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Accounting for both parameter and model structure uncertainty in crop model predictions of phenology: A case study on rice

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ABSTRACT

We consider predictions of the impact of climate warming on rice development times in Sri Lanka. The major emphasis is on the uncertainty of the predictions, and in particular on the estimation of mean squared error of prediction. Three contributions to mean squared error are considered. The first is parameter uncertainty that results from model calibration. To take proper account of the complex data structure, generalized least squares is used to estimate the parameters and the variance-covariance matrix of the parameter estimators. The second contribution is model structure uncertainty, which we estimate using two different models. An ANOVA analysis is used to separate the contributions of parameter and model uncertainty to mean squared error. The third contribution is model error, which is estimated using hindcasts. Mean squared error of prediction of time from emergence to maturity, for baseline +2 °C, is estimated as 108 days², with model error contributing 86 days², followed by model structure uncertainty which contributes 15 days² and parameter uncertainty which contributes 7 days². We also show how prediction uncertainty is reduced if prediction concerns development time averaged over years, or the difference in development time between baseline and warmer temperatures.

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1. Introduction

Rice is the principal food crop in Sri Lanka, with about 20% of the population engaged in rice cultivation (Department of census and statistics, 2012). Global warming trends will impact rice production, and have already been found to affect rice phenology and growth in China (Tao et al., 2006).

Crop models are often the tools of choice for estimating the impact of climate change on crop development and production (Masutomi et al., 2009; Matthews, 1995; Parry et al., 2004). Uncertainty information is essential in all prediction studies, but perhaps especially so when predicting behavior of complex systems such as climate or crops, where predictions ineluctably have substantial error (Holzkämper et al., 2015; Tebaldi and Knutti, 2007).

There have been numerous studies of uncertainty in crop models, using various different approaches. A fundamental choice is whether or not to treat the simulated values as random variables. One common approach is to consider the simulated values as fixed, ignoring uncertainty in the model equations or parameter values. One uses agreement of this fixed model with hindcasts in order to calculate mean squared error or some other measure of agreement with the data (Basso et al., 2016; Bouman and van Laar, 2006; Timsina and Humphreys, 2006; Wallach et al., 2014; Yang et al., 2014). The implicit assumption is that the errors of simulated values based on past data is indicative of the distribution of errors for new predictions.

An alternative approach is to explicitly consider the model structure and/or parameters as random variables, with some distribution. Uncertainty in this case includes uncertainty in the simulated values. There have been studies where parameter uncertainty is propagated through the model to obtain uncertainty in simulated values (Aggarwal, 1995). Recently there have been

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several studies where multiple crop models have been applied using a common protocol, and where the variability between models is taken as a measure of model uncertainty (Asseng et al., 2013; Bassu et al., 2014; Li et al., 2015; Rosenzweig et al., 2013). Taking account of both model and parameter uncertainty in the same study has not been done for crop models, though there have been studies of this type with climate models (Monier et al., 2014).

The variability in simulated values due to model structure and parameter uncertainty does not represent all the uncertainty in predictions. It ignores the fact that in general even the best model, calibrated with a large amount of data to eliminate parameter uncertainty, is not a perfect predictor. That is, there is a model error term that also contributes to prediction uncertainty. The model error term is not normally considered in studies that use multi-crop model ensembles, but it is taken into account in other settings. In standard regression analysis, the mean squared error of prediction includes both the effect of parameter uncertainty and the variance of model error (Myers, 2007). In Bayesian regression, one calculates both the distribution of the parameters and the variance of residual error (Gelman et al., 2004; Omlin and Reichert, 1999). (Wallach et al., n.d.) propose a framework to quantify prediction which includes parameter uncertainty, model uncertainty, explanatory variable uncertainty and model error.

Thus in some studies, model structure and model parameters have been treated as fixed, while in others they have been treated as random quantities. Treating the model and parameters as fixed or random implies somewhat different definitions of uncertainty; uncertainty just in the agreement between simulated and observed values in the first case, uncertainty also in the simulated values in the second. Each approach has its advantages and drawbacks. A major advantage of the random approach is that it allows one to study how uncertainty varies depending on the quantity being predicted. One does multiple simulations (using multiple models and/or parameters for each model) for each specific prediction, and calculates the simulation variance specifically for that prediction. This is based just on simulations, not on data. In principle one could also model hindcast errors as a function of covariates, but this would be based on data, and is usually impractical for crop models because of the limited amount of data available.

A major difficulty associated with treating the model and parameters as random variables is that one must specify a distribution for each. As to the distribution of parameter values, if the parameters are estimated using frequentist estimation, then that approach furnishes an estimate of the variance-covariance matrix of the parameter estimators (Nissanka et al., 2015; Seber and Wild, 1989). A Bayesian approach to calibration produces directly the distribution of the parameters (Gelman et al., 2004; Iizumi et al., 2009; Wallach et al., 2012). In practice however, crop model calibration is often done using an ad hoc approach, which does not provide any information on parameter uncertainty (Ahuja and Ma, 2011). Then one must rely on expert opinion to obtain parameter uncertainties (Aggarwal, 1995). If one does use a standard statistical approach, there is the difficulty of taking the often complex data structure into account. If there is dependence among model errors that is ignored, this in general leads to underestimation of parameter uncertainty (Seber and Wild, 1989).

The objective of this paper is to illustrate an overall approach to uncertainty estimation that combines several of the methods described above, which have not previously been employed together. Our approach treats models and parameters as random variables, includes model error, takes account of the complex data structure in estimating parameter uncertainty and takes into account the effect of averaging or differencing on uncertainty.

We will specifically consider the problem of predicting development times of rice in Sri Lanka for temperatures that are on average 2 °C warmer than current temperatures. This is

approximately the average monthly temperature increase predicted by an average of multiple GCMs at mid-century for scenario RCP8.5, for the concerned area of Sri Lanka (Zubair et al., 2015). We consider just two models, DSSAT for rice (Alocilja and Ritchie, 1988; Jones et al., 2003) and APSIM-Oryza (Gaydon et al., 2012a, 2012b). These are the models that were used in a model intercomparison study in South Asia organized as part of the AgMIP project (Hillel and Rosenzweig, 2015).

2. Materials and methods

2.1. The data

The data here are from two sites in Sri Lanka; the Rice Research and Development Institutes (RRDI) at Batalagoda (7°32' N, 80°27' E), and Mahailuppallam (8°06' N, 80°27' E). The data are either from detailed field experiments or from Coordinated Rice Variety Trials (CRVT), and concern both the maha season (spans approximately mid-November to February), and the yala season (South-West monsoon, spans approximately mid-May to September). The rice variety is Bg300, which is widely used in Sri Lanka. Altogether there are 27 year-site-season combinations, from the period 2000–2010.

For Batalagoda, the range of maximum temperature (T_{max}) in the weather file (Jan 1, 2000–31 Dec 2010) is 23.4 °C to 38.1 °C with 80% of the values between 29.1 °C and 33.6 °C. The range of minimum temperatures (T_{min}) is between 13.9 °C and 28.9 °C, with 80% of the values between 20.9 and 24.9. The values for Mahailuppallam, for the period Jan 1, 2000–31 Dec 2008, are similar. The range of T_{max} is 23.6 °C to 37.8 °C, with 80% of the values in the range 29.3 °C to 34.6 °C. The range of T_{min} is 15.4 °C to 27.3 °C, with 80% of the values in the range 20.6 °C to 25.3 °C.

Seeds were soaked for one day until germination began, and then the germinating seeds were broadcast in the field at a rate of around 350 plants/m². After broadcasting, emergence could be seen in general in three days.

The date of panicle initiation (PI) was determined by dissecting the main culm of 5 plants from each plot in order to see if the panicle primordia were visible using a hand-held magnifying glass. The date of PI was taken as D-10 days, where D is the date when the primordia were first visible. Heading date of an individual plant was defined as the date when the panicle of the main stem first becomes visible as it comes out of the leaf sheath. Heading date for the crop was defined as the first date when 50% heading is observed in a demarcated area (0.5 m² or 1 m in a row). To determine heading date, visual observations were made daily around 9.00–10.00 am. The day of physiological maturity was only determined in the detailed experiments. In the CRVT experiments the day of harvest was recorded, but this coincided closely with physiological maturity. The standard deviations of the replicates for days of heading or maturity were in the range 0.6–3 days. Recommended Department of Agriculture (DOA) management was followed in all fields. Further experimental details can be found in (Nissanka et al., 2015).

2.2. The APSIM-Oryza model for rice phenology

The APSIM-Oryza model for rice (Gaydon et al., 2012a; Gaydon et al., 2012b; Zhang et al., 2004), hereafter referred to as APSIM, uses the plant routines including the phenology sub model of ORYZA2000 with the water and nitrogen routines of APSIM.

According to this model the development rate depends on degree days (DD), calculated from daily T_{min} (°C) and T_{max} (°C) temperatures. First, hourly temperature is calculated as

$$T_i = (T_{min} + T_{max})/2 + (T_{max} - T_{min}) \times \cos(0.2618 \times (i - 14))/2 \quad (1)$$

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