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Uncertainty in wheat phenology simulation induced by cultivar parameterization under climate warming

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A R T I C L E I N F O

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A B S T R A C T

Rigorous calibration of crop phenology models, providing both best-estimate parameters and estimates of parameter uncertainty, is essential for evaluating how crops will respond to future environmental and management changes. Least squares parameter estimation is a widely used approach to calibration of nonlinear models, and there are many software packages available for implementing this approach. However, these packages are rarely if ever used for complex phenology models because of technical difficulties. The purpose of this research is to overcome these difficulties, in particular the issue of a model which is a discontinuous function of the parameters. The calculations were conducted with the WheatGrow phenology model, but the approach is applicable to other complex phenology models. The approach was used to calibrate WheatGrow phenology for 4 widely used cultivars in the main winter wheat production region of China. The resulting fit to the data was quite good (root mean squared error (RMSE) of 3–4 days for flowering and maturity). The coefficients of variation (CV) of the parameters ranged from 6% to 40%. Furthermore, the model was used to predict the effect of warming on phenology, and the uncertainty in those predictions. The results showed that each degree of warming reduced the time from sowing to flowering by 7–8 days for the spring cultivars and 3–4 days for the winter cultivars. The time form flowering to maturity is hardly affected. In addition, the higher the temperature, the larger the uncertainty in the predictions. Comparison with variability in multi-model ensembles suggests that parameter uncertainty is less than the model uncertainty.

1. Introduction

Wheat (*Triticum aestivum* L.) is the third most important agricultural food and feed crop in the world behind maize and rice, and an essential source of carbohydrates for millions of people. In China wheat plays a significant role in the diet of the majority of people. It accounts for about 10.9% of China's total planting area and approximately 17.3% of China's total crop production (FAOSTAT, 2014). The anticipated rise in demand for food in the future has further promoted wheat production (Ortiz et al., 2008) and spurred research, including the use of modelling to evaluate the impact of climate change on wheat production (Asseng et al., 2015; Lv et al., 2013), and potential and achievable wheat yields across regions (Abeledo et al., 2008; Ma et al., 2016; Schierhorn et al., 2014; Wu et al., 2006).

Simulation of crop phenology is a central aspect of crop models. Crop phenology controls the life cycle of crops and the partitioning of assimilates between crop organs. It also determines the timing of various agronomic management practices (Menzel et al., 2006). Phenology has been shown to change as temperature has risen in recent decades, a process that occurs worldwide in most crops (Zhang et al., 2013). The accelerated developmental rate caused by climate warming is often associated with a harmful effect on production, particularly for agricultural crops for which sunlight, water and nutrient resources would be consequently reduced (Challinor et al., 2007). Alterations in the duration of crop growth are thus an important indicator of agricultural vulnerability to climate warming and have captured great attention. A number of modelling studies have shown that future crop productivity will strongly depend on the magnitude of the change in the duration of crop growth brought on by climate warming (Asseng et al., 2015; Palosuo et al., 2011; Zhao et al., 2015). Accurate modelling of crop phenology is therefore essential to evaluation of management options and crop response to climate and management changes (Craufurd et al.,

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2013; He et al., 2017; Liu et al., 2016; Wang et al., 2013).

Several of the key parameters that specify cultivar phenological differences in current phenology models are not directly related to measurable quantities (Liu et al., 2000). These parameters are obtained by calibration, i.e. by fitting the model to field data. It is important that calibration provide not only good estimates of the model parameters, but also estimates of the uncertainty in the parameter values, which can be used to estimate the uncertainty in predictions due to parameter uncertainty. Several recent studies have focused on differences in prediction between models, as a measure of the consequences of model structure uncertainty (Asseng et al., 2013; Bassu et al., 2014; Li et al., 2015). Few studies however have attempted to quantify the uncertainty caused by model parameterization and its response to climate change. One recent study investigated the uncertainty which was induced by cultivar parameterization in canola (He et al., 2017). No attempts seem to have been made to quantify the uncertainty caused by model parameterization for wheat.

There are two quite different approaches to quantify the uncertainty in statistics, corresponding to the two major paradigms of frequentist and Bayesian statistics (Stark, 2015). In frequentist statistics, parameters are fixed quantities, but their estimators are random variables, and uncertainty refers to the distribution of the parameter estimators. In Bayesian statistics, the parameters are themselves random variables, and uncertainty quantifies our knowledge about them. Most work on parameter uncertainty in crop models has been based on a Bayesian approach (Dumont et al., 2014) or on GLUE, a Bayesian-like approach (He et al., 2010). A Bayesian approach is relatively simple to implement, even for complex models, because it does not require the model to have any particular mathematical properties. However, in the Bayesian approach, one must define prior information about the parameters. If there is well-documented quantitative prior information, it is advantageous to take it into account. In most cases, however, the prior information is rather vague, and so its quantification is quite subjective. This is problematic, since the calculated uncertainties may depend strongly on the chosen priors (Stark, 2015). GLUE has the same issue of priors, plus other additional subjective features (He et al., 2010). The frequentist approach requires no such subjective input, which is an important advantage, though there can be a model user effect, as found by Confalonieri et al. (2016). A very common frequentist approach is least squares (Motulsky and Christopoulos, 2004; Seber and Wild, 1989). There are many software packages which calculate least squares parameter estimates and associated uncertainties, but they usually require the model to be continuous, which is often not the case for phenology models. As a result, least squares parameter estimation for phenology models often uses an ad hoc criterion of goodness of fit, and a trial and error search for the best fit parameters (Jin and Shi, 2006; Xiong et al., 2007). Other studies have used specially programmed algorithms, such as simulated annealing (Ferreyra, 2004) or a genetic algorithm (Dai et al., 2009). None of these calculate uncertainty information. Standard statistical least squares algorithms, with uncertainty estimation, seem to have been used only for the simplest phenology models (Wallach et al., 2017).

The first goal of this study is methodological. The goal is to show how a standard frequentist approach can be used to estimate parameters and parameter uncertainty for complex phenology models, based on existing statistical software. The specific software we use is the nonlinear least squares (nls) function of the R statistical programming language (Bates and Chambers, 1992; R Core Team, 2013). The specific model studied is WheatGrow, but our approach could be applied to other models. The statistical approach is not new. In fact, the goal is to take advantage of existing theory and methods in statistics, which have been thoroughly tested and are based on known principles. The innovation here is in coupling these approaches to complex phenology models. The major difficulty to overcome is the existence of discontinuities in the model outputs as a function of the parameters. The second goal of this paper is to apply the methodology to obtain estimated parameters and associated uncertainties for the WheatGrow phenology model, for four common wheat cultivars in the main winter wheat production region of China. The model has previously only been calibrated by trial and error (Huang et al., 2013). Having reliable parameter values is important for building up a data base of parameter values for this model and for using the model for prediction. In particular, we estimate the effect of warming on wheat phenology in the region of interest.

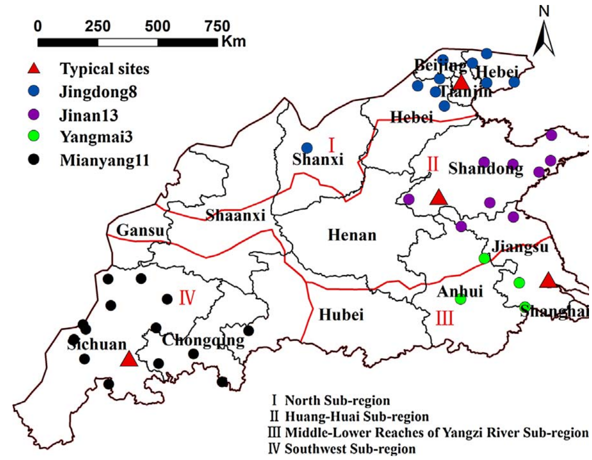

Fig. 1. Map of the study region of China and the locations of the study sites (circles and triangles). In each sub region, data for only a single variety was used, as indicated. The red triangles indicate the single site in each region used to investigate prediction uncertainty.

2. Materials and methods

2.1. Study sites and sources of observed data and model input variables

The study region was located between 102°46′–122°11′E and 28°13′–41°10′N, covering 14 major winter wheat production provinces and municipalities in China. The whole study region was divided into four sub-regions based on geography and climate, two northern sub-regions, namely the North Sub-region (NS) and the Huang-Huai Sub-region (HHS), and two southern sub-regions, namely the Middle-Lower Reaches of the Yangzi River Sub-region (MYS) and the Southwest Sub-region (SWS) (Fig. 1). The study region accounts for more than 85% of the total wheat planting area in China and more than 90% of the total wheat grain yield in the country (National Bureau of Statistics of China, 2012).

In each sub region, one variety planted at different sites during the period 1981–2010 was selected (Fig. 1). The total number of sites and site-year combinations for each variety, plus additional information, are shown in Table 1. One of the study sites in each sub-region was chosen to investigate prediction uncertainty under various warming scenarios (Table 1). Each study site provided sowing day, day when 50% of plants first flowered and maturity day for each year. Durations from sowing to flowering and sowing to maturity were used for calibration. Normal local management practices were followed at each site. In all experiments, weeds, pests and diseases were properly controlled, and fertilizers were applied to eliminate any nutrient deficiency. Observed daily weather data, including maximum and minimum temperatures, sunshine hours and rainfall, were obtained from the China Meteorological Administration for each site-year.

2.2. The WheatGrow model

The WheatGrow model used in this study was developed by the National Engineering and Technology Center for Information Agriculture, Nanjing Agricultural University. It can simulate the daily