Phenomics data processing: Extracting temperature dose-response curves from repeated measurements

Lukas Roth[a,*], Hans-Peter Piepho[b], Andreas Hund[a]

[a]*ETH Zurich, Institute of Agricultural Sciences, Universitätstrasse 2, 8092 Zurich, Switzerland*
[b]*University of Hohenheim, Institute for Crop Science, Biostatistics Unit, Fruwirthstrasse 23, 70593 Stuttgart, Germany*

Summary

Temperature is a main driver of plant growth and development. New phenotyping tools enable quantifying the temperature response of hundreds of genotypes. Yet, particularly for field-derived data, the process of temperature response modelling bears potential flaws and pitfalls with regard to the interpretation of derived parameters. In this study, climate data from three growing seasons with differing temperature distributions served as starting point for a wheat stem elongation growth simulation, based on a four-parametric Wang-Engel temperature response function. To extract dose-responses from the simulated data, a novel approach to use temperature courses with high temporal resolution was developed. Linear and asymptotic parametric modelling approaches to predict the cardinal temperatures were investigated. An asymptotic model extracted the base and optimum temperature of growth and the maximum growth rate with high precision, whereas simpler, linear models failed to do so. However, when including seasonally changing cardinal temperatures, the prediction accuracy of the asymptotic model was strongly reduced. We conclude that using an asymptotic model based on temperature courses with high temporal resolution is suitable to extract meaningful parameters from field-based data. Consequently, applying the presented modelling approach to high-throughput phenotyping data of breeding nurseries may help selecting for climate suitability.

Keywords: growth, high-throughput field phenotyping, stem elongation, wheat (Triticum aestivum).

1. Introduction

Already in 1996, van Haren noted that the knowledge of crop responses to weather extremes is incomplete and not explicitly included in crop models. Today, high-throughout field phenotyping (HTFP) potentially enables to quantify crop growth—and consequently crop response—of hundreds of genotypes under field conditions (Araus et al., 2018). Understanding crop responses to environmental factors is essential to secure global food demands: Improvement in wheat yields stagnated on a global scale in the past three decades (Brisson et al., 2010; Laidig

*Corresponding author: lukas.roth@usys.ethz.ch

et al., 2017). It was suspected that for Europe, the changing climate increasingly impacts wheat yields (Brisson et al., 2010). Mitigating these changes in plant breeding to improve yield requires understanding crop responses to environmental factors (Ramirez-Villegas et al., 2015). A main driver of plant growth and development is temperature (Porter and Gawith, 1999).

1.1. Approaches to quantify temperature responses under controlled conditions

The effects of changes in temperature on crops are well studied in controlled environments, but the translation of insights to the field is not straightforward. The temperature response of developmental processes is usually studied by exposing plants to different temperature regimes—often during rather short time period of their life cycle. Two different approaches are used: one can either (1) expose different plants of the same genotype to different temperatures (Slafer and Rawson, 1995; Hund et al., 2012; Reimer et al., 2013), or (2) apply short phases of different temperatures to the same plant. Examples of the latter approach are the studies on leaf growth performed in the indoor platform 'Phenoarch', summarized by Parent and Tardieu (2012). This approach requires that the temperature response is measured at a constant growth phase, during which growth is linear when the temperature remains constant. Hence, response-pattern can be observed non-destructively on the same plant, offering a high throughput. In such experiments, the conditions of all but one covariate may be kept constant. Furthermore, the reversibility of the process can be tested by repeatedly applying the same conditions during the course of the experiment.

In general, developmental processes follow some sort of peak function in response to increasing temperatures, i.e., there is a base temperature T_{min} at which growth starts, an optimal temperature T_{opt} at which growth reaches its maximum rate r_{max}, and a maximum temperature T_{opt} at which growth stops (Porter and Gawith, 1999). Depending on the research field, different models are used to approximate such functions—for an overview see, e.g., Wang et al. (2017); Parent et al. (2019) for plants, and Rebaudo et al. (2018); Rebaudo and Rabhi (2018) for ectoterms (i.e., animals whose regulation of body temperature depends on external sources). In their work, Wang et al. (2017) distinguish four types of temperature response functions with increasing complexity. Clearly, type 4 functions (linear or curvilinear functions with three cardinal temperatures) are most appropriate to describe temperature responses. Among the most widely used type 4 functions for plants are the Wang-Engel cardinal temperature function (Wang et al., 2017) and a modified version of the reaction rates equation from Johnson et al. (1942) applied to different growth processes in a variety of major crops by Parent and Tardieu (2012). We will refer to these different response functions in detail further down.

1.2. Cardinal temperatures of wheat

For wheat, meta-analyses summarizing cardinal temperatures of different developmental processes are to some extent controversial. Porter and Gawith (1999) summarized 65 studies with regard to the minimum (T_{min}), optimum (T_{opt}) and maximum (T_{max}) temperature. Mean cardinal temperatures for shoot growth were 3.0 °C (T_{min}), 20.3 °C (T_{opt}) and > 20.9 °C (T_{max}). Notably, T_{opt} and T_{max} were very close together in many studies.

In contrast to the comparably low T_{opt} summarized by Porter and Gawith (1999), Parent and Tardieu (2012) reported a significantly higher T_{opt} of 27.7 °C when summarizing 8 studies and own data. We speculate that the discrepancies between the two studies are caused by the fact that the former is based mainly on studies using long-term exposure of individual plants, and the latter on studies that applied short-term changes in temperatures on a growing organ. In the present study we will use the more conservative, i.e., lower, temperature optimum reported by Porter and Gawith (1999).

There is evidence that cardinal temperatures are not constant during the lifetime of a crop: Slafer and Rawson (1995) examined T_{min} and T_{opt} for leaf appearance rates of vernalized winter wheat plants within three phases, i) after vernalization up to the terminal spikelet, ii) from the terminal spikelet up to heading, and iii) from heading to anthesis. The authors found that, averaged across cultivars, T_{min} was -1.9 °C, 1.2 °C and 8.1 °C, while T_{opt} was $<$ 22 °C, 25 °C and $>$ 25 °C for the three different phases, respectively. In addition, the cultivars differed substantially for the two parameters. Consequently, one may assume that particularly the base temperature may change cultivar-specific throughout the season. Nevertheless, the estimates from Slafer and Rawson (1995) of cardinal temperatures and their changes were derived from a controlled environment study. The benefits of controlled environment phenotyping lies in the ability to test a wide range of temperature regimes while keeping other influential factors, such as vapor pressure deficit and light, constant. However, plants usually do not experience such conditions in the field, as discussed by Slafer and Rawson (1995).

1.3. Approaches to quantify temperature responses with high-throughput in the field

Under field conditions, the temperature regimes are distinctly different from the controlled-environment studies considered so far. The environmental covariates in the field follow an annual and diurnal pattern to which plants adjust their life cycle. HTFP offers the possibility to assess crop growth under such more realistic conditions with high temporal and spatial resolution (Rebetzke et al., 2019). Hence, one can use the temperature course during the season to quantify the genotype-specific temperature responses. Still, such studies are sparse. Grieder et al. (2015) extracted the base temperature and response to increasing temperatures at early growth stages before terminal spikelet formation. The authors were able to extract heritable slopes and intercepts of linear responses. Kronenberg et al. (2020a) were able to extract heritable response traits for the stem elongation phase based on data from three seasons. Again, the authors used linear regressions of growth versus temperature as model. Kronenberg et al. (2020a) argued that the recorded average temperatures in the measuring intervals were well below the optimum temperature of 27.7 °C reported by Parent and Tardieu (2012), which would justify approximating a curvilinear with a linear function. However, the optimum temperature of 20.3 °C summarized by Porter and Gawith (1999) is distinctly lower. Following those results, it is likely that growth reached its optimum during several hours of the day during their measurement period. Therefore, the extracted temperature response (slope) may be greatly affected by the optimum temperature and maximum growth rate at this temperature. Thus, modelling plant response to temperature based on HTFP-derived data bears several challenges, e.g.,

the comparably sparse measuring frequency, the unpredictable range of temperatures, the changes of cardinal temperatures during the measuring period, and confounding effects between earliness and seasonal temperature development.

1.4. Research aims

HTFP data are characterized by irregular and long trait measurement intervals but regular and short covariate measurement intervals. Our main research question was how to parameterize genotype-specific temperature response pattern from such HTFP data. Using the stem elongation phase of winter wheat as an example, we aimed to evaluate a new modelling approach with regard to its suitability. Therefore, we simulated the temperature-response in the stem elongation phase using a Wang-Engel response function. The chosen parameters were based on existing literature on cardinal temperatures in winter wheat (Porter and Gawith, 1999; Parent and Tardieu, 2012) and enhanced with realistic temperature recordings of the stem elongation phase at the FIP site (Kronenberg et al., 2020a). To evaluate the strengths and limitations of our approach, we added changing cardinal temperatures, shifts in the start and end of the elongation phase, measurement noise, and spatial field inhomogeneities to our simulation.

2. Background

2.1. Parametric versus semi-parametric approaches

Semi-parametric approaches (e.g., using P-splines) are often favored to extract traits related to growth processes from HTFP time series (van Eeuwijk et al., 2019), as they avoid the daunting task of modeling explicitly the—potentially unknown—influence of time-dependent covariate courses. In a previous research, we have shown that semi-parametric approaches are suitable to extract timing of key stages and quantities at defined time points or periods from simulated HTFP data. Those data were generated using a dose-response curve that was unknown to the model being fitted, and corresponding covariate dependencies masked by a “smoothing” part in the model (Roth et al., 2021).

In contrast, to extract temperature responses, one cannot avoid modeling a dose-response curve explicitly, as one is interested in its parameters. Consequently, we hereafter propose a parametric approach. Although our focus is on HTFP data, the approach is also directly applicable to indoor platform data, but additionally considers HTFP specific characteristics.

In comparison to greenhouse or climate chamber data, HTFP data have two major drawbacks: (i) Field-based measurements are notoriously noisy due to environmental and soil inhomogeneities and measurement errors; (ii) the suitability of measured trait time series and covariate courses to answer a research question depends on the good luck of the scientist to catch a meaningful season. Research in agriculture has already addressed some of these limitations with the development of highly specialized experimental designs and matching statistical analysis. We could already show that following these principles is of advantage for HTFP as well (Roth et al.,

2021). For brevity, we therefore focus on the extraction of response traits from time series but refrain from further processing to adjusted genotype means. To allow determining and comparing the performance of non-linear and linear models, we use a simulation that is parametrized based on real field data.

2.2. Temperature response functions

The linear temperature response model used in Grieder et al. (2015) and Kronenberg et al. (2020a) is defined as

$$r_{\text{linear}}(T) = a \cdot (T - T_{\text{min}}), \tag{1}$$

where T is the temperature, a is the slope of the response, and T_{min} the base temperature. Note that such a model causes negative growth rates r for $T < T_{\text{min}}$ and does not include an optimum temperature T_{opt}. Therefore, it is likely that the extracted temperature response (slope) is affected by the optimum temperature and maximum growth rate at this temperature. Additionally, using such a Type 1 response will come to its limitation when data ranges span a whole growing season where temperatures also expand to supra-optimal ranges (Parent et al., 2019). In the crop model community, models describing the response to temperature vary widely, but most of them consider an optimum temperature beyond which the growth rate levels off (Bonhomme, 2000; Parent et al., 2010; Wang et al., 2017).

Arrhenius type functions were shown to adequately describe the dose-response relationship between temperature and growth across a wide range of temperatures and species (Parent et al., 2010; Parent and Tardieu, 2012). However, it was disputed whether this approach allows for a mechanistic interpretation of the different model parameters (Clavijo Michelangeli et al., 2016). Evidently, research in wheat mainly focused on determining cardinal temperatures such as the lower and upper base temperature of growth T_{min} and T_{max} and the optimum temperature T_{opt} where the growth rate r is maximal (Porter and Gawith, 1999). Wang et al. (2017) could show that using the Wang-Engel temperature function (Wang and Engel, 1998) allows to adequately replace an Arrhenius type functions to describe growth rates using these cardinal temperatures,

$$r_{\text{Wang-Engel}}(T) = r_{\text{max}} \cdot \left(\frac{(2(T - T_{\text{min}})^{\alpha}(T_{\text{opt}} - T_{\text{min}})^{\alpha} - (T - T_{\text{min}})^{2\alpha}}{(T_{\text{opt}} - T_{\text{min}})^{2\alpha}} \right)^{\beta} \tag{2}$$

$$\alpha = \frac{\ln(2)}{\ln\big((T_{\text{max}} - T_{\text{min}})/(T_{\text{opt}} - T_{\text{min}})\big)} \tag{3}$$

$$\beta = 1, \tag{4}$$

where T is the temperature, r_{max} the maximum growth rate at the temperature optimum T_{opt}, T_{min} the lower base temperature and T_{max} the upper base temperature of growth.

The Wang-Engel temperature function is a Type 4 response (Wang et al., 2017) in regards that it is based on three cardinal temperatures T_{min}, T_{max} and T_{opt}. If aiming to extract genotype-specific cardinal temperatures as well as the maximum growth rate r_{max} from HTFP data, this would require to fit a four-parametric non-linear

model with parameters that have interdependent constrains (e.g., $T_{\min} < T_{\text{opt}}$). In our experience, extracting meaningful parameters by fitting such a model to noisy HTFP data is practically impossible for different reasons, i.e., (i) the optimum temperature T_{opt} and maximum growth rate $r_{\max}$ are closely correlated, (ii) for field experiments performed in target environments (without stress treatments), the maximum temperature $T_{\max}$ is typically outside the range of observed data, and (iii) proximity of cardinal temperatures $T_{\min}$ and T_{opt} may prevent model conversions. Some authors have reacted to these restrictions by fixing one or multiple parameters and normalizing growth rates (Parent and Tardieu, 2012).

As a previously unconsidered alternative, we propose a Type 2 response that integrates an optimum temperature (Wang et al., 2017) to approximate the Arrhenius type functions of Parent and Tardieu (2012) based on an asymptotic model (Figure 1c),

$$r = r_{\max} \cdot (1 - \exp(-\exp(lrc) \cdot (T - T_{\min}))) \tag{5}$$

$$r_{\text{asym}}(T) = \begin{cases} r, & r > 0 \\ 0, & \text{otherwise} \end{cases}, \tag{6}$$

where T is the temperature, $r_{\max}$ is the maximum growth rate (and therefore the asymptote of the curve), $T_{\min}$ the base temperature where the growth rate is zero, and lrc characterizes the steepness of the response as the natural logarithm (l) of the rate (r) constant (c), thus lrc. The proposed asymptotic model does not consider a maximum temperature and therefore supra-optimal range, and has no inflection point (Paine et al., 2012). It requires to fit a three-parametric non-linear model.

2.3. Combining irregular and long trait measurement intervals with constant and short covariate measurement intervals

Independent of the specific dose-response model, one can describe a phenotype y at time point t (Figure 1a) as the result of such a dose-response model $r()$ (Figure 1c) dependent on a temperature course T_t (Figure 1b)

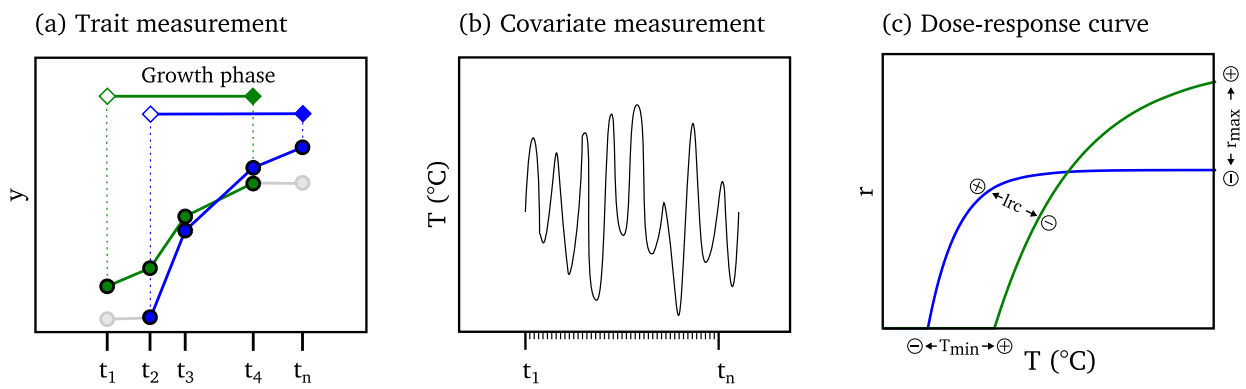

Figure 1: Schematic drawing of trait measurements with irregular and long intervals (a), covariate measurements with short and constant intervals (b), and the asymptotic dose-response model based on a maximum growth rate ($r_{\max}$), minimum temperature ($T_{\min}$), and steepness of the response (lrc) (c).

and a genotype-specific set of crop model parameters θ, e.g., $\theta = (T_{\text{min}}, T_{\text{opt}}, T_{\text{max}}, r_{\text{max}})$,

$$y_t = \int_{t_0}^{t} r(T_{t'}, \theta)\, dt', \tag{7}$$

where t_0 is the time point were growth started and therefore a timing of key stage trait that needs to be determined beforehand. Trait and covariates such as canopy height and temperatures are only measured at certain points in time, dependent on the measurement interval Δm. We therefore may discretize Equation 7 to

$$y_t = \sum_{t'=t_0}^{t} r(T_{t'}, \theta) \cdot \Delta m, \tag{8}$$

where t' are measurement time points with $(t' = t_0, t_0 + \Delta m, t_0 + 2\Delta m, \ldots, t)$, e.g., days.

Note that fitting Equation 8 to data implies the same measurement interval for traits y_t and temperatures $T_{t'}$. Although the goal of HTFP is to measure at small measurement intervals, unfavorable weather conditions may prevent regular measurements at all times, while registering covariates is weather-independent and done with constant high frequency. Outdoor phenotyping therefore produces trait measurements with irregular and long measurement intervals Δm_d (e.g., measurements every 3–4 days) but covariate measurements with constant and short measurement intervals Δm_h (e.g., hourly measurements). Therefore, before applying Equation 8 to data, an aggregation step is required.

A common technique is to align trait and covariate measurements by aggregating the covariate values to a mean (e.g., Kronenberg et al., 2017, 2020a),

$$y_t = \sum_{d=t_0}^{t} \left(r\left(\overline{T}_d, \theta\right) \cdot \Delta m_d \right), \tag{9}$$

where $\overline{T}_d$ is the mean of all covariate measurements made in the time period between successive trait measurement time points d where $(d = t_0, t_0 + \Delta m_1, t_0 + \Delta m_1 + \Delta m_2, \ldots, t)$. In this study, we propose an alternative approach: One may also apply the dose-response function r to each covariate value T_{dh} where h indexes covariate values between successive trait measurement time points d, $(h = 1, \ldots, n_d)$, and sum up the responses to the trait measurements,

$$y_t = \sum_{d=t_0}^{t} \left(\sum_{h=1}^{n_d} r\left(T_{dh}, \theta\right) \cdot \Delta m_h \right). \tag{10}$$

In the following, the first method is denoted the T_{mean} method and the second method the T_{course} method.

3. Materials and Methods

3.1. Simulation of canopy height data

The canopy growth of wheat genotypes was simulated using a growth function g_T that was based on the Wang-Engel dose-response model of Equation 4 parameterized with four genotype-specific dose-response crop

model parameters $\theta^C = (T_{\min}, T_{\text{opt}}, T_{\max}, r_{\max})$. This model was extended with time points for the start and end of growth, parameterized with two genotype-specific timing traits $\theta^T = (t\text{PH}_{\text{start}}, t\text{PH}_{\text{stop}})$. An environment inhomogeneity factor u and a measurement error e were added, leading to the model

$$y_{it} = g_T(t, \theta_i^C, \theta_i^T; T_{dh}) + u_{it} + e_t\,, \tag{11}$$

where y_{it} is the measured canopy height (phenotype) for the ith genotype at campaign time points t in intervals of three days ($t = 1, 4, 7, \ldots, T$), θ_i^C and θ_i^T are genotype-specific crop growth model parameters respectively timing traits, T_{dh} are hourly (h) temperature readings nested in measurement days (d), u_{it} a time point and genotype-specific inhomogeneity error (i.e., simulating the influence of other covariates than temperature) and e_t a time point specific measurement error (i.e., simulating random measurement errors). The growth function g_T was specified as an implementation of Equation 10 based on the Wang-Engel function of Equation 4,

$$g_T(t, \theta^C, \theta^T; T_{dh}) = \sum_{d=1}^{t} \begin{cases} \sum_{h=1}^{72} r_{\text{Wang-Engel}}(T_{dh}, \theta^C) & t\text{PH}_{\text{start}} < d < t\text{PH}_{\text{stop}} \\ 0, & \text{otherwise}\,. \end{cases} \tag{12}$$

The genotype-specific traits θ_i^C and θ_i^T and the errors u_{it} and e_{it} were simulated using normal distributions ($\sim \mathcal{N}(\mu, \sigma^2)$) for genotype traits respectively first order auto-correlations ($\sim \text{AR}_1(\sigma, \rho)$) for the errors. Specific μ and σ^2 were chosen based on literature if available, and otherwise based on own field data (Roth, 2021). Corresponding sources and chosen distributions for all simulation input parameter are summarized in Table 1. Two alternative simulations were performed: One with changing cardinal temperatures with time (indicated with '→' in Table 1), and one with fixed cardinal temperatures (set to the mean of changing cardinal temperatures indicated in Table 1).

Canopy growth was simulated for a measurement interval of three days for a period between the 15th of March and 20th of July based on temperature courses of three years (Figure 2). A total of 1,000 differing genotypes were assumed, resulting in 3,000 genotype time series. As temperature data source, real weather data of three consecutive years at the ETH research station of agricultural sciences in Lindau Eschikon, Switzerland (47.449 N, 8.682 E, 556 m a.s.l.) were used.

3.2. Extracting dose-response curves

To extract the Wang-Engel dose-response curve parameters $T_{\min}$, T_{opt} and $r_{\max}$, the linear and asymptotic growth response models (Equation 1 and 6) were fitted to canopy height data between $t\text{PH}_{\text{start}}$ and $t\text{PH}_{\text{stop}}$ for two covariate options, T_{mean} based on averaged temperatures between measurements (Equation 9), and T_{course} based on temperature courses with a period of one hour (Equation 10).

Maximum-likelihood optimization was used to fit Equation 9 to a set of t data points, $X_t = (\bar{T}_t, y_t - y_{(t-1)})$. Fitting Equation 10 to data required modifying the definition of the data set so that $X_t = (\vec{T}_t, y_t - y_{(t-1)})$, where $\vec{T}_t$ is a vector of covariate readings between trait measurement time points $t-1$ and t.

Table 1: Model input parameters for the simulation.

		Values	Source
θ_i^T	$\mathcal{N}(\mu, \sigma^2)$	$\mu_{T_{\min}} = 1.5 \rightarrow 9.5$ °C	Porter and Gawith (1999) (Terminal spikelet→Anthesis)
		$\sigma_{T_{\min}} = 2$ °C	Assumption
		$\mu_{T_{\text{opt}}} = 10.6 \rightarrow 21$ °C	Porter and Gawith (1999) (Terminal spikelet→Anthesis)
		$\sigma_{T_{\text{opt}}} = 2$ °C	Assumption
		$\mu_{T_{\max}} = 30 \rightarrow 35$ °C °C	Porter and Gawith (1999) (Anthesis −1/+4 °C)
		$\sigma_{T_{\max}} = 2$ °C	Assumption
		$\mu_{r_{\max}} = 1.05$ mm h^{-1}, $\sigma_{r_{\max}} = 0.12$ mm h^{-1}	Roth (2021)
θ_i^{PH}	$\mathcal{N}(\mu, \sigma^2)$	2016: $\mu_{t\text{PH}_{\text{start}}} = 108$ d, $\sigma_{t\text{PH}_{\text{start}}} = 2.8$ d	Kronenberg et al. (2020a)
		2017: $\mu_{t\text{PH}_{\text{start}}} = 103$ d, $\sigma_{t\text{PH}_{\text{start}}} = 3.0$ d	Kronenberg et al. (2020a)
		2018: $\mu_{t\text{PH}_{\text{start}}} = 101$ d, $\sigma_{t\text{PH}_{\text{start}}} = 3.1$ d	Roth (2021)
		2016: $\mu_{t\text{PH}_{\text{stop}}} = 165$ d, $\sigma_{t\text{PH}_{\text{stop}}} = 2.5$ d	Kronenberg et al. (2020a)
		2017: $\mu_{t\text{PH}_{\text{stop}}} = 162$ d, $\sigma_{t\text{PH}_{\text{stop}}} = 3.5$ d	Kronenberg et al. (2020a)
		2018: $\mu_{t\text{PH}_{\text{stop}}} = 158$ d, $\sigma_{t\text{PH}_{\text{stop}}} = 4.0$ d	Roth (2021)
u_{it}	AR(1)	$\rho = 0.9$, $\sigma = 0.003$ m d^{-1}	Assumption
e_t	AR(1)	$\rho = 0.3$, $\sigma_m = 0.01$ m	Roth et al. (2020)

→ connects lower and upper limit of cardinal temperature ramps

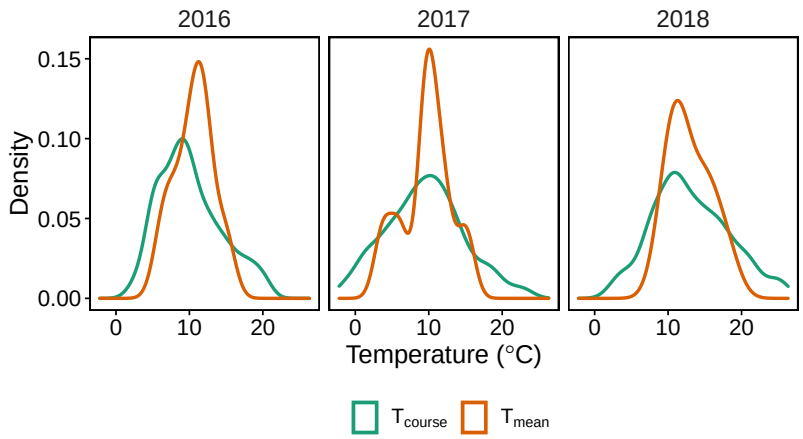

Figure 2: Measured temperatures in the stem elongation phase of winter wheat at the FIP site on an hourly scale (T_{course}) and aggregated to a 3-day scale (T_{mean}).

As an independent random measurement errors was assumed, the maximum-likelihood optimization parameter σ was fixed to the well-known measurement error of the device, herein the simulation input σ_m (Table 1). Parameters were optimized in R using the method L-BFGS-B of the function *optim*.

To allow examining the effect of noise caused by inhomogeneities and measurement errors, the extraction was once performed on raw simulated data, once on data contaminated with the measurement error e, and once with both measurement and inhomogeneities errors e and u. Bias, variance, root-mean squared error (RMSE) and Pearson's correlation were calculated after extracting the parameters T_{min}, lrc and r_{max} for the asymptotic model and a (slope) and T_{min} for the linear model.

4. Results

Aggregating measured temperatures at the FIP site to hourly means (T_{course}) and 3-day means (T_{mean}) reveled sever differences in their distribution (Figure 2): Temperatures close to the cardinal temperatures T_{min} and T_{opt} were frequent for T_{course}, but almost absent for T_{mean}. Simulating the stem elongation by combining the T_{course} measurements with a Wang-Engel dose-response function resulted in an average final height slightly higher than observed for elite varieties under field conditions (Kronenberg et al., 2020b), but realistic individual plant height time series with characteristic starts, stops, and lag phases (Figure 3). Fitting the asymptotic model based on T_{course} to the simulated data converged for 96% of all genotypes. All other models converged for all genotypes. In a preliminary run, we also tried to fit the Wang-Engel model to simulated data, but failed to extract meaningful parameters. This was partly due to the complexity of defining valid non-overlapping ranges for the cardinal temperatures, but mainly because the model did not converge in most cases.

Based on the RMSE, the maximum growth rate r_{max} and base temperature T_{min} were best estimated with the asymptotic dose-response model (Equation 5 and 6) based on T_{course} covariates (Table 2). While the variance was drastically lower for both parameters if using T_{course}, the bias slightly increased for r_{max} but decreased for T_{min}. The RMSE, bias and variance of the linear model for the parameter T_{min} was much higher than for the asymptotic model.

Introducing a systematic measurement error e did not affect the slope estimated by the linear model; extracted values correlated 1:1 for the simulation with and without noise (Table 3). In contrast, the Pearson's r for T_{min} was close to zero, but a Spearman's rank correlation revealed nevertheless a high robustness of the extracted ranking to noise. The asymptotic model was more susceptible to noise than the linear model (Table 3). Using temperature courses instead of mean temperatures was of benefit for the parameters r_{max} and T_{min}, but of disadvantage for lrc.

Correlating simulated versus predicted parameter values revealed further differences between the methods (Figure 4): While the asymptotic model based on T_{course} was able to extract r_{max} and T_{min} with very strong correlations to the input values, the same model based on T_{mean} yielded only moderate correlations for r_{max} and T_{min}.

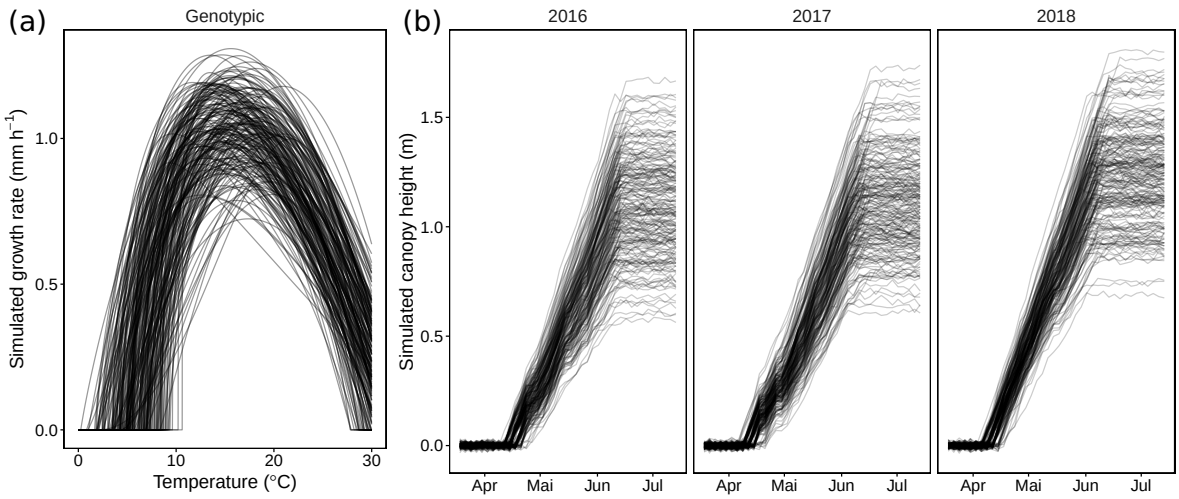

Figure 3: Simulated growth rates (a) and canopy heights (b) for 100 out of 1000 simulated genotypes and three years. Simulated growth rates are based on a Wang-Engel dose-response curve model.

Table 2: Bias, variance and root-mean squared error for the linear and asymptotic model based on mean temperature and temperature courses for simulated data without noise.

Parameter	Model	Bias	Var	RMSE
r_{max}	Asymptotic T_{mean}	0.0805	0.0347	0.103
	Asymptotic T_{course}	0.0949	0.00309	0.0959
T_{min}	Linear T_{mean}	9.21	1.96e+08	10.6
	Asymptotic T_{mean}	0.764	2.24	1.04
	Asymptotic T_{course}	-0.352	0.575	0.439
a (slope)	Linear T_{mean}	0.0657	0.00272	0.0657

Table 3: Pearson's and Spearman's correlation between parameters extracted on simulated data with systematic measurement error noise and without noise.

Model	Parameter	Pearson's r	Spearman's r
Linear T_{mean}	a (slope)	1.00	1.00
	T_{min}	0.00	0.88
Asymptotic T_{mean}	r_{max}	0.61	0.79
Asymptotic T_{course}	r_{max}	0.85	0.92
Asymptotic T_{mean}	T_{min}	0.60	0.66
Asymptotic T_{course}	T_{min}	0.77	0.72
Asymptotic T_{mean}	*lrc*	0.69	0.73
Asymptotic T_{course}	*lrc*	0.46	0.70

Table 4: Bias, variance, root-mean squared error and Pearson's correlation of the asymptotic model based on temperature courses with simulated noise due to measurement errors and field and environment inhomogeneities.

Parameter	Noise	Bias	Var	RMSE	Correlation
r_{max}	-	0.0949	0.00309	0.0959	0.89
	e	0.0971	0.119	0.114	0.3
	$e+u$	0.0964	0.116	0.113	0.3
T_{min}	-	-0.352	0.575	0.439	0.92
	e	-0.108	5.55	1.27	0.48
	$e+u$	-0.112	5.67	1.28	0.47

e: systematic measurement error noise
u: field and environment inhomogeneities

The parameter r_{max} extracted by the asymptotic model based on T_{mean} was not only correlated with the simulated r_{max}, but also moderately related to T_{opt}. Using T_{course} reduced this moderate bias for the parameter estimates of r_{max} but introduced a new weak bias for the parameter estimates of T_{min} towards T_{opt}. The asymptotic model additionally allowed estimating T_{opt} using *lrc* as proxy with a high correlation to input values.

For the linear model, both parameter estimates of slope and T_{min} were uncorrelated with the corresponding simulated input parameter (Figure 4b). Instead, the slope was related to r_{max}, T_{min} and T_{opt}, while T_{min} based on the estimated intercept was not correlated to any input parameter. Both the linear and asymptotic model were not affected by supra-optimal temperatures: the input parameter T_{max} that defined growth in the supra-optimal range above T_{opt} was uncorrelated with any extracted parameter.

Adding noise to the simulated growth time series led to increased variances for the parameter estimates of r_{max} and T_{min} based on the asymptotic model (Table 4). While the RMSE drastically increased by a factor of three for T_{min} and the correlation to input values dropped below 0.5, it remained low for r_{max} while the correlation with input parameter dropped to 0.3. The bias for r_{max} remained unchanged, while the bias for T_{min} decreased. Adding additional noise caused by highly auto-correlated spatial inhomogeneities did not further decrease the RMSE or increase the variance and bias.

Simulating changing cardinal temperatures for all genotypes alike decreased correlations of extracted parameters for all models (Figure 4c). The differences between T_{mean} and T_{course} for the asymptotic model disappeared: While both models were able to extract r_{max} with moderate correlations, they failed to extract T_{min}. The curvature parameter *lrc* was now moderately correlated with T_{min} and T_{opt} for T_{mean} and weakly correlated with T_{min} and T_{opt} for T_{course}. The slope extracted by the linear model was moderately related to T_{min} and weakly to r_{max} and T_{opt}. Again, T_{max} was uncorrelated with any extracted parameter.

5. Discussion

Although the growth of simulated canopies was based on a Wang-Engel temperature dose-response curve, using a corresponding model to extract parameters turned out to be not suitable, mainly because of failed con-

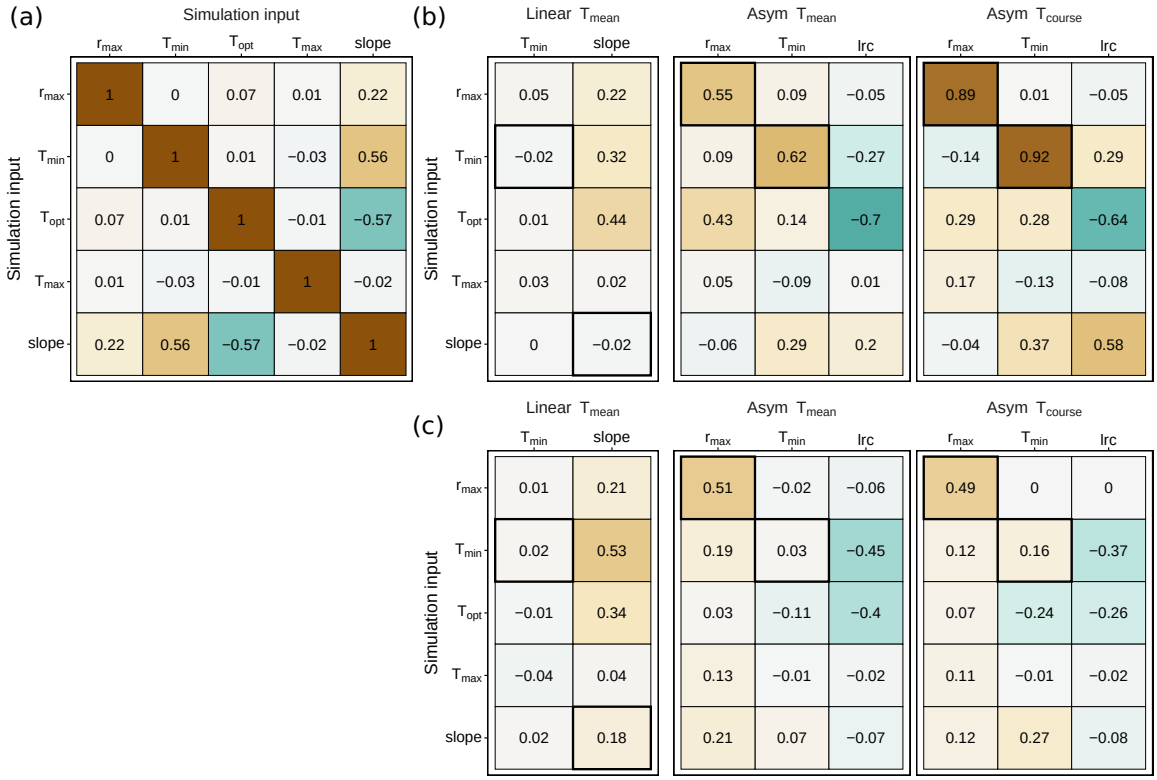

Figure 4: Pearson's correlations of simulated data versus extracted temperature response parameters. Provided are results for the simulation without noise (a) versus extracted temperature response parameters with fixed cardinal temperatures (b) and changing cardinal temperatures with time (c) for the linear model based on mean temperature (Linear T_{mean}) and the asymptotic growth model based on mean temperature (Asym T_{mean}) and temperature courses (Asym T_{course}). Note that the slope is derived from the relation slope $= r_{\text{max}}/T_{\text{opt}}-T_{\text{min}}$ and therefore not an independent input parameter of the simulation. Black bold boxes indicate correlations between predicted and true values for identical parameters.

vergence. Presumably, non-existing measurements at supra optimal temperatures ($\gtrsim$ 30 °C, Figure 2) prevented estimating the required parameter T_{max}. As suspected, the asymptotic model performed better with percentages of converged time series close to 100%. Using temperature courses instead of aggregated mean values allowed estimating independent parameters with higher correlations to input parameters, to the cost of a slightly decreased convergence rate. Especially the parameter T_{min} profited from taking temperature courses into account (Table 2), which indicates that in the early phase where stem elongation starts the distribution of temperatures and therefore temperature courses are essential to describe temperature responses ($\lesssim$ 5 °C, Figure 2). Additionally to T_{min}, the asymptotic model will extract the maximum growth rate r_{max} and the parameter *lrc* which is related to the optimum temperature T_{opt}, and therefore allow to fully describe temperature responses between the lower base temperature T_{min} and optimum temperature T_{opt}. A limitation of the proposed asymptotic approach may be the high optimum temperatures: Although the extracted base temperature T_{min} and maximum growth rate r_{max} were strongly correlated with input parameters, they were also slightly biased by the optimum temperature T_{opt}.

Noise and environment inhomogeneities reduced the correlation to input parameters drastically, independent on whether RMSE stayed stable or not (Table 4). It seems reasonable to assume that this reduction in correlation will lead to reduced heritabilities of measured traits in HTFP. The simulation was not including a randomized field experiment set-up, but only independent genotype time series. Nevertheless, we assume based on our previous study on two other intermediate traits (Roth et al., 2021) that also for dose-response curve traits it is essential to follow the three principles of experimental design, i.e., replication, randomization and blocking (Kempton, 1984). Such an experimental design will allow to process the extracted plot-based parameters using, e.g., linear mixed models to compensate for measurement errors and environment inhomogeneities and therefore ensure the overall heritability.

Simulating changing cardinal temperatures drastically reduced the ability of the asymptotic model to extract meaningful cardinal temperatures (Figure 4c). We suspect that this effect was overamplified by the simulation and that supposed cardinal temperature ramps in Porter and Gawith (1999) may be too extreme for wheat elite cultivar sets. Nevertheless, in the worst case that cardinal temperature ramp assumptions were justified, the asymptotic model would yield less heritable parameters than in the optimum case of fixed cardinal temperatures, but not introduce additional biases.

In contrast, one may conclude that using a 'simple' linear model to avoid the complexity of curvy dose-response models is not advisable. The results of this study demonstrated that the extracted linear response to temperature (slope) was similarly related to both cardinal temperatures T_{min} and T_{opt} but also to the maximum growth rate r_{max}, while unrelated to the simulated slope (Figure 4b). Thus, the apparent temperature response is mainly driven by cardinal temperatures. When fitting a linear model to a wide temperature range, with significant number of hours in temperature ranges beyond the optimum (Figure 2), it will inevitably compensate for both the maximum growth rate at the optimum and the base temperature of growth. Using a linear model if cardinal temperatures are not fixed is even more harmful: The relation of the slope may switch from T_{opt} towards

$T_{\min}$ (Figure 4c). Depending on the examined genetic material, applying a linear model may therefore lead to completely different conclusions. Eventually, one has to review existing literature that refers to slopes as temperature responses (e.g., Kronenberg et al., 2020a) being at least partly affected by growth at optimum temperature, maximum growth rate, and changing cardinal temperatures.

Using modeling we aimed to simulate different aspects of temperature-response during the important phase of stem elongation of wheat. A major advantage of this approach is that it can be used to test different approaches to parameterize temperature-response. This approach is particularly valuable as other factors such as, e.g., the effect of drying soil, extremely low vapor pressure deficit, or low radiation, do not have to be included. For real field data, such influences will have to be considered to improve the model.

6. Conclusion

Adequate models to quantify the different aspects of growth response to temperature may greatly improve our understanding of crop adaptation to certain climatic scenarios. Asymptotic models represent a valid choice if sampling winter wheat genotypes in an environment where the decrease in growth after reaching an optimum temperature is negligible. Using temperature courses with high temporal resolution as covariate input for the model fit instead of aggregated mean temperatures is advisable. Changing cardinal temperatures—related to advancing phenology—may reduce the ability to extract parameters with an asymptotic model but will not severely bias results. Nevertheless, measurement noise and environment and field inhomogeneities may significantly increase the variance of extracted parameters. Care should be taken if interpreting existing literature based on linear temperature growth response models, as extracted response reactions may be strongly biased by base and optimum temperature, maximum growth rate at optimum temperature, and changing cardinal temperatures with time. As supra optimal temperatures before flowering are hardly ever reached in a temperate climate, we conclude that models including maximal temperatures will neither deliver any benefit under these conditions.

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Declaration of Competing Interest

The authors declare no conflict of interest.

CRediT authorship contribution statement

Lukas Roth: Conceptualization, Methodology, Software, Formal analysis, Visualization, Writing - Original Draft. **Hans-Peter Piepho**: Conceptualization, Methodology, Writing - Review & Editing. **Andreas Hund**: Conceptualization, Supervision, Project administration, Funding acquisition, Writing - Review & Editing.

Data availability

Data and source code that support the findings of this study are openly available in the ETH gitlab repository at https://gitlab.ethz.ch/crop_phenotyping/htfp_data_processing and archived in the ETH research collection (http://doi.org/10.5905/ethz-1007-385).

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