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A procedure for ranking parameter importance for estimation in predictive mechanistic models

Craig R. Elevitch[a,*], C. Richard Johnson Jr.[b]

[a] Agroforestry Net, 76-5921 Mamalahoa Hwy, #5, Holualoa, HI, 96725, United States
[b] School of Electrical and Computer Engineering, Frank HT Rhodes Hall, Cornell University, Ithaca, NY, 14853, USA

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ABSTRACT

We begin with a mechanistic model that is considered to be a reasonably good predictor of the real-life system with a set of parameters determined from prior biophysical studies and expert knowledge. For complex mechanistic growth models, it is usually advantageous to numerically estimate a subset of the 'most important' parameters (i.e., those that most influence dynamic model behavior) based on data and fix the others at their estimated *a priori* values. Determining a reduced-order parameter subset for end-user estimation can be challenging, often relying heavily on expert knowledge and trial-and-error. A straightforward but oversimplified method relies on one-at-a-time (OAT) sensitivity of model outputs to changes in individual parameters. However, this commonly used method fails to account for how simultaneous changes in multiple parameters can significantly impact model outputs in unpredictable ways due to model nonlinearities. Additionally, hidden relationships between parameters can prevent consistent identifiability of parameters from different initial estimates. Rather than analyzing the effect of individual parameter variation on the model outputs, we evaluate the importance of parameters to the curvature of the quadratic cost function (sum squared difference between reference and model output sequences). This analysis is carried out by calculating the matrix of second-order partial derivatives of the cost function (aka Hessian matrix) with respect to the model parameters. Calculating the cost function Hessian allows analysis of changes in multiple parameters simultaneously. The method is presented as an analytic, reproducible procedure for determining a ranking for parameter importance. The procedure is demonstrated on a limited version of the Yield-SAFE predictive agroforestry growth model. For the analysis, 12 model parameters are considered with their nominal values set to those given in a published implementation of Yield-SAFE. The Hessian was calculated at 2^{12} (= 4096) locations systematically selected in the neighborhood of the nominal parameter setting, each generating a parameter ranking determined by the relative contribution of each parameter to the cost function curvature. The top ranked 6 parameters were the same for 4091 of 4096 locations, suggesting that this procedure has potential to guide modelers in recommending the most important parameters for estimation given reasonably good initial parameter estimates and real data.

1. Introduction

An increasing number of tree growth models are very complicated (Weiskittel et al., 2011; Pretzsch et al., 2015). When modeling intraspecific interactions between trees or trees and crops grown in close proximity (e.g., in tree polycultures and agroforestry), complexity can increase significantly beyond individual or monospecific tree growth models due to the interactions between species (Monteith et al., 1991; van der Werf et al., 2007). In tree modeling as well as in biophysical modeling of natural processes in general, model complexity can become problematic, particularly when accurate prediction of outcomes is of primary importance (Ljung, 1999; Cox et al., 2006; Sivakumar, 2008). For agroforestry and other crop growth modeling in general, outcomes prediction has become particularly timely. Agroforestry is increasingly seen as an important means to regenerate degraded lands and address climate change challenges while producing economically viable crops (Verchot et al., 2007; Jose, 2009; Jat et al., 2016; Hillbrand et al., 2017; Toensmeier, 2016; Schoeneberger et al., 2017; Elevitch et al., 2018). Predictive modeling can extend existing knowledge into novel crop combinations in new environments and justify investment in agroforestry for both producers and policymakers (Malézieux et al., 2009).

Problems encountered in model predictive accuracy include propagation of model error between interconnected model components, uncertainty in parameter (model constant) values, and inadequate data

* Corresponding author.
E-mail addresses: cre@agroforestry.org (C.R. Elevitch), crj2@cornell.edu (C.R. Johnson).

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for parameterization and validation (Beck, 1983; Young and Ratto, 2009). When accurate prediction is of primary importance to the modeler, reduction in the number of estimated parameters is desirable (Sjöberg et al., 1995; Gupta and Sharma, 2019). The number of parameters estimated can be reduced if variations in some parameters (or combinations of parameters) contribute little to the model output(s). The degree of contribution is a combination of richness of the frequencies in the inputs and parameter sensitivities of the model structure (Yao et al., 2003; Gutenkunst et al., 2007; Crout et al., 2009; Li and Vu, 2013). Additionally, the model structure (including interactions between submodels) can inadvertently render some parameters unidentifiable (Bellman and Åström, 1970; Beck, 1983; Young, 1983; Hengl et al., 2007; Vilela et al., 2009).

In order to reduce complexity in predictive models, many model reduction schemes have been developed. In general, model reduction methods approximate the most important dynamics of the system by considering the relationship between inputs and outputs (Schilders, 2008). Methods for reducing the complexity are well-studied and straightforward for linear models, less straightforward for linear approximations of nonlinear models, and most challenging for reducing nonlinear models to simpler nonlinear models (Ljung, 2010). Mechanistic models are usually in the latter category, engendering a range of model reduction approaches.

Model reduction techniques such as Proper Orthogonal Decomposition (POD) project high dimensional data onto a lower dimensional space to derive low dimension models that capture most of the dynamics of the full model (Hinze and Volkwein, 2005; Kerschen et al., 2005; Schilders, 2008). Although POD can be applied to nonlinear models, it yields an approximating linear manifold, which may be considered a serious limitation in its application to nonlinear models (Kerschen et al., 2005). Also based upon analysis of dynamic modes, Young and Ratto (2009) present a seven-phase strategy for reducing the complexity of mechanistic models termed Data-Based Mechanistic (DBM) modeling. After implementing a computational version of the model, the process begins with stochastic analysis using Monte-Carlo simulations to determine the relative importance of different submodels in explaining the dominant model behavior. From this step, a process called “dominant mode analysis” is performed over a user-defined parameter range to determine a low order approximation of the original model. This process generates a mapping of the unreduced model to a reduced-order model called the Dynamic Emulation Model (DEM) that can replace the full model over a range of parameter values (Young, 2011). All of the analysis is done in the absence of experimental data, with the original model serving as a surrogate for the ‘true system.’ A disadvantage of this approach is the lack of a biophysical interpretation of the resulting DEM model.

Recognizing that many process-based models are “over-parameterised [and] may have poor predictive performance,” Cox et al. (2006) followed by Crout et al. (2009) and others approach model reduction by setting signals in the model to fixed nominal values and evaluating how well each model version performs. The signals considered are chosen by the modeler, but generally have a mechanistic interpretation. An exhaustive search of all possible combinations of signal replacements with constant values are assessed in order to determine which model dynamics may be excluded from the model without significantly degrading performance. According to Crout et al. (2009), “The work of Cox et al. (2006) is distinct from the data based mechanistic modelling of Young et al. (e.g. Young, 1998, 1999) in that it operates directly on the formulation of the original model, rather than synthesizing a simplified linearised stochastic model using data sets generated from the original process based model.”

Of these model reduction approaches, the method presented here is most similar to that of Cox et al. (2006) and Crout et al. (2009) in that it preserves the mechanistic model structure. However, rather than considering signals within the model, analysis is done with respect to input-output behavior of the whole model, where inputs are the measurable exogenous drivers of the mechanistic model and outputs are only those signals that we are interested in predicting accurately and which can be readily measured. This approach may conflict with other modeling preferences such as maintaining the biophysical interpretation of internal model signals or parameter values, in exchange for accurate prediction of outputs. Such input-output analysis has been carried out in developing models for highly complex systems such as industrial processes and machines for the purpose of control since the 1970′s (Balakrishnan and Peterka, 1969; Åström and Eykhoff, 1971; Eykhoff, 1981). In this field, models may be described as ‘black box’ which are composed of well-understood mathematical expressions or ‘grey box’, composed of mechanistic descriptions of the physical processes, which are frequently nonlinear and not well understood mathematically (Ljung, 1996).

As for control systems where accurate prediction is essential, accurate prediction may be the primary goals of the modeler. For example, accurate prediction of tree and crop growth has practical importance in developing and evaluating crop combinations, management planning, and risk assessment for agroecosystems with wide-ranging potential benefits in mitigating risks associated with climate change (Malézieux et al., 2009). In this framework, submodel parameters are estimated using empirical data related to the whole system (Landsberg and Sands, 2011). Such numerically estimated parameters are seen only as a means to adjust model fit and may lose their physical interpretation (Ljung, 1999).

Others have also acknowledged a shift away from physically interpretable parameters in developing complex models. Valentine and Mäkelä (2005) state, “In principle, the values of … parameters may be estimated by lower-level process models. Alternatively, the physiological and morphological parameters combine, under reasonable assumptions, into a set of aggregate parameters, whose values can be estimated from inventory data with a statistical fitting procedure.” In other words, the individual parameters may lose their physical interpretation through the fitting to empirical data, but the suite of identified parameters combine into ‘aggregate’ parameters that are used to more accurately model the overall system dynamics.

To summarize, this system identification framework that underlies the approach taken here

- Output prediction is of primary importance (rather than the understanding of internal mechanisms).
- Signals within the model are no longer necessarily assumed to have physical interpretations.
- Biophysical parameter interpretations may no longer be valid.

Given these relaxations from an input-output predictive modelling perspective, we use input-output system analysis approaches to develop a procedure to rank parameters in terms of their importance to model output prediction. Additionally, the procedure presented here includes tests for parameter identifiability in the reduced parameter set.

2. Approach

The procedure presented here begins with a number of assumptions:

1 The mechanistic, predictive model of interest is trusted based on prior studies.
2 There exists an ‘nominal’ parameter setting that gives an acceptable fit to data (even sparse data).
3 The primary objective is accurate prediction of outputs.
4 Model developers wish to recommend a minimum number of model parameters for estimation to model users that will result in a good fit to measured data.

In other words, we begin with a mechanistic model that we consider to be a good representation of the real system whose outputs we wish to

predict, and we have a parameter setting where the model is believed to perform well. Because of nonlinearities, it is important to note that the analysis is only valid for the neighborhood of a specific parameter setting, as parameter importance to the output may change across the feasible range of parameter values.

2.1. Model class, Hessian, and goodness-of-fit

The procedure presented here was developed for application to mechanistic models constructed from deterministic descriptions (submodels) characterizing the underlying growth dynamics considered by the modeler to be of importance such as interception and conversion of solar energy, biomass growth, and transpiration (Buck-Sorlin, 2013). Each submodel is a well-studied dynamic process with its own inputs and outputs described by a set of differential or difference equations. Submodel outputs are often inputs to other submodels (Buck-Sorlin, 2013) and the same parameters may occur in multiple submodels (Cox et al., 2006). Mathematical representations for the dynamic processes within and between submodels are drawn from the extensive body of work in environmental physics (e.g., Campbell and Norman, 2012; Monteith and Unsworth, 2013), quantitative agronomy (e.g., Vries and de, 1989; Villalobos and Fereres, 2016), and other fields.

We represent a model by

$$y(n) = f(u(n), \theta) \tag{1}$$

where $f(\bullet)$ is the mechanistic model, $y(n)$is a vector of outputs, $u(n)$ is a vector of inputs, θ is a vector of m parameters, and n is time. When the model parameters are set to a nominal setting (accepted by modelers and determined by numerical estimation from data, prior studies of component submodels, and expert knowledge), the parameter vector is denoted by θ_0 and the output denoted by $y_0(n)$. For the purposes of analysis, we also introduce the identifier, which is identical to the model in mathematical structure but with parameters set to *a priori* estimates $\theta_j \neq \theta_0$, denoted by

$$y_j(n) = f(u(n), \theta_j) \tag{2}$$

As a reminder, we are assuming that the model with nominal parameters θ_0 is a reasonably good predictor of reality according the modelers, i.e., that we can take y_0 to be a surrogate for the real system, a reference output sequence, an approach taken by others (e.g., Young, 2012). Therefore the error between the reference model and the identifier at time n for the analysis is

$$r(n) = y_0(n) - y_j(n) \tag{3}$$

leading to the average quadratic cost function over Nsteps (from time $n - N + 1$ to time n)

$$V_N(n) = \frac{1}{N} \sum_{i=n-N+1}^{n} \frac{1}{2} r^2(i) \tag{4}$$

The matrix of second partial derivatives of $V_N(n)$ with respect to the model parameters is called the Hessian. Under conditions of continuity of a function f, the Hessian can be determined analytically, yielding an expression that can be calculated at any time n. The Hessian matrix of the second partial derivatives of a function f is of the form

$$H(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_m} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x^2 \partial x_m} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_m \partial x_1} & \frac{\partial^2 f}{\partial x_m \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_m^2} \end{bmatrix} \tag{5}$$

We are interested in the average Hessian of (4), which contains information about how parameters affect the curvature of the cost function over N steps, an $m \times m$ matrix

$$H(V_N) = \frac{1}{2N} \sum_{i=1}^{N} \begin{bmatrix} \frac{\partial^2 r^2(i)}{\partial x_1^2} & \frac{\partial^2 r^2(i)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 r^2(i)}{\partial x^1 \partial x_m} \\ \frac{\partial^2 r^2(i)}{\partial x_2 \partial x_1} & \frac{\partial^2 r^2(i)}{\partial x_2^2} & \cdots & \frac{\partial^2 r^2(i)}{\partial x^2 \partial x_m} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 r^2(i)}{\partial x_m \partial x_1} & \frac{\partial^2 r^2(i)}{\partial x_m \partial x_2} & \cdots & \frac{\partial^2 r^2(i)}{\partial x_m^2} \end{bmatrix} \tag{6}$$

where the x_k are the individual parameters. The eigenvalues and eigenvectors of $H(V_N)$, which are important in ranking parameter importance to the cost function curvature in the neighborhood of the nominal parameter setting, are determined by the solution to

(7)$H^*X = X^*D$

where D is the $m \times m$ diagonal matrix of eigenvalues λ_k and X is an $m \times m$ matrix whose columns are the corresponding eigenvectors X_k.

With the Hessian calculated a method to order the importance of the parameters to the cost function curvature is needed. In addition to the magnitude of the eigenvalues, we are interested in the projections of the eigenvectors onto the parameter axes multiplied by their associated eigenvalues (Johnson, 1988). Based on this reasoning, the measure for ranking the importance of parameters to the Hessian curvature is assigned to be the 1-norm of the projections of the eigenvectors onto each parameter axis multiplied by their respective eigenvalues. That is, the combined magnitude of the eigenvector projections on the parameter axes for the ith parameter Λ_i is defined as

$$\begin{aligned} \Lambda_i &= \| DX_i^T \|_1 \\ &= \left\| \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_m \end{bmatrix} [X_i^T] \right\|_1 \end{aligned} \tag{8}$$

where X_i is the ith column of the eigenvector matrix$X$.

Finally, the normalized root mean squared error (NRMSE) goodness-of-fit measure will be used in the procedure below to compare the fit of an estimated output with the reference output (MathWorks, 2018)

$$NRMSE(y(N)) \equiv \left(1 - \frac{\sqrt{\sum_{i=1}^{N} (y_0(i) - y(i))^2}}{\sqrt{\sum_{i=1}^{N} \left(y_0(i) - \frac{\sum_{j=1}^{N} y_0(j)}{N} \right)^2}} \right) \times 100\% \tag{9}$$

where $y_0(i)$ is the reference sequence, $y(i)$ is the comparison sequence, and N is the number of data points. The possible range of NRMSE values is 100 % (perfect fit) to $-\infty$. The threshold NRMSE value for an acceptable fit depends upon the context and, ultimately, user preferences. A user may consider a $>$ 90 % fit is good enough in a certain setting, while another calls for a $>$ 99 % fit (as applied in the example of Section 3.2).

2.2. Input class

Model inputs include environmental data such as solar radiation, temperature, rainfall, wind speed, relative humidity, and soil nutrients. Historical weather data are available for locations around the world from various databases (https://www.ncdc.noaa.gov/cdo-web/, http://koeppen-geiger.vu-wien.ac.at/shifts.htm, http://archive.ceda.ac.uk/). However, data may not be available for the duration (many years) or the sampling interval (e.g., day, month, year) required by the model. A range of stochastic weather data generators has been developed for climate studies that are available for generation of synthetic weather data. Such synthetic data are widely used for crop growth modeling purposes (Ailliot et al., 2015) and have been made widely available (e.g., Palma, 2017).

2.3. Consistent identifiability

A model is uniquely identifiable if for any parameterization θ^*, the model has identical outputs for any input and time to the model parameterized by $\hat{\theta}$ if and only if $\theta^* = \hat{\theta}$ (Walter, 2012). One may begin characterizing the problem of determining identifiability by establishing the model class, input class, and a criterion for comparison (Åström and Eykhoff, 1971). Identifiability has been well-studied for linear systems (Ljung, 1999; Walter, 2012) and classes of nonlinear systems (e.g., Vilela et al., 2009).

Due to the complex nonlinear nature of many mechanistic models and frequently noisy data, theoretical identifiability may be much less of a concern than practical identifiability, the ability to uniquely identify parameters in practice (Walter, 2012). For our purposes, a model-specific concept is introduced: consistent identifiability. We begin with the *a priori* parameters θ_j and numerically estimate a subset of parameters χ_j based upon input-output data resulting in estimated parameters $\hat{\theta}_j$. χ_j is *consistently identifiable* if numerical estimation with the same input-output sequences yields $\hat{\theta}_j$ for any initialization in the neighborhood of θ_j. Since it is not possible to test every point within a certain distance of θ_j, in practice one can vary each parameter in χ_j plus/minus a small percentage away from their θ_j values and run the numerical estimation from those initializations.

2.4. The Hessian-informed Reduced-Order Parameter Estimation (HIROPE) procedure

This procedure for determining a reduced-order space for parameter estimation is based upon analytic evaluation of the average Hessian of the quadratic cost function at an *a priori* parameter setting θ_j in the neighborhood of an accepted nominal setting θ_0. The conceptual basis of the HIROPE procedure for a linear model and the simple 3-parameter logistic equation is presented in detail in Elevitch (2018, Chapter 2).

2.4.1. Model prerequisites

Application of the procedure has the following prerequisites

a Full deterministic process equations are defined.
b Conditions on parameters are determined, including mathematical and 'realism' constraints. This may be set by modelers (e.g., all parameters are positive real), or by model itself (e.g., prohibiting output of negative biomass).
c If model input-output equations are not twice continuously differentiable with respect to the parameters of interest, acceptable differentiable analytic approximations are substituted.
d The general class of model inputs is known and ample input data at the model time step can be accessed.
e A parameter optimization algorithm is implemented.

A list of symbols used in this analysis and associated notes for the example described in detail in Section 3 (for the Yield-SAFE model) is given in Table 1.

2.4.2. Steps of the HIROPE procedure

The steps of the model reduction procedure are outlined here (for a detailed description see Elevitch, 2018, Chapter 2). The procedure is summarized graphically in Fig. 1. Note that in this analysis, we have nominal parameters θ_0 and the *a priori* estimates θ_j are selected in the neighborhood of θ_0. For convenience, here we assume that all elements of θ_j are ± 5 % away from θ_0.

Step 1. Compare goodness-of-fit of y_0 with the estimated output y_j. For inputs u_i, compare output y_0 for a parameter set θ_0 with the output y_j for the *a priori* θ_j parameter set using the NRMSE goodness-of-fit measure (9). If the fit meets the criterion, move to Step 6 (validation).

Step 2. Compute Hessian $H_{i,j}$ and its eigenvectors and eigenvalues. Compute $H_{i,j}$for θ_j using data sequences u_i, y_0, and y_j from simulation of Step 1 and determine its eigenvectors and eigenvalues.

Step 3. Generate Λ_k parameter ranking. From the computed $H_{i,j}$,rank parameters using the formula (8), which leads to reduced-order parameter sets $\chi_{j,k}$.

Step 4. Confirm consistent identifiability. Beginning with highest ranked reduced-order parameter set $\chi_{j,1}$ containing only one parameter, optimize the parameter value from two nearby locations (e.g., ± 5 % from its *a priori* value), with all other parameters in θ_j fixed to their original estimated values to calculate a $\hat{\theta}_j$.

Step 5. Check goodness-of-fit of y_0 and $\hat{y}_j$. Using the current $\hat{\theta}_j$, generate $\hat{y}_j$ and calculate the NRMSE value relative to y_0. If fit criterion (NRMSE ≥ 99 %) is met, then move to the next step for validation. If optimization on the first candidate parameter set does not meet the NRMSE criterion, then repeat Step 4 for the next candidate parameter set, and so on, until either the fitting criterion is met for the optimization and validation inputs (success) or not (failure of procedure). In case of failure, revise fit criterion or model.

Step 6. Validation. Validate the optimized parameter set using a number of different input sequences from the same location and calculating their NRMSE values. If the validating input data also results in an acceptable NRMSE value, then the model optimization procedure is considered successful, otherwise return to Step 4. One may proceed to the next candidate parameter set if one wishes to see if there is improvement.

3. Results

This section demonstrates the HIROPE procedure applied to the Yield-SAFE model (van der Werf et al., 2007). The Yield-SAFE model may be the most widely used multistory agroforestry model designed for predictive purposes. It was developed as "a very parameter sparse, yet process-based model" providing "the best chance that robust parameter values can be identified" (van der Werf et al., 2007). Despite Yield-SAFE's parsimoniousness, it is recognized that only a subset of parameters can reasonably be estimated (Palma et al., 2017).

Developed by the Silvoarable Agroforestry for Europe (SAFE) project during the 2000's, the Yield-SAFE model estimates biomass yields of tree rows integrated with arable crops (Dupraz et al., 2005;, van der Werf et al., 2007; Graves et al., 2010). The model consists of mechanistic descriptions of tree and crop growth in a two-story planting configuration driven by environmental inputs (solar radiation, temperature, and precipitation), i.e., it is an input-output model that includes both plant growth and interactions between trees and crops. Recently, Yield-SAFE was augmented with several new submodels, including vapor pressure deficit input (to predict transpiration), modified water uptake, and the effect of the trees on temperature and wind speed, among others (Palma et al., 2016, 2018b). As an initial case study, the analysis below is based upon the original version of Yield-SAFE described in van der Werf et al. (2007) and implemented in Microsoft Excel (Burgess et al., 2014). The analysis is expected to be extendable to the recently introduced more complex versions of Yield-SAFE as well as other process-based models that meet the procedure criteria.

The Yield-SAFE model is described in detail in van der Werf et al. (2007). The model includes seven state Eq. (1) tree biomass; (2) tree leaf area; (3) number of shoots per tree; (4) crop biomass; (5) crop leaf area index; (6) soil water content; and (7) heat sum. The model runs on a daily time step and is driven by exogenous inputs of solar radiation, temperature, and precipitation. For the purposes of the present analysis, water and soil nutrients will be considered sufficient and non-limiting to potential growth, which is consistent with the initial parameter calibration assuming non-drought stress conditions undertaken by the Yield-SAFE team (van der Werf et al., 2007; Keesman et al., 2011; Palma et al., 2017). This type of simplification often applied to crop

Table 1
Symbols used for models, parameterizations, parameter initializations, and inputs with notes related to model simulations in Section 3.

Symbol	Description	Notes for simulations of Section 3 (Yield-SAFE model)
M	The model as described by the modelers	Models for tree (M_t), crop(M_c), tree/crop combination (M_{tc}), denote Yield-SAFE models
N		Number of time steps in simulation (days for Yield-SAFE)
Θ	Vector of model parameters considered for estimation (symbols)	Dimension 1 x d. $d = 12$ for M_{tc}
θ_0	Nominal parameter values	Dimension 1 x d. $d = 12$ for M_{tc}
θ_j	*A priori* parameter values with each element located at +5% or –5% of its nominal value	Dimension 1 x d. $j = 1, 2, \ldots, 2^d$
$\hat{\theta}_j$	*A priori* parameter values with some or all parameters optimized, and others fixed at their θ_j values	Dimension 1 x d. $j = 1, 2, \ldots, 2^d$
$\hat{\hat{\theta}}_j$	*A priori* parameter values that meet model fit criterion with some or all parameters optimized, and others fixed at their θ_j values	Dimension 1 x d. $j = 1, 2, \ldots, 2^d$
u_i	Inputs	First column is solar radiation (MJ m^{-2}) and second is temperature (°C). Index i is associated with location L_i. A 2 x N array.
y_0	Nominal or reference model output(s)	Biomass (g $tree^{-1}$ for M_t; g m^{-2} for M_c; both outputs for M_{tc}), with θ_0 and reference input u_i, 2 x N for M_{tc}.
y_j	*A priori* output(s)	Generated with θ_j and reference input u_i, 2 x N for M_{tc}.
$\hat{y}_j$	*A priori* output(s) with some or all parameters optimized	Generated with $\hat{\theta}_j$ and reference input u_i, 2 x N for M_{tc}.
$\hat{\hat{y}}_j$	*A priori* output(s) that meet model fit criterion with some or all parameters optimized	Generated with $\hat{\hat{\theta}}_j$ and reference input u_i, 2 x N for M_{tc}.
V	Loss function $V_N(u_i, \theta_j, y_0, y_j)$ (defined in (4))	Value computed from analytical expression using u_i, θ_j, y_0, and y_j over N steps. A scalar quantity.
$H_{i,j}$	Hessian of loss function $H(V_N(u_i, \theta_j, y_0, y_j))$ (defined in (6))	Derived from analytical expression of $V_N(u_i, \theta_j, y_0, y_j)$. Values computed over N steps. Dimension is d x d.
X_k	Eigenvectors of $H_{i,j}$	Dimension is d x 1.
λ_k	Eigenvalues of $H_{i,j}$	A scalar.
Λ_k	Ranking value for parameter k (defined in (8))	Computed from $H_{i,j}$ by ranking parameters by summing the 1-norm of the eigenvector projections scaled by their respective eigenvalues onto each parameter axis. A scalar quantity.
$\chi_{j,k}$	Candidate reduced parameter sets (k) for optimization from *a priori* parameter set θ_j	Computed from parameter rankings for all parameters in Θ. Dimension is d x d.

growth model analsis is based upon Liebig's Law of the Minimum, which states that plant growth is limited by the scarcest resource (van Ittersum and Rabbinge, 1997; van der Ploeg et al., 1999). The growth equations used here are based upon the Excel implementation by Burgess et al. (2014) without management interventions such as tree thinning and pruning (or the water and soil modules, as previously mentioned). See Fig. 2 for a graphical depiction of the tree-crop combination model with tree parameters listed in Table 2 and crop parameters in Table 3.

3.1. Yield-SAFE project's parameterization methods

Due to lack of input-output data for two-story agroforestry configurations, the Yield-SAFE developers have parameterized their model based on yield tables, other models (such as STICS, see Brisson et al., 2003), and field data for monocultures (single-species plantings) of the tree and crop species of interest. Van der Werf et al. (2007) described how parameters are determined through a two-step process

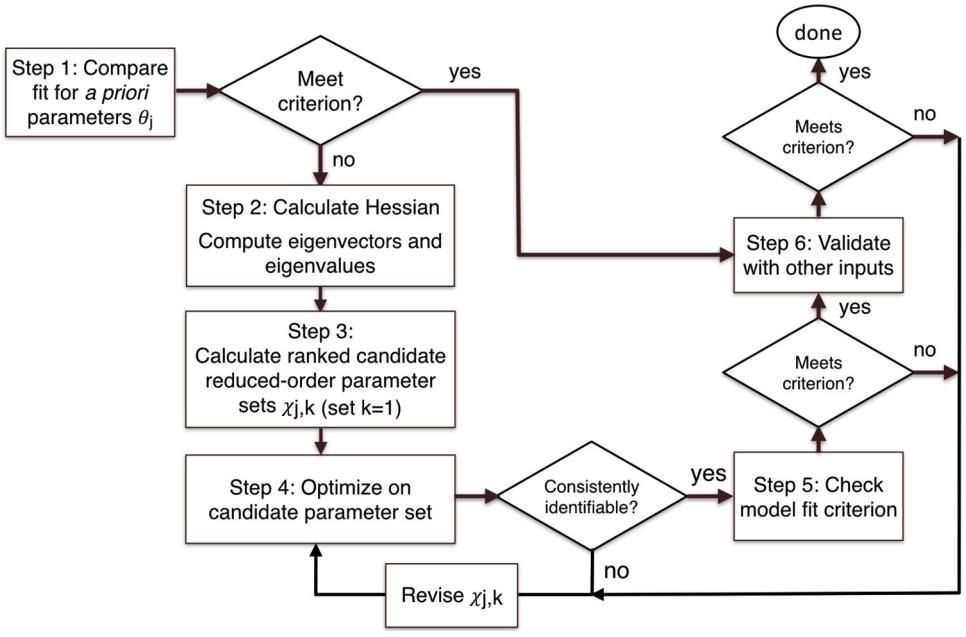

Fig. 1. The 6-step Hessian-informed reduced-order parameter estimation (HIROPE) procedure.

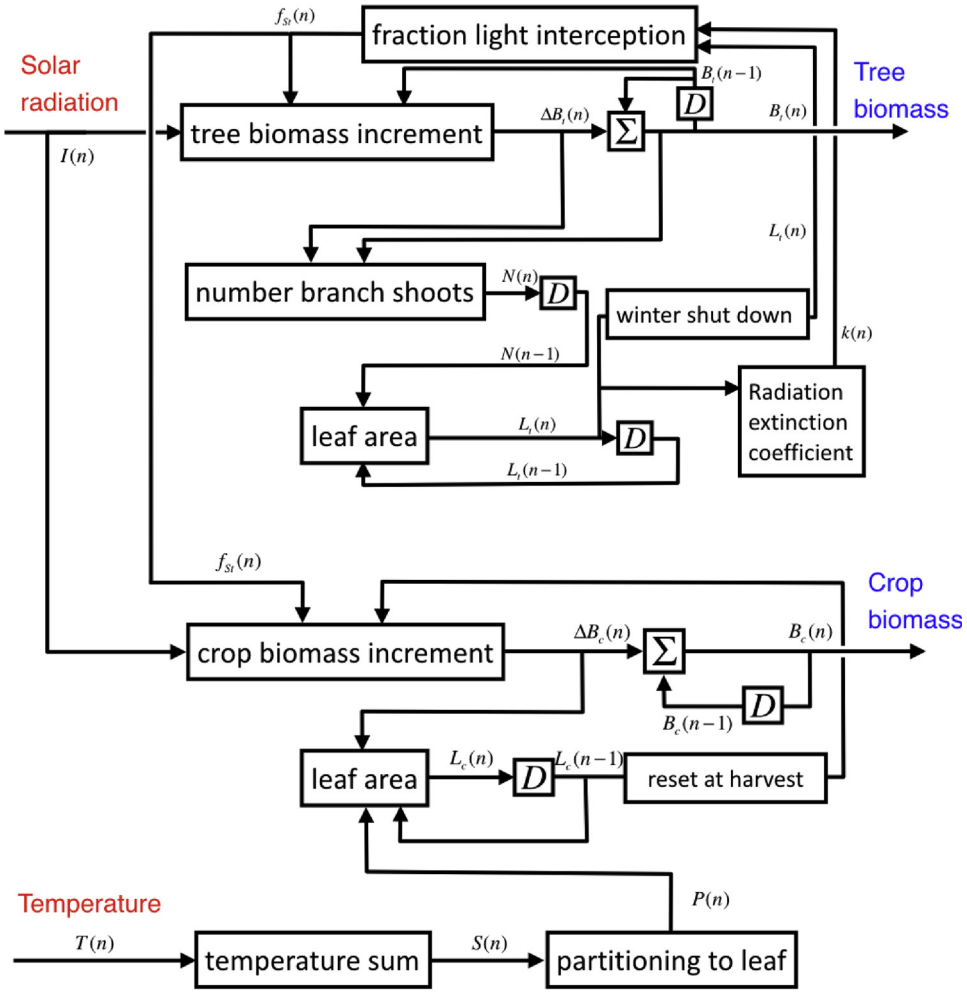

Fig. 2. Yield-SAFE tree-crop combination model, non-water-limiting case.

Table 2
Parameters used in Yield-SAFE tree growth model in the non-water limiting case and accepted parameter values given for poplar in Yield-SAFE Excel implementation (Burgess et al., 2014).

Symbol	Description	Units	Poplar1 (Graves 2010)
ε_t	Radiation use efficiency	g MJ^{-1}	1.4086
α	Attrition rate of standing biomass	day^{-1}	0.0001
L_m	Maximum leaf area	m^2	500
$B_t(0)$	Initial biomass per tree	g $tree^{-1}$	100
N(0)	Initial number of shoots per tree	$tree^{-1}$	0.6225
R	'Ratio' related to leaf and shoot maxima	–	200000
τ	Time constant of leaf area growth	days	10
k_t	Light extinction coefficient	–	0.8
k_a	Light extinction "a" coefficient	–	10
k_b	Light extinction "b" coefficient	–	0.4
DOYbudb	Day-of-year of bud burst	–	100
DOYleaff	Day-of-year of leaf fall	–	300
ρ	Tree stand density (user-assigned constant based on planting configuration)	trees m^{-2}	0.0156

1) Curve fitting to accepted yield tables for tree monocultures and accepted model yields for arable crop monocultures (using least squares optimization and manual adjustments).
2) Fine-tuning of certain parameters for a specific site based upon monoculture growth data.

In later publications regarding Yield-SAFE parameterization, no specific, reproducible methods for parameter estimation are given (Keesman et al., 2011; Palma et al., 2017). A reproducible procedure is presented here for determining a lower dimensional subspace for parameter estimation that may benefit model users who would like to parameterize the model for new crops and environments.

3.2. Inputs and validation

In order to acquire the needed input data, the Yield-SAFE developers draw on simulated climate data to drive their model, and have developed the web portal CliPick ("Climate Change Web Picker," http://home.isa.utl.pt/~joaopalma/projects/agforward/clipick/) to access climate data generated by a number of climate modeling projects (Palma, 2015, 2017; Palma et al., 2018a). The data sets available through CliPick include a number of future climate scenarios as well as climate data simulated based upon historical measurements of atmospheric aerosols (van Meijgaard et al., 2012). As Palma et al. (2017) state, "There are indications that the simulated climate can be used for calibration purposes with minor loss of quality in comparison to real data." The basis for using historical data to simulate climate data is documented in Lamarque et al. (2011). Various data sequences extracted from a historical climate scenario were used for the optimization and validation simulations conducted here (Table 4). Typical input-output sequences for a 20-year period are depicted in Fig. 3.

Table 3
Crop model parameters and initial conditions for the crop in the non-water limiting case (Burgess et al., 2014).

Symbol	Description	Units	Annual grass
ε_c	Potential growth	g MJ^{-1}	0.3
T_0	Temperature threshold	°C	0
P_0	Partition to leaves at emergence	–	0.8
S_1	T-sum at which partitioning starts to decline	°C days	1600
S_2	T-sum at which partitioning to leaves = 0	°C days	1840
σ	Specific leaf area	$m^2\,g^{-2}$	0.021
k_c	Radiation extinction coefficient	–	0.4
DOYsow	Day-of-year of sowing	–	−107
DOYharv	Day-of-year of harvest (if threshold not reached)	–	243
S_0	Temperature sum to emergence	°C days	150
S_h	Temperature sum to harvest	°C days	3200
$B_c(0)$	Initial crop biomass	g m^{-2}	0
$L_c(0)$	Initial leaf area	$m^2\,m^{-2}$	0.1

Table 4
Input sequence source from Norwich, UK (Lat: 52.6628 Long: 1.2283) used for simulations. All data were imported through the CliPick portal.

Symbol	Source data set	Start date	Length (days)
$u_{1,1}$	Hist KNMI-RACMO22E	31-12-51	7306
$u_{1,2}$	Hist KNMI-RACMO22E	31-12-66	7306
$u_{1,3}$	Hist KNMI-RACMO22E	31-12-86	7306
$u_{1,4}$	A1B - HadCM3Q0	31-12-51	7306
$u_{1,5}$	A1B - HadCM3Q0	31-12-71	7306

3.3. Yield-SAFE model implementation and parameter estimation

The tree and crop combination growth model was implemented in the MATLAB® System Identification Toolbox™ to take advantage of advanced optimization routines and the ability to easily run multiple simulations. Nominal parameters θ_0 for poplar and annual grass (Tables 2 and 3) and input $u_{1,1}$ (Table 4 model object defined the model equations and the nlgreyest parameter estimation function was used with the default optimization settings. The default optimization algorithm used is the Trust-Region Reflective Newton method for nonlinear least-squares (Ljung, 2018).

The analytic Hessian was derived from the cost function expression (see Elevitch, 2018 for full details). A twice continuously differentiable symbolic expression for the cost was first coded in MATLAB, using approximations for discontinuous functions in the growth equations where necessary. The Hessians of the symbolic cost function expressions (for a certain time step) were then derived using MATLAB's hessian function with respect to the parameters of interest. The eigenstructure of the calculated Hessian for the nonlinear models was determined using the eig function.

3.4. HIROPE applied to Yield-SAFE combination model

Application of the HIROPE procedure to the separate tree and crop models is presented in detail in Elevitch (2018, Chapter 3). Here we present the main results for the combined tree and crop model (in the non-water limited case). For the example presented here, the *a priori* parameter values θ_1 are set –5 % away from their nominal values (Table 5).

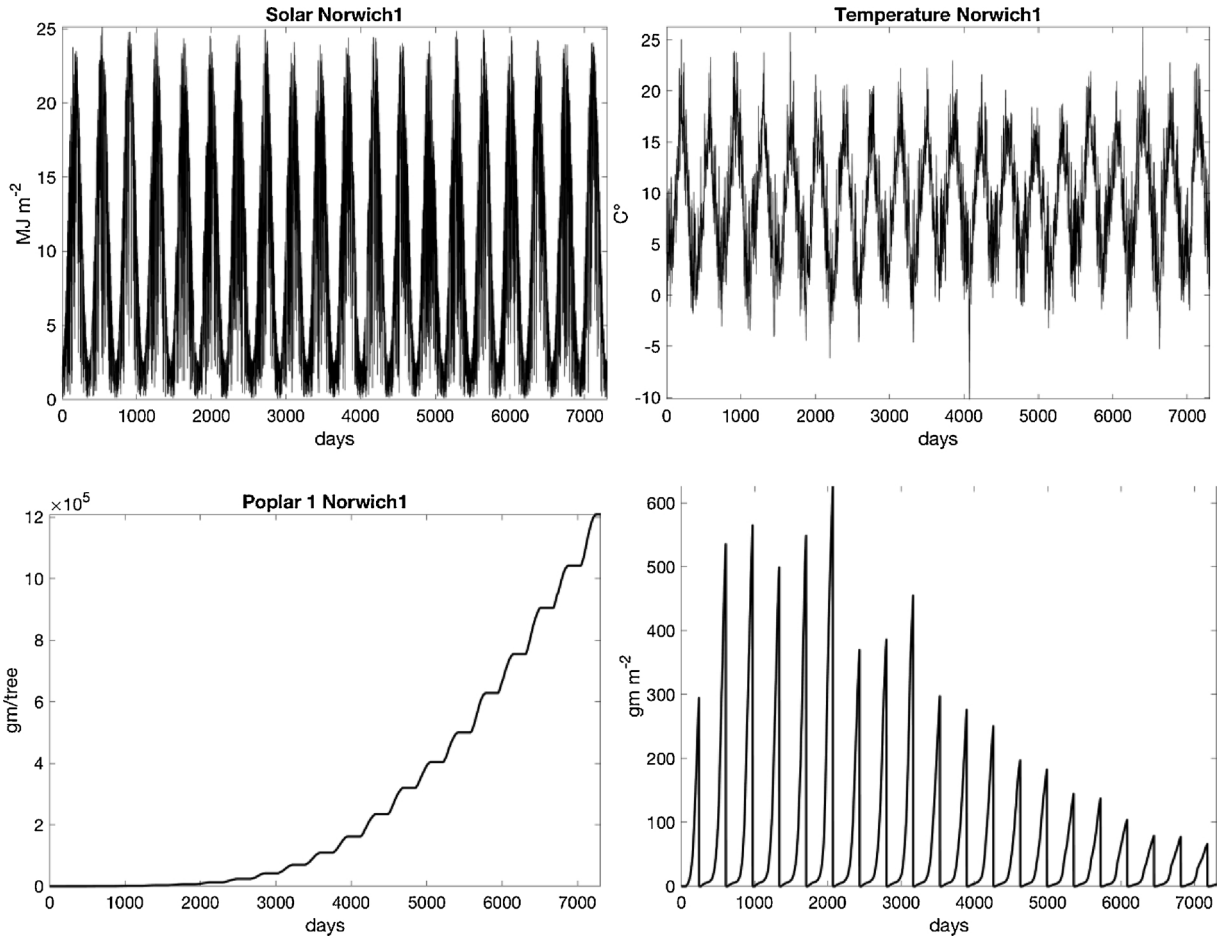

Fig. 3. Solar radiation and temperature inputs $u_{1,1}$ (top), and combination model outputs y_0 for tree growth (bottom left) and crop growth (bottom right) with θ_0 for Poplar and annual grass.

Table 5
Nominal parameters θ_0 and *a priori* settings θ_1 for combination model.

Tree Parameters	Units	θ_0	θ_1	Crop Parameters	Units	θ_0	θ_1
ε_t	g MJ^{-1}	1.4086	1.33817	ε_c	g MJ^{-1}	0.3	0.285
α	day^{-1}	0.0001	0.000095	T_0	°C	0.5	0.475
L_m	m^2	500	475	P_0	–	0.8	0.76
$B_t(0)$	g $tree^{-1}$	100	95	S_1	°C days	1600	1520
N(0)	$tree^{-1}$	0.6225	0.591375	S_2	°C days	1840	1748
R	–	200000	190000	k_c	–	0.4	0.38

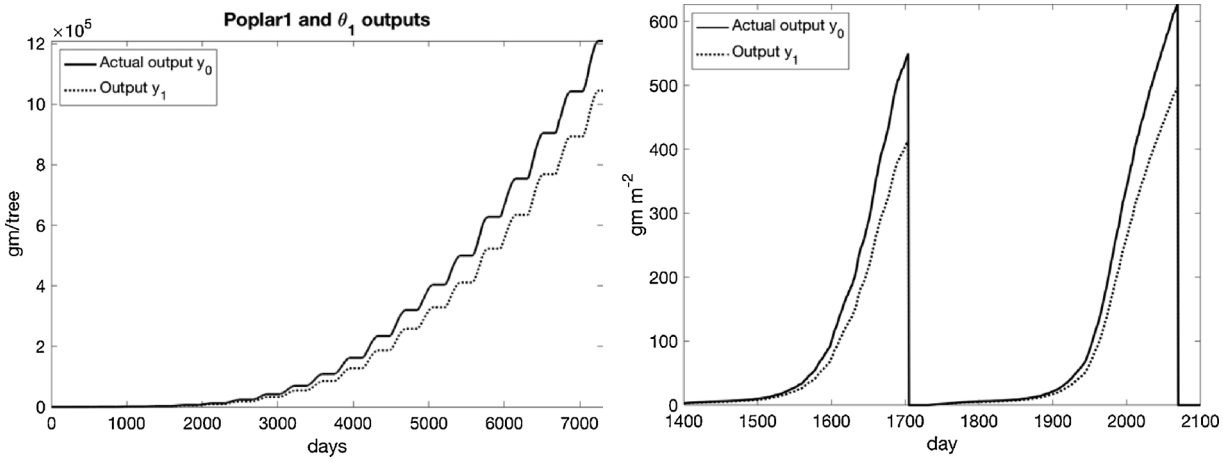

Fig. 4. Outputs y_0 and y_1 for tree (left) and crop (right, n = 1400–2100) models driven by $u_{1,1}$. The NRMSE values are 79.09 % and 73.45 %, respectively, indicating parameter must be adjusted to achieve an acceptable fit.

Table 6
Eigenvectors and eigenvalues of the Hessian**Error! Reference source not found.**. The eigenvector directions X_i are labelled according the parameter axes, ordered by their relative eigenvalues (in absolute value) λ_i.

	Eigenvalue					
	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6
	−7.25e+05	6.61e+05	1.52e+05	9.38e+04	−3.28e+04	1.72e+03
	Eigenvector					
Axis	X_1	X_2	X_3	X_4	X_5	X_6
ε_t	−0.3786	0.8203	−0.0001	0.4257	−0.0003	−0.0000
R	0.8749	0.1659	−0.0000	0.4521	0.0022	−0.0000
L_m	−0.3020	−0.5469	−0.0001	0.7791	0.0019	−0.0000
k_c	0.0008	−0.0005	−0.8790	0.0010	−0.4764	0.0069
ε_c	0.0013	−0.0008	0.4767	0.0021	−0.8788	0.0037
α	−0.0102	−0.0227	0.0000	−0.0862	−0.0002	0.0000
S_2	0.0000	−0.0000	−0.0050	0.0000	−0.0135	−0.6487
S_1	0.0000	−0.0000	−0.0041	−0.0000	−0.0155	−0.5327
P_0	0.0000	−0.0000	−0.0021	−0.0000	−0.0192	0.5435
$B_t(0)$	0.0005	0.0002	−0.0000	0.0060	−0.0001	−0.0000
N(0)	−0.0005	−0.0002	0.0000	−0.0061	0.0001	0.0000
T_0	0.0000	−0.0000	−0.0000	0.0000	−0.0000	−0.0003
	Eigenvalue					
	λ_7	λ_8	λ_9	λ_{10}	λ_{11}	λ_{12}
	−7.15e+02	−6.25e+02	4.54e+02	−2.93e+02	2.80e+02	8.76e-09
	Eigenvector					
Axis	X_7	X_8	X_9	X_{10}	X_{11}	X_{12}
ε_t	−0.0000	0.0058	0.0116	−0.0000	−0.0501	−0.0000
R	−0.0001	0.0065	0.0111	0.0000	−0.0504	−0.0000
L_m	−0.0001	0.0078	0.0100	0.0000	−0.0507	−0.0000
k_c	0.0173	0.0001	−0.0001	−0.0034	−0.0000	0.0000
ε_c	0.0213	0.0002	−0.0001	−0.0032	−0.0000	0.0000
α	−0.0001	0.0582	0.2687	−0.0000	−0.9573	−0.0000
S_2	−0.2213	−0.0002	0.0000	0.7280	0.0000	0.0003
S_1	−0.5508	−0.0006	0.0000	−0.6424	0.0000	0.0003
P_0	−0.8043	−0.0009	0.0001	0.2395	0.0000	−0.0000
$B_t(0)$	0.0011	−0.9944	−0.0684	0.0000	−0.0802	−0.0000
N(0)	−0.0002	0.0873	−0.9606	0.0000	−0.2637	−0.0000
T_0	−0.0002	−0.0000	0.0000	−0.0000	0.0000	−1.0000

Table 7
Λ_i values and their associated ranking based upon Hessian eigenstructure.

Ranking	Parameter	Submodel	Λ
1	ε_t	tree	8.57e+05
2	R	tree	7.86e+05
3	L_m	tree	6.54e+05
4	k_c	crop	1.50e+05
5	ε_c	crop	1.03e+05
6	α	tree	3.09e+04
7	S_2	crop	2.69e+03
8	S_1	crop	2.64e+03
9	P_0	crop	2.53e+03
10	$B_t(0)$	tree	1.77e+03
11	N(0)	tree	1.67e+03
12	T_0	crop	1.44e+00

3.4.1. Step 1 compare goodness-of-fit of y_0 with the estimated output y_1

For this 2-output model, each output is compared with the reference. The goodness-of-fit measures are well below the cut-off of 99 % (Fig. 4).

3.4.2. Step 2 Compute $H_{i,j}$ and its eigenvectors and eigenvalues

Parameter scaling was employed prior to differentiation and the analytic Hessian with respect to the 12 parameters of interest was derived using MATLAB's hessian function. The average Hessian calculated for N = 5475 (15 years) was calculated, with its eigenvalues and eigenvectors given in Table 6.

3.4.3. Step 3 generate Λ parameter ranking

Based on Table 6 and Eq. (8), the Λ values and associated parameter ranking for θ_1 setting are shown in Table 7.

This leads to a set of candidate parameter vectors $\chi_{1,k}$ for estimation (Table 8).

3.4.4. Step 5 check goodness-of-fit of y_0 and $\hat{y}_1$

To compress the procedure steps for presentation here, the optimization algorithm was run from θ_1 for the first seven $\chi_{1,k}$ and the model fit for each was evaluated. Fig. 5 shows the goodness-of-fit measure NRMSE for the first seven $\chi_{1,k}$. Both outputs meet the > 99 % fit criterion for $\chi_{1,5}$–$\chi_{1,7}$. Since the reduced-order set $\chi_{1,7}$ gives a bigger margin above 99 %, we proceed with this optimized parameter set.

3.4.5. Step 4 confirm consistent identifiability

$\chi_{1,7}$ has seven estimated parameters, therefore, consistent identifiability is tested from 2^7 or 128 *a priori* ± 5 % variations of the θ_1 parameter values. All estimates converge to the same location $\hat{\hat{\theta}}_1$ within 0.00464 %, as shown in Table 9. This confirms consistent identifiability for $\chi_{1,7}$.

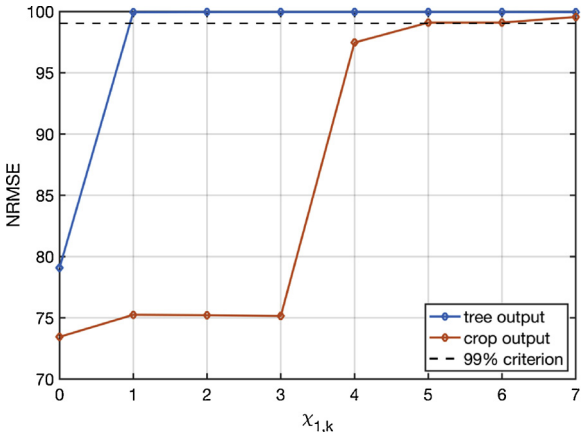

Fig. 5. NRMSE values for unoptimized parameters (shown at 0) and the first seven $\chi_{1,k}$ optimized parameter sets. Both outputs meet the > 99 % criterion for $\chi_{1,5}$–$\chi_{1,7}$.

Table 9
Step 4 for the first three candidate parameter sets.

	Units	Optimized on $\chi_{1,7}$	*A priori* values	Nominal
		$\hat{\hat{\theta}}_1$ (for all 128 a priori sets with ± 5% values)	θ_1	θ_0
Max % param. diff.		0.00464 %	–	–
ε_t	g MJ^{-1}	1.3860	1.3382	1.4086
α	day^{-1}	9.0478e-05	9.5000e-05	0.0001
L_m	m^2	495.86	475.00	500
$B_t(0)$	g $tree^{-1}$	95	95	100
N(0)	$tree^{-1}$	0.59137	0.59137	0.6225
R	–	189840	190000	200000
ε_c	g MJ^{-1}	0.30055	0.28500	0.3
T_0	°C	0.475	0.475	0.5
P_0	–	0.76	0.76	0.8
S_1	°C days	1520	1520	1600
S_2	°C days	2060.7	1748	1840
k_c	–	0.41551	0.38	0.4
NRMSE tree		99.96 %	79.09 %	100 %
NRMSE crop		99.51 %	73.45 %	100 %

3.4.6. Step 6. Validation

Validation of $\hat{\hat{\theta}}_1$ with other four other inputs from the test location was successful (Table 10).

3.4.7. Comprehensive ranking all 4096 θj

To systematically extend the analysis to the space around θ_1, Λ_k are calculated for all 2^{12} (4096) combinations of *a priori* parameters set at ± 5 % of their nominal values. Table 11 shows the parameter

Table 8
$\chi_{1,k}$ candidates for reduced-order parameter estimation for combination model.

Par.	Sub-model	$\chi_{1,1}$	$\chi_{1,2}$	$\chi_{1,3}$	$\chi_{1,4}$	$\chi_{1,5}$	$\chi_{1,6}$	$\chi_{1,7}$	$\chi_{1,8}$	$\chi_{1,9}$	$\chi_{1,10}$	$\chi_{1,11}$	$\chi_{1,12}$
ε_t	tree	X	X	X	X	X	X	X	X	X	X	X	X
R	tree		X	X	X	X	X	X	X	X	X	X	X
L_m	tree			X	X	X	X	X	X	X	X	X	X
k_c	crop				X	X	X	X	X	X	X	X	X
ε_c	crop					X	X	X	X	X	X	X	X
α	tree						X	X	X	X	X	X	X
S_2	crop							X	X	X	X	X	X
S_1	crop								X	X	X	X	X
P_0	crop									X	X	X	X
$B_t(0)$	tree										X	X	X
N(0)	tree											X	X
T_0	crop												X

Table 10
Fit measures with validation inputs from the test location for $\hat{\hat{\theta}}_1$ optimized on $\chi_{1,7}$.

		Tree model output		Crop model output	
Input	Use	NRMSE	Cost $g^2\ tree^{-2}$	NRMSE	Cost $g^2\ m^{-2}$
$u_{1,1}$	Optimization	99.96 %	5.3672e+04	99.51 %	4.5973e-01
$u_{1,2}$	Validation	99.93 %	9.2455e+04	99.50 %	5.0933e-01
$u_{1,3}$	Validation	99.96 %	3.4066e+04	99.41 %	7.7433e-01
$u_{1,4}$	Validation	99.81 %	5.1725e+05	99.09 %	9.7463e-01
$u_{1,5}$	Validation	99.77 %	6.6030e+05	99.06 %	9.8339e-01

rankings across all parameter sets. The top six parameters are the same for 4091 of 4096 θ_j (with k_c and $B_t(0)$ switching places 5 times), suggesting robustness of parameter choice for the highest-ranking parameters. The rankings of the next five lower ranked parameters are mixed. The lowest ranked parameter is the same for all θ_j.

It is interesting to note that OAT parameter sensitivity analysis carried out by the Yield-SAFE modelers led to somewhat different results. Of the 12 model parameters considered here, Keesman et al. (2011) found tree model ε_t, L_m, and N(0) to be dominant, while ε_c and k_c were dominant for the crop model. Of these five parameters, four are in the top five ranking carried out through the HIROPE procedure. Parameter N(0) is one of the lowest ranked parameters according to our analysis. It should also be noted that the Keesman et al. (2011) OAT analysis was carried out on data for monocultures of trees and crops, rather than trees and crops grown together in a multistrata planting, which may account for the difference in results.

Figs. 6 and7 show graphically the Λ_i values for the top eight ranked parameters (selected by the previous analysis of θ_1).

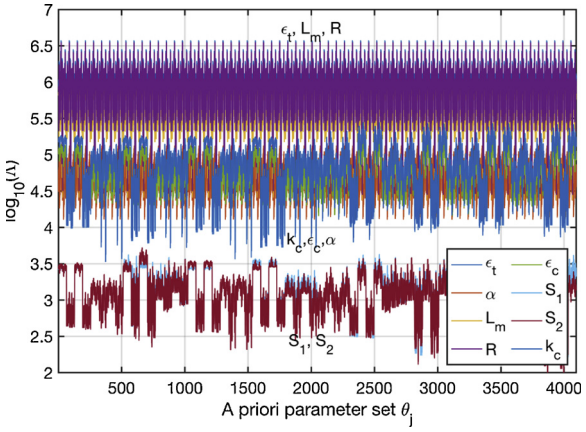

Fig. 6. The Λ_k values ($\log_{10}$ scale) for the highest ranked six parameters of the combination model are consistent across all 4096 *a priori* estimates θ*j*.

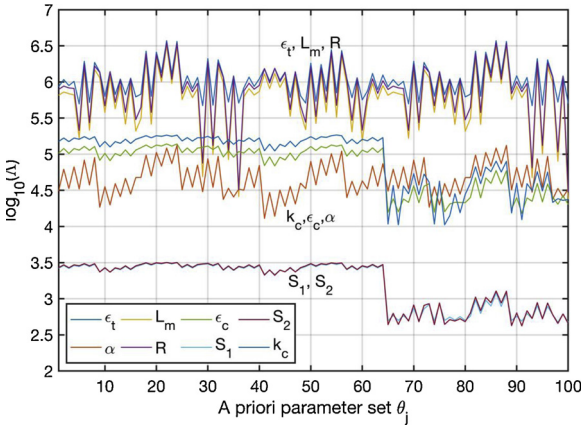

Fig. 7. 6 (Close up of Fig. 6) Λ_k for highest ranked six parameters of the combination model across 100 *a priori* estimates θ*j*.

4. Conclusions

Reduced-order parameter estimation based on the Hessian of the cost function in this early investigation uses foundational systems theory, straightforward mathematics, and off-the-shelf simulation and optimization software, and is by no means a state-of-the-art implementation. Rather, the research presented here is meant to illustrate the value of *a priori* investigation of parameter identifiability through a conceptual framework. The potential of a systematic, reproducible approach to determining the importance of parameters in a complex model illuminates an area of model development that can otherwise be shrouded in guesswork and trial-and-error. Although the OAT analysis by the Yield-SAFE modelers led to somewhat similar ranking of the most important parameters (Keesman et al., 2011), the HIROPE procedure gives a higher confidence in the ranking as it accounts for the effects of simultaneous changes in multiple parameters, while also adding confirmation of consistent identifiability.

Initial tests of the HIROPE procedure on the Yield-SAFE model described here gave a consistent parameter ranking in the neighborhood of a nominal setting for the 12-parameter, non-water limiting tree-crop combination model. Additional investigation is needed to test the procedure on more complex implementations of Yield-SAFE (with other connecting submodels included) and with other plant growth models before any definitive conclusions can be made about the applicability of HIROPE. Further refinement of the procedure will be needed. Additionally, the definition of the ranking metric Λ proposed here proved to be an effective measure for relative parameter influence on the cost function, however, this formulation deserves further study, especially as the number of parameters increases. Also, as the number

Table 11
Occurrence of parameter ranking for all 4096 *a priori* estimates θ*j*.

		Ranking											
Par.	Sub-model	1	2	3	4	5	6	7	8	9	10	11	12
ε_t	tree	4096	0	0	0	0	0	0	0	0	0	0	0
R	tree	0	3967	61	28	40	0	0	0	0	0	0	0
L_m	tree	0	0	3925	65	58	48	0	0	0	0	0	0
k_c	crop	0	113	42	2560	914	462	0	5	0	0	0	0
ε_c	crop	0	0	60	84	2375	1577	0	0	0	0	0	0
α	tree	0	16	8	1359	709	2004	0	0	0	0	0	0
S_2	crop	0	0	0	0	0	0	481	386	1253	1285	691	0
S_1	crop	0	0	0	0	0	0	892	534	1793	626	251	0
P_0	crop	0	0	0	0	0	0	110	528	718	822	1918	0
$B_t(0)$	tree	0	0	0	0	0	5	2283	476	162	868	302	0
N(0)	tree	0	0	0	0	0	0	330	2167	170	495	934	0
T_0	crop	0	0	0	0	0	0	0	0	0	0	0	4096

of model parameters increases, the Hessian computational demand increases quadratically. An iterative or 'successive' method of reducing the number of parameters for the analysis such as suggested by Cox et al. (2006) may be considered.

The procedure proposed here is only a small part of model development (although it does involve a considerable amount of work). Real data are required to validate model predictions and give a model credibility. Even more important, one should confirm which output measurements are needed for model parameterization before undertaking field study. Analysis of consistent identifiability such as that included in HIROPE may suggest which output measurements are needed for parameter identification.

Author contributions

This article presents portions of C.R.E.'s PhD dissertation carried out with guidance of C.R.*J*. C.R.E. and C.R.*J*. designed the research; C.R.E. performed the research, conducted simulations, and analyzed the data; and C.R.E. and C.R.*J*. wrote the paper.

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Declaration of Competing Interest

None.

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