How well do crop models predict phenology, with emphasis on the effect of calibration?

Running head: Crop model phenology prediction

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ABSTRACT

Plant phenology, which describes the timing of plant development, is a major aspect of plant response to environment and for crops, a major determinant of yield. Since climate change is projected to alter crop phenology worldwide, there is a large effort to predict phenology as a function of environment. Many studies have focused on comparing model equations for describing how phenology responds to weather but the effect of crop model calibration, also expected to be important, has received much less attention. The objective here was to obtain a rigorous evaluation of prediction capability of wheat crop phenology models, and to analyze the role of calibration. The 27 participants in this multi-model study were provided experimental data for calibration and asked to submit predictions for sites and years not represented in those data. Participants were instructed to use and document their "usual" calibration approach. Overall, the models provided quite good predictions of phenology (median of mean absolute error of 6.1 days) and did much better than simply using the average of observed values as predictor. Calibration was found to compensate to some extent for differences between models, specifically for differences in simulated time to emergence and differences in the choice of input variables. Conversely, different calibration approaches led to major differences in prediction error between models with the same structure. Given the large diversity of calibration approaches and the importance of calibration, there is a clear need for guidelines and tools to aid with calibration. Arguably the most important and difficult choice for calibration is the choice of parameters to estimate. Several recommendations for calibration practices are proposed. Model applications, including model studies of climate change impact, should focus more on the data used for calibration and on the calibration methods employed.

Introduction

Global change is placing unprecedented pressure on food security (Campbell et al., 2018; Godfray et al., 2010; Wheeler & von Braun, 2013). The search for ways to increase the volume and efficiency of food production needs to account for the effects of climate change on agricultural production systems (Porter, Howden, & Smith, 2017). Modeling is an important tool in projecting and understanding the trajectory of food production under future climates (Asseng et al., 2019; Bindi, Palosuo, Trnka, & Semenov, 2015; Carberry et al., 2013; Hochman, Gobbett, & Horan, 2017; Parry, Rosenzweig, Iglesias, Livermore, & Fischer, 2004). One of the likely effects of climate change will be an increase in air temperature (IPCC, 2014). Temperature directly affects plant growth through a number of pathways, one of which is phenology (Went, 2003). Phenology describes the cycles of biological events in plants. These events include seedling emergence, leaf appearance, and flowering. Matching the phenology of crop varieties to the climate in which they grow is a critical crop production strategy (Hunt et al., 2019; Rezaei, Siebert, & Ewert, 2015; Rezaei, Siebert, Hüging, & Ewert, 2018). Thus, understanding and improving our ability to simulate phenology with crop models is an important activity in preparing for and adapting to global change. Process-based models similar to those for crops can be used for natural vegetation, so crop models can serve as examples for studies of phenology in ecosystems (Piao et al., 2019).

Crop model evaluation is an essential aspect of modeling, assessing whether model performance is acceptable for the intended use of the model. For studies of phenology two major questions are a) how accurate are current models for the prediction of crop development stages? and b) what determines model accuracy and what does that imply about how accuracy can be improved? We use here prediction in the sense of determining outputs (dates of development stages) from known inputs (weather, soil, management). The problem of predicting future events, with unknown weather, is not considered.

There have been numerous evaluation studies of crop model simulations, including but not restricted to phenology, both of individual models and of multi-model ensembles. The typical procedure is to first calibrate the model using a part of the available field data and then to evaluate it using the remaining data. Most crop model evaluation studies focusing on crop phenology have had relatively little data for calibration or evaluation. (Andarzian, Hoogenboom, Bannayan, Shirali, & Andarzian, 2015) for example, used data from one location covering five growing seasons and two or three sowing dates per year. Out of these data, one year was used for calibration and the other two years of data to evaluate the model. (Yuan, Peng, & Li, 2017) used one year of data for calibration and the second year of data from the same location for evaluation of the rice crop model ORYZA. Hussain, Khaliq, Ahmad, & Akhtar (2018) tested four models using data from two locations with two years of data, 11 crop planting dates, and three varieties. Paucity of data means that model parameters are estimated with relatively large uncertainty and model evaluation is quite uncertain.

Another common feature of crop model evaluation is that the data are often such that model error for the evaluation data cannot be assumed to be independent of model error for the calibration data. That holds for the examples listed above since the evaluation and calibration data come from the same sites. In such cases, the evaluation does not give an unbiased estimate of how well the model will predict for other sites not included in the calibration data. Since usually the model is meant for use over a range of sites, this clearly reduces the usefulness of the evaluation information.

A third feature often found in crop model evaluation is that the range of situations from which the calibration data are drawn (the "training population") is often different than the range of conditions from which the evaluation data are drawn (the "evaluation population"). For example, Hussain et al. (2018) used data from an experiment that included a range of crop stresses to calibrate their model. They used data from the least stressed treatment in the calibration process and evaluated the resultant model on the remaining planting dates at the same location. The evaluation data thus represented a different range of conditions than the calibration data. In a multi-model ensemble study of the effect of high temperatures on wheat growth (S. Asseng et al., 2015) detailed crop measurements were provided for one planting date and the models were evaluated using other planting dates, some with additional artificial heating. Again, the evaluation data represented a much larger range of temperatures than represented in the calibration data. While the capacity of crop models to extrapolate to conditions quite different than those of the calibration data is obviously of interest, it is a rather different type of evaluation than the case where the training and evaluation populations are similar.

Thus, evaluation of crop phenology models to date has mainly concerned situations that would tend to make prediction difficult, because of small amounts of data for calibration and differences between the training and target populations. Furthermore, the quality of the evaluation is often questionable, because of the relatively small amounts of data and the non-independence of the errors for the calibration and evaluation situations. There is thus a need for more rigorous assessments of simulation capability of crop phenology models in the well-defined situation where the calibration and evaluation data can be assumed to come from the same underlying population. The first objective of this paper is, therefore, to evaluate how well crop models predict wheat phenology in such a case. To ensure the rigor of the evaluation, we create a situation where the model errors for the calibration and simulation data can be assumed independent.

The emphasis in model evaluation studies is often on the role of model structure, i.e. model equations (Maiorano et al., 2017; Svystun, Bhalerao, & Jönsson, 2019; Wang et al., 2017), and not on model calibration. Clearly however the simulated values depend on the parameter values estimated by calibration and therefore on the calibration approach. (Confalonieri et al., 2016) found that the model user, responsible for calibration, had a very large effect on predictive quality. In a wide-ranging survey, (Seidel, Palosuo, Thorburn, & Wallach, 2018) found that there is a wide diversity of calibration strategies used for crop models. The second objective of this study was therefore to obtain detailed information about the calibration strategies in use for phenology models and to better understand the effect of calibration methodology in determining predictive capability for phenology. This is of practical interest not only for stand-alone phenology models, but also for crop models more generally, since crop models are often calibrated first just for phenology, and then separately for biomass increase and partitioning and soil processes.

Materials and Methods

Experimental data

The data were provided by ARVALIS – Institut du vegetal, a French agricultural technical institute. They run multi-year multi-purpose trials at multiple locations across France, which include variety trials. The data here are from the two check varieties, *Apache* which is a common variety grown throughout France and Central Europe and *Bermude*, mainly grown in Northern and Central France. The trials have three repetitions and follow standard agricultural practices, with N fertilization calculated to be non-limiting. Thus, both the calibration and evaluation data are drawn from sites in France where winter wheat is grown, subject to standard management.

The observed data used in model calibration and evaluation are the dates of two development stages, namely beginning of stem elongation (growth stage 30 on the BBCH and Zadoks scales (Zadoks, Chzang, & Konzak, 1974) and middle of heading (growth stage 55 on the BBCH and Zadoks scales). These stages are of practical importance because they can easily be determined visually and are closely related to the recommended dates for the second and third nitrogen fertilizer applications.

The data were divided into three categories (table 1). One part, the calibration data (14 environments i.e. site-year combinations), was provided to participants for calibration. A second part, the evaluation data (eight environments), was not given to participants. The division of the data was such that the calibration and evaluation data had no sites or years in common. The only way to achieve this was have a third category, “other” (from 13 environments), with data that were not revealed to participants but were used neither for calibration nor evaluation. These environments had either the site or the year in common with the calibration data. Errors for these environments cannot be assumed to be independent of errors for the calibration data, and so they were not used for evaluation. All conclusions about predictive capability are based on the evaluation data. The individual observed values for the evaluation and other hidden data are not presented here because they will be used again in a subsequent study where all groups will be asked to use the same calibration approach.

Table 1.

Environments (site-year combinations) that provided the data. C= calibration data. E = evaluation data. O = other hidden data.

Site (longitude,latitude)	Harvest year						
	2010	2011	2012	2013	2014	2015	2016
FORESTE (3.20,49.82)			E	E	OO*	O	
MERY 4.02,48.33)	C	C		O	C	C	
ROUVRES 5.09,47.28)			E	E	O	O	
CESSEVILLE[1] (0.90,49.15)		C					
IVILLE[1] (0.90,49.15)			E				
VILLETTES[1] (0.90,49.15)				E			
EPREVILLE[1] (0.90,49.15)					C		
CRESTOT[1] (0.90,49.15)						C	
OUZOUER (1.52,47.90)		O	E	E	O	O	
BIGNAN (-2.73,47.88)	C	C	O	O	C	C	
BOIGNEVILLE (2.38,48.33)			O	O	C	C	C

*There were two sowing dates at FORESTE in 2014. [1] These are separate sites that are geographically close to one another and share a single weather station.

The background and input information provided to the modelers for all environments included information about the sites (location, soil texture, field capacity, wilting point), management (sowing dates, sowing density, irrigation and fertilization dates and amounts), and daily weather data (precipitation, minimum and maximum air temperature, global radiation and potential evapotranspiration). Initial soil water and N content were not measured in these experiments, but best guesses were provided by the experimental scientist. If any models required other input data, modeling groups were asked to derive those values in whatever way that seemed appropriate.

The range of observed days from sowing to development stages BBCH30 and BBCH55 for the two varieties for each category of data (calibration, evaluation, other hidden data) is shown in figure 1. The spread from minimum to maximum in the evaluation data is between 24 and 27 days depending on stage and variety. The spread is larger for the calibration data, and in fact, the calibration data cover the range of the evaluation data and the range of other hidden data. Thus, the models are not being used to extrapolate outside the observed values of the calibration data.

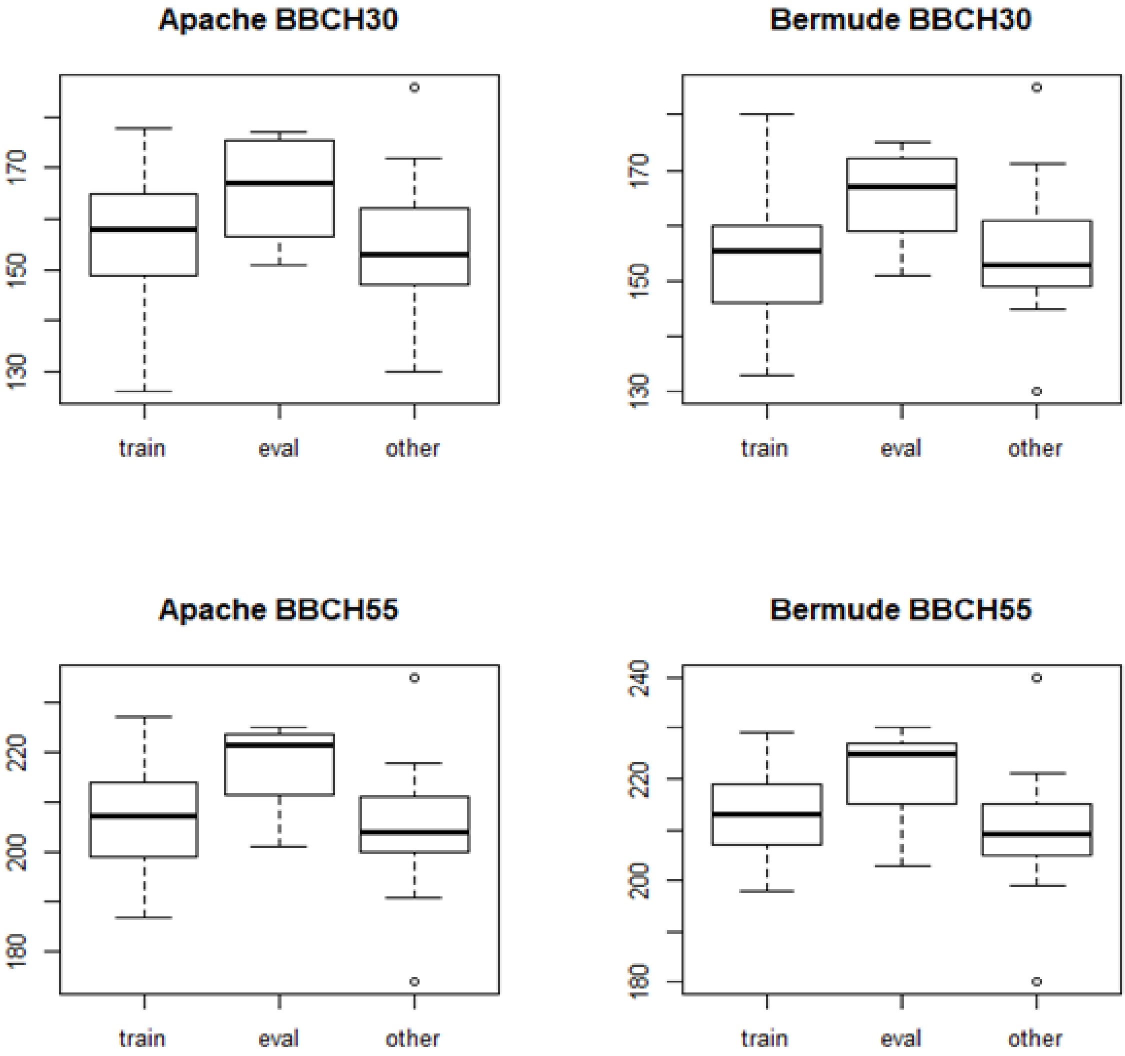


Figure 1

Boxplots of calibration, evaluation and other data for development stages BBCH30 and BBCH50 and varieties Apache and Bermude. The y-axis shows days from sowing to the indicated development stage. Boxes indicate the lower and upper quartiles.

The solid line within the box is the median. Whiskers indicate the most extreme data point, which is no more than 1.5 times the interquartile range from the box, and the outlier dots are those observations that go beyond that range.

Crop models

Twenty-seven modeling groups participated in this study, noted M1-M27. The four groups M2, M3, M4, and M5 all used the same model structure (i.e. models with the same name), denoted as model structure S1. The four models M7, M12, M13, and M25 also shared a common model structure, denoted as S2. As will be seen, different groups using the same model structure had different results. The model versions for the same model structure differed in some cases, but the differences are not in the basic phenology equations implemented, and therefore, should have no or only a negligible effect on the simulated development stages. Some differences in results may have resulted from different values for the parameters that were not fit to the calibration data, although this was not recorded. The differences in calibration approach were recorded, and this certainly led to differences in simulated values. Since even groups using the same model structure obtained different results, we refer to the 27 contributions as different models, In the presentation of the results the models are anonymized and are identified simply as M1 to M27. It would be misleading to use the names of the model structures, since the results depend on both model structure and on the approach to calibration. Information about the model structures is given in Supplementary table S1.

Two of the models (M9, M18) only simulated days to development stage BBCH55 and not to stage BBCH30. Results for these two models are systematically included with the results for the other models, but averages over development stages for these two models only refer to BBCH55. This is not repeated explicitly every time an average over development stages is discussed.

In addition to the individual model results, we show the results for the model ensemble mean (“e-mean”) and the model ensemble median (“e-median”). We also define a very simple predictor, denoted “naive”, which was calculated as the average of the observations in the calibration data for prediction. The naive model thus predicts that all days from sowing to stage BBCH30 (BBCH55) will correspond to the average of days from sowing to BBCH30 (BBCH55) in the calibration data, separately for each variety. The naive model predictions for days from sowing to BBCH30 and BBCH55 are respectively 155.9 days and 206.9 days for variety Apache, and 156.1 days and 213.1 days for variety Bermude.

Calibration and simulation experiment

The participants were provided with observed phenology data (dates of BBCH30 and BBCH55) only for the calibration environments. The participants were asked to calibrate their model using those data, and then to use the calibrated model to simulate phenology for all environments (i.e. calibration, evaluation and hidden data environments). No guidelines for calibration were provided. Participants were instructed to calibrate their model in their “usual way” and fill out a questionnaire explaining what they did (Supplementary table S2).

Evaluation

A common metric of error is mean squared error (MSE). We calculated MSE for each model, each development stage (BBCH30 and BBCH55) and for each variety, as well as averaged over stages and varieties. This was done separately for the calibration and evaluation data. For example, MSE for model m, for predicting BBCH30, variety Apache, based on the evaluation data, is:

$$MSE_{eval,m}^{BBCH30,Apache} = (1/8)\sum_{i\in eval}\left(y_i^{BBCH30,Apache} - \hat{y}_{i,m}^{BBCH30,Apache}\right)^2 \qquad (1)$$

where the sum is over the eight environments used for evaluation and $y_i^{BBCH30,Apache}$ and $\hat{y}_{i,m}^{BBCH30,Apache}$ are respectively the observed value and value simulated by model m for evaluation environment *i*, development stage BBCH30 and variety Apache. For $MSE_{eval,m}^{all}$, the average is over the eight evaluation environments, both stages and both varieties, so overall 32 predictions.

Mean squared error can be shown to be the sum of three positive terms, namely squared bias, the difference in variance between the observed and simulated values and a term related to the correlation between observed and simulated values (Kobayashi & Salam, 2000). We specifically examined the bias, defined as the average over observed values minus the average over simulated values.

The mean absolute error (MAE) is of interest as a more direct measure of error, that does not give extra weight to large errors as MSE does. For example, MAE for model m for predicting BBCH30, variety Apache, based on the evaluation data, is:

$$MAE_{eval,m}^{BBCH30,Apache} = (1/8)\sum_{i\in eval}\left|y_i^{BBCH30,Apache} - \hat{y}_{i,m}^{BBCH30,Apache}\right|$$

We also look at modeling efficiency (EF) defined for model m as

$$EF_m = 1 - MSE_m / MSE_{naive}$$

where MSE_m is MSE for model m and MSE_{naive} is MSE for the naive model defined above. EF is a skill measure, which compares the predictive capability of a model to that of the naive model. Since the naive model makes the same prediction for all environments, it does not account for any of the variability between environments. A model with $EF \le 0$ is a model that does no better than the naive model, and so would be considered to be a very poor predictor. A perfect model, with no error, has modeling efficiency of 1.

Results

Goodness-of-fit and prediction error

Summary statistics for MSE averaged over both varieties and over both development stages, for the calibration and evaluation data, are shown in table 2. Summary MSE values for the calibration data for each development stage and variety separately are shown in Supplementary table S7, and results for each individual model are given in Supplementary figure S1.

Table 2

Summary statistics of MSE (days²) averaged over both varieties and over both development stages.

MSE (days²)	Minimum	1st quartile	Median	Mean	3rd quartile	Maximum
Calibration data	15	28	47	77	63	426
Evaluation data	20	35	62	79	111	235

In most cases, the bias for the calibration data is quite small. Considering absolute bias for both development stages and both varieties, the median value was 2 days (Supplementary table S8). In cases where the bias is relatively large, it is often of opposite sign for BBCH30 and BBCH55, as in the examples of figure 2.

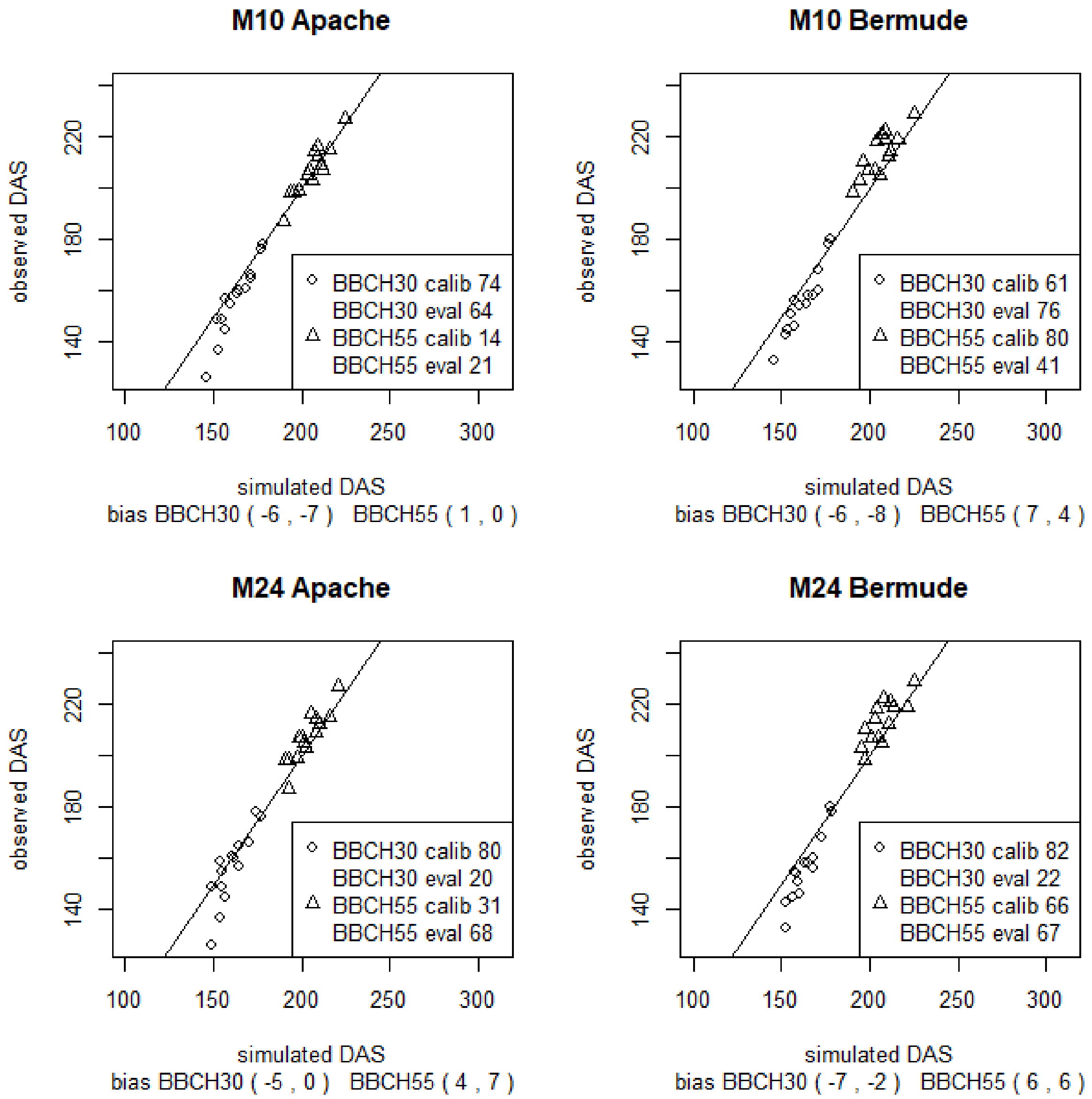
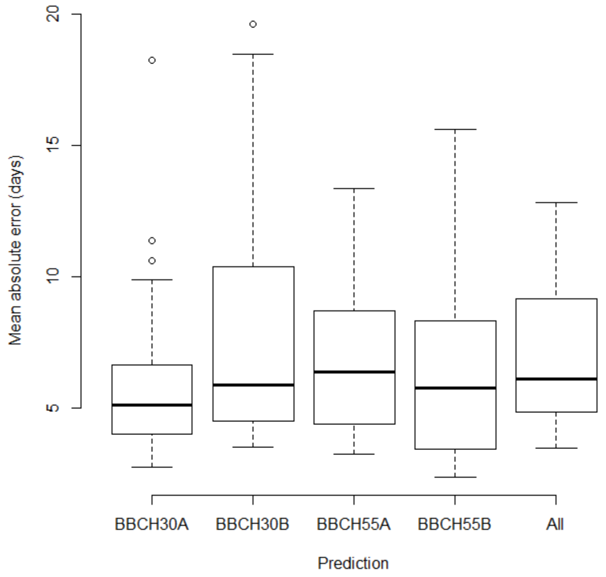


Figure 2

Observed vs. simulated days after sowing (DAS) for calibration data for models M10 and M24. The legend shows MSE (days²) for each stage and for calibration and evaluation data. (The individual evaluation results are not displayed). In the subtitles, bias values (days) for each stage are shown. The first number in parentheses is for the calibration data, the second number is for the evaluation data.

Figure 3 and Supplementary tables S4-S6 show results for each development stage and variety and averaged over development stages and varieties for the evaluation data. Results for each model are given in Supplementary table S3. The median of MAE for the evaluation data is 6.1 days. The median of overall efficiency is 0.62, signifying that half of the models have MSE values for the evaluation data that are at most 38% as large as that of the naive predictor. Only two models have negative values of EF, indicating that one would do better to predict using the average of the calibration data. For the four individual predictions (two development stages, two varieties), the median of MAE ranges from 5.1 to 6.4 and the median of EF ranges from 0.6 to 0.8. The ensemble models e-median and e-mean, though not the best predictors, are among the best, with e-median being rated second best and e-mean fourth best. The range of results among individual models is appreciable. The mean absolute errors for the evaluation data averaged over all predictions (MAE_{eval}^{all}) go from 3.5 to 13 days. The MSE_{eval}^{all} values vary by over a factor of 10, from a minimum of 20 days² to a maximum of 235 days².



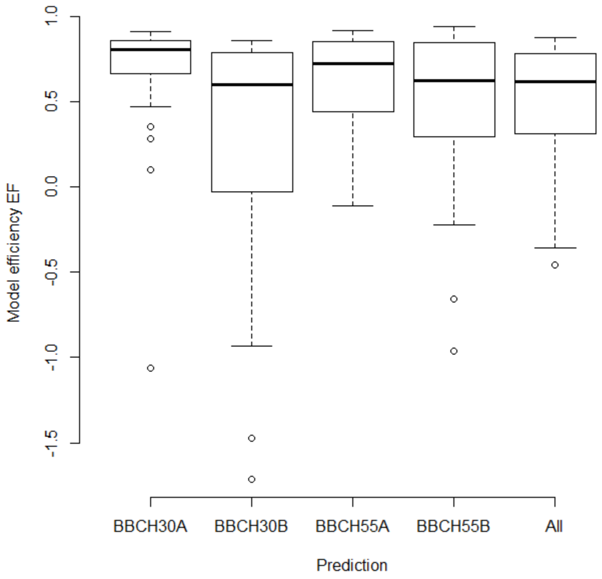


Figure 3

Box and whisker diagrams of absolute errors for evaluation data for each prediction and on average (top panel) and modeling efficiency for each prediction and on average (bottom panel). BBCH30A and BBCH30B refer respectively to prediction of days to BBCH30 for variety Apache and variety Bermude. BBCH55A and BBCH55B refer respectively to prediction of days to BBCH55 for variety Apache and variety Bermude. The variability comes from differences between models.

The relationship between overall MSE for the evaluation data and overall MSE for the calibration data is quite close (adjusted R²=0.70, figure 3). That is, much of the variability between models in MSE for the evaluation data can be explained by the variability in the calibration data, which further emphasizes the importance of calibration.

The four models that have model structure S1 and the four models that have model structure S2 are identified in figure 4. Models with the same structure have different MSE values; the differences are particularly large for S1. The models with structure S1 are ranked 3rd, 9th, 14th and 27th best for overall evaluation MSE among the 27 individual models. The models with structure S2 are ranked 4th, 8th, 17th and 18th est.

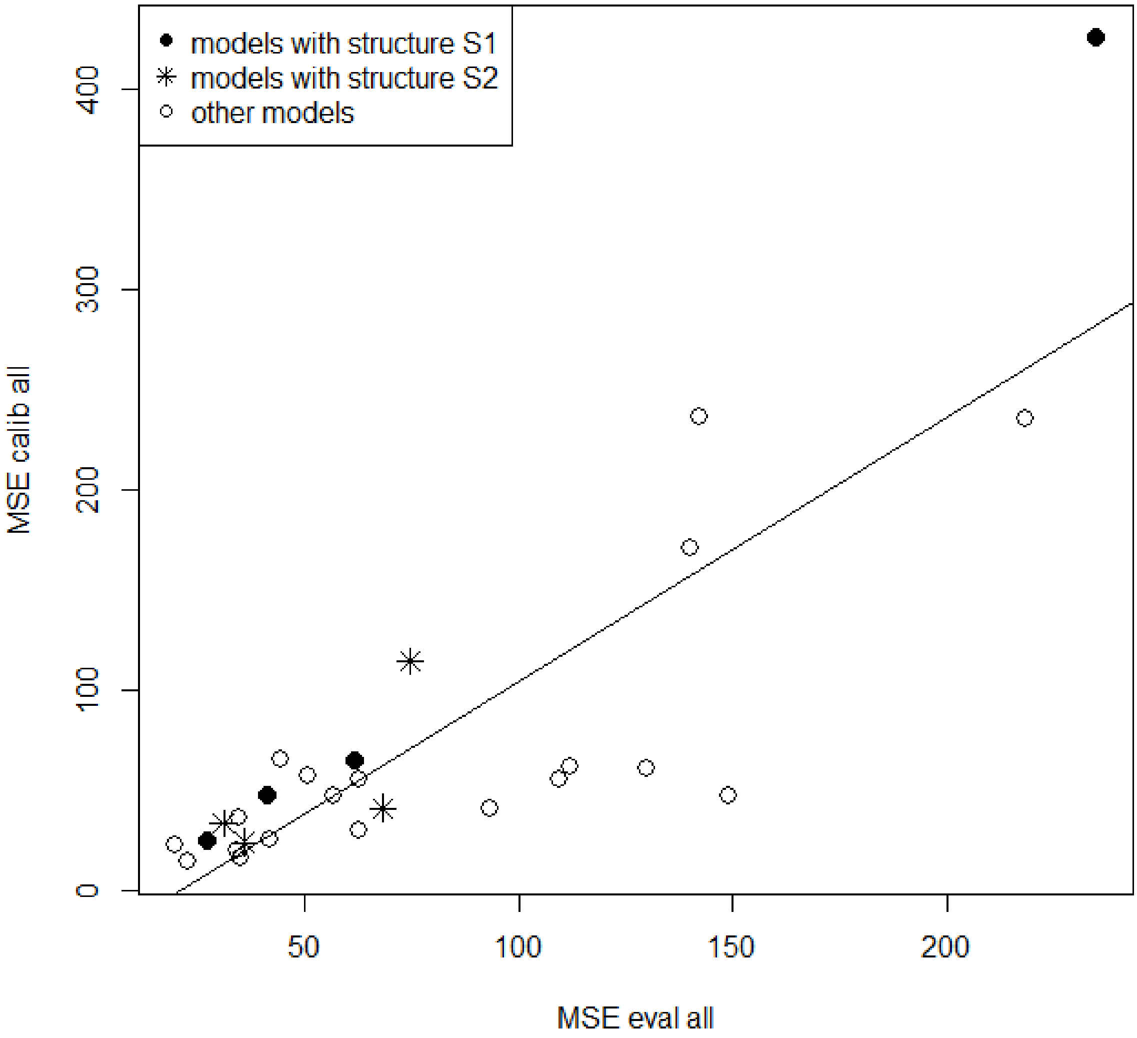


Figure 4

Mean squared error (MSE) for the calibration data, averaged over environments, development stages and varieties (MSE_{calib}^{all} days²), as related to MSE for the evaluation data (MSE_{eval}^{all}, days²). The regression line MSE_{calib}^{all} = -27.6 + 1.32 MSE_{eval}^{all} is shown (R²=0.70). ● indicates models with structure S1. ⁎ indicates models with structure S2. ○ indicates other models.

Twenty-one models simulated and reported time from sowing to emergence. For these models, we can separate simulated time from sowing to BBCH30 (sow_30) into two contributions, the simulated time from sowing to emergence (sow_em) plus the simulated time from emergence to BBCH30 (em_30), so that sow_30=sow_em+em_30. Figure 5 shows results from two environments, typical of essentially all environments and both varieties, for the relation between em_30 or sow_30 and sow_em. The average slope of the regression em_30=a+b*sow_em over all environments (including calibration, evaluation and other environments) and both varieties is b=-1.04, so that each day increase in simulated days to emergence is on average associated with a 1.04 day decrease in simulated time from emergence to BBCH30. The negative correlation between sow_em and em_30 leads to a between-model variance for sow_30 (average variance 92 days^2) that is smaller than the sum of the variances of sow_em (average variance 20 days^2) and em_30 (average variance 101 days^2). The right panels of figure 5 show that different models could simulate almost exactly the observed value of sow_30 with quite different values of sow_em.

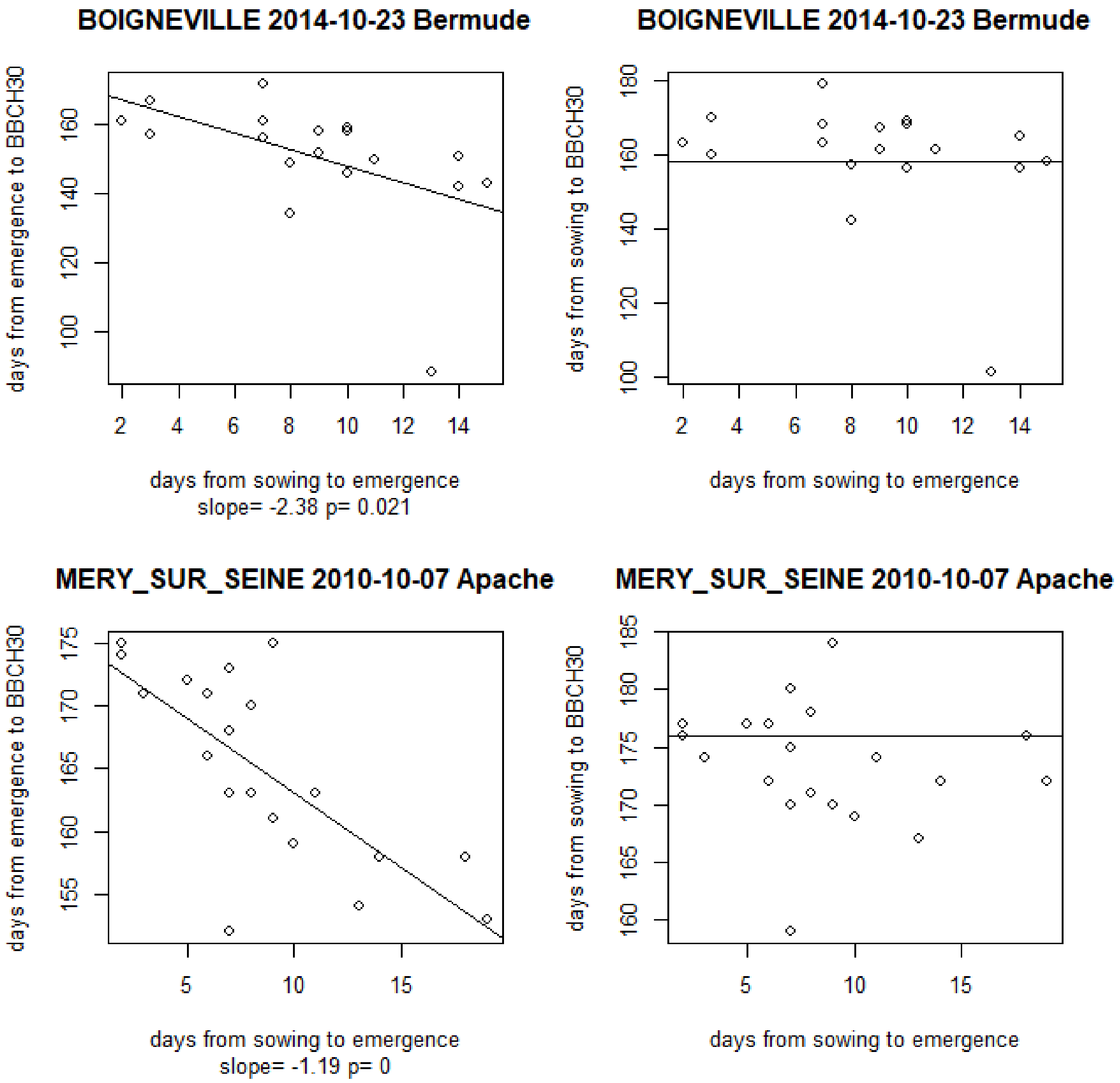


Figure 5

Relation between simulated days from emergence to BBCH30 and simulated days from sowing to emergence as reported by 21 crop models for two environments (left panels). Relation between simulated days from sowing to BBCH30 and simulated days from sowing to emergence for the same environments (right panels). The slope of the linear regression line and the p-value for testing slope=0 are shown for the left panels. The observed days from sowing to BBCH30 is shown as a horizontal line in the right panels.

Calibration approaches

Each participant was asked to calibrate the model in the "usual" way, using the calibration data provided. The questionnaire about calibration focused on three aspects of calibration; the choice of parameters to estimate, the criterion of error to be minimized and the software used. The choices of the participants are summarized in table 3 and choices for each model are shown in Supplementary table S9.

Table 3

Summary of calibration approaches. Numbers are number of models with indicated choice. The specific models associated with each choice are shown in Supplementary tables S3 and S9. More information about the software is presented in Supplementary table S10.

Number of parameters[1]	Minimum 1st Quartile Median Mean 3rd Quartile Maximum 1.00 2.00 3.00 3.63 4.50 9.00
Which parameters	Thermal time to a single development stage 16 Thermal time to two or more development stages 6 Related to vernalization 11 Related to photoperiod 11 Related to effect of temperature (e.g. base temperature) 6 Related to phyllochron 6 Related to tiller appearance 2 Related to time to emergence 3 Parameters unrelated to calibration data[2] 6
Objective function	Sum of squared errors or of root mean squared errors 21 Sum of absolute errors 2 Concentrated likelihood 1 No single explicit objective function 3
Software[3]	Trial and error 10 DIRECT-L (Gablonsky & Kelley, 2001; Johnson, n.d.) 2 Ucode (E. P. Poeter, Hill, Banta, Mehl, & Christensen, 2005; Eileen P. Poeter & Hill, 1999) 3 DE Optim (Mullen, Ardia, Gil, Windover, & Cline, 2011) 3 PEST (Doherty, Hunt, & Tonkin, 2010) 2 SCE (Duan, Gupta, & Sorooshian, 1993; Houska, Kraft, Chamorro-Chavez, & Breuer, 2015) 2 GLUE (Beven & Binley, 2014; J. He, Jones, Graham, & Dukes, 2010) 1 DREAM (J. A. Vrugt et al., 2009; Jasper A. Vrugt, 2016) 2 Wrote code [4] 4

[1] Summary of number of estimated parameters for models M1-M27. [2] these are parameters that do not affect simulated days to BBCH30 or BBCH55. [3] Some modeling groups used more than one software package. [4]. Modeling groups that wrote their own software.

The choice of parameters to estimate was based on expert judgement in most cases. The participants declared that they chose parameters known to affect phenology in the model, or more specifically parameters expected to have a major effect on time to BBCH30 and BBCH55 and expected to differ between varieties. Five participants did a sensitivity analysis to aid in the choice of parameters to estimate. The number of estimated parameters ranged from 1 to 9. In almost all cases, the number of parameters to estimate was decided a priori. In three cases, the number was the result of testing the fit with different numbers of parameters. In one of those cases the Akaike Information Criteria (AIC, Akaike, 1973) and adjusted R^2 were used to test whether additional parameters should be estimated.

Almost all modeling groups estimated one or more parameters that represent thermal time between development stages (table 6). Some adjustments were necessary for models that did not explicitly calculate time of BBCH30 or BBCH55. In model M2, for example, a new parameter was added to the model, and estimated, representing the fraction of thermal time from double ridge to heading at which BBCH30 occurs. Thirteen groups estimated a parameter related to the effect of photoperiod. Ten groups estimated a parameter related to vernalization. Six groups modified one or more parameters related to the temperature response (for example model M6 estimated *Tbase*, the temperature below which there is no development). Only three models modified parameters related to the time from sowing to emergence, and only one model modified a parameter related to the effect of water stress. Six models included among the parameters to estimate, parameters that have no effect on the variables furnished as calibration data. Such parameters included thermal times for development stages after BBCH55, potential kernel growth rate, kernel number per stem weight and the temperature below which there is 50% death due to cold (Supplementary table S9).

Most modeling groups defined the sum of squared errors or the sum of root mean squared errors as the objective function to be minimized, where the sum is over the two stages. (In all cases, the calibration was done separately for the two varieties). Two groups minimized the sum of absolute errors. Calibration for model M21 was based on maximizing the concentrated likelihood (Seber & Wild, 1989) assuming a normal distribution of errors with possibly different error variances for the two development stages. In this case, the objective function involves a product of errors for the two outputs, rather than a sum. Four of the participants (M15, M16, M17, M18) did not define an explicit objective function to be minimized. In these cases, the parameter values were chosen to obtain a “good fit” to the data by visual inspection. Finally, two of the models (M7, M8) divided the calibration into two steps. In these cases three of the parameters were used to fit the BBCH30 data, and then in another step another parameter was used to fit the BBCH55 data.

Minimizing the sum of squared errors is a standard statistical approach to model calibration, which has highly desirable properties if certain assumptions about model error are satisfied, including equal variance of model error for all data points and non-correlation of model errors. Only one model took into account the possibility that the error variances are different for BBCH30 and BBCH55, and none of the modeling groups took into account possible correlations between errors for BBCH30 and BBCH55 in the same field. Based on the errors for all the data and all the models, it was found that there is a highly significant difference in variance between errors for BBCH30 (variance of error 100.7 days^2) and BBCH55 (variance of error 67.3 days^2). Also, the correlation between the error for BBCH30 and the error for BBCH55 in the same field is 0.53 and highly significant. However, if only results for a single model are considered, then for most models the differences in variance and the correlation are not significant.

Two models defined a posterior probability of the parameters equal to the likelihood times the prior probability, as usually assumed in a Bayesian approach. The parameters used for prediction were those that maximized the posterior probability (i.e., the estimated mode of the posterior distribution). In both cases, the likelihood was assumed Gaussian with independent errors, and the prior distribution was assumed uniform between some minimum and maximum value. This approach is equivalent to minimizing the mean squared error, with constraints on the parameter values.

Seven participants simply used trial and error to search for the optimal parameters. The other participants used software specifically adapted to minimizing the objective function, either written specifically for their model or, in most cases, available from other sources (Supplementary table S10).

Discussion

The challenge in this study was to predict the time from sowing to beginning of stem elongation and to heading in winter wheat field trials performed across France. This is a problem of practical importance, since these two development stages are important for wheat management (e.g. fertilization). The evaluation concerned years and sites not included in the calibration data, making this one of the most rigorous evaluations to date of how well crop models simulate phenology.

Twenty-seven modeling groups participated in the exercise. Most models predicted times to stem elongation and heading quite well (median MAE of 6 days). Half the models had MSE values of prediction that were 36% or less than MSE of a naive predictor. It must be kept in mind that this study is a rather favorable situation for prediction, with a substantial amount of calibration data and predictions for environments similar to those of the calibration data.

The results for each individual model depend on the model equations, the values of the fixed parameters and the calibration approach which determines the values of the estimated parameters, and on the interactions among those elements. A full, detailed analysis of each model is beyond the objectives of this study. We focused on the calibration approaches used and its relation to errors for the calibration and evaluation data.

The results show that calibration can, in some cases, compensate for differences in model equations and/or values of fixed parameters. Compensation is usually discussed in the context of single models. For example, equifinality, which is a well-known phenomenon of complex models, means that different combinations of parameter values, and thus different quantitative descriptions of processes, can lead to the same results for outputs because there is compensation between the processes (Beven, 2006; D. He et al., 2017). However, this phenomenon has not been described in the context of multi-model studies. Here, we have an example of compensation for differences between models in the way they partition days from sowing to BBCH30 into days from sowing to emergence plus days from emergence to BBCH30. Models with longer simulated times from sowing to emergence tend to have a shorter simulated time from emergence to development stage BBCH30 and vice versa. In fact, each extra day from sowing to emergence is associated on average with almost exactly one less day from emergence to BBCH30. The result is that models with quite different simulated days from sowing to emergence can have nearly identical times from sowing to BBCH30. This can be expressed in terms of model uncertainty, as quantified by between-model variance. The variance of days from sowing to BBCH30 is less than the sum of variances of days from sowing to emergence and days from emergence to BBCH30. That is, calibration reduces, but does not eliminate, model uncertainty for the variable provided for calibration.

We don't have observed time to emergence, but in any case the models with different simulated days to emergence can't all be right. This is an example of how models can get the right answer (correct days to BBCH30) for the wrong reasons (wrong days to emergence), illustrating the problem pointed out for example by (Challinor, Martre, Asseng, Thornton, & Ewert, 2014). The same compensation of errors between sowing to emergence and emergence to BBCH30 will not be appropriate for all environments. This is one of the main reasons that extrapolation to populations different than the training population is dangerous.

Another indication of compensation induced by calibration is the fact that after calibration, models with quite different choices for the variables that affect development can have very similar levels of prediction error. The most important inputs that determine spring wheat phenology are daily temperature and photoperiod (Aslam et al., 2017) and for winter wheat it is also necessary to include the process of vernalization, i.e. the effect of low winter temperatures on development (Li et al., 2013). Five of the best eight predicting models here, with MSE_{eval}^{all} < 40 days², do use all three of those variables (daily temperature, photoperiod, vernalizing temperatures) as inputs. Two of the best eight models however do not use vernalizating temperatures, and one of those best eight does not use photoperiod. The choice of input variables is a fundamental aspect of model structure. In fact, MSE can be expressed as a sum of two terms, the first of which depends only on the choice of the model input variables and not on any other aspects of structure, while the second measures the distance between the model used and the optimal model for those inputs (Wallach, Makowski, Jones, & Brun, 2019). It seems that calibration can lead to similar values of MSE for prediction even for quite different choices of input variables.

While models with different structures can give similar results thanks to calibration, our results also show that models with the same structure can provide different results, if different calibration approaches are used. This is illustrated here by the results for two groups of models sharing the same structure. There are major differences in prediction error between models with the same structure depending on how calibration was done. Much previous work on improving the predictive capability of crop models has focused on the model equations, for instance the way temperature is taken into account in various processes (Maiorano et al., 2016; Wang et al., 2017). Here we show that models with quite different structures can have very similar prediction accuracy, thanks to calibration using the same data, while models with the same model structure can have very different levels of prediction error, if the calibration methods differ. This means that model comparison studies may often be comparing calibration approaches as much or more as they are comparing model equations. This is in line with the conclusions of Confalonieri et al. (2016), who argued that one should not speak of evaluation of a model but rather of a model-user combination; a major role of the user is in determining the method of calibration.

The choice of objective function for calibration can have an effect on quality of prediction. While most participants defined an explicit objective function (e.g. minimizing sum of squared errors, or some closely related criterion) three models (see Supplementary table S9) did not have an explicit quantitative objective function. Those models all had relatively large values of overall MSE for the evaluation data (MSE_{eval}^{all}), having 15th, 16th, and 18th largest MSE_{eval}^{all} values out of the 25 models that predicted both BBCH30 and

BBCH55. These results suggest that the lack of a quantitative objective function can be a drawback since then one does not have a clear criterion for judging the results of calibration.

There was a large diversity of choices of parameters to estimate by calibration, and this had in certain cases an important effect on prediction error. One rather unexpected observation was that several participants included parameters that have no effect on the variables furnished as calibration data among the parameters to estimate. The data cannot in those cases give any information about the parameter value. At best, including such parameters among the parameters to estimate is useless, and those parameters will simply have final values exactly equal to their initial values. However, there may also be serious disadvantages to including such parameters. It gives the erroneous impression that one is estimating parameters that cannot in fact be estimated, it increases computation time and it can cause problems for the parameter estimation algorithm. The very poor fit of model M5 to the calibration data seems to be directly related to the fact that for this model, several parameters unrelated to the calibration data were chosen to be fitted. The software used here was PEST (Doherty et al., 2010), with the singular value decomposition option, which allows one to deal with non-estimable parameters, but at the cost of introducing bias in the estimated parameter values. Obviously, one should not include non-estimable parameters among the parameters to estimate.

The choice of parameters to estimate may be the principal cause of bias in fitting the calibration data for some models. If a model includes an additive constant term, and squared error is minimized, bias will be 0 for the calibration data. Even for more complex models, calibration can bring bias close to 0, as illustrated here by the fact that many of the models had very small biases for the calibration data. Eliminating bias is important, since squared bias is one component of MSE, and therefore the bias necessarily adds on to MSE (Kobayashi & Salam, 2000). If one does not have a parameter with a nearly additive effect for each of the development stages BBCH30 and BBCH55, the elimination of bias for both outputs is not assured. Model M24 estimated only a single parameter. In such a case, at best one can estimate a parameter value that gives the best compromise between errors in BBCH30 and BBCH55. This may lead to a negative bias for one of those outputs and more or less corresponding positive bias for the other. This is exactly the behavior illustrated in figure 2. Model M10 also had fairly large biases. Here three parameters were estimated, but one is unrelated to the observed data and a second concerns time to emergence, which was only allowed to vary in a limited range. Apparently in this case also there was not enough flexibility to eliminate bias for both development stages. Models with large bias for the calibration data tended to have large MSE values for the evaluation data (Supplementary figure S2). This suggests that the parameters to estimate should include one parameter that is nearly additive (i.e. that adds an amount that is nearly the same for all environments) for each observed output, and that is not too limited in the allowed range of values.

The calibration choices here suggest other recommendations for calibration. One concerns the specific choice for the objective function. Among the models that defined a likelihood or a sum of squares criterion, all but one assumed that all model errors had equal variance and were independent. One should probably take into account unequal variances and correlation of simulation errors for BBCH30 and BBCH55 in the same field. A second recommendation concerns the software. There does not seem to be any clear connection between the software used for calibration and the predictive quality of the resulting calibrated model. Various different software solutions were used by the best predicting models, but largely the same software solutions were also found among the models with the largest prediction errors. A problem that may arise concerns the test for convergence to the parameter values that minimize the chosen objective function. Having such a test allows the user to have confidence that the best parameter values have been found. With trial and error, there is no such test, which is a major drawback of this approach. Algorithms to estimate a Bayesian posterior distribution normally test convergence to the posterior distribution, which may not be relevant if one is using just the mode of the distribution. It would be good practice to adopt a software option that includes an appropriate test of convergence.

Overall, we have shown in a rigorous evaluation of prediction for new environments that most of the 27 crop models tested, given calibration data, provide good predictions of phenology in winter wheat and explain much of the variability between environments. Calibration has a major effect on predictive quality. Calibration reduces variability between models for outputs used for calibration, but may lead to models getting the right answer for the wrong reason. Calibration can compensate to some extent for different choices of input variables. Poor practices of calibration can seriously degrade predictive capability. Arguably the most difficult aspect of calibration, and yet the least studied, is the choice of parameters to estimate. Unlike the choice of objective function and of software, there is little guidance here from other fields. Furthermore, the problem is specific to each model, since each model has a different set of parameters. Given the large diversity of calibration approaches and the importance of calibration, there is a clear need for guidelines and tools to aid model users with respect to calibration. Model applications, including model studies of climate change impact, should focus more on the data used for calibration and on the calibration methods employed.

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