied to crop models. The specific problems of crop models include the large number of parameters compared to the amount of field data and the complex structure of that data (several variables, at various dates). On the other hand, there is often outside knowledge about many of the parameter values (from controlled environment studies, similar crops, etc.). The chapter begins with a basic introduction to the principles and methods of parameter estimation. Then the specific case of complex crop models is considered. A number of approaches to parameter estimation that have been or could be used are described and illustrated. Included here is the Bayesian approach to parameter estimation, which is particularly adapted to the efficient use of the outside information.

5. Data assimilation. In-season information about crop growth, for example from satellite photos, is becoming increasingly available. This information can be used to adjust a crop model to reflect the specific trajectory of the field in question. This chapter discusses and illustrates how this adaptation can be done. In particular, variants of the Kalman filter approach are explained and illustrated.

6. Representing and optimizing management decisions. Improving crop management is a major use of crop models. The first part of this chapter concerns how to express management decisions, and discusses in particular decision rules, which express decisions as functions of weather or state of the crop. The second part of the chapter presents and discusses algorithms for calculating optimal decisions. The problem is very complex because of the multiple decisions and the uncertainty in future climate, but efficient algorithms exist.

7. Using crop models for multiple fields. One is often faced with the problem of running a crop model for multiple fields, for example in order to predict regional yields or nitrogen leaching for each field in a watershed. This chapter discusses the specific problems posed by this use of crop models. A major problem is that in general one cannot obtain all the necessary input variables for every field. The chapter presents the different solutions that have been proposed for each type of input data.

II. Applications

8. Introduction to Section II

9. Fundamental concepts of crop models. This chapter discusses the way crop models represent a crop–soil system, with examples from five different crop models.

10. Crop models with genotype parameters. The existence of multiple varieties for each crop, and the fact that many new varieties are developed each year, is a problem specific to crop models. It is important that models be variety specific, but this raises the problem of how to identify and estimate the variety specific parameters. This chapter discusses the approaches that have been proposed.

11. Model assisted genetic improvement in crops. This chapter covers the very new field of the use of crop models in plant breeding. It explains the different ways in which crop models can contribute to selection and includes examples of such uses.

12–20. Case studies. These chapters illustrate a diversity of applications of crop models, and show how the methods presented in Section I can be useful.

Section I
Methods

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Chapter 1
The two forms of crop models

D. Wallach

1. Introduction

Crop models are mathematical models which describe the growth and development of a crop interacting with soil. They can be viewed in two different, complementary ways. First, a crop model can be seen as a system of differential or difference equations, which describe the dynamics of the crop–soil system. Second, the model can be thought of as a set of equations for responses of interest as functions of explanatory variables. We present and discuss these two viewpoints in this chapter. As we shall see, the different methods described in this book may call for one or the other of these viewpoints.

2. A crop model is a dynamic system model

The general form of a dynamic system model in discrete time is

$$\begin{aligned} U_1(t+\Delta t) &= U_1(t) + g_1\left[U(t), X(t); \theta\right] \\ &\vdots \\ U_S(t+\Delta t) &= U_S(t) + g_S\left[U(t), X(t); \theta\right] \end{aligned} \tag{1}$$

where t is time, Δt is some time increment, $U(t) = [U_1(t), \ldots, U_S(t)]^T$ is the vector of state variables at time t, $X(t)$ is the vector of explanatory variables at time t, θ is the vector of parameters and g is some function. For crop models, Δt is often one day. The state variables $U(t)$ could include for example leaf area index (leaf area per unit soil area), biomass, root depth, soil water content in each of several soil layers, etc. The explanatory variables $X(t)$ typically include initial conditions (such as initial soil moisture), soil characteristics (such as maximum water holding capacity), climate variables (such as daily maximum and minimum temperature) and management variables (such as irrigation dates and amounts). Chapter 9 contains an overview of the processes generally described by crop models.

The model of Eq. (1) is dynamic in the sense that it describes how the state variables evolve over time. It describes a system in the sense that there are several state variables that interact.

To illustrate, we present a very simplified crop model with just 3 state variables, namely the temperature sum *TT*, plant biomass *B* and leaf area index *LAI*. The equations are:

$$TT(j+1) = TT(j) + \Delta TT(j)$$

$$B(j+1) = B(j) + \Delta B(j)$$

$$LAI(j+1) = LAI(j) + \Delta LAI(j)$$

with

$$\Delta TT(j) = \max\left[\frac{T\mathrm{MIN}(j) + T\mathrm{MAX}(j)}{2} - T_{\mathrm{base}},\ 0\right] \tag{2}$$

$$\begin{aligned} \Delta B(j) &= RUE(1 - \mathrm{e}^{-K \cdot LAI(j)})I(j) & TT(j) &\le TT_{\mathrm{M}} \\ &= 0 & TT(j) &> TT_{\mathrm{M}} \end{aligned} \tag{3}$$

$$\begin{aligned} \Delta LAI(j) &= \alpha \Delta TT(j) LAI(j) \max[LAI_{\max} - LAI(j), 0] & TT(j) &\le TT_{\mathrm{L}} \\ &= 0 & TT(j) &> TT_{\mathrm{L}} \end{aligned} \tag{4}$$

The index j is the day. The model has a time step Δt of one day. The explanatory variables are $T\mathrm{MIN}(j)$, $T\mathrm{MAX}(j)$ and $I(t)$ which are respectively minimum and maximum temperature and solar radiation on day j. The parameters are T_{base} (the baseline temperature for growth), RUE (radiation use efficiency), K (excitation coefficient, which determines the relation between leaf area index and intercepted radiation), α (the relative rate of leaf area index increase for small values of leaf area index), $LAI_{\max}$ (maximum leaf area index), TT_{M} (temperature sum for crop maturity) and TT_{L} (temperature sum at the end of leaf area increase).

2.1. The elements of a dynamic system model

2.1.1. State variables U(t)

The state variables play a central role in dynamic system models. The collection of state variables determines what is included in the system under study. A fundamental choice is involved here. For example, if it is decided to include soil mineral nitrogen within the system being studied, then soil mineral nitrogen will be a state variable and the model will include an equation to describe the evolution over time of this variable. If soil mineral nitrogen is not included as a state variable, it could still be included as an explanatory variable, i.e. its effect on plant growth and development could still be considered. However, in this case the values of soil mineral nitrogen over time would have to be supplied to the model; they would not be calculated within the model. The limits of the system being modeled are different in the two cases.

The choice of state variables is also fundamental for a second reason. It is assumed that the state variables at time t give a description of the system that is sufficient for calculating the future trajectory of the system. For example, if only root depth is included among the state variables and not variables describing root geometry, the implicit assumption is that the evolution of the system can be calculated on the basis of just root depth. Furthermore, past values of root depth are not needed. Whatever effect they had is assumed to be taken into account once one knows all the state variables at time t.

Given a dynamic model in the form of Eq. (1), it is quite easy to identify the state variables. A state variable is a variable that appears both on the left side of an equation, so that the value is calculated by the model, and on the right side, since the values of the state variables determine the future trajectory of the system.

2.1.2. Explanatory variables and parameters ($X(t)$, θ)

The explanatory variables likewise imply a basic decision about what is important in determining the dynamics of the system. In the chapter on model evaluation, we will discuss in detail how the choice of explanatory variables affects model predictive quality. Briefly, adding additional explanatory variables has two opposite effects. On the one hand, added explanatory variables permit one to explain more of the variability in the system, and thus offer the possibility of improved predictions. On the other hand, the additional explanatory variables normally require additional equations and parameters which need to be estimated, which leads to additional error and thus less accurate predictions.

Explanatory variables and parameters can be recognized by the fact that they appear only on the right-hand side of Eq. (1). They enter into the calculation of the system dynamics but are not themselves calculated. The difference between explanatory variables and parameters is that explanatory variables are measured or observed for each situation where the model is applied, or are based on measured or observed values. Thus for example maximum soil water holding capacity is measured for each field, or perhaps derived from soil texture, which would then be the measured value. Potentially at least, an explanatory variable can differ depending on the situation while a parameter is by definition constant across all situations of interest.

2.2. The random elements in the dynamic equations

We have written the dynamic equations as perfect equalities. In practice however they are only approximations. The actual time evolution of a state variable in a system as complex as a crop–soil system can depend on a very large number of factors. In a crop model this is generally reduced to a small number of factors; those considered to be the most important. The form of the equation is also in general chosen for simplicity and may not be exact. Thus the equations of a crop model should actually be expressed as

$$U_i(t + \Delta t) = U_i(t) + g_i\,[U(t), X(t); \theta] + \eta_i(t), \quad i = 1, \ldots, S \tag{5}$$

where the error $\eta_i(t)$ is a random variable. This is a stochastic dynamic equation.

Another major source of uncertainty in the dynamic equations comes from the explanatory variables and in particular climate. When crop models are used for prediction, future climate is unknown and this adds a further source of uncertainty about the time evolution of the system.

3. A crop model is a response model

We can integrate the differential equations or difference equations of the dynamic system model. Often we talk of "running" the model when the equations are embedded in a computer program and integration is done numerically on the computer. For the difference equations, one simply starts with the initial values at $t = 0$ of the state variables, uses the dynamic equations to update each state variable to time $t = \Delta t$, uses the dynamic equations again to get the state variable values at $t = 2\Delta t$, etc. up to whatever ending time one has chosen.

The result of integration is to eliminate intermediate values of the state variables. The state variables at any time T are then just functions of the explanatory variables for all times from $t = 0$ to $t = T - \Delta t$ i.e. after integration the state variables can be written in the form

$$U_i(T) = f_{i,T}\,[X(0), X(\Delta t), X(2\Delta t), X(3\Delta t), \ldots, X(T - \Delta t); \theta], \quad i = 1, \ldots, S \tag{6}$$

In general, there are a limited number of model results that are of primary interest. We will refer to these as the model response variables. They may be state variables at particular times or functions of state variables. The response variables may include: variables that are directly related to the performance of the system such as yield, total nitrogen uptake or total nitrogen leached beyond the root zone; variables that can be used to compare with observed values, for example leaf area index and biomass at measurement dates; variables that help understand the dynamics of the system, for example daily water stress.

We note a response variable Y. According to Eq. (6) the equation for a response variable can be written in the form

$$Y = f(X; \theta) \tag{7}$$

where X stands for the vector of explanatory variables for all times from $t = 0$ to whatever final time is needed and θ is the same parameter vector as in Eq. (1). When we want to emphasize that the model is only an approximation, we will write $\hat{Y}$ in place of Y.

3.1. The random elements in the response equations

Since the dynamic equations are only approximate, the response equations are also only approximate. Including error, the equation for a response variable can be written

$$Y = f(X;\theta) + \varepsilon \tag{8}$$

where ε is a random variable. For the moment we ignore the uncertainty in X. Since the response equations derive directly from the dynamic equations, ε is the result of the propagation of the errors in Eq. (5). However, it is not obligatory to first define the errors in the dynamic equations and then derive the errors in the response equations. An alternative is to directly make assumptions about the distribution of ε. In this case, Eq. (8) is treated as a standard regression equation. If there are several response variables to be treated, then one is dealing with a (generally non-linear) multivariate regression model.

The error arises from the fact that the explanatory variables do not explain all the variability in the response variables, and from possible errors in the equations. In addition there may be uncertainties in the explanatory variables, in particular climate when the model is used for prediction.

4. Working with crop models. Which form?

In developing and working with crop models, both the dynamic equations and response equations are used, though for different objectives one will in general concentrate on one or the other.

During the initial development of a crop model one generally works with the dynamic equations. Several reasons have led to the use of dynamic crop models. First, we have a great deal of information about the processes underlying crop growth and development, and the dynamic equations allow us to use this information in studying the evolution of the overall crop–soil system. A second reason is that they allow us to break down the very complex crop–soil system into more manageable pieces and to model each of those pieces separately. It is possible to develop response models directly, without the intermediate step of dynamic equations. However, such models are in general limited to much simpler representations of a crop–soil system than is possible with dynamic crop models. The individual dynamic equations in crop models may also be quite simple, but their combination and interaction in the overall model results in complex response equations.

Historically, researchers have had two quite different attitudes towards crop models. On the one hand, a crop model can be considered a scientific hypothesis. Testing the hypothesis involves both forms of a crop model. The dynamic equations represent the hypothesis, which is tested by comparing the response equations with observations. The second attitude is that crop models are engineering tools. They are useful in relating outputs to inputs, but it is not necessary that the dynamic equations mimic exactly the way the system functions. The dynamic equations are simply a way of deriving useful input–output relationships. In this case, the response equations are of main interest and the evaluation of the model measures the quality of the input–output relationships. Evaluation is treated in Chapter 2.

Especially from an engineering perspective, the general behavior of the model responses as functions of the explanatory variables is of interest and importance. However, the response equations are in general not available as analytic expressions, but only after numerical integration of the dynamic equations. It is thus difficult to analyze the effect of input variables on response variables directly from the model equations. This has led to the use of sensitivity analysis, which is the study of how input factors (both explanatory variables and parameters) affect the outputs of a response model. This topic is treated in Chapter 3.

A major problem with crop models is obtaining the values of the parameters. The complexity of crop models means that there are in general, many (often a hundred or more) parameters. The amount of experimental data on the other hand is in general limited because experimentation on crop systems is necessarily lengthy and expensive in terms of land, equipment and manpower. If we consider just the response equations, then we have a regression problem involving simultaneously all the parameters in the model, and their estimation from the experimental data may be impossible or at least lead to large errors. However, the fact that a crop model has two forms often leads to additional information that can be used for parameter estimation. In particular, one often assumes that the dynamic equations have validity beyond the range of conditions described by the response model. This implies that one can do experiments on some processes under other conditions than those where the crop model will be used. For example, the temperature dependence of some processes may be studied in controlled temperature environments. The result is additional data, independent of the data on the overall system, that can be used to estimate parameters. The problem of parameter estimation for crop models is discussed in Chapter 4.

A specific problem related to crop models is that for each crop species there are in general many varieties, and plant breeders add new varieties each year. From a crop model perspective, this greatly exacerbates the problem of parameter estimation, since at least some of the model parameters vary from variety to variety. A possible solution is to use both the dynamic and response forms of a crop model. Some varietal parameters can be obtained from studies on the individual processes, others can be estimated from the response equations. This approach is discussed in Chapter 10. One can also treat this problem at a more fundamental level, by seeking to relate the model parameters more closely to genetic information (see Chapter 11).

A very promising approach to improving crop models is data assimilation, where one injects in-season data into the model and adjusts the values of the state variables or the parameters to that data. Assimilation is based on Eq. (5). It is necessary to have an estimate of error in the dynamic equations, in order to determine the respective weights to give to the data and to the model when combining those two sources of information. Data assimilation is treated in Chapter 5.

Testing different possible crop management strategies is a major use of crop models. One aspect of this use is mathematical optimization of management strategies. Chapter 6 presents two different approaches to optimization. Optimization by simulation is based on the response form of crop models. Here, management strategies are parameterized. Optimization consists of calculating the values of the management parameters that maximize an objective function, which in general depends on a small number of model response variables such as yield or grain protein content. The second approach treats optimization as a control problem. Here, the dynamic equations are used to calculate the transition probabilities from one time step to the next, as a function of explanatory variables including management decisions.

5. Conclusions

The fact that crop models exist in two forms, as dynamic equations and as response equations, is both a complication and an advantage. One complication is that in general this leads to quite complex models. A second is that model error must be treated at two levels, that of the dynamic equations and that of the overall system response.

The advantage is that the model can be developed and analyzed at two levels. One can study the individual processes and the overall system, and results from both can be integrated into the model. This allows us to profit from knowledge of how the system functions in order to better understand and manage crop–soil systems. The connection between processes and the overall system can also be used to test and improve our knowledge of the processes.