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A FRAMEWORK FOR UNCERTAINTY EVALUATION AND ESTIMATION IN DETERMINISTIC AGRICULTURAL MODELS

Esther Meenken[1], David Wheeler[2], Martin Espig[1], Hamish Brown[3], Edmar Teixeira[3], Chris Triggs[4]

[1]AgResearch, Lincoln Research Centre
1365 Springs Road, Private Bag 4749, Lincoln 7608
esther.meenken@agresearch.co.nz
[2]AgResearch, Ruakura Agricultural Centre
Private Bag 3123, Hamilton 3240
[3]Plant and Food Resesarch, Canterbury Agriculture & Science Centre,
Private Bag 4704, Lincoln 7608
[4]The University of Auckland,
Private Bag 92019, Auckland 1142

Abstract

If decisions are made without adequate acknowledgment of uncertainty, the chance of undesirable outcomes are either understated or overlooked. There has been increasing recognition that uncertainty in deterministic model results needs to be systematically considered and this includes understanding the environment in which the model operates, and that the sources of uncertainty and the reasons for the uncertainty are identified. We present a system for quantitative uncertainty evaluation (UE) that facilitates exploration of how the components of a model contribute together to the overall model output uncertainty. A key aspect is a structure that classifies the types of uncertainty that can be introduced by each model component. A systematic sequence of tasks is used to carry out a case-study. This formal structure and systematic sequence for quantitative uncertainty evaluation provides a common language for what a UE encompasses, and a starting point for carrying out such an evaluation. Identifying and discussing components of uncertainty provide an opportunity to target resources to reduce the overall size of uncertainty.

Introduction

Biophysical agricultural models are used to inform and support farm-level decision making, agronomic research, breeding strategies, and government policy (Rosenzweig, Jones et al. 2013). Colloquially known as crop models, they are simplified mathematical representations of physiological and physical processes that occur in plants (e.g. leaf appearance rates) and soils (e.g. mineralization of N) in response to environmental (e.g. temperature and rainfall) and management (e.g. sowing dates and irrigation) drivers. Crop models can be integrated into wider decision making tools such as catchment tools or applied to areas of food security and climate change impact and adaptation assessments (Boote, Jones et al. 1996, Sinclair and Seligman 2000, Jamieson, Brooking et al. 2007, Cooper, van Eeuwijk et al. 2009, Hochman, Van Rees et al. 2009, Bezlepkina, Adenäeur et al. 2010, Teixeira, Fischer et al. 2013, Holzworth, Huth et al. 2014).

These models have multiple forms of uncertainty that are inherent in the way that they are built, how they run and how they are used. There has been increasing recognition that:

1. The impact of uncertainty on deterministic model results needs to be systematically considered to ensure outcomes derived from model estimates can be achieved,
2. An assessment of uncertainty in its widest sense also means understanding the

environment in which the model operates, and
3. The sources of uncertainty AND the reasons for the uncertainty need to be identified.

(Refsgaard, Henriksen et al. 2005, McFarland 2008, Guillaume 2011, Wallach, Makowski et al. 2014, Meenken, Triggs et al. 2015, Uusitalo, Lehikoinen et al. 2015)

When uncertainty in a deterministic model is discussed, uncertainty is often due to both quantitative and qualitative sources. The focus of this paper is on quantitative uncertainty evaluation. For a discussion of some other types of uncertainties to consider see (Espig, Finlay-Smits et al. 2020, Wheeler, Meenken et al. 2020). Quantifiable uncertainties include[1]:

1. Input parameter uncertainty (e.g. soil type, nitrogen amount, etc.),
2. data uncertainty (e.g. weather data) (Sharifi, Meenken et al. 2020),
3. scaling/aggregation uncertainty (model used at a scale it was not calibrated for),
4. structural uncertainty (e.g. deliberate simplification or incomplete understanding of real world processes),
5. epistemic uncertainty (intrinsic, random variation of a real-world process even when the conditions are fully specified),
6. unknown unknowns,

(e.g. (O'Hagan, Kennedy et al. 1999, Kennedy and O'Hagan 2001, Katz 2002, Spiegelhalter and Best 2002, O'Hagan 2006, Cressie and Wikle 2011, Gupta, Clark et al. 2012).

The development of methods to quantify uncertainty in deterministic models is an active area of research and many tools are in common use including statistical objective functions, multi-model ensembles, sensitivity analysis and emulators (Saltelli, Chan et al. 2000, Gauch, Hwang et al. 2003, O'Hagan 2006, Asseng, Ewert et al. 2013, Wallach, Makowski et al. 2014, Teixeira, Brown et al. 2015). Which techniques will provide most insightful will vary depending on the objectives and specific properties of the model, and there is no single technique that can fully quantify all these types of uncertainties. In most situations, a selection of techniques will likely be helpful and should be combined to provide a heuristic view of the model, and even simply describing these uncertainties can provide a more complete picture of the information the model provides to decision makers. To make UE cleaner and easier to achieve, in this paper we outline a UE framework that carefully and systematically builds up information, objectives and analyses.

Definitions of model components

We identified five key components in a deterministic model. These were:

State equations Z which define the processes that make up the model, representing either experimentally derived relationships or theoretical constructs. State equations are mathematical equations that describe the underlying scientific processes of the model. Although the coefficients of these equations may have been derived via a calibration process during the model building phase (O'Hagan 2006), these coefficients and the equations to which they relate are distinct from the input parameters as they are usually constant for all scenarios under which

[1] Some qualitative sources of uncertainty include bug fixes, improved methodologies, the addition of new features; when the model is a 'black box' (e.g. when model is not fully disclosed); user error (e.g. inaccurate input information) and when the model doesn't reflect the way users such as farmers see their system.

the model might be expected to simulate crop responses. For example, the thermal-time calculation used to drive phenological development of lucerne (Teixeira, Moot et al. 2009) or the vernalisation requirement for wheat (Brooking 1996).

Independent input information to the model that does not change during the development of the crop is denoted as θ. Examples of input parameters in an agricultural setting could be soil type, cultivar or other 'scenario' indicators as considered by Teixeira, Brown et al. (2015) and Holzkämper and Klein et al. (2015). These are typically the inputs a user can manipulate.

Time varying environmental or managerial inputs such as temperature, rainfall and/or irrigation are represented by E_t. This may link to database information that is accessed as directed by the user.

Response or calibration data, possibly for multiple variables and/or scenarios, is denoted (C_t). This represents the situation when data is available that can be used to directy assess simulated outputs. This could be available only as a single vector outcome (e.g. yield at the end of the simulation process for a selection of scenarios) or the outcome from a single scenario. C_t is distinct from data used during the model building phase to construct the Z. It can be thought of as test data or independent validation data. In the case study below, C_t acts within the modelling process itself upon the estimated real, unknown target quantity r_t, for example during data assimilation (Gordon, Salmond et al. 1993, Thacker and Lacey 1996, Lewis, Lakshmivarahan et al. 2006, Bulygina and Gupta 2009, Candy 2009, Cressie and Wikle 2011). Note that data used to describe mechanisms and validate the model are also present in the framework via their contribution toward Z.

Residual variation (ε) between the prediction and the real world that remains once the model and data have been considered. This can include both aleatory uncertainty and the unknown unknowns.

Thus the real world (r) at time (t) is represented by the model $f(\bullet)$ which has the above components[2], such that:

$$r_t = f((g(Z, \theta, E_t), C_t)\varepsilon) \tag{1}$$

Each of these components have an uncertainty associated with them. This model can be implemented using a Bayesian approach to estimate target measures (discussed below). In order to carry out most UE tasks this full implementation to Bayesian modelling is not needed, but this framing of the problem is invaluable when considering what could/should be considered, and how the tasks relate to each other, the model and the other available resources.

Case-study

The Wheat Development Model SIRIUS.

The crop model SIRIUS (Brooking, Jamieson et al. 1995, Jamieson, Brooking et al. 1995, Jamieson, Brooking et al. 1995, Brooking 1996, Jamieson, Brooking et al. 1996, Jamieson, Semenov et al. 1998a, Jamieson, Brooking et al. 1998b) is summarised by He, Le Gouis et al. (2012). SIRIUS is a dynamic, deterministic computer simulation model for representing the phenological development of a wheat plant through time as realised by the number of fully extended leaves. It has a discrete nature such that on each day there is a well-defined set of states by which each state variable may either remain in its current state or update according to environmental cues. The sub-model used in this example applies only to spring wheat. State equations Z are used to predict the (observable) state variable leaf number (ln_t) on day t based

[2] Details in a journal paper currently in preparation

on calculations that simulate the rate of leaf appearance (*phyllochron*$_t$), number of organs (*primordia*$_t$) and the possible final number of leaves given daylength and developmental progress ($flnt_t$, fln_t). $t = 1$ is the day the grain is sown, as this is the stage at which its apical meristem germinates and becomes sensitive to temperature. SIRIUS simulates the plant's development based on mean daily environmental information. The simulations depend on input parameters θ that describe cultivar specific characteristics and responses to environmental signals, and observable environmental information E_t where TT = mean daily thermal time and PP = daily photoperiod. He, Le Gouis et al. (2012) describe how, for spring wheat, the state equations, environmental data and input parameters simulate the effects of thermal time and photoperiod to express vegetative development. The state equations (5) – (9) are

$$ln_t = \min(fln_{t-1}, \frac{TT_t}{phyllochron_t} + ln_{t-1}) \quad (2)$$

$$phyllochron_t = b * bp \quad (3)$$

where $b = \begin{cases} 0.75 \; if \; ln_t \leq 2 \\ 1 \;\; if \; ln_t > 2 \leq 8 \\ 1.3 \; if \; ln_t > 8 \end{cases}$,and *bp* is a cultivar specific value for baseline phyllochron (the rate of leaf development at 2–8 leaves).

$$flnt_t = lmin + (ps * (ppsat - PP_t) * s) \quad (4)$$

where $s = \begin{cases} 1 \; if \; PP_t \leq ppsat \\ 0 \; otherwise \end{cases}$ and *ps* and *ppsat* are cultivar specific values for rate of development in response to photoperiod the photoperiod at which full response occurs.

$$primordia_t = pe + pn * ln_t \quad (5)$$

where *pe* is the number of primordia in the seed at sowing and *pn* is the number of primordia present in the meristem on per leaf basis.

$$flnt_t = \begin{cases} \min\left(flnt_t, primordia_t\right) if \; primordia_t < \left(flnt_{t-1} + pe\right) \\ fln_{t-1} otherwise \end{cases} \quad (6)$$

where each state variable excepting ln_t is treated as an unobservable latent variable throughout the day to day simulation of the wheat plant development. At the completion of the vegetative development phase, the state variable fln_t is observable once the onset of spikelets is seen.

UE sequence of tasks

A simple UE was developed using a sequence of tasks to provide uniform information about deterministic model uncertainty[2]. This may be beneficial to modellers as well as users of models who seek to understand the source of uncertainty. Tasks may be carried out in a sequence as described next, with some analysis details and figures below:

1. *State objectives:* The objective is to provide robust, data-driven credible intervals. This could be achieved by fitting a Bayesian data assimilation model to explore not only whether the model ends up with accurate estimates of flag leaf date, but also whether it correctly simulates the development of each leaf through time. This should help provide prediction and credible intervals that use multiple sources of information including the model, expert opinion and data. The model is visualised in Figure 2.

2. *Identify model components:* Table 1 summarises the state variables, input parameters, and observed variables in SIRIUS as described above. It also acknowledges the presence of aleatory uncertainty.
3. *Curate available information:* Data, expert opinion, and other quantitative and qualitative information can both *inform* and *describe* how each model component may introduce uncertainty to model simulations (Table 2). If no information is available this is immediately clear.
4. *Confirm/redefine objectives:* With the current data and a Bayesian data assimilation model we should be able to achieve the objective.
5. *Generate and analyse data:* A brief outline of the analysis is discussed below.
6. *Visualise and communicate results:* See Figure 3 and discussion next.

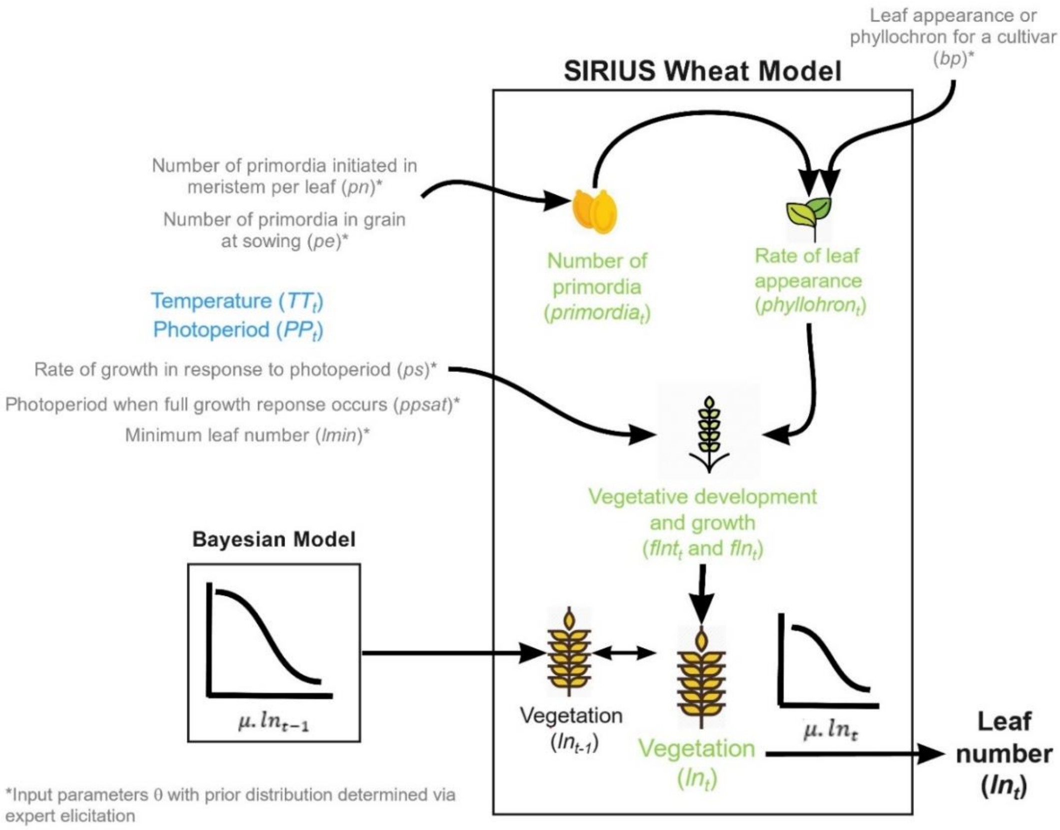

Figure 1: Visualisation of Bayesian Model for SIRIUS

Table 1: Model components and types and sources of uncertainty for SIRIUS[3]

Input Parameter	Observed Data		Structural		Remaining variation
	Calibration Data	Environmental/ Management Data	Model Form	State Equation	
θ	C_t	E_t	*g()*	Z_t	ε
ps	LN_t	PP_t	*relationship between inputs, e.g. could be visualised by a model wiring diagram.*	$phyllochron_t$	*inherent randomness*
ppsat		TT_t		$primordia_t$	*unknown unknowns*
lmin				$flnt_t$	
pn				fln_t	
pe				ln_t	
bp					

Table 2: Component specific information

Model Component	How uncertainty might be introduced	How uncertainty might be evaluated	Quantitative and Qualitative Information		
			State-space identification	Data	Expert Opinion
Appropriate values for input parameters		This information can be used in sensitivity analysis to assess potential model outcomes and the sensitivity of the model to changes in cultivar due to base phyllochron (*bp*).	$r = f(Z_t, \boldsymbol{\theta}, E_t, C_t, \varepsilon)$		There is expert opinion regarding the correct value of *bp* for different cultivars, ranging from 90-110.
Measured data with which to update or assess model simulations	Scaling, aggregation, bias, sampling and other types of measurement uncertainty. Aleatory uncertainty may or may not be able to be differentiated from measurement uncertainty.	Calibration, validation, verification and data assimilation can provide information around how well the simulated data reflects the measured data. Measurement error and aleatory uncertainty tied up in statistics such as rmse's, standard errors or credible intervals.	$r = f(Z_t, \theta, E_t, \boldsymbol{C_t}, \boldsymbol{\varepsilon})$	Measured observations of flag in Southland crops for one cultivar are available.	
Measured data with which to update or assess model simulations	Same as above	Same as above but information is available through time rather than at a single point.	$r = f(Z_t, \theta, E_t, \boldsymbol{C_t}, \varepsilon)$	Measured observations of LN at weekly intervals under climate controlled conditions are available	
Real world environmental data indicating appropriate values for model input information.	Sensor uncertainty such as bias or precision problems, distance from weather station to crop, aggregation.	Sensitivity analysis.	$r = f(Z_t, \theta, \boldsymbol{E_t}, C_t, \varepsilon)$	Weather station data in Lincoln, Canterbury, New Zealand from 1950-present are available	
A potential missing mechanism	Lack of understanding; ignorance.		$r = f(\boldsymbol{Z_t}, \theta, E_t, C_t, \varepsilon)$		The developmental phase between imbibition and emergence may not be correctly specified.
Could be either an incorrect model specification of input information	$\boldsymbol{Z_t}$: Lack of understanding of mechanism in a novel environment. $\boldsymbol{E_t}$ Incorrect environmental data.	$\boldsymbol{Z_t}$ The importance of structural uncertainty can be explored via sensitivity analysis by e.g. introducing a random component to model runs.	$r = \boldsymbol{f}(\boldsymbol{Z_t}, \boldsymbol{\theta}, \boldsymbol{E_t}, C_t, \varepsilon)$	Simulated data for wheat grown in Southland, New Zealand, consistently underestimates the time of anthesis	

[3] Note the use of italics for all parameters and variables, the use of lower case for state variables and input parameters, and the use of upper case for observed variables.

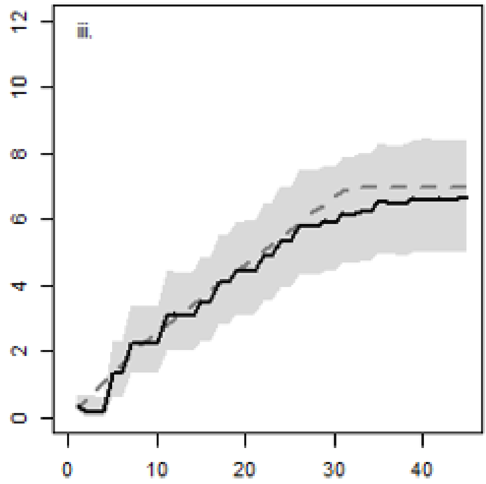

Figure 2: Process model predictions (bold dashed line), data (light dotted lines) and hybrid (bold solid line) predictions. X-axis = day, y axis = leaf number.

A Bayesian hierarchical model (Gelman, Carlin et al. 2006, Candy 2009, Cressie and Wikle 2011) was used to combine incoming data with the process model SIRIUS[4]. The model and fitted results are visualised in Figures 2 and 3. This approach allows expert opinion (e.g. about the input parameters shown in Table 1), and subject observations, to be integrated to determine the uncertainty in deterministic model predictions throughout the duration of their simulations. This allows a probabilistic description of inputs and model structures to explore model sensitivity. It gives users and decision makers real time predictions that are a combination of up-to-date information and an underlying process understanding. The results indicate that as the leaf number increases so too does the confidence in the estimate. Referring back to the state-space model component formulation in eq.8., we can see that we have a better understanding of how calibration data C_t relates to the model (i.e. observed leaf count closely follows the simulated leaf count, however, it is not a perfect match). This also provides insights to intrinsic, random variation ε. In order to build a more complete uncertainty evaluation more work is required to describe uncertainties that relate to model structure, input parameters, and environmental data. Possible objectives include:

1. Structural uncertainty $r_t = f((g(\boldsymbol{Z_t}, \theta, E_t), C_t), \varepsilon)$: Assess the size and direction of bias of model simulated values for *fln* by collecting new calibration data for a new location, potentially to guide new research/calibration efforts,
2. Input parameter uncertainty $r_t = f((g(Z_t, \boldsymbol{\theta}, E_t), C_t), \varepsilon)$: carry out a sensitivity analysis to assess whether the model is also sensitive to changes in *bp*, or carry out a sensitivity analysis to assess whether the model is not sensitive to changes in *pe*,
3. Environmental input data uncertainty $r_t = f((g(Z_t, \theta, \boldsymbol{E_t}), C_t), \varepsilon)$: Carry out a sensitivity analysis to assess the impact (in number of days of error in day of flag leaf estimation) of spatial bias in thermal time (TT) input data.

A range of analysis and sampling techniques that are useful to achieve the above are not reviewed in this paper but can be found in e.g. (Saltelli, Chan et al. 2000, Wallach, Makowski et al. 2014, Douglas-Smith, Iwanaga et al. 2020).

[4] Details in a journal paper currently in preparation

Summary

By explicitly describing a structure that encompasses model components and how they contribute uncertainty to model outputs, and systematically working through a defined sequence of tasks to describe and quantify that uncertainty we have achieved at least five important outcomes. Firstly, if the model had formerly not been fully disclosed, the model is no longer a black box since the model structure has been explicitly described. Second, each model component has been equally considered as a potential focus for uncertainty evaluation from the outset. Third, the model has been subjected to a formal process to help demonstrate both that it is trustworthy and that it is, to some degree, fit for purpose. Fourth, formal UE activities can provide a natural platform to curate and compile many types of information and data, including expert knowledge. This would provide an improved platform for decision and policy makers to assess model outputs and their implication, resulting in improved decision making. Fifth, fitting the process model with data via a Bayesian model formally grounds the uncertainty modelling technique used in statistical theory. Although the full extension of the formalisation will not always be necessary, it is there underlying the UE framework proposed here.

In this paper we have proposed a systematic approach in understanding and determining and communicating uncertainty from multiple sources in deterministic model, that enables improved identification of sources and the reasons for uncertainty. This provides an opportunity to target resources to reduce the overall size of uncertainty, for example, through better data acquisition or remodelling specific parts of the model.

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