**CONFIDENCE INTERVAL ESTIMATION FOR AN EMPIRICAL
MODEL QUANTIFYING THE EFFECT OF SOIL MOISTURE
AND PLANT DEVELOPMENT ON SOYBEAN (GLYCINE MAX
(L.) MERR.) LEAF CONDUCTANCE**

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Abstract: In this work, we address uncertainty analysis for a model, presented in a separate paper, quantifying the effect of soil moisture and plant age on soybean (*Glycine max* (L.) Merr.) leaf conductance. To achieve this we present several methods for confidence interval estimation. Estimation of confidence intervals for model parameters and predictions is investigated using asymptotic theory, Monte Carlo methods, and bootstrap methods. A computationally feasible solution for estimating confidence intervals for model parameters via asymptotic theory is unattainable. Confidence intervals for model

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predictions under water-stressed environmental conditions when using asymptotic theory and Monte Carlo methods are artificially large due to underlying false assumptions of normality. For this model, where the residuals exhibit heteroscedasticity, the confidence intervals estimated by the wild bootstrap method appear the most realistic of the methods investigated. Of the three methods presented for estimating 95% confidence intervals for model predictions, it is our opinion that the bootstrap method is the most reliable.

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1. Introduction

Increasingly, scientists and modelers are recognizing the importance of confidence intervals associated with model predictions. Often the quantitative methods utilized for model calibration yield only point estimates for model parameters. Given that the data upon which calibration is based typically includes some degree of error and variability, an associated confidence interval for the model parameter estimate is necessary to understand the reliability of the parameter estimate. Further, since uncertainty in parameter values propagate to uncertainties in model prediction, confidence intervals associated with the predictions are also critical.

However, many methods exist to estimate these confidence intervals and there is a lack of consensus on which method is appropriate for general application. We evaluate herein several methods for the estimation of confidence intervals applied to the model characterizing total leaf conductance (g_ℓ) presented in a recent paper, [16]. In that paper two distinct soybean (*Glycine max* (L.) Merr.) genotypes (Haskell and N01-11771) were studied to characterize the effect of water stress on total leaf conductance under four different watering scenarios. In general, Experiment A subjected the soil to single or multiple drying cycles by withholding water to reach approximately 10% of soil water capacity. Experiment B was also subjected to one or more drying cycles. Both Experiments A and B were stressed during different developmental periods in order to explore the influence of stress during those periods on the final yield. At the desired developmental stage, water was withheld until soil water content measurements reached the desired level and then held at or near those levels as long as desired before returning them to field capacity, either briefly or for the duration of the season. Soil moisture deficits in Experiments A and B could be

Table 1: Parameter estimates for each case and the associated SSE values.

	2008		2009	
Parameter	Haskell	N01-11771	Haskell	N01-11771
α_0	-1.5696×10^0	-1.4458×10^0	-3.1455×10^{-1}	-1.5080×10^{-1}
α_1	8.8589×10^{-2}	8.2528×10^{-2}	4.0108×10^{-2}	3.4635×10^{-2}
α_2	-9.4632×10^{-4}	-8.6359×10^{-4}	-3.5844×10^{-4}	-3.0155×10^{-4}
α_3	2.9296×10^{-6}	2.6251×10^{-6}	7.6305×10^{-7}	5.8973×10^{-7}
β_1	1.1386×10^3	8.8798×10^2	1.2073×10^3	8.5345×10^2
β_2	-1.9524×10^0	-1.3563×10^0	-2.0879×10^0	-6.8660×10^0
β_3	-2.9004×10^1	-7.4450×10^1	-1.1315×10^1	-1.6028×10^1
SSE	1.9310×10^7	1.4852×10^7	8.9006×10^6	9.2991×10^6
No. data pts	592	592	486	487
Normalized SSE	3.2619×10^4	2.5087×10^4	1.8314×10^4	1.9095×10^4

crudely maintained by adding smaller quantities of water less frequently than Experiments C and D, which were both well-watered throughout the growing season. Experiment C was irrigated with 76 mm of water per week in the 2008 growing season and 38 mm in the 2009 growing season. The different amounts of irrigation required to maintain soil moisture near field capacity varied based on evaporative demand related to differing weather conditions. The fourth experiment, D, unlike the other three did not have polyethylene sheeting covering the surface of the soil, so it received precipitation exposure as well as irrigation water sufficient for a total of 76 mm per week during 2008 and 38 mm in 2009. The purpose of this experiment was to determine the effect, if any, of the polyethylene sheeting. By comparing the data from Experiments C and D, it was concluded that the polyethylene sheeting did not have a statistically significant effect on conductance measurements. For all treatments, well-watered conditions were applied to keep soil moisture near field capacity early in the growing season to facilitate plant establishment.

Data included soil moisture content and measurements of total leaf conductance during the 2008 and 2009 growing seasons in a controlled water stress field located at the USDA-ARS Plant Science Research Unit field site in Raleigh, NC, USA. These data were utilized to construct a model quantifying the response of total leaf conductance to soil moisture and plant age. Estimates for the seven unknown parameters of that model are presented in Table 1. However, these values are only point estimates and it is important to understand the accuracy and reliability of these parameter values. Confidence intervals for the parameter estimates provide an indication of this reliability.

We begin by applying traditional asymptotic theory to establish confidence intervals for the estimated parameters. However, as shown in the Results section, this method does not provide a computationally feasible solution. We then describe bootstrap methods in general and choose in particular the wild bootstrap, which is applicable to our case where the residuals exhibit heteroscedasticity.

Figs 5, 6, 9, and 10 of Matthews et al. (2013) [16] illustrate the model predictions of conductance as a function of plant age. The individual conductance data points exhibit significant scatter, as is typical for many biological data sets. Therefore, it is useful for a model to not only provide point estimates, but also the associated confidence intervals for the model predictions.

Three different methodologies are explored to determine confidence intervals for the model predictions. We begin by applying traditional asymptotic theory to establish confidence intervals for the model predictions. Then confidence intervals are estimated using Monte Carlo simulations. Finally, the wild bootstrap method is used to ascertain confidence intervals for model predictions.

2. Materials and Methods

2.1. Model Formulation

As described by Matthews et al. (2013), we suggest that total leaf conductance (g_ℓ) can be modeled by a relation of the form

$$g_\ell(t, w_2; \theta) = f(t; \theta) \cdot h(w_2; \theta) \quad (2.1)$$

where $f(t; \theta)$ is a scaling function valued between 0 and 1 that depends on plant age (t) and $h(w_2; \theta)$ is a function describing conductance with units of $\text{mmol m}^{-2} \text{s}^{-1}$ based on soil water content (w_2).

To model the total leaf conductance data using (2.1), we employed a polynomial

$$f(t; \theta) = \alpha_0 + \alpha_1 t + \alpha_2 t^2 + \alpha_3 t^3 \quad (2.2)$$

to define the plant age dependency. Here t is the days after planting (DAP) and α_k for $k = 0, \dots, 3$ are coefficients estimated through a least squares fit to data.

The conductance-dependence on soil moisture is defined as a Gompertz-like function

$$h(w_2; \theta) = \beta_1 e^{\beta_2 e^{\beta_3 w_2}} \quad (2.3)$$

where β_1 is the maximum allowable conductance, β_2 sets the displacement of the sigmoidal curve along the w_2 axis, and β_3 represents the extent of dependence of conductance on w_2 [17]. The complete set of parameters for this model is given by

$\theta = [\alpha_0, \alpha_1, \alpha_2, \alpha_3, \beta_1, \beta_2, \beta_3]$ and is estimated as detailed in Matthews et al. (2013) using the cost functional

$$\begin{aligned} SSE &= \sum_{k_1=1}^{n_1} \sum_{k_2=1}^{n_2} [y_{k_1, k_2} - g_\ell(t_{k_1}, w_{2, k_2}; \theta)]^2 \\ &= \sum_{k=1}^n [y_k - g_\ell(e_k; \theta)]^2 \end{aligned} \quad (2.4)$$

where SSE represents the sum of squared error, y_k for $k = 1, \dots, n$ are the measured leaf conductances and $g_\ell(t_{k_1}, w_{2, k_2}; \theta) = g_\ell(e_k; \theta)$ are modeled values given by (2.1). Here e_k denotes the unique input associated with the measurement (t_{k_1}, w_{2, k_2}) .

2.2. Confidence Intervals for Parameter Estimates

Table 1 presents estimated parameters for the model described in (2.1)-(2.3). These values are only point estimates and it is important to understand the accuracy and reliability of these parameter values. Now we describe two different methods for establishing confidence intervals for the estimated parameters: asymptotic theory and the bootstrap method.

2.2.1. Asymptotic Theory

We let n denote the number of data points, p the number of estimated parameters, and $\hat{\theta}$ the estimated parameter vector. Then, define the $n \times p$ sensitivity matrix $\chi(\hat{\theta})$ to have components

$$\chi_{i,j}(\hat{\theta}) = \left. \frac{\partial g_\ell(e_i; \theta)}{\partial \theta_j} \right|_{\theta=\hat{\theta}} \quad (2.5)$$

for $i = 1, \dots, n$ and $j = 1, \dots, p$. The variance-covariance matrix V may then be estimated as

$$V = s^2 \left(\chi^T(\hat{\theta}) \chi(\hat{\theta}) \right)^{-1} \quad (2.6)$$

where the variance estimate is $s^2 = \frac{SSE}{n-p}$, with SSE defined in (2.4).

Often, a $1 - \alpha$ joint inference region for estimated parameters within a nonlinear model can be adequately approximated via the inequality

$$(\theta - \hat{\theta})^T V^{-1} (\theta - \hat{\theta}) \leq pF(p, n-p; \alpha) \quad (2.7)$$

where F represents the F distribution [18, 3]. The associated $1 - \alpha$ confidence interval for an individual estimated parameter $\hat{\theta}_j$ is

$$\hat{\theta}_j \pm \sqrt{V_{jj}} t(n-p; \alpha/2) \quad (2.8)$$

where t represents the Student's T distribution.

2.2.2. Bootstrap Method

As an alternative to the asymptotic theory to derive confidence intervals for the estimated parameters, we turn to a form of bootstrapping. This nonparametric approach to statistical inference substitutes intensive computation for more traditional asymptotic results and can be used to derive confidence intervals [10]. In particular, we apply the bootstrap to the residuals of our model. This method treats the model dependent variables (i.e., soil moisture, plant age) as fixed rather than random because they may be a product of experimental design.

Assume that the experimental data $(y_1, e_1), \dots, (y_n, e_n)$ are from an underlying observation process

$$Y_k = g_\ell(e_k; \theta_0) + \epsilon_k \quad (2.9)$$

for $k = 1, \dots, n$ where the errors ϵ_k are assumed to be independent and identically distributed (iid) from a distribution F with mean 0 and constant variance, and θ_0 is the “true” parameter value.

First, the ordinary least squares estimate $\hat{\theta}$ is obtained by minimizing (2.4). Then, the residuals

$$u_k = y_k - g_\ell(e_k; \hat{\theta}) \quad (2.10)$$

for $k = 1, \dots, n$ are computed. Bootstrapped data values $\bar{y}_k^m$ are formed by

$$\bar{y}_k^m = g_\ell(e_k; \hat{\theta}) + \bar{u}_k^m \quad (2.11)$$

where $\bar{u}_k^m$ is an element randomly selected with replacement from the residual vector u and $m = 1, \dots, M$ where M is a sufficiently large number. Thus, each bootstrap error term $\bar{u}_k^m$ can take on n possible values; that is, the values in u , each with probability $1/n$. Finally, the ordinary least squares estimate $\hat{\theta}^m$ is determined by

$$\hat{\theta}^m = \underset{\theta}{\operatorname{argmin}} \sum_{k=1}^n [\bar{y}_k^m - g_\ell(e_k; \theta)]^2. \quad (2.12)$$

In the results presented here, we chose $M = 1000$. This technique of bootstrapping the residuals and re-estimating the parameter vector θ M times is referred to as residual bootstrapping [9, 13, 10].

However, the residual bootstrap as described is not valid if the error terms ϵ_k are not iid because if the heteroscedasticity is of an unknown form, it cannot be emulated with the bootstrap distribution [13, 7]. Note that if the residuals are iid, a plot of residual values versus the associated model predictions will appear random [8, 4, 2].

Consider next the case where the experimental data $(y_1, e_1), \dots, (y_n, e_n)$ are from an underlying observation process

$$Y_k = g_\ell(e_k; \theta_0) (1 + \epsilon_k) \quad (2.13)$$

for $k = 1, \dots, n$ where the ϵ_k are iid from a distribution F with mean 0 and non-constant variance, and θ_0 is the “true” parameter value.

Several sophisticated variants of bootstrapping exist to address this case of heteroscedastic residuals. Among the many options are the generalized least squares (GLS) method and the wild bootstrap. GLS is well documented as a good theoretical alternative approach to parameter estimation in the presence of non-constant variance [11, 4, 6, 1]. Briefly, in GLS, one searches for θ which minimizes

$$SSE = \sum_{k=1}^n \hat{w}_k [y_k - g_\ell(e_k; \theta)]^2 \quad (2.14)$$

where $\hat{w}_k$ are weights designed to give greater weight to observations with smaller variance. Unfortunately, in practice, the GLS method often does not achieve the theoretical advantages. Because the weights $\hat{w}_k$ are unknown and

must be estimated, there is a possibility that the GLS regression may in fact “miss” the data entirely [18].

Hence, the method chosen to address heteroscedastic residuals is the wild bootstrap method. This method was originally proposed by Wu and rigorously expanded by Liu as a general method for resampling residuals in the presence of error variance heteroscedasticity [19, 12]. The method is referred to as wild because n different distributions are estimated from only n observations. The procedure is identical to that described above for the residual bootstrap with the exception that (2.11) is replaced by

$$\bar{y}_k^m = g_\ell(e_k; \hat{\theta}) + h(u_k)v_k \quad (2.15)$$

where $h(u_k)$ is a transformation of the k th residual and v_k is a random variable from a distribution satisfying $E(v_k) = 0$, $E(v_k^2) = 1$, and $E(v_k^3) = 1$.

2.3. Confidence Intervals for Model Predictions

Figs 5, 6, 9, and 10 of Matthews et al. (2013) illustrate the model predictions as compared to data as a function of plant age. The individual conductance data points exhibit significant scatter, as is typical for many biological data sets. Therefore, it is useful for a model to not only provide point estimates, but also the associated confidence intervals for the model predictions. Here we describe three distinct methods to determine confidence intervals for model predictions: asymptotic theory, Monte Carlo method, and the bootstrap method.

2.3.1. Asymptotic Theory

Consider the gradient vector

$$\nabla g_\ell(t, w_2; \theta) = \begin{bmatrix} \frac{\partial g_\ell(t, w_2, \theta)}{\partial \alpha_0} \\ \frac{\partial g_\ell(t, w_2, \theta)}{\partial \alpha_1} \\ \frac{\partial g_\ell(t, w_2, \theta)}{\partial \alpha_2} \\ \frac{\partial g_\ell(t, w_2, \theta)}{\partial \alpha_3} \\ \frac{\partial g_\ell(t, w_2, \theta)}{\partial \beta_1} \\ \frac{\partial g_\ell(t, w_2, \theta)}{\partial \beta_2} \\ \frac{\partial g_\ell(t, w_2, \theta)}{\partial \beta_3} \end{bmatrix} \quad (2.16)$$

where the elemental definitions are explicitly given in (3.1) through (3.7). The $1 - \alpha$ confidence interval for the conductance prediction can then be defined as

$$g_\ell(t, w_2, \theta) \pm t(n - p; \alpha/2) \sqrt{\nabla^T g_\ell(t, w_2; \hat{\theta}) \text{cov}(\hat{\theta}) \nabla g_\ell(t, w_2; \hat{\theta})} \quad (2.17)$$

which is commonly known as the delta method [18, 10]. The matrix $\text{cov}(\hat{\theta})$ is calculated as indicated in (3.10).

2.3.2. Monte Carlo Method

A different method to estimate confidence intervals for model predictions involves Monte Carlo simulations. This method utilizes the estimated parameter vectors summarized in Table 1. Under the assumption that these estimated parameters originate from a normal distribution where the mean is the estimated parameter vector $\hat{\theta}$ and the covariance amongst parameters is quantified by the estimated covariance matrix $\text{cov}(\hat{\theta})$, 1000 parameter vectors $\hat{\theta}_m$ for $m = 1, \dots, 1000$ are randomly chosen. Then, the associated model predictions $g_\ell(t, w_2; \hat{\theta}_m)$ are calculated. Hence, for each e_k , $k = 1, \dots, n$, there are 1000 model predictions $g_\ell(e_k; \hat{\theta}_m)$. These 1000 predictions are sorted in ascending order and, using the percentile method to establish the 95% confidence interval, the 25th and 975th predictions are selected as the lower and upper bounds, respectively.

Occasionally the randomly selected vectors were infeasible. In particular, we define $\beta_2 < 0$ and $\beta_3 < 0$. If by chance the random selection procedure produced a parameter vector which did not meet these criteria, a new vector was randomly selected until the criteria were met. Also, occasionally a randomly selected parameter vector would result in a negative conductance prediction g_ℓ , which is also infeasible. Upon this event, a new vector was randomly selected until a positive prediction g_ℓ was achieved.

2.3.3. Bootstrap Method

As described in (2.12), applying the wild bootstrap method yields the estimated parameter vectors $\hat{\theta}^m$ for $m = 1, \dots, 1000$. Using these estimated parameter vectors, the associated model predictions $g_\ell(t, w_2; \hat{\theta}^m)$ can be calculated. Hence, for each e_k , $k = 1, \dots, n$, there are 1000 model predictions $g_\ell(e_k; \hat{\theta}^m)$. These 1000 predictions are sorted in ascending order, and using the percentile method to establish the 95% confidence interval for model predictions, the 25th and 975th predictions are selected as the lower and upper bounds, respectively.

3. Results

In this section we present the results of efforts to establish confidence intervals for parameter estimates and model predictions for the leaf conductance model described in (2.1)-(2.3). To obtain confidence intervals for parameter estimates, we separately applied asymptotic theory and bootstrap methods. To establish confidence intervals for model predictions asymptotic theory, Monte Carlo methods, and bootstrap methods were utilized.

In the interest of space, the results presented below focus mainly on the case of the Haskell soybean genotype from the 2008 growing season, as all cases showed analogous results. Detailed results of the remaining cases (Haskell in 2009, and N01-11771 in 2008 and 2009) may be found in Matthews (2010) [15].

3.1. Confidence Intervals for Parameter Estimates

3.1.1. Asymptotic Theory

Calculating (2.6) was the first step taken to approximate confidence intervals for the estimated parameters. Partial derivatives of the model, as described in (2.1), with respect to each of the parameters are

$$\chi_{i,1} = \frac{\partial g_\ell(e_i; \theta)}{\partial \alpha_0} = \beta_1 e^{\beta_2} e^{\beta_3 w_{2,i}} \quad (3.1)$$

$$\chi_{i,2} = \frac{\partial g_\ell(e_i; \theta)}{\partial \alpha_1} = t_i \beta_1 e^{\beta_2} e^{\beta_3 w_{2,i}} \quad (3.2)$$

$$\chi_{i,3} = \frac{\partial g_\ell(e_i; \theta)}{\partial \alpha_2} = t_i^2 \beta_1 e^{\beta_2} e^{\beta_3 w_{2,i}} \quad (3.3)$$

$$\chi_{i,4} = \frac{\partial g_\ell(e_i; \theta)}{\partial \alpha_3} = t_i^3 \beta_1 e^{\beta_2} e^{\beta_3 w_{2,i}} \quad (3.4)$$

$$\chi_{i,5} = \frac{\partial g_\ell(e_i; \theta)}{\partial \beta_1} = (\alpha_0 + \alpha_1 t_i + \alpha_2 t_i^2 + \alpha_3 t_i^3) e^{\beta_2} e^{\beta_3 w_{2,i}} \quad (3.5)$$

$$\chi_{i,6} = \frac{\partial g_\ell(e_i; \theta)}{\partial \beta_2} = \beta_1 (\alpha_0 + \alpha_1 t_i + \alpha_2 t_i^2 + \alpha_3 t_i^3) e^{\beta_2} e^{\beta_3 w_{2,i}} e^{\beta_3 w_{2,i}} \quad (3.6)$$

$$\chi_{i,7} = \frac{\partial g_\ell(e_i; \theta)}{\partial \beta_3} = \beta_1 \beta_2 w_{2,i} (\alpha_0 + \alpha_1 t_i + \alpha_2 t_i^2 + \alpha_3 t_i^3) e^{\beta_2} e^{\beta_3 w_{2,i}} e^{\beta_3 w_{2,i}} \quad (3.7)$$

These values yield the $n \times p$ sensitivity matrix

$$\chi = \begin{bmatrix} \chi_{1,1} & \chi_{1,2} & \chi_{1,3} & \chi_{1,4} & \chi_{1,5} & \chi_{1,6} & \chi_{1,7} \\ \chi_{2,1} & \chi_{2,2} & \chi_{2,3} & \chi_{2,4} & \chi_{2,5} & \chi_{2,6} & \chi_{2,7} \\ \vdots & & & & & & \vdots \\ \chi_{n,1} & \chi_{n,2} & \chi_{n,3} & \chi_{n,4} & \chi_{n,5} & \chi_{n,6} & \chi_{n,7} \end{bmatrix}. \quad (3.8)$$

This matrix χ was formed for the case of the Haskell genotype for the 2008 growing season. Using the parameter values indicated in Table 1 for this case we have

$$\chi^T \chi = \begin{bmatrix} 1 \times 10^9 & 2 \times 10^{11} & 5 \times 10^{13} & 1 \times 10^{16} & 4 \times 10^6 & 4 \times 10^8 & -6 \times 10^7 \\ 2 \times 10^{11} & 5 \times 10^{13} & 1 \times 10^{16} & 3 \times 10^{18} & 1 \times 10^9 & 1 \times 10^{11} & -2 \times 10^{10} \\ 5 \times 10^{13} & 1 \times 10^{16} & 3 \times 10^{18} & 6 \times 10^{20} & 3 \times 10^{11} & 3 \times 10^{13} & -4 \times 10^{12} \\ 1 \times 10^{16} & 3 \times 10^{18} & 6 \times 10^{20} & 2 \times 10^{23} & 6 \times 10^{13} & 7 \times 10^{15} & -1 \times 10^{15} \\ 4 \times 10^6 & 1 \times 10^9 & 3 \times 10^{11} & 6 \times 10^{13} & 3 \times 10^4 & 3 \times 10^6 & -4 \times 10^5 \\ 4 \times 10^8 & 1 \times 10^{11} & 3 \times 10^{13} & 7 \times 10^{15} & 3 \times 10^6 & 6 \times 10^8 & -5 \times 10^7 \\ -6 \times 10^7 & -2 \times 10^{10} & -4 \times 10^{12} & -1 \times 10^{15} & -4 \times 10^5 & -5 \times 10^7 & 7 \times 10^6 \end{bmatrix}.$$

Note that the order of magnitude of the entries in $\chi^T \chi$ varies from 10^4 to 10^{23} , which is a difference of 19 orders of magnitude. Based on the singular value decomposition of $\chi^T \chi$, the rank of $\chi^T \chi$ is 4. Since this matrix is not full rank, we can not compute $(\chi^T \chi)^{-1}$ as required by the linear approximation parameter confidence interval formula in (2.8). The remaining cases, the Haskell genotype in 2009 and the N01-11771 genotype in both 2008 and 2009, yielded similar results. Therefore, asymptotic theory as applied to this problem does not provide a computationally feasible solution for estimating confidence intervals for model parameters.

3.1.2. Bootstrap Method

As shown in Fig. 1, the pattern of residuals versus the associated model predictions in all cases does not appear random, and therefore we conclude that the residuals are heteroscedastic. Hence, we employ the wild bootstrap method to estimate confidence intervals for parameter estimates. There are many options for how one may choose to define $h(u_k)$ and the distribution of v_k from

Figure 1: Conductance predictions versus residuals. (a) Haskell genotype in 2008, (b) N01-11771 genotype in 2008, (c) Haskell genotype in 2009, and (d) N01-11771 genotype in 2009.

(2.15). A simple choice for $h(u_k)$, and the one we chose, is the identity relation $h(u_k) = u_k$. A commonly employed two-point distribution for v_k is

$$v_k = \begin{cases} \frac{-(\sqrt{5}-1)}{2} & \text{with probability } p = (\sqrt{5} + 1)/(2\sqrt{5}) \\ \frac{\sqrt{5}+1}{2} & \text{with probability } 1 - p \end{cases} \quad (3.9)$$

[14, 13, 7]. Clearly this distribution satisfies the aforementioned requirements $E(v_k) = 0$, $E(v_k^2) = 1$, and $E(v_k^3) = 1$, although the proof is omitted. Fig. 2 depicts the histograms of bootstrapped parameter estimates of $\alpha_0 - \alpha_3$ and $\beta_1 - \beta_3$ for the case of the Haskell genotype during the 2008 growing season. The results from the other three cases are analogous.

From the bootstrap simulations, there are M estimates of θ . The percentiles of these histograms may be used to construct confidence intervals for the original estimate $\hat{\theta}$ [9]. Since in these studies $M = 1000$, the vector of M estimates is ordered and the 25th and 975th entry define the 95% confidence interval for each parameter. Table 2 summarizes the 95% confidence intervals for each parameter for each of the four studies.

The results of the bootstrap method may also be used to approximate the

Figure 2: Histograms of bootstrapped parameter estimates of $\alpha_0 - \alpha_3$ and $\beta_1 - \beta_3$ for the Haskell genotype in 2008. Vertical lines on each indicate the original parameter estimate values summarized in Table 1.

parameter covariance matrix using the relation

$$\text{cov}(\hat{\theta}) = \frac{1}{M-1} \sum_{m=1}^M \left(\hat{\theta}^m - \hat{\theta}_{boot} \right)^T \left(\hat{\theta}^m - \hat{\theta}_{boot} \right) \tag{3.10}$$

Parameter	2008		2009	
	Haskell	N01-11771	Haskell	N01-11771
α_0	-1.7179×10^0 -1.4282×10^0	-1.5934×10^0 -1.2953×10^0	-6.0004×10^{-1} -1.4438×10^{-2}	-4.5386×10^{-1} 1.6120×10^{-1}
α_1	8.2446×10^{-2} 9.4965×10^{-2}	7.6065×10^{-2} 8.8577×10^{-2}	2.6568×10^{-2} 5.2630×10^{-2}	2.1278×10^{-2} 4.7835×10^{-2}
α_2	-1.0351×10^{-3} -8.6433×10^{-4}	-9.4650×10^{-4} -7.7608×10^{-4}	-5.3074×10^{-4} -1.7310×10^{-4}	-4.8244×10^{-4} -1.2584×10^{-4}
α_3	2.5929×10^{-6} 3.2960×10^{-6}	2.2639×10^{-6} 2.9574×10^{-6}	-5.2958×10^{-9} 1.4689×10^{-6}	-1.6015×10^{-7} 1.3166×10^{-6}
β_1	1.0313×10^3 1.5240×10^3	8.6112×10^2 9.1654×10^2	9.8532×10^2 2.0365×10^3	8.0699×10^2 9.3165×10^2
β_2	-2.5096×10^0 -1.6331×10^0	-1.8148×10^0 -1.0441×10^0	-2.4663×10^0 -1.8831×10^0	-1.1856×10^1 -4.2127×10^0
β_3	-4.1250×10^1 -1.6210×10^1	-9.5787×10^1 -5.5021×10^1	-1.6197×10^1 -6.7589×10^0	-2.0605×10^1 -1.2013×10^1

Table 2: 95% confidence intervals derived from the wild bootstrap method using the percentile method for each case.

where

$$\hat{\theta}_{boot} = \frac{1}{M} \sum_{m=1}^M \hat{\theta}^m \quad (3.11)$$

is the mean of all M bootstrapped parameter vector estimates [4]. Using the definition given by (3.10) for the covariance matrix, the standard errors for each of each of the $j = 1, \dots, p$ estimated parameters are [10]

$$SE(\hat{\theta}_j) = \sqrt{\text{cov}(\hat{\theta})_{jj}}. \quad (3.12)$$

Recall that (2.8) defined confidence intervals for the estimated parameters as motivated by asymptotic theory. The bootstrap method was investigated because of the matrix singularity which did not provide a computationally feasible solution for the covariance matrix via sensitivities based methods. However, since the covariance matrix may be estimated from the bootstrap method as in (3.10), the confidence intervals as derived directly from the bootstrap method and as estimated with asymptotic theory may be compared. In (2.8), the substitution of $SE(\hat{\theta}_j)$ for $\sqrt{V_{jj}}$ yields our confidence intervals. The 95% confidence intervals for the estimated parameters computed with the asymptotic theory method are summarized in Table 3.

Parameter	2008		2009	
	Haskell	N01-11771	Haskell	N01-11771
α_0	-1.7208×10^0 -1.4184×10^0	-1.6000×10^0 -1.2915×10^0	-6.1111×10^{-1} -1.7978×10^{-2}	-4.5839×10^{-1} 1.5680×10^{-1}
α_1	8.2113×10^{-2} 9.5065×10^{-2}	7.6007×10^{-2} 8.9049×10^{-2}	2.6916×10^{-2} 5.3299×10^{-2}	2.1196×10^{-2} 4.8073×10^{-2}
α_2	-1.0344×10^{-3} -8.5829×10^{-4}	-9.5068×10^{-4} -7.7650×10^{-4}	-5.3858×10^{-4} -1.7831×10^{-4}	-4.8254×10^{-4} -1.2056×10^{-4}
α_3	2.5705×10^{-6} 3.2887×10^{-6}	2.2757×10^{-6} 2.9745×10^{-6}	1.9926×10^{-8} 1.5062×10^{-6}	-1.4961×10^{-7} 1.3291×10^{-6}
β_1	8.4866×10^2 1.4286×10^3	8.6019×10^2 9.1577×10^2	5.9334×10^2 1.8213×10^3	7.9065×10^2 9.1624×10^2
β_2	-2.3845×10^0 -1.5203×10^0	-1.7355×10^0 -9.7705×10^{-1}	-2.3913×10^0 -1.7845×10^0	-1.0726×10^1 -3.0061×10^0
β_3	-4.1648×10^1 -1.6360×10^1	-9.5104×10^1 -5.3795×10^1	-1.6094×10^1 -6.5349×10^0	-2.0306×10^1 -1.1750×10^1

Table 3: 95% confidence intervals derived from (2.8) and (3.12) applying wild bootstrap simulations for each case.

3.2. Confidence Intervals for Model Predictions

3.2.1. Asymptotic Theory

The matrix $\text{cov}(\hat{\theta})$ is calculated as indicated in (3.10) and for the Haskell genotype in 2008 is

$$\begin{bmatrix} 3 \times 10^{-14} & 8 \times 10^{-12} & 6 \times 10^{-10} & 1 \times 10^{-8} & 2 \times 10^{-5} & 4 \times 10^{-8} & 1 \times 10^{-6} \\ 8 \times 10^{-12} & 2 \times 10^{-9} & 1 \times 10^{-7} & 3 \times 10^{-6} & 6 \times 10^{-3} & 1 \times 10^{-5} & 3 \times 10^{-4} \\ 6 \times 10^{-10} & 1 \times 10^{-7} & 1 \times 10^{-5} & 3 \times 10^{-4} & 4 \times 10^{-1} & 7 \times 10^{-4} & 2 \times 10^{-2} \\ 1 \times 10^{-8} & 3 \times 10^{-6} & 2 \times 10^{-4} & 6 \times 10^{-3} & 1 \times 10^1 & 2 \times 10^{-2} & 5 \times 10^{-1} \\ 2 \times 10^{-5} & 6 \times 10^{-3} & 4 \times 10^{-1} & 1 \times 10^1 & 2 \times 10^4 & 3 \times 10^1 & 8 \times 10^2 \\ 4 \times 10^{-8} & 1 \times 10^{-5} & 7 \times 10^{-4} & 2 \times 10^{-2} & 3 \times 10^1 & 5 \times 10^{-2} & 1 \times 10^0 \\ 1 \times 10^{-6} & 3 \times 10^{-4} & 2 \times 10^{-2} & 5 \times 10^{-1} & 8 \times 10^2 & 1 \times 10^0 & 4 \times 10^1 \end{bmatrix}. \quad (3.13)$$

Similar covariance matrices were calculated for the remaining three cases (N01-11771/2008, Haskell/2009, N01-11771/2009).

Table 4 summarizes the percentages of data points covered by the estimated 95% confidence intervals computed with (2.17) for each respective case. The values reported in Table 4 include both the fitted and validation data points. Fig. 3 graphically depicts the estimated 95% confidence interval along with mean conductance data for the Haskell genotype in 2008. Analogous figures for the N01-11771 genotype in 2008, the Haskell genotype in 2009, and the N01-11771 genotype in 2009, may be found in Matthews (2010) [15].

Figure 3: 95% confidence intervals computed with (2.17) (dotted lines) compared to mean data by date (solid lines) using the asymptotic theory method for the Haskell genotype in 2008.

Table 4: Percentage of data points covered by estimated 95% confidence intervals computed using (2.17), the asymptotic theory method.

Study year	Genotype	Expt. A	Expt. B	Expt. C	Expt. D	Total
2008	Haskell	38.18	42.91	45.27	42.57	42.23
2008	N01-11771	17.57	15.54	16.89	12.84	15.71
2009	Haskell	50.82	69.17	87.50	84.84	73.16
2009	N01-11771	20.49	18.33	18.95	17.21	18.75

3.2.2. Monte Carlo Method

Table 5 summarizes the percentages of data points covered by the estimated 95% confidence intervals computed by this Monte Carlo method for each respective case. Fig. 4 is analagous to Fig. 3 of the previous section. Similar figures for the N01-11771 genotype in 2008, the Haskell genotype in 2009, and the N01-11771 genotype in 2009, may again be found in [15].

Figure 4: 95% confidence intervals computed with Monte Carlo methods (dotted lines) compared to mean data by date (solid lines) for the Haskell genotype in 2008.

Table 5: Percentage of data points covered by estimated 95% confidence intervals computed with Monte Carlo methods.

Study year	Genotype	Expt. A	Expt. B	Expt. C	Expt. D	Total
2008	Haskell	41.22	46.62	45.61	47.30	45.19
2008	N01-11771	16.55	15.20	16.55	12.84	15.29
2009	Haskell	56.15	72.08	89.92	80.74	74.80
2009	N01-11771	21.31	22.08	21.77	20.08	21.31

3.2.3. Bootstrap Method

Table 6 summarizes the percentages of data points covered by the estimated 95% confidence intervals computed by the percentile method with bootstrap simulations. Fig. 5 is analagous to Figs 3 and 4 from the asymptotic and Monte Carlo methods, respectively. Similar figures for the N01-11771 genotype in 2008, the Haskell genotype in 2009, and the N01-11771 genotype in 2009, may be located in [15].

Figure 5: 95% confidence intervals computed with percentile methods and bootstrap simulations (dotted lines) compared to mean data by date (solid lines) for the Haskell genotype in 2008.

Table 6: Percentage of data points covered by estimated 95% confidence intervals computed with percentile methods and bootstrap simulations.

Study year	Genotype	Expt. A	Expt. B	Expt. C	Expt. D	Total
2008	Haskell	19.26	13.85	12.50	10.47	14.02
2008	N01-11771	16.89	14.86	16.89	12.50	15.29
2009	Haskell	16.80	16.67	14.11	13.93	15.37
2009	N01-11771	18.44	17.08	17.74	15.98	17.32

4. Discussion

A simple, empirical model adequately representing the trends in total leaf conductance under a variety of water stress scenarios is presented in Matthews et al. (2013) [16]. In this work, two different methodologies, asymptotic theory and wild bootstrap, were applied to estimate 95% confidence intervals for the estimated parameters of this leaf conductance model. Additionally, asymptotic theory, Monte Carlo, and wild bootstrap methods were applied to estimate 95% confidence intervals for the model predictions.

We found that asymptotic theory as applied to this problem does not provide a computationally feasible solution for estimating confidence intervals for model parameters. The underlying problem of singularity of the $\chi^T \chi$ matrix is quite common for inverse problems with nonlinear models. A method to handle singularity of the Fisher Information Matrix ($\chi^T \chi$) as a result of poor parameter identifiability and estimability has recently been introduced in [5]. This algorithm determines which parameter axes lie closest to the ill-conditioned directions of $\chi^T \chi$ and then implements a reduced-order estimation by fixing these associated parameter values at prior estimates. Because reasonable ranges for the estimated parameters in this application are unknown, we were unable to employ this method.

Although we were unable to calculate the variance-covariance matrix via asymptotic theory, we were successful using bootstrap methods to identify this matrix. We then proceeded to use this matrix to estimate 95% confidence intervals for the model parameters based on both asymptotic theory (2.8) and the percentile method with bootstrapped simulations. Comparison of Tables 2 and 3 reveals that, in general, the confidence intervals derived from the asymptotic methods summarized in (2.8) and (3.12) are, for the most part, slightly larger in size and negatively shifted compared to those using the percentile method with the bootstrap simulation results. In practice, the confidence intervals from the percentile method with the bootstrap simulation results are likely more reliable. The asymptotic theory method inherently makes a number of assumptions and approximations mainly regarding the estimation of the covariance matrix and

the assumption regarding the distribution choice of (2.8), whereas the percentile method bypasses these assumptions.

We have presented three different methods for estimating confidence intervals for model predictions. The obvious question is: which method is best? Unfortunately, the answer is not so simple. Initially one may be tempted to review Tables 4 through 6 and choose the method which has the highest coverage of data points, as this is the most conservative method. Ideally, given a perfect model, a 95% confidence interval would cover 95% of the data points. However, as is typical with many biological data sets, there is a large degree of scatter amongst measurements in the data sets under consideration. Therefore, achievement of 95% coverage by any methodology would likely imply huge confidence intervals which are not particularly useful in application. Hence, a more detailed examination of the estimated confidence intervals is warranted.

Recall that both the asymptotic theory and Monte Carlo methods rely on the assumption that the model parameters are normally distributed. Table 7 presents the p-values from the Lilliefors's test for normality performed on the estimated parameters from the wild bootstrap simulations, as bootstrapping reveals the true distribution of the parameters. In each of the four genotype and growing season cases, there is at least one parameter which violates the normality assumption at the $\alpha = 0.1$ level.

For both the 2008 and 2009 growing seasons, the coverages determined by all three methods for the N01-11771 genotype are remarkably similar (see Tables 4 through 6). However, comparing the values for the Haskell genotype in the 2008 growing season, Tables 4 through 6 illustrate that the estimated 95%

Table 7: P-values from Lilliefors's test for normality on estimated parameter distributions from wild bootstrap simulations for each case. * indicates normality is rejected.

	2008		2009	
Parameter	Haskell	N01-11771	Haskell	N01-11771
α_0	0.1749	> 0.5	> 0.5	> 0.5
α_1	0.1940	> 0.5	> 0.5	> 0.5
α_2	0.1548	> 0.5	> 0.5	> 0.5
α_3	0.0724*	> 0.5	> 0.5	> 0.5
β_1	< 10^{-4} *	0.4355	< 10^{-4} *	< 10^{-4} *
β_2	0.0006*	0.0640*	< 10^{-4} *	< 10^{-4} *
β_3	> 0.5	> 0.5	0.3234	0.0197*

confidence intervals using the asymptotic theory and Monte Carlo methods are much larger than those estimated via the bootstrap method, as seen through their greater percentage of covered data points. Figures 3 through 5 reiterate this difference in size of estimated confidence interval. Fig. 6 compares the estimated CI half-lengths normalized by the value of leaf conductance prediction for the three methodologies as applied to the Haskell genotype during the 2008 growing season. In these histograms, a value of one indicates that the estimated CI half-length is the same magnitude as the prediction. For example, if we had a total leaf conductance prediction of $50 \text{ mmol m}^{-2} \text{ s}^{-1}$ and value of 1, this implies that the estimated confidence interval is $50 \pm 50 \text{ mmol m}^{-2} \text{ s}^{-1}$. We note that the asymptotic theory and Monte Carlo methods tend to have larger estimated CIs, when normalized by prediction magnitude, than the bootstrap method, which explains the better coverage of data points indicated in Tables 4 and 5.

Figure 7 shows the CI half-lengths as a function of soil moisture content for each of the three methods. Excluding the maximum soil moisture content value, there is a noticeable pattern of CI half-length as a function of soil moisture content. Fig. 9 helps to explain this pattern. Here the sensitivity of g_ℓ to the β_j parameters is plotted as a function of soil moisture content. Note that these sensitivities have been normalized to allow for inter comparison. At values lower than approximately $0.023 \text{ m}^3 / \text{m}^3$, g_ℓ is more sensitive to β_2 , and after this

Figure 6: Histograms of CI half-lengths normalized by prediction for the Haskell genotype in 2008 using (a) asymptotic theory, (b) Monte Carlo, and (c) bootstrap methods.

Figure 7: Plot of CI half-lengths as a function of soil moisture, w_2 , for the Haskell genotype during the 2008 growing season.

point, β_1 is the most sensitive parameter of the β s. In Fig. 7 there is a similar pattern with an inflection point at approximately $0.023 \text{ m}^3 / \text{m}^3$.

However, at the maximum soil moisture content value in Fig. 7, there is clearly no pattern in CI half-length based on soil moisture content. Fig. 8 plots only these unexplained cases as a function of days after planting. Now the pattern for these is clearly visualized. Fig. 10 helps to explain this relation of CI half-lengths at saturated soil moisture content to days after planting. Here the sensitivity of g_ℓ to the α_j parameters is plotted as a function of soil moisture content.

For the Haskell genotype in the 2008 growing season, the normality of α_3 , β_1 , and β_3 are rejected, as shown in Table 7. The impact of this violation in this case manifests in the over-prediction of the estimated 95% confidence intervals using both the asymptotic theory and Monte Carlo methods.

Figure 8: Plot of CI half-lengths as a function of days after planting, for the Haskell genotype during the 2008 growing season, where soil moisture content was maximized.

Figure 9: Sensitivity of g_l to β_1 , β_2 , and β_3 as a function of soil moisture content for the Haskell genotype during the 2008 growing season.

Figure 10: Sensitivity of g_l to α_0 , α_1 , α_2 , and α_3 as a function of days after planting for the Haskell genotype during the 2008 growing season.

The results for the Haskell genotype in the 2009 growing season are similar. Tables 4 through 6 again show that the estimated 95% confidence intervals using the asymptotic theory and Monte Carlo methods are much larger than those estimated via the bootstrap method. The relationships between estimated CI half-lengths with soil moisture content and days after planting, are nearly identical to the 2008 growing season results. For this case, Table 7 indicates that β_1 and β_2 are not normally distributed according to the Lilliefors's test. Again, the violation of the normality assumption results in the over-prediction of the estimated 95% confidence intervals using both the asymptotic theory and Monte Carlo methods.

5. Conclusions

The simple model proposed in Matthews et al. (2013) has room for improvement and additional measures are suggested as future work. However, the value of this model is its simplicity coupled with a quality representation of the response of leaf conductance to varying soil moisture. The utility of the estimated confidence intervals for both parameters and model predictions is directly affected by the quality of the model calibration and accuracy of the resultant predictions. Therefore, model improvement may propagate improvement in coverage of data points. Specifically, it could result in figures closer to

the desired 95% in Tables 4 through 6.

Potential impacts of climate change include periods of drought as well as the greater possibility of extreme precipitation events. Additionally, agronomists desire crops with higher productivity using the same amount or even less water to accommodate the needs of an ever-increasing population. Because of the importance of correctly characterizing photosynthetic processes within these contexts, it is imperative that the response of conductance to drought and extreme precipitation events be well understood and applicably modeled. The model presented in Matthews et al. (2013) effectively quantifies the response of total leaf conductance to soil moisture and plant age. Understanding the uncertainties associated with the model parameters and predictions is critical for proper utilization of the model.

As applied to the model herein, using bootstrap methods to estimate confidence intervals appears to be very promising. Computational issues confronted when applying the classical asymptotic theory are bypassed and fewer assumptions, any of which could be false, are required for implementation as compared to asymptotic theory and Monte Carlo methods. This field of research in the statistical community is still very active and novel methods are still being discovered. Further exploration of the many versions of available bootstrap methods is warranted.

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