Evaluation of non-linear wheat development models and optimization methods for their parameter determination

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Abstract

Predicting certain crop phenological stages is important for scheduling agricultural practices and predicting crop responses to climate change. In this study, we developed three different wheat phenological models, a polynomial model and two sigmoid and exponential mixed (SEM) models developed by different parameter determination methods (the Nelder-Mead and augmented Lagrange multiplier methods), and determined which of these models is the most effective for predicting the flowering date in wheat. Five winter wheat cultivars were cropped in western Japan for four years; we split the cultivation data for model calibration and validation. The SEM models showed higher precision in root mean square error (RMSE; 3–5 days) than the polynomial model when using the validation data. The models developed using the Nelder-Mead and augmented Lagrange multiplier methods showed similar RMSE values (Mean ± SD: 4.24 ± 0.59 and 4.16 ± 0.36, respectively). On the other hand, in the context of validity, the model developed using the Nelder-Mead method showed an unnatural development response to changes in environmental variables; thus, we found that the model developed using the augmented Lagrange multiplier method would be more realistic and effective to express the response of wheat growth to environmental factors. The results of our study shed new light on the optimization methods used in crop development models and on the advantages of using the augmented Lagrange multiplier method for determining the parameters of a non-linear crop development model.

Key words: Augmented Lagrange multiplier method, Crop development model, Parameterization, Phenology, Wheat

1. Introduction

Predicting certain crop phenological stages is useful for agricultural management practices, such as optimal scheduling of spraying or predicting crop yields (Mkhabela et al., 2016). For example, in wheat, it is important to know the time of flowering in order to schedule fungicide application for the control of Fusarium head blight. Palosuo et al. (2011) investigated the yield of eight wheat cultivars using crop growth simulation models. Furthermore, the technique of predicting crop phenology is used for investigating future crop yield in response to global warming (He et al., 2015; Li et al., 2015; Tubiello et al., 2000). For example, Li et al. (2015) predicted the future yield of rice under a range of climatic conditions by using the rice phenological model.

The crop phenological model usually expresses crop daily development using some important meteorological factors, such as temperature or photoperiod, as mathematical functions (Yin et al., 1995). A number of models expressing daily crop growth have been developed and used for predicting certain growth stages, such as germination, heading, or flowering, by calculating daily growth up to the particular growth stage of interest (Nakazono et al., 2014; Yin et al., 1995, 1997). For example, one of the simplest models to understand current crop development is the so-called thermal time model that accumulates the temperature data from a certain growth stage (Tollenaar et al., 1979).

The process of developing crop phenological models is divided into two steps: 1) defining the algorithm for a crop growth stage using a mathematical equation that includes several environmental factors as variables, and 2) determining the parameters defined by the 1) step. To date, a variety of models have been developed and grouped into linear and non-linear models (Ritchie, 1991; Streck et al., 2003; Wang and Engel, 1998; Yan and Wallace, 1998). Xue et al. (2004) developed thermal time and non-linear models for predicting leaf appearance in wheat, and they reported that a non-linear model could predict target stages more accurately than a thermal time model. However, different types of non-linear models, such as polynomial models, sigmoid models, and more complex models, are suitable for wheat. Nevertheless, the advantages and disadvantages of these models have not been completely clarified yet.

The determination of the coefficients of a crop model is another important process in its construction. In the case of a developmental model expressed as a linear combination,
such as a polynomial model, it is relatively easy to determine the coefficients, since the linear least square method can be applied by solving the normal equation. However, in the case of sigmoid or exponential models, it is not possible to determine the coefficients like in the case of a polynomial model since the objective function cannot be transformed into a normal equation; thus, other optimization methods are necessary to determine the coefficients of the models other than the polynomial ones. In a previous study, He et al., (2017) reported the uncertainty caused by parameterization of the agricultural production systems simulator (APSIM)-canola model using the Bayesian optimization method, but there is still a lack of information about optimization methods that should be used for determining the coefficients of crop models. We believe that in developing a non-linear crop phenological model, choosing the adequate optimization method is just as important as defining a good algorithm of crop development, while many researchers have been solely concerned about developing a good algorithm for expressing crop development.

The purpose of this study was to evaluate different non-linear crop models for the better understanding of crop phenological models. Specifically, we developed three winter-wheat phenological models (a polynomial model and two sigmoid and exponential mixed (SEM) models developed by two different optimization methods) for predicting the flowering date in wheat as a case study. Although a number of phenological models are used in wheat, the polynomial and SEM models were selected since these models were frequently used for crop growth models, especially in Japan. As for the optimization methods, we used the Nelder-Mead and augmented Lagrange multiplier methods to determine the coefficients of the selected models. The Nelder-Mead method is one of the most commonly used in determining the coefficients of the SEM model (Horie and Nakagawa, 1990; Maruyama et al., 2010; Nakazono et al., 2014; Onogi et al., 2016) while the other has not been used so far. We chose the winter wheat phenological model since wheat experiences relatively longer days during cultivation than rice or soybean, making the prediction error clear in case of model failure. Since farmers need to schedule fungicide application for the prevention of Fusarium head blight after the flowering date in Japan, we calibrated the wheat development model for predicting the flowering date from the seeding date. Furthermore, we simulated the change in daily wheat development ratio in response to the changes in temperature and photoperiod to evaluate the validity of the models developed in terms of actual wheat development.

2. Materials and Methods

The sowing and flowering dates were collected at Yamaguchi University (34°14′N, 131°46′E, 20 m above sea level), located in Yamaguchi, Japan. The five winter cultivars (Norin 61, Iwainodaichi, Kinuhime, Akitakko, and Kitahonami) were cultivated during the 2012 and 2015 growing seasons. The winter habit (Crock 1989, Gotoh 1979) of the experimental cultivars varies widely (degree II in Norin 61, degree IV in Iwainodaichi and Kinuhime, degree V in Akitakko, and degree VI in Kitahonami). Norin 61 is a spring variety, but it is usually cultivated in winter in western Japan. In total, 22 cultivation datasets were collected from each cultivar. The sowing dates were always between October and December, and the flowering dates were between the beginning of April and May during the four years of field experiments. These cultivars were hand-seeded at a row spacing of 20 cm and at a sowing rate of 100 seeds m⁻². The fertilizer containing 16 g m⁻² of N, 10 g m⁻² of P₂O₅, and 8 g m⁻² of K₂O was applied as a basal application in all growing seasons. In addition, for Kinuhime, we collected 20 samples from the farmland at Higashihiroshima (34°50′N, 132°87′E, at 270–300 m above sea level, sowed in November and December, 2016) and 9 samples from Fukuyama (34°50′N, 133°39′E, at 1 m above sea level, sowed between October and December in 2016 and 2017); both of these sites are located in Hiroshima, Japan. The flowering at the study site began towards the middle of April to the beginning of May. The flowering time is defined as the time when 50% of the heads begin to flower in a study area.

We constructed simple wheat phenological development models from the response functions of temperature and photoperiod, using the data from Yamaguchi for calibrating the models. The 22 cultivation datasets were divided into four segments according to the four sowing years (2012–2015) to conduct a four-fold cross-validation, wherein three segments were used for calibration (16–17 datasets) and the remaining one (5–6 datasets) was saved for validation. The temperature data for Yamaguchi was obtained from the meteorological station of the Japanese Meteorological Agency (AMEDAS: Yamaguchi, http://www.data.jma.go.jp/biob/stn/etrn/index.php), while the temperature data for Fukuyama and Higashihiroshima were obtained from the data loggers (Climatec Inc. C-HPT-5-JM and T&D Corporation RTR-502, respectively) set at the farmland. The data loggers were set in a plastic box (at approximately 1.5 m from the ground) that had a forced draft fan. The average air temperatures in Fukuyama and Yamaguchi showed similar patterns, and the average air temperature of Higashihiroshima was approximately 0.5–3.5 lower than the other sites (Fig. 1).

We referred to the method of the developmental index (DVI) to express the change in wheat development (de Wit et al., 1970; Horie and Nakagawa, 1990; Yin et al., 1997), and calculated DVI by accumulating the daily development rate (DVR) as follows

$$DVI_i = \sum_{i=1}^{n} DVR_i$$

$$DVR_i = f(x(1), \cdots, x(n), T_i, P_i)$$

where $DVI_i$ is the developmental index on day $n$, and $DVR_i$ is the developmental rate on day $i$, which is a function of the daily mean temperature ($T$) and photoperiod ($P$). In this study, we defined $DVI = 0$ at the seeding date and $DVI = 1$ at the flowering date.

In this study, we developed polynomial and sigmoid and exponential mixed models for expressing the $DVR$ of each cultivar. The polynomial model (Kawakata, 2012) was described as follows:

$$DVR_i = X_1 + X_2 T_i + X_3 T_i^2 + X_4 P_i + X_5 P_i^2$$
where $X_i$, $X_j$, $X_k$, and $X_l$ are the coefficients, $T_i$ ($°C$) is the daily mean temperature and $P_i$ (h) is the photoperiod of day $i$. The SEM model was used in several previous studies (Horie and Nakagawa, 1990; Maruyama et al., 2010; Nakazono et al., 2014; Yin et al., 1997). In this study, we referred to the approach of Maruyama et al. (2010) and Nakazono et al. (2014) to predict the flowering or heading time in wheat as follows:

$$DVR = C \times f(T_i) \times f(P_i)$$

$$f(T_i) = \frac{1}{1 + \exp[-A(T_i - T_0)]}$$

$$f(P_i) = 1 - \exp[-B(P_i - P_0)]$$

where $A$, $B$, and $C$ are the coefficients, $T_0$ ($°C$) is the base temperature, and $P_0$ (h) is the base photoperiod; these were the inflection points of each growth model. The SEM model has a mixed function of the temperature function, which shows a sigmoidal relationship with temperature, and of the photoperiod function, which shows an exponential relationship with photoperiod (Angus et al., 1981; Xue et al., 2004). We also concluded that there were no development ($DVR = 0$) if $DVR$ was below 0 in the SEM model.

To determine the parameter values of each model, we input the original meteorological data of each day from the seeding date to the flowering date for each cultivar under study and accumulated the $DVR$ values until $DVR$ became greater than 1 and determined the parameters by minimizing the root mean square error (RMSE) of the estimated and actual flowering dates. RMSE is one of the most commonly used criteria for evaluating predictive models; we calculated it as follows:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (S_i - O_i)^2}$$

where $O_i$ and $S_i$ are the observed and simulated wheat flowering dates, respectively, and $n$ is the number of samples. In this study, we calculated the RMSE of the three proposed models in case we applied them on the training and validation data.

In the case of the polynomial model, we used the least-square method to determine the five parameters used in the model employing QR decomposition by referring to a previous study (Kawakata, 2012). QR decomposition (also called as QR factorization) is one of the most commonly used method for solving normal equation, and it involves decomposing a matrix into an orthogonal matrix and an upper triangular matrix to determine the unique parameters of the model (Daniel et al., 1976). In the case of the SEM model, finding the least square solution by using the normal equation was not directly applicable; thus, we used the Nelder-Mead and augmented Lagrange multiplier methods to determine the parameters of the model.

The Nelder-Mead method is one of the most commonly used optimization methods in non-linear programming, and most studies (Horie and Nakagawa, 1990; Maruyama et al., 2010; Nakazono et al., 2014; Onogi et al., 2016) that used the SEM model adopted this approach to determine the parameters of the model. Moreover, it is one of the traditional optimization methods used for multidimensional unconstrained minimization, also known as the downhill simplex method (Lagarias et al., 1998). For a function of $N$ parameters, the optimization algorithm is based on comparing the objective function at the $N+1$ vertices of a simplex and compares the worst vertex through three basic steps — reflection, contraction, and expansion (Klein and Neira, 2014; Nelder and Mead, 1965). The advantage of this method is that it does not require partial derivatives of the objective function (Cryer et al., 2015). Thus, a wide range of studies have applied this method for determining some coefficients of crop models so far; however, the method requires initial values for making a first simplex, while the final values of

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Fig. 1. (a) Seasonal variation in monthly mean air temperature during the growing seasons in 2016–2017 (average) in Fukuyama (solid line), in 2012–2015 (average) in Yamaguchi (dotted line), and in 2016 in Higashihiroshima (dashed line). (b) Seasonal variation in monthly mean photoperiod between October and the following September in Yamaguchi. The variations in the case of Fukuyama and Higashihiroshima were abbreviated because the latitudes of Fukuyama and Higashihiroshima (34°50’ N) and Yamaguchi (34°14’ N) are not very different from one another.
the parameters and precision of model prediction can reportedly change depending on the initial values selected (Nakano et al., 2015). In addition, sometimes an unnatural coefficient for crop growth can be determined in the preliminary test. Considering this, we set 15 patterns of the initial values for each crop model in reference to the results of the previous studies (Maruyama et al., 2010; Nakazono et al., 2014) and our preliminary test, when determining model parameters, and finally adopted the models that gave the lowest RMSE value in the training dataset.

The augmented Lagrange multiplier method is another optimization method for non-linear programming. This method uses partial derivatives of the objective function for determining model parameters (Rockafellar, 1976). In general, in the augmented Lagrange multiplier method, the objective function is modified by adding the terms that describe the constraints of the model, and it is augmented by the constraint of inequations through a set of non-negative multiplicative Lagrange multipliers (Gavin and Scruggs, 2016). This optimization method has been widely used in different sectors, such as financial engineering (Zhang et al., 2006) and computer science (Peng and Wu, 2010); it has the additional advantage of avoiding an unnatural coefficient determined by setting constraints. To date, a variety of non-linear crop growth models have been developed, but, to our knowledge, no study has ever used the augmented Lagrange multiplier method for determining the parameters of a crop model. Here, we set the constraints on the parameters of SEM as \(\{0.1 < A < 1; 0.1 < B < 1; 0 < C < 100; 8 < P_x < 11; 0 < T_x < 15\}\) on the basis of the results of the previous studies (Maruyama et al., 2010; Nakazono et al., 2014) and our preliminary test.

In addition, we investigated the changing pattern of DVR accompanied by the changes in temperature and photoperiod to evaluate the validity of the proposed models. The parameters of the model for each cultivar were determined by using the data of the corresponding wheat planted in 2012–2014. Regarding the model for Kinuhime, we used the data collected at Higashihiroshima (20 datasets) and Fukuyama (9 datasets) as the test data and checked the accuracy of the flowering dates predicted by the SEM models developed by the Nelder-Mead or augmented Lagrange multiplier method at each site. All analyses were conducted using the R software version 3.2.4. The “Rsolnp” package (Ghalanos and Theussl, 2012) was used for determining the parameters using the augmented Lagrange multiplier method.

### 3. Results

Tables 1 and 2 show the prediction accuracy of the three models proposed on the basis of the training and validation data obtained from the four-fold cross-validation. In the case of the Kinuhime and Akitakko cultivars, both polynomial models showed more than 20 days of RMSE using the training data; therefore, we did not continue to evaluate the model using the validation data. However, the polynomial model showed relatively good precision in cultivars Norin 61 and Iwainodaichi among the three models in the training data (Table 1).

When applying the three models to the validation data, we found that the polynomial models showed the lowest RMSE for the cultivar Iwainodaichi (RMSE: approximately 2 days) among the three models tested, while they showed the worst level of performance, especially for the cultivar Kitahonami (RMSE: approximately 12 days) (Table 2). On the other hand, both SEM models showed the RMSE of each cultivar with values ranging between 3 and 5 days (Table 2), and few cases showed a difference of more than 10 days similar to polynomial models (Fig. 2). In fact, we found that the SEM models developed by the Nelder-Mead method showed relatively similar RMSE values compared with the model developed by the augmented Lagrange multiplier method (Table 2). However, in the case of the cultivar Kinuhime cultivated in Higashihiroshima, the model developed by the augmented Lagrange multiplier method showed lower RMSE (2.78) than the model developed by the Nelder-Mead method (RMSE: 9.01), while in Fukuyama, both models predicted the flowering date approximately 4 days in RMSE (Fig. 3). We found that both models predicted the flowering date earlier than the actual date in Higashihiroshima, but the model developed by Nelder-Mead method seemed to predict the flowering date earlier than the other method (Fig. 3).

Figure 4 shows a variation in the DVP predicted the three models constructed in response to temperature and photoperiod for the five cultivars under study. We found that in the case of the cultivars Kinuhime and Akitakko, DVP became lower than 0 under certain conditions of temperature and photoperiod,

### Table 1. Comparison of root mean square error (RMSE) values of three crop development models using the training data of four-fold cross-validation for five wheat cultivars collected in Yamaguchi.

| Cultivar   | Polynomial model | SEM model (NM*) | SEM model (ALM**) |
|-----------|------------------|-----------------|-------------------|
| Norin61   | 2.49             | 3.02            | 3.33              |
| Iwainodaichi | 1.29             | 3.74            | 4.12              |
| Kinuhime  | > 20             | 3.46            | 3.75              |
| Akitakko  | > 20             | 2.80            | 3.42              |
| Kitahonami| 4.42             | 3.40            | 3.69              |

Mean ± SD: 2.74 ± 1.58*** 3.29 ± 0.37 3.66 ± 0.31

*NM: Nelder-Mead method

**ALM: Augmented Lagrange multiplier method

***The mean RMSE was calculated for all cultivars, except for the Kinuhime and Akitakko cultivars.

### Table 2. Comparison of the root mean square error (RMSE) of three crop development models using the validation data of four-fold cross-validation in five wheat cultivars collected in Yamaguchi.

| Cultivar   | Polynomial model | SEM model (NM*) | SEM model (ALM**) |
|-----------|------------------|-----------------|-------------------|
| Norin61   | 4.31             | 3.54            | 3.65              |
| Iwainodaichi | 1.95             | 5.13            | 4.62              |
| Kinuhime  | NA               | 4.07            | 4.22              |
| Akitakko  | NA               | 4.47            | 4.00              |
| Kitahonami| 12.03            | 4.02            | 4.30              |

Mean ± SD: 6.10 ± 5.27 4.24 ± 0.59 4.16 ± 0.36

*NM: Nelder-Mead method

**ALM: Augmented Lagrange multiplier method
according to the polynomial model (Fig. 4). On the other hand, both SEM models showed similar patterns of DVR change in response to the two variables; further, DVR increased with an increase in temperature or photoperiod in all cultivars, except for Iwainodaichi, in which case, the model developed by the Nelder-Mead method showed a decrease in DVR with increasing temperature. In addition to Iwainodaichi, we observed obvious differences between the SEM models developed by the two optimization methods; for example, in Akitakko, the DVR model developed by the Nelder-Mead method showed a rapid increase.
Fig. 4. Relationships among daily mean air-temperature, photoperiod, and development rate ($DVR$) determined by three different models in five wheat cultivars. NM denotes the results of the sigmoid and exponential mixed (SEM) model using the Nelder-Mead method, and ALM denotes the results of the SEM model using the augmented Lagrange multiplier method for determining crop model coefficients. The parameters of the model for each cultivar were determined by using the data of the corresponding cultivar sowed between 2012 and 2014 in Yamaguchi.

Fig. 5. Relationships between daily mean air-temperature and development rate ($DVR$) determined by the Nelder-Mead method and the augmented Lagrange multiplier method in Akitakko (left) and Kinuhime (right) wheat cultivars for two given photoperiods (11 h and 13 h). The $DVR$ in Akitakko wheat cultivar determined by the Nelder-Mead method was constantly 0 when the photoperiod was 11 h. The parameters of the model for each cultivar were determined by using the data of the corresponding cultivar sowed between 2012 and 2014 in Yamaguchi.
in DVR at mean ambient temperature of 9–10 °C, while the model developed by the augmented Lagrange multiplier method showed a relatively smooth growth curve with increasing temperature (Fig. 5).

4. Discussion

Overall, we found that the polynomial model yielded an RMSE value greater than 12 days in case of the cultivar Kitahonami with the validation data. The polynomial model can reportedly predict rice phenological stages effectively (Kawakata, 2012); however, our results suggest that the SEM model would predict the flowering date more accurately than the polynomial model in the studied wheat cultivars, (RMSE from 3 to 5 days), except for Iwainodaichi. In France, Bogard et al. (2014) developed a hybrid wheat phenological model that combined weather variables and wheat QTL information; their model predicted the heading date with an RMSE value of approximately 5 to 9 days. In the model developed by the Nelder-Mead method, Maruyama et al. (2010) reported that their approach could predict the heading date in wheat with an RMSE of approximately 5 days; further, Nakazono et al. (2014) used the same algorithm and predicted the heading date in wheat with an RMSE value ranging from 4 to 6 days for different cultivars. Considering earlier studies, our model could predict the flowering date in wheat, at least, as accurately as predicted by these previous studies.

The SEM model developed by the Nelder-Mead method showed similar precision with the validation data from Yamaguchi compared with the model developed by the augmented Lagrange multiplier method (Table 2). This result indicates that the augmented Lagrange multiplier method can substitute for the Nelder-Mead method for optimizing non-linear models. Particularly, the result of the test data in Higashihiroshima showed that the model developed by the augmented Lagrange multiplier method predicted the flowering date in wheat more precisely (RMSE: 2.78) than the model developed by the Nelder-Mead method (RMSE: 9.01), indicating that the SEM model developed by the former method was more applicable in the sites other than the site from where the training data was obtained.

In terms of the validity of the models constructed here, the polynomial models showed a variety of patterns of DVR changes in response to environmental conditions. For example, the modeling of the cultivars Kinuhime and Akitakko showed a sharp decrease in DVR with increasing temperature (Fig. 4); this might not happen in reality, in the way wheat actually grows. Considering the performance of the model (Table 2), it is likely that it might work well at specific sites under specific conditions, but it cannot be applied to different places or under a wide range of climatic conditions. Higher-order polynomial models can show more smooth response curve against the temperature or photoperiod, but the parameters of higher order are difficult for interpretation in the biological context (Yan and Hunt, 1999).

The SEM growth model developed by the Nelder-Mead method also showed some cases of rapid changes in DVR under slight changes of temperature or photoperiod. For example, in the cultivar Akitakko, DVR showed a rapid increase (between 9 and 10 °C) in temperature (Fig. 5). It has been reported that the wheat growth response to temperature would be relatively smooth (Li et al., 2008), and the rapid development was limited under the conditions of warm temperature and long photoperiod (>14 h) (Robertson 1968; Angus et al., 1981). Slafier and Rawson (1995) reported that wheat growth became relatively fast with an increase in temperature or photoperiod; however, in the cultivar Iwainodaichi, the model developed by the Nelder-Mead method showed that DVR decreased as the temperature increased (Fig. 4); this is not supported by the data on the actual wheat growth patterns.

The SEM model developed by the augmented Lagrange multiplier method, on the other hand, can set constraints in coefficients, so that we can prevent the model from having unnatural coefficients. Our models developed by the augmented Lagrange multiplier method showed a consistent increase in DVR in response to an increase in temperature and photoperiod (Fig. 4). For practical purposes, it is important that a crop phenological model be applied to a variety of places under varying climatic conditions; thus, the ability of a model to set constraints in some coefficients would be a great advantage. The coefficients determined for a crop model tend to be dependent on the training data, but the ability to set constraints leads to the generation of more flexible models that are also applicable in the sites different from where the training data was obtained. For example, Figure 3 shows that the model developed by the Nelder-Mead method estimated the flowering date for the cultivar Kinuhime earlier than the actual date, while it showed higher DVR values under both 11-h and 13-h photoperiods than the DVR determined by the augmented Lagrange multiplier method (Fig. 5). These results suggested that the model developed by the Nelder-Mead method overestimated the DVR of the cultivar Kinuhime, and that the growth curve determined by the augmented Lagrange multiplier method would be more applicable to Higashihiroshima. Since we only showed the case of Kinuhime for validating whether the model could be used for different places, further study is necessary to test whether the augmented Lagrange multiplier method would be reliable for determining the coefficients of non-linear crop models, although the relationships among weather variables and development rate show its potential advantage (Fig. 4).

Precision model improvement can be reached by changing the algorithms describing wheat growth. Especially, in our study, we defined wheat growth in a single model, but the actual DVR of wheat could vary for different growth stages; thus, defining the different growth models according to wheat growth stages would clearly be one of the options for improving models. For example, Wu et al. (2017) tried splitting wheat growth into four stages (seedling to germination, germination to stem elongation, stem elongation to flowering, and flowering to maturation). Based on this division, they developed phenological models and showed that they could predict each stage within 2 to 5 days of the actual dates. In addition, winter wheat needs a vernalization period, so that a model that includes a vernalization function would naturally predict the flowering date more precisely. Streek et al. (2003) modified the Wang and Engel model (WE model) by including such vernalization function, and they reported an
RMSE of 5–6 days for the modified model, corresponding to a 45% decrease in the RMSE value obtained using the original WE model. Furthermore, in rice, a hybrid model evaluation including genomic prediction was conducted recently (Onogi et al., 2016), and this approach is also applicable to other crop models. Indeed, the training data used for calibrating the model for cross-validation in this study was only 16–17 datasets; therefore, it is likely that the precision of each model can be substantially improved simply by using more data, if it can be obtained.

5. Conclusion

In this study, we constructed and evaluated three different wheat phenological models (polynomial model and SEM models developed by the Nelder-Mead and augmented Lagrange multiplier methods) in five wheat cultivars. We found that the SEM model predicted the flowering date in wheat more precisely than the polynomial models. In addition, we found that the model developed by the Nelder-Mead method showed similar performance compared with the model developed by the augmented Lagrange multiplier method. However, in the context of model validity, the model developed by the augmented Lagrange multiplier method would be more realistic and effective for expressing wheat growth response to environmental factors. As is the case with other crop modeling studies, we need a certain amount of data for calibrating the model, but we believe that the methodology used in this study can be applied to other crop models. Although additional research is necessary to confirm our results with other types of crops and different environmental conditions, we trust that our study contributes to select and develop more effective crop models for conducting future studies in this field.

Acknowledgments

We thank Dr. Yoshitaka Kurose for giving instructive comments on our research and also thank Dr. Hideki Ueyama and Mr. Tatsuya Sato for helping us to collect the cultivation and weather data in the field. We are also grateful for all those who helped with fieldwork and gave us constructive comments. This research was supported by the grants from a Project of the Bio-oriented Technology Research Advancement Institution (Bio-TARAI) and the special scheme project on regional developing strategy.

References

Angus JF, Mackenzie DH, Morton R, Schafer CA, 1981: Phasic development in field crops II. Thermal and photoperiodic responses of spring wheat. *Field Crops Research* 2, 269–283. https://doi.org/10.1016/0378-4290(81)90078-2

Bogard M, Ravel C, Paux E, Bordes J, Balfourier F, Chapman S, Le Gouis J, Allard V, 2014: Predictions of heading date in bread wheat (*Triticum aestivum L.*): using QTL-based parameters of an ecophysiological model. *Journal of Experimental Botany* 65(20), 5849–5865.

Crofts HJ, 1989: On defining a winter wheat. *Euphytica* 44(3), 225–234.

Cryer SA, Havens PL, Hillger DE, van Wesenbeeck JJ, 2015: An improved indirect procedure for estimating pesticide volatility from field trials. *Journal of Environment Quality* 44(5), 1513. https://doi.org/10.2134/jeq2015.03.0125

Daniel JW, Gragg WB, Kaufman L, Stewart GW, 1976: Reorthogonalization and stable algorithms for updating the Gram-Schmidt QR factorization. *Mathematics of Computation* 30(136), 772–795.

de Wit CT, Brouwer R, De Vries FP, 1970: The simulation of photosynthetic systems. *Proceedings of the IBP/PP Technical Meeting*, 14–21 September, 1969, Trebon, Czech Republic, pp. 47–70.

Gavin HP, Scruggs JT, 2016: Constrained optimization using Lagrange multipliers. Retrieved from http://people.duke.edu/~hpavgin/cee201/LagrangeMultipliers.pdf

Ghalanos A, Theussl S, 2012: Rsolnp: general non-linear optimization using augmented Lagrange multiplier method. *R Package Version 1.16*

Gotoh T, 1979: Genetic studies on growth habit of some important spring wheat cultivars in Japan, with special reference to the identification of the spring genes involved. *Japanese Journal of Breeding* 29(2), 133–145.

He D, Wang E, Wang J, Lilley J, Luo Z, Pan X, Pan Z, Yang N, 2017: Uncertainty in canola phenology modelling induced by cultivar parameterization and its impact on simulated yield. *Agricultural and Forest Meteorology* 232, 163–175. https://doi.org/10.1016/j.agrformet.2016.08.013

He L, Asseng S, Zhao G, Wu D, Yang X, Zhuang W, Jin N, Yu Q, 2015: Impacts of recent climate warming, cultivar changes, and crop management on winter wheat phenology across the Loess Plateau of China. *Agricultural and Forest Meteorology* 200, 135–143. https://doi.org/10.1016/j.agrformet.2014.09.011

Horie T, Nakagawa H, 1990: Modelling and prediction of developmental process in rice. I. Structure and method of parameter estimation of a model for simulating developmental process toward heading. *Japanese Journal of Crop Science* 59(4), 687–695. (in Japanese) https://doi.org/10.1626/jcs.59.687

Kawakata T, 2012: Calculation of crop developmental rate using a polynomial expression with linear least squares solution. *Climate in Biosphere* 12, 52–58. (in Japanese) https://doi.org/10.2480/cib.12.5.2

Klein K, Neira J, 2014: Nelder-Mead Simplex optimization routine for large-scale problems: A distributed memory implementation. *Computational Economics* 43(4), 447–461. https://doi.org/10.1007/s10614-013-9377-8

Lagarias JC, Reeds JA, Wright MH, Wright PE, 1998: Convergence properties of the Nelder-Mead Simplex method in low dimensions. *SIAM Journal on Optimization* 9(1), 112–147. https://doi.org/10.1137/S1052623496303470

Li L, McMaster GS, Yu Q, Du J, 2008: Simulating winter wheat development response to temperature: Modifying Malo’s exponential sine equation. *Computers and Electronics in Agriculture* 63(2), 274–281. https://doi.org/10.1016/j.compag.2008.03.006

Li T, Hasegawa T, Yin X, Zhu Y, Boote K, Adam M, Bregaglio S, Buis S, Confolonieri R, Fumoto T, Gaydon D, Marcaida M, Nakagawa H, Oriol P, Ruane AC, Ruget F, Singh B, Singh U, Tang L, Tao F, Wilkens P, Yoshida H, Zhang Z, Bouman B, 2015: Uncertainties in predicting rice yield by current crop models under a wide range of climatic conditions. *Global Change Biology* 21(3), 1328–1341. https://doi.org/10.1111/gcb.12758

Maruyama A, Kurose Y, Ohba K, 2010: Modeling of phenological development in winter wheat to estimate the timing of phenological events. *Theussl S, Le Gouis J, Allard V*, 2014: Predictions of heading date development in field crops II. Thermal and photoperiodic conditions.
heading and maturity based on daily mean air temperature and photoperiod. *Journal of Agricultural Meteorology* **66**(1), 41–50. https://doi.org/10.2480/agrmet.66.1.7

Mkhabela M, Ash G, Grenier M, Bullock P, 2016: Testing the suitability of thermal time models for forecasting spring wheat phenological development in western Canada. *Canadian Journal of Plant Science* **96**(5), 765–775. https://doi.org/10.1139/cjps-2015-0351

Nakano S, Kumagai E, Shimada S, Sameshima R, Ohno H, Homma K, Shiraiwa T, 2015: Modeling of phenological development stages and impact of elevated air temperature on the phenological development of soybean cultivars in Japan. *Japanese Journal of Crop Science* **84**(4), 408–417. (in Japanese) https://doi.org/10.1626/jcs.84.408

Nakazono K, Ohno H, Yoshida H, Sasaki K, Nakagawa H, 2014: Modeling phenological development in wheat. *Japanese Journal of Crop Science* **83**(3), 249–259. (in Japanese) https://doi.org/10.1626/jcs.83.249

Nelder JA, Mead R, 1965: A simplex method for function minimization. *The Computer Journal* **7**(4), 308–313. https://doi.org/10.1093/comjnl/7.4.308

Onogi A, Watanabe M, Mochizuki T, Hayashi T, Nakagawa H, Hasegawa T, Iwata H, 2016: Toward integration of genomic selection with crop modelling: the development of an integrated approach to predicting rice heading dates. *Theoretical and Applied Genetics* **129**(4), 805–817. https://doi.org/10.1007/s00122-016-2667-5

Palosuo T, Kersebaum KC, Angulo C, Hlavinka P, Moriondo M, Olesen JE, Patil RH, Ruget F, Rumbaur C, Takač J, Trnka M, Biná M, Čaldař B, Ewert F, Ferriese R, Mirschel W, Şaylan L, Šiška B, Rötter R, 2011: Simulation of winter wheat yield and its variability in different climates of Europe: A comparison of eight crop growth models. *European Journal of Agronomy* **35**(3), 103–114. https://doi.org/10.1016/j.eja.2011.05.001

Peng Z, Wu D, 2010: A partial parallel splitting augmented Lagrangian method for solving constrained matrix optimization problems. *Computers and Mathematics with Applications* **60**(6), 1515–1524. https://doi.org/10.1016/j.camwa.2010.06.035

Ritchie JT, 1991: Wheat phasic development. In: *Modeling Plant and Soil Systems* (ed. by Hanks RJ, Ritchie JT). American Society of Agronomy, Madison (WI), pp. 31–54.

Robertson, GW, 1968: A biometeorological time scale for a cereal crop involving day and night temperatures and photoperiod. *International Journal of Biometeorology* **12**(3), 191–223.

Rockafellar RT, 1976: Augmented Lagrangians and applications of the proximal point algorithm in convex programming. *Mathematics of Operations Research* **1**(2), 97–116. https://doi.org/10.1287/moor.1.2.97

Slafer GA, Rawson HM, 1995: Photoperiod × temperature interactions in contrasting wheat genotypes: Time to heading and final leaf number. *Field Crops Research* **44**(2–3), 73–83. https://doi.org/10.1016/0378-4290(95)00077-1

Streck NA, Weiss A, Xue Q, Stephen Baenziger P, 2003: Improving predictions of developmental stages in winter wheat: A modified Wang and Engel model. *Agricultural and Forest Meteorology* **115**(3–4), 139–150. https://doi.org/10.1016/S0168-1923(02)00228-9

Tollenaar M, Daynard TB, Hunter RB, 1979: Effect of temperature on rate of leaf appearance and flowering date in maize. *Crop Science* **19**(3), 633. https://doi.org/10.2135/cropsciresearch1979.0011183X001900030022x

Tubiello FN, Donatelli M, Rosenzweig C, Stockle CO, 2000: Effects of climate change and elevated CO2 on cropping systems: model predictions at two Italian locations. *European Journal of Agronomy* **13**, 179–189. Retrieved from www.elsevier.com/locate/eja

Wang E, Engel T, 1998: Simulation of phenological development of wheat crops. *Agricultural Systems* **58**(1), 1–24. https://doi.org/10.1016/S0308-521X(98)00028-6

Wu L, Feng L, Zhang Y, Gao J, Wang J, 2017: Comparison of five wheat models simulating phenology under different sowing dates and varieties. *Agronomy Journal* **109**(4), 1280. https://doi.org/10.2134/agronj2016.10.0619

Xue Q, Weiss A, Baenziger PS, 2004: Predicting leaf appearance in field-grown winter wheat: Evaluating linear and non-linear models. *Ecological Modelling* **175**(3), 261–270. https://doi.org/10.1016/j.ecolmodel.2003.10.018

Yan W, Hunt LA, 1999: An equation for modelling the temperature response of plants using only the cardinal temperatures. *Annals of Botany* **84**(5), 607–614.

Yan W, Wallace DH, 1998: Simulation and prediction of plant phenology for five crops based on photoperiod x temperature interaction. *Annals of Botany* **81**(6), 705–716. https://doi.org/10.1006/anbo.1998.0625

Yin X, Kropff MJ, Horie T, Nakagawa H, Centeno HGS, Zhu D, Goudriaan J, 1997: A model for photothermal responses of flowering in rice. I. Model description and parameterization. *Field Crops Research* **51**(3), 189–200. https://doi.org/10.1016/S0378-4290(96)03456-9

Yin X, Kropff MJ, McLaren G, Visperas RM, 1995: A nonlinear model for crop development as a function of temperature. *Agricultural and Forest Meteorology* **77**(1–2), 1–16. https://doi.org/10.1016/0168-1923(95)00226-Q

Zhang K, Yang XQ, Teo KL, 2006: Augmented Lagrangian method applied to American option pricing. *Automatica* **42**(8), 1407–1416. https://doi.org/10.1016/j.automatica.2006.01.017