Simulation of crop growth, time to maturity and yield by an improved sigmoidal model

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Models that accurately estimate maximum crop biomass to obtain a reliable forecast of yield are useful in crop improvement programs and aiding establishment of government policies, including those addressing issues of food security. Here, we present a new sigmoidal growth model (NSG) and compare its performance with the beta sigmoidal growth model (BSG) for capturing the growth trajectories of eight crop species. Results indicated that both the NSG and the BSG fitted all the growth datasets well ($R^2 > 0.98$). However, the NSG performed better than the BSG based on the calculated value of Akaike’s information criterion (AIC). The NSG provided a consistent estimate for when maximum biomass occurred; this suggests that the parameters of the BSG may have less biological importance as compared to those in the NSG. In summary, the new sigmoidal growth model is superior to the beta sigmoidal growth model, which can be applied to capture the growth trajectory of various plant species regardless of the initial biomass values at the beginning of a growth period. Findings of this study will be helpful to understand the growth trajectory of different plant species regardless of their initial biomass values at the beginning of a growth period.

The growth of plants is driven by numerous functions and involves numerous physiological and ecological processes12. The complete growth trajectory of a plant often resembles a sigmoidal curve34 that begins with a slow rate of increase, transitions to a log increase in growth rate and ends with a decrease in the rate of increase ending in zero growth when maximum biomass is reached. Although many growth models have been proposed for plants, such as the logistic, Richards and Gompertz growth models15, these models do not accurately predict the amount of maximum biomass present when the asymptotic line of the model trajectory, $w_{\text{max}}$, is reached.

To address this deficiency, the beta distribution function to describe the trajectory of plant growth rate was introduced67:

$$\frac{dw}{dt} = c_m \left( \frac{t_e - t}{t_e - t_m} \right) \left( \frac{t - t_b}{t_m - t_b} \right)^{t_m - t_b \delta}$$

(1)

where $w$ is the biomass at time $t$, $\delta$ is a constant, $c_m$ is the maximum growth rate, reached at time $t_m$, $t_b$ and $t_e$ represent times of starting and ending growth, respectively. When $t_b$ and $\delta$ are set as 0 and 1, respectively, the beta function can be simplified as follows:

$$\frac{dw}{dt} = c_m \left( \frac{t_e - t}{t_e - t_m} \right) \left( \frac{t}{t_m \delta} \right)^{t_m - t_e \delta}$$

(2)

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For example, the estimates of $t_e$ respectively). These results suggest that the estimates of days of age (Fig. 2), the observed values of (Wild.) (Table 3).

Datasets of eight crop species to estimate the timing and the maximum biomass when growth ceases. Comparing it with the beta sigmoidal growth (BSG) model. We evaluated both the models using observed growth

Curves to those obtained by the leaf-growth model8. In addition, the performance of the BSG is superior to other traditional growth models (e.g., Gompertz and von Bertanffy growth models) for its flexibility, outcompeting the exponential and logistic 8. In this study, we developed and tested a new sigmoidal growth (NSG) model by

Although the BSG is slightly different from the leaf-growth model9, the BSG can produce similar growth curves to those obtained by the leaf-growth model. In addition, the performance of the BSG is superior to other traditional growth models (e.g., Gompertz and von Bertanffy growth models) for its flexibility, outcompeting the exponential and logistic. In this study, we developed and tested a new sigmoidal growth (NSG) model by comparing it with the beta sigmoidal growth (BSG) model. We evaluated both the models using observed growth datasets of eight crop species to estimate the timing and the maximum biomass when growth ceases.

**Results**

Results showed the new sigmoidal growth (NSG) and the beta sigmoidal growth (BSG) provided good fits for all eight crop species well ($R^2 > 0.98$) (see Table 1). The fitted curves of the NSG and BSG were generally close to each other before reaching the maximum biomass (Figs 1 and 2). The NSG performed better than the BSG based on the calculated values of Akaike’s information criterion (AIC) for the growth datasets (Table 1). The negative estimate of $t_b$ from the NSG was observed only for peanut *Arachis hypogaea* L., whereas the estimates of $t_b$ from the BSG were negative for six species. The estimated values of $t_b$ from the BSG were higher than the NSG for all eight-crop species (Table 2). Similarly, the calculated values of maximum biomass ($w_{max}$) of the BSG were all higher than those of the NSG except for the growth of Adzuki bean *Vigna angularis* (Wild.) Ohwi et Ohashi (Table 3).

For example, the estimates of $t_b$ from the BSG for Mung bean reached 311 days, which was more than four times of that from the NSG. Because the observed value of biomass remained steady when the Mung bean reached 80 days of age (Fig. 2), the observed values of $t_b$ and $w_{max}$ were around 80 days and 40 g that compare well with the NSG model but not the BSG model that seriously overestimated the time/yield end points (311 days and 202 g, respectively). These results suggest that the estimates of $t_b$ and calculated value of $w_{max}$ from the BSG for is not reliable for some cases.

**Discussion**

Results indicated that both the NSG and the BSG can fit the growth datasets of crop species well, and NSG performed better than the BSG based on the calculated values of AIC (Table 1). The parameter $t_b$ in the NSG is equivalent to the parameter $T_{min}$ in Eq. (5), the lower threshold of temperature for the growth rate of bacteria. Ratkowsky et al.10 have pointed out that the parameter $T_{min}$ in degrees Kelvin is a conceptual temperature representing an intrinsic feature of the organism. In the study of Ratkowsky et al.10, a total of 13 estimates of $T_{min}$ from the Eq. (5) are negative with lower than 273 K among all 16 bacterial cultures. Accordingly, the estimates of $t_b$ from the NSG can also assume negative values. As a result, estimates of $t_b$ from the NSG were negative for the growth of peanut.

Although it observed that $t_b$ could represent the beginning of the growth period at which the growth rate is set to zero. However, our results showed that the estimates of $t_b$ from the BSG were negative except for the Adzuki bean and Mung bean. Furthermore, the estimates of $t_b$ from the BSG are not reliable for some cases (Table 2). For the BSG, the parameters of $t_b$ and $t_e$ represent the replacement of the lower and upper bounds, respectively, in the beta distribution function with four parameters. Consequently, the biological functions used for the parameters

| Number of Species | Latin name           | English name | NSG          | BSG          |
|-------------------|----------------------|--------------|--------------|--------------|
| 1                 | *Helianthus annuus*  | Sunflower    | 0.998        | 0.998        |
|                   | L.                   |              | 50.09        | 53.4         |
| 2                 | *Arachis hypogaea*   | Peanut       | 0.997        | 0.997        |
|                   | L.                   |              | −1.61        | −1.14        |
| 3                 | *Glycine max* (L.)   | Black soybean| 0.996        | 0.995        |
| Merr.             |                      |              | 15.05        | 15.74        |
| 4                 | *Psium sativum*      | Garden pea  | 0.996        | 0.998        |
|                   | L.                   |              | 17.21        | 18.35        |
| 5                 | *Vigna angularis*    | Adzuki bean | 0.997        | 0.982        |
| (Willd.)          |                      |              | −9.13        | 16.66        |
| 6                 | *Vigna radiata* (L.) | Mungbeans   | 0.999        | 0.985        |
| R. Wilczek        |                      |              | −17.81       | 26.07        |
| 7                 | *Gossypium* spp.     | Cotton      | 0.994        | 0.996        |
|                   |                      |              | 38.2         | 34.08        |
| 8                 | *Sorghum bicolor* (L.)| Moench | 0.996        | 0.996        |
|                   | Moench               | Sweet sorghum| 58.16        | 56.62        |

Table 1. Akaike’s information criterion (AIC) and R square values of the two growth models for the datasets of crop species. NSG and BSG represent the new sigmoidal growth model and the beta sigmoidal growth model in Eq. (4), respectively.

$$w = w_{max} \left(1 + \frac{t_e - t}{t_e - t_m}\right)\left(\frac{t}{t_m}\right)^{\frac{t_e - t}{t_e - t_m}} (0 \leq t < t_e)$$

where $t_e$ is the time when biomass reaches the value of $w_{max}$. In particular, the biomass $w$ equals zero when $t = 0$ in Eq. (3). This assumption matches the growth trajectory of many plants; however, exceptions do occur. To address this issue, only assumed $\delta = 1$ in Eq. (1) and then derived a more flexible beta sigmoidal growth model (BSG) in Eq. (4) to capture the growth trajectory of various plant species regardless of the initial biomass values.

$$w = c_m \cdot (t - t_b) \cdot \frac{2t_e - t_m - t}{2t_e - t_m - t_b} \left(\frac{t - t_b}{t_m - t_b}\right)^{\frac{t_e - t_b}{t_e - t_m}}$$

Although the BSG is slightly different from the leaf-growth model8, the BSG can produce similar growth curves to those obtained by the leaf-growth model. In addition, the performance of the BSG is superior to other traditional growth models (e.g., Gompertz and von Bertanffy growth models) for its flexibility, outcompeting the exponential and logistic8. In this study, we developed and tested a new sigmoidal growth (NSG) model by comparing it with the beta sigmoidal growth (BSG) model. We evaluated both the models using observed growth datasets of eight crop species to estimate the timing and the maximum biomass when growth ceases.
of \( t_b \) and \( t_e \) are artificially provided in the BSG model. The BSG fits the growth datasets of the eight crop species well \( (R^2 > 0.98) \) (Table 1) through the flexibility of the beta distribution function, however, the parameters used to derive the BSG are not biologically accurate. Consequently, the estimates of \( t_b \) and \( t_e \) from the BSG are not biologically relevant in some cases, which is confirmed by the overestimated \( w_{\text{max}} \) compared to the observed values. On the contrary, the observed values of \( t_e \) and \( w_{\text{max}} \) compared well with the estimates of NSG model. Therefore, we concluded the NSG is better than the BSG and other traditional sigmoidal growth models, which can be applied to capture the growth trajectory of various plant species regardless of the initial biomass values at the beginning of the growth period.

Methods
Model derivation. Ambient temperature is the principal variable that determines the developmental growth rate of poikilotherms, including plants, which occurs in a range between the lower and upper developmental temperature threshold determined for each species. A nonlinear model was proposed to describe the effect of temperature on the growth rate of bacteria:

\[
\dot{r} = c(T - T_1)(1 - e^{k(T - T_2)})
\]

where \( r \) is the growth rate, \( c \) and \( K \) are constants, \( T_1 \) and \( T_2 \) is the minimum and maximum temperature for growth, respectively. After replacing the temperature with time, we derived a new sigmoidal growth model (NSG) by integrating Eq. (5) as follows:

\[
w = \frac{1}{3} \xi(t) + \frac{c^2(\varphi(t) + \theta(t)\eta(t) - 16\eta(t))}{4k^2}
\]
With \( \eta(t) = e^{k(T-t)} \), \( g(t) = c^2t^3 - 3c^2t^2t_0 + 3c^2t_0^2t \), \( \varphi(t) = -8k^2t^2 + 16k^2t_0 - 8k^2t_0^2 + 16kt - 16kt_0 \) and \( \theta(t) = (2k^2t^2 - 4k^2t_0 + 2k^2t_0^2 - 2kt + 2kt_0 + 1)e^{k(T-t)} \) where \( w \) is the biomass at time \( t \); \( c \) and \( k \) are constants; \( t_0 \) and \( t_f \) represent the starting and ending time of growth.

**Parameter estimation.** The parameters of the BSG and the NSG were estimated using the Differential Evolution by optimizing the problem and the Nelder-Mead algorithms by non-linear optimization problems.
Table 3. Estimated value of maximum biomass of the new and beta sigmoidal growth models for the growth datasets of crop species. NSG and BSG represent the new sigmoidal growth model and the beta sigmoidal growth model in Eq. (4), respectively.

| Species         | NSG Maximum biomass (g) | BSG Maximum biomass (g) |
|-----------------|--------------------------|--------------------------|
| Sunflower       | 310.69                   | 924.76                   |
| Peanut          | 41.90                    | 177.78                   |
| Black soybean   | 47.97                    | 54.09                    |
| Garden pea      | 86.07                    | 93.56                    |
| Adzuki bean     | 23.36                    | 22.92                    |
| Mung bean       | 33.92                    | 202.84                   |
| Cotton          | 88.49                    | 90.26                    |
| Sweet sorghum   | 186.24                   | 186.40                   |

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Acknowledgements

We thank to the China Scholarship Council (CSC) for supporting Lei Chen studies in Japan. The paper was supported by Henan Province Science and Technology projects (No. 132102110021, 142300410007 and 142102110028).

Author Contributions

Lei Chen, Ming-Fu Yu and Jun-He Liu conceived and designed the experiment, Qi-Jie Xu and Pei-Jian Shi wrote the article. Yan Yan, Lei Chen, Pei-Jian Shi and Abid Ali performed the data analysis. Jun-He Liu, Abid Ali and Pei-Jian Shi modified the paper. All authors reviewed the manuscript.

Additional Information

Competing Interests: The authors declare no competing interests.

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