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Estimating uncertainty in crop model predictions: Current situation and future prospects

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ABSTRACT

In this introductory paper to the special issue on crop model prediction uncertainty, we present and compare the methodological choices in the studies included in this issue, and highlight some remaining challenges. As a common framework for all studies, we define prediction uncertainty as the distribution of prediction error, which can be written as the sum of a bias plus a predictor uncertainty term that represents the random variation due to uncertainty in model structure, model parameters or model inputs. Several themes recur in many of the studies: Use of multi-model ensembles (MMEs) to quantify model structural uncertainty; Emphasis on uncertainty in those inputs related to prediction of regional results or climate change impact assessment; Simultaneous consideration of multiple sources of uncertainty; Emphasis on exploring the variability of uncertainty over space or time; Use of sensitivity analysis techniques to disaggregate the separate contributions to prediction uncertainty. Relatively new approaches include the estimation of both the bias and predictor uncertainty terms of prediction error, the construction of MMEs specifically designed to explore the uncertainty in model structure, the use of emulators for sensitivity analysis and the exploration of ways to reduce prediction uncertainty other than through model improvement. Major remaining challenges are standardization of approaches to quantifying uncertainty in model structure, parameters and inputs, going beyond studies of specific sources of uncertainty to estimation of overall prediction uncertainty, comparing and combining validation and uncertainty studies, and evaluation of uncertainty estimates. Looking forward, we suggest that assessment of prediction uncertainty should be a standard part of any modelling project. The studies here will contribute toward that goal.

1. Introduction

The practice of crop modeling has undergone an important evolution in recent years, with a growing acknowledgement and characterization of uncertainty in crop model predictions (Rötter et al. 2011; Rosenzweig et al. 2013; Asseng et al. 2013). One new approach to have come from this work is the use of multi-model ensembles (MMEs), following the impulsion of the Agricultural Modeling and Improvement Project (AgMIP) (Rosenzweig et al. 2013) and the European knowledge hub on Modelling European Agriculture with Climate Change for Food Security (MACSUR). A major focus of MME modeling is to obtain information on prediction uncertainty; the variability between outcomes simulated by different models is a measure of the prediction uncertainty due to uncertainty in model structure. Thus the widespread use of MMEs has shifted the equilibrium of modeling studies from a rather one-sided emphasis on prediction to a more balanced viewpoint where both prediction and information on prediction uncertainty are major goals.

Once variability becomes a major issue, other sources of uncertainty besides model structure need to be considered. There is uncertainty not only in model structure, but also in the values of the model parameters and in the values of the input variables. Furthermore, it is clear that the variability between multiple simulations is not sufficient for appreciating prediction uncertainty. There is also the possibility that all models have some common bias, which also contributes to prediction uncertainty. Additional sources of uncertainty can be important for specific uses of models. A new frontier in analysis of crop model prediction uncertainty is combining and comparing different sources of uncertainty, firstly in order to evaluate overall prediction uncertainty, and secondly to identify the most important contributions to that uncertainty.

The goal of this special issue (SI) is to highlight recent progress in the estimation of crop model prediction uncertainty, with emphasis on the use of MMEs. Most of the articles consider not only structure uncertainty, based on the MME results, but also uncertainty due to one or more other sources. The articles illustrate the range of prediction problems that can be addressed, the sources of uncertainty that can be important and procedures for taking multiple sources of uncertainty into account. Several of the papers furthermore show how prediction uncertainty due to multiple sources of uncertainty can be disaggregated, in order to identify the contribution from each source. The problem of reducing prediction uncertainty is also considered in several of the papers.

Each paper in this SI treats uncertainty for one specific problem, and covers multiple aspects of estimating uncertainty that arise for that problem.

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That is, the articles are objective-oriented. However, it is also useful to present a methodology-oriented view of these studies. That is the purpose of this introduction. We decompose the problem of uncertainty estimation into individual components, and show how each component is treated in the different studies. The sections of this introduction correspond to separate aspects or components of the problem of estimating prediction uncertainty.

In the following section we present a rigorous statistical definition of model uncertainty. This is important in order to provide a common framework for understanding and comparing the various studies on uncertainty. In the subsequent section we discuss the important distinction between uncertainty and variability. Next we discuss the various sources of uncertainty that contribute to overall simulation uncertainty, pointing out which are addressed by the articles in this SI. Then the way that the articles treat the problem of disaggregating overall uncertainty, in order to quantify the contributions of different sources of uncertainty, is discussed. The following section concerns paths toward the reduction in uncertainty that are proposed in the articles. Some of the remaining challenges in the evaluation of crop model uncertainty are discussed in the next to last section, followed by conclusions.

2. Defining uncertainty

In Challinor et al. (2013) uncertainty is defined as follows: "… uncertainty … is used to denote a lack of predictive precision due to either inherent limitations to predictability (e.g. due to unknown future greenhouse gas emissions) or to a lack of predictive skill (e.g. errors in the design of a model)." It is important to complement this narrative with a precise statistical definition of prediction uncertainty, in order to have a common framework for analyzing different studies and to avoid ambiguity and misunderstanding in comparing approaches and results. We use the definition of Wallach et al. (2016c), which is also explicitly adopted by two of the papers in this SI (Wallach, et al 2017, Alderman and Stanfill 2017). According to this definition, uncertainty is the distribution of errors of prediction e, where

$$e = Y - f(X; \theta) \tag{1}$$

In this equation Y is the true value of the quantity being predicted and f(X;θ) is the predictor (model) that is used, which is a function f (the model equations) of input variables X and parameters θ. Of course we don't know, for each prediction, what the error will be. If we did, we would simply correct to give perfect predictions in each case. But we can hope to estimate the distribution of that error, based on past experience and on our knowledge of uncertainties in the prediction. That is, estimating prediction uncertainty means estimating how predictions are distributed around the true value. A simple summary of the distribution of prediction error is the mean squared error of prediction, defined as

$$MSEP(X) = E\{[Y - f(X; \theta)]^2\}$$

While the full distribution of e contains of course more information, the summary MSEP has the advantage that it expresses prediction uncertainty as a single number.

Two quite different approaches to uncertainty arise depending on whether we treat the predictor f(X;θ) as fixed or random. If fixed, the variability in e comes only from the variability in Y. The distribution of e represents the errors for different Y values. Treating the predictor as fixed means that we are looking at the error for a specific model, with a specific parameter vector, and assuming that the input variables are perfectly well known. This is of course of major interest; we are in fact often interested in how well a specific model, with a specific parameter vector, predicts.

When f(X;θ) is considered fixed, prediction error can be estimated based on past error. If we assume that past agreement between model and observations is indicative of future agreement, then we can use that past agreement to estimate the distribution of prediction error e or certain aspects of that distribution. In particular, consider the mean squared error (MSE) of simulated values compared to observations

$$MSE = \sum [Y_i - f(X_i; \theta)]^2$$

where the sum is over observations. This is an estimate of E(MSEP(X)), where the expectation is over the range of predictions of interest. Evaluating MSE for a model is usually referred to as model "evaluation" or model "validation", not as "model uncertainty". However, it is also clearly related to model uncertainty as we have defined it.

The second possibility is to treat one or all of model structure, model parameter vector and model inputs as random variables, i.e. they are not assumed to be fixed but rather have some distribution of possible values. Then the predictor f(X;θ) is a random function, and e has a distribution not only because of the variability in Y, but also because of the variability of f(X;θ). This approach is appropriate when we want to take into account explicitly the uncertainty in model structure and/or parameter values and/or input values. In this case e is not a measure of how well a specific predictor performs, but rather a more general measure of how well we can predict given the current state of uncertainty about structure, parameters and inputs. More specifically, it measures the distribution of error when prediction uses a model structure chosen at random from a distribution of model structures, a parameter vector chosen at random from a distribution of parameter vectors and an input vector chosen at random from a distribution of approximations to the true input vector.

We can write model error as the sum of two terms

$$\begin{aligned} e &= \{Y - E[f(X; \theta)]\} + \{E[f(X; \theta)] - f(X; \theta)\} \\ &= \text{bias} + \text{predictor uncertainty} \end{aligned} \tag{2}$$

Since the predictor is treated as a random function, it has an expectation, which is the value averaged over the distributions of structures, parameter vectors and approximations to the inputs. The above equation simply adds and subtracts that expectation. The advantage of doing so is to separate e into a term that depends on the true value Y (the bias term), and a second term that just depends on the random variation in the predictions (the predictor uncertainty). It is important to note the distinction between "prediction uncertainty", which is the distribution of model error and which includes the bias term, and "predictor uncertainty", which only concerns the random variability of the predictor.

Using the expression in Eq. (2), it is easily shown that MSEP(X) also separates into 2 terms:

$$\begin{aligned} MSEP(X)_{random} &= E[(Y - f(X; \theta))^2] \\ &= \{Y - E[f(X; \theta)]\}^2 + \{E[f(X; \theta)] - f(X; \theta)\}^2 \\ &= \text{squared bias} + \text{predictor variance} \end{aligned} \tag{3}$$