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ABSTRACT

The ability of 'digital agriculture' to support on-farm decision making is predicated on the real-time combination of observations and prior knowledge into an integrated digital environment. The mathematical discipline that seeks to provide this integration is known as model data assimilation (DA), with demonstrated benefits including improved predictive reliability, and the capacity to identify unexpected changes in field conditions and potential measurement errors. Despite routine adoption in other fields, the delayed adoption of DA in agriculture is due to the need to express end-of-season outcomes such as yield, update forecasts of these outcomes throughout the growing season as data become available, and enhance forecast reliability. To overcome these challenges, three guiding principles are introduced, providing a means to operationalize crop model DA for robust on-farm decision support. We apply the guiding principles using a South Australian viticulture case study. Our case study involves application of an iterative form of a widely used DA algorithm (ensemble Kalman filter) to dynamically update both static parameters and states associated with a grapevine simulation model. Daily weather data as well as fortnightly ground-based leaf area index (LAI) data are used for assimilation. It is shown how crop model DA can lead to not only significant improvements in forecasts of LAI but also to forecasts of end-of-season yield. The guiding principles also enable observations of greatest value to be identified throughout the season. This study highlights the role that formal crop model DA can play in agricultural decision support through enhancing situational awareness in real time.

1. Introduction

The ability of 'digital agriculture' to support on-farm decision making (sometimes referred to as 'decision agriculture'; Leonard et al., 2017) is predicated on the real-time combination of observations and prior knowledge into a unified digital environment. Optimal 'fusion' of observations and prior knowledge is the aim of the mathematical discipline of model data assimilation (DA). While DA has been fundamental to advances in fields such as numerical weather prediction (Navon, 2009), its application to support decisions in agriculture remains rare. This delayed adoption reflects unique challenges facing practitioners in applying DA for on-farm decision support. As a result, much of the potential of DA in the agricultural context is yet to be realized.

Process-based models are widely used for decision support in agriculture (Wallach et al., 2006). Crop models are particularly well suited to agricultural decision support due to their ability to simulate key end-of-season outcomes and their sensitivity to both management decisions such as irrigation rates, and exogenous factors that are outside of the grower's control such as climate/weather (Knowling et al., 2021). The ability of crop models to effectively support decision making is dependant on the reliability of simulated outputs that pertain to

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decision-relevant performance metrics (herein referred to as 'quantities of interest' or QoI such as crop yield).

Crop models by themselves are limited in their ability to reliably inform on-farm decisions (Wallach et al., 2006; Wallach, 2011). This is in part due to the high levels of complexity of crop growth and development processes, and the heterogeneity of applications. The reliability of simulated outputs can be enhanced by 'conditioning' a model based on observation data. This involves updating uncertain model input parameters and/or states through reducing the discrepancy between observation data and their simulated counterparts. Formal conditioning is often achieved via DA by updating model parameters and/or states in a dynamic sense as observations become available. This allows simulated outputs to continuously reflect observed conditions.

The combination of crop models and DA have shown significant promise (e.g., Pauwels et al., 2007; Xiao et al., 2009; Mansouri et al., 2014; Tewes et al., 2020a, b). For example, many studies show how crop model DA can improve forecasts of state variables such as leaf area index (LAI) and soil moisture (e.g., Linker and Ioslovich, 2017; Lei et al., 2020). However, there remain unique challenges facing practitioners in applying crop model DA to support on-farm decision making. Challenges include the expression of end-of-season QoI (Knowling et al., 2021) and how insights gained through DA map to these QoI in real time throughout the season. There also remain more general challenges surrounding forecast reliability (e.g., Ines et al., 2013; Hu et al., 2017). Guidance to overcome these challenges (a detailed description given in Section 2.2) is currently limited for applying crop model DA to on-farm decision support.

The objectives of this study are as to: (1) develop guiding principles for effective crop model DA in the context of on-farm decision support and (2) demonstrate the guiding principles on a real-world viticulture case study. Briefly, the guiding principles address the need to express end-of-season QoI and how these QoI change throughout the season as more data are collected, as well as to enhance forecast reliability. Viticulture represents an ideal agriculture application area because of the complexity of biophysical processes involved in grapevine growth and development (Laurent et al., 2021), highlighting the need to combine both biophysical knowledge derived from crop models and field observations to provide integrated situational awareness and predictive capacity.

2. Crop model data assimilation and its challenges and opportunities for on-farm decision support

2.1. Overview of model data assimilation

Formal model DA involves three main components: a process-based model (Section 2.1.1), observation data (Section 2.1.2) and the DA procedure (Section 2.1.3). Here we provide a brief overview of DA and its components, with a focus on its application in conjunction with crop models towards end-of-season QoI estimation throughout the growing season. For more details, the reader is referred to the reviews of Jin et al. (2018) and Huang et al. (2019).

2.1.1. Process-based models

Process-based models represent a mathematical description of our understanding of the relationships between key quantities that control system behaviour. In the context of crop models, this commonly includes relationships across the soil-plant-atmosphere continuum associated with soil water dynamics, radiation use efficiency, crop phenology, and so forth (Wallach et al., 2006). These relationships have often been developed from decades of scientific development but have not necessarily been adapted to specific applications; in this way, a process-based model (herein referred to as 'model') serves to provide 'prior knowledge', independent of those that can be derived from observation data being collected.

For deployment in DA, a model must be capable of propagating forward system states (that can be observed), subject to initial system states, forcing variables and static parameter estimates. Mathematically:

$$h_{t+1} = g(h_t, p, q_t) \tag{1}$$

where g represents the action of a model in simulating the evolution of a dynamic system within an 'assimilation cycle' from time t to $t+1$, h_t and h_{t+1} are system states (e.g., LAI, soil moisture) at time t and $t+1$, respectively, p are static parameters (i.e., time-invariant on the scale of a season, e.g., thermal time thresholds, soil permeability), and q_t are forcing variables operating within the period t to $t+1$, such as climate/weather variables (e.g., temperature, rainfall) and decision levers (e.g., date and severity of canopy trimming, irrigation rate). Note that the time index t does not necessarily represent an individual unit of time; it can represent an arbitrary number of time units, e.g., days corresponding to irregular sampling events.

It should be noted that model inputs—p, q_t and h_t—are uncertain. Model input ('prior') uncertainty requires explicit specification. Uncertainty in model inputs will result in uncertainty in model outputs—h_{t+1}—to the extent that model outputs are sensitive to model inputs. A model is therefore also responsible for propagating uncertainty forward in time. Uncertainty quantification is a key aspect of DA (Section 2.1.3).

The suitability of process-based models, and in particular, crop models to agricultural decision support has been discussed previously (Wallach et al., 2006; Knowling et al., 2021). Crop models typically run on a daily basis. They require as inputs daily forcing variables, static parameters and decision levers (examples above). Crop model outputs include daily states (examples above) and fluxes (e.g., carbon assimilation, infiltration), as well as summary variables (e.g., yield).

2.1.2. Observation data

The role of observation data within DA is to capture key characteristics and dynamics of the system under investigation. Observation data therefore provide a basis for 'ground-truthing' the model and keeping the model 'current' (i.e., in line with current real observed conditions) through the process of DA. Observation data provide information related to system behaviour that can be used to condition uncertain model inputs towards reducing uncertainty in QoI such as end-of-season yield.

Some level of physical correspondence between observations and model simulated counterparts is required for observation data to be used for DA. However, for example, while LAI observations can be used to update LAI model states, it is important to consider that there will inevitably exist a difference between how LAI is represented by observations and the model (e.g., different spatial scale, treatment of non-canopy matter per area). Such correspondence may also be established or improved by observation pre-processing and/or model post-processing. These considerations are critical given that computation of the discrepancy between observations and model simulated counterparts (termed 'innovation' in DA parlance) is a key aspect of DA (Section 2.1.3).

Observation data are also subject to uncertainty, e.g., due to measurement noise. This uncertainty requires explicit specification within formal DA. Observation uncertainty is sometimes inflated to account for a lack of correspondence between observations and model simulated counterparts in an effort to account for effects of model misspecification on the DA process (Wallach, 2011).

Examples of observational data that are widely used for DA in agriculture include canopy size (e.g., LAI) and soil moisture. These data can be derived from both proximal sensing (e.g., De Bei et al., 2016; Yu et al., 2021) and remote sensing (e.g., Ballesteros et al., 2015; Bégué et al., 2010). Other less conventional observation data types include sap flow rates and stem radial variability (e.g., Corell et al., 2014; Scholasch, 2018).

2.1.3. Data assimilation

The role of the DA procedure in general terms is to bring together insights from the model and the data. This is achieved by updating model states and/or parameters in a way that optimally combines the model (e.g., simulated states before conditioning) with observations.

DA is often formulated in terms of Bayesian updating. This involves estimating in a sequential sense an ensemble of model states and/or static parameters over discrete time intervals to reduce model misfit and drive the ensemble towards a posterior condition (note that static parameters, while time-invariant in *simulation* time, can be updated sequentially, in *real* time as new data are assimilated). Bayesian updating involves two main steps: forecast and analysis. The forecast step involves propagating states and their uncertainty forward in time, giving rise to a 'prior' ensemble of states during the current assimilation cycle. The analysis step then involves solving an inverse problem to condition states and/or parameters, thereby reducing uncertainty and giving rise to a 'posterior' ensemble of states for the current assimilation cycle. This posterior state ensemble then becomes the prior state ensemble for the next assimilation cycle.

Suppose we have a parameter-state vector as $x_{t+1} = [p_s;\ h_{t+1};\ h_t]$. A general Bayesian formulation of the estimation problem takes the form:

$$p(x_{t+1}|d_{t+1}) = \frac{p(d_{t+1}|x_{t+1})p(x_{t+1})}{p(d_{t+1})} \tag{2}$$

where $p(x_{t+1}|d_{t+1})$ is the posterior probability density function (PDF) of x_{t+1} given a set of observations d_{t+1}; $p(d_{t+1}|x_{t+1})$ is the likelihood PDF that describes the deviation of model simulation results from observations; and $p(x_{t+1})$ is the prior distribution of x_{t+1}, and $p(d_{t+1})$ is the PDF of field observations (also called the 'evidence' term).

There are different ways in which DA problems can be formulated. For example, they can involve the estimation of states, estimation of parameters or joint estimation of states and parameters. Moreover, states can be estimated either at the end of a cycle (i.e., final states) or at the beginning of a cycle (i.e., initial states). While the approach of estimating final states is not constrained by the physics embedded in the model, it is nevertheless necessary when it is computationally infeasible to propagate the entire ensemble forward in time. It is therefore common in fields like numerical weather prediction (Navon, 2009). The latter approach of estimating initial states involves, at the completion of the analysis process, propagating the posterior ensemble of initial states (and perhaps static parameters) forward in time; the resulting simulated state ensemble is then used as the prior initial state estimates for the next DA cycle. In this way, the assimilation process maintains coherence with the model physics, yet at the computational expense of propagating the ensemble forward through the model. The additional computational expense of this approach is unlikely to serve as a limit when using crop models due to their run times. The reader is referred to Alzariee et al. (2021) for an overview of several popular cases in the context of environmental modelling.

Several algorithms enable the DA estimation problem to be solved using a Bayesian formulation. Popular examples include the Ensemble Kalman Filter (EnKF; Evensen, 1994; 2003), the Particle Filter (Gordon et al., 1993) and 4D-Var (Lorenc et al., 2000), all of which have shown promise in agriculture due to their ability to capture model non-linearity and relative computational efficiency (e.g., Pauwels et al., 2007; Xiao et al., 2009; Mansouri et al., 2014).

DA can also be achieved in a 'direct' fashion. Direct DA involves replacing prior or 'background' realizations of model states or forcing variables (e.g., rainfall, irrigation rate) with observation data plus measurement error (Evensen, 2003).

2.2. Challenges and opportunities

As discussed in the Introduction, although the benefits of DA are well-known and the methods have been applied in a broad range of fields, several unique challenges face practitioners in applying crop model DA to support on-farm decisions. Below we discuss in detail three significant challenges, as well as opportunities that currently exist to overcome these challenges.

2.2.1. Expression of decision-relevant quantities

A prerequisite for model-based decision support in general terms is the expression of QoI that drive decision-making. Despite this, the expression of decision-relevant QoI in crop modelling studies, where QoI are often end-of-season outcomes such as yield, remains a challenge (Knowling et al., 2021). This is evidenced by many previous crop model DA studies forecast state variables only. For example, Linker and Ioslovich (2017) showed that assimilation of LAI data into AquaCrop (Steduto et al., 2009) using an extended Kalman filter (Brown and Hwang, 1997) led to a considerable improvement in predictive reliability of LAI later in the season for potato in Denmark.

Without expressing and forecasting QoI, the outcomes of DA are likely to be of limited value to decision makers (e.g., growers, advisors). For example, it is likely that growers or their advisors will be more interested in what improved LAI forecasts mean in terms of yield, harvest timing and/or various quality measures, rather than in terms of LAI itself. This reflects the limited transferability of insights gained through DA from observed state variables to unobserved variables including QoI. The fact that assimilation of observations of a particular state variable may not lead to improved forecasts of other variables has been acknowledged (e.g., Pauwels et al., 2007; Linker and Ioslovich, 2017). The extent to which insights gained from DA are transferable between observed and unobserved variables is a function of their similarity in terms of spatial scale, temporal characteristics, etc.

The expression of decision-relevant QoI has remained a challenge due to the widespread adoption of crop models (or other process-based models that do not simulate physical processes across the soil-plant-atmosphere continuum) that are not capable of simulating end-of-season QoI. For example, only a subset of crop models are capable of simulating end-of-season QoI such as yield for perennial crops such as grapevine (Moriondo et al., 2015; Knowling et al., 2021). While several DA studies do in fact use crop models that can simulate end-of-season QoI, this capability is not always utilized (e.g., Linker and Ioslovich, 2017; Lei et al., 2020), perhaps due to the unrealized potential of DA for decision support more generally.

To overcome this challenge, a model that is capable of simulating end-of-season QoI must be adopted. The availability of many crop models that can simulate end-of-season QoI suggests that there exists a significant opportunity to address this challenge. This is notwithstanding the adoption of such models by practitioners (e.g., advisors) has been limited due to practical factors such as usability and availability of supporting documentation (Rossi et al., 2014). While these factors do not serve as an immediate barrier to crop model DA, greater adoption of such models would benefit the uptake of crop model DA.

2.2.2. Real-time mapping to decision-relevant quantities

Building on the need to express decision-relevant QoI, effective model-based decision support also requires the mapping of insights gained through DA to QoI on a regular basis throughout the growing season. Such mapping facilitates enhanced situational awareness through continual evaluation of QoI throughout the season. Mapping of insights to QoI in such a way, however, represents a challenge. This is evidenced by the fact that, of the relatively few crop model DA studies that do forecast QoI, they map insights to QoI only via a single 'after the fact' snapshot (i.e., post-season, after assimilating all observations within the season). For example, Chen and Cournede (2014) showed that the variance of winter wheat yield was considerably reduced after assimilating leaf biomass estimates into STICS (Brisson et al., 2008) using a convolution particle filter (Kitagawa, 1996).

Without continually mapping insights to QoI, the outcomes of DA are likely to be of limited value to decision makers. Frequent, decision-relevant insights on the other hand, are expected to enhance situational awareness, which empowers growers and their advisors to make better decisions. In addition, mapping insights to QoI can provide a basis for comparing the informativeness of different observation data types, observations made at different times, etc. For example, the variance surrounding decision-relevant QoI has been used widely as a metric for evaluating the 'worth' of observation data in areas such as hydrology (e.g., Dausman et al., 2009; Partington et al., 2020). Such analyses are expected to create value for a grower or advisor through guiding the design of data collection practices.

Fig. 1 shows schematically how expressing decision-relevant QoI, and mapping insights gained through DA to these QoI, broadcasts across real and model time. How continual mapping of insights to QoI contrasts with a traditional DA approach is also shown in Fig. 1.

Mapping insights to end-of-season QoI is particularly challenging due to the additional complexity required as part of the interface between a crop model and a DA algorithm (orange arrows; Fig. 1). This likely explains why previous studies that use models capable of expressing QoI do not map insights to QoI. Previous studies often 'statically link' DA algorithms within crop models, meaning that the DA algorithm is embedded within a model's time-stepping routine (e.g., Ines et al., 2013; Zhuo et al., 2020). Such an approach precludes the flexibility necessary to map insights to end-of-season QoI throughout the season.

It follows that this challenge can be addressed by adopting a non-intrusive (i.e., model-independent) DA algorithm. Non-intrusiveness in this context means that the algorithm can interface with a model of arbitrary complexity, and where model runs and pre- and post-processing are undertaken by the DA algorithm itself through configuration files that communicate with model input and output files (Doherty, 2015). Only recently has a non-intrusive tool for real-world-scale DA been developed (Alzraiee et al., 2021). This publicly available and open-source tool therefore provides a significant opportunity to address this challenge.

Mapping insights to end-of-season QoI also requires that a model be run to the end-of-season, regardless of current stage in the growing season. This incurs a cost in terms of computational time. However, due to the short run times (in the order of 1 s) typically associated with crop models, this is not expected to represent a barrier to mapping insights to QoI.

It is worth noting that the need to map insights to QoI is somewhat unique to crop model DA. This is because the QoI being forecast in this context are time-integrated variables, in contrast to state variables, which often represent QoI when predicting a dynamic system into the future. Crop model DA is therefore characteristically different to other typical DA application areas, where frequently collected observation data are similar in nature to QoI, such as the situation in numerical weather prediction (Navon, 2009).

2.2.3. Enhancing reliability

Model-based decision support is also underpinned by predictive reliability. Achieving and enhancing reliability, which involves reducing forecast bias and overconfidence (i.e., uncertainty underestimation) (Friedman, 1997; Knowling et al., 2019), still remains a challenge in many predictive modelling contexts including agriculture. This is evidenced by previous crop model DA studies that report forecast bias and/or overconfidence (e.g., Ines et al., 2013; Hu et al., 2017).

To the extent that a grower's or advisor's decisions are informed by forecasts of QoI that lack reliability, such decisions are likely to be compromised, and therefore lead to undesirable outcomes. For example, a model may indicate that the probability of an undesirable crop yield is sufficiently low from a decision maker's perspective. However, where yield forecasts are biased and/or overconfident, and where the 'true' probability of an undesirable crop yield is higher, then decisions informed by these forecasts are naïve to precisely the outcomes that the decision maker is trying to avoid.

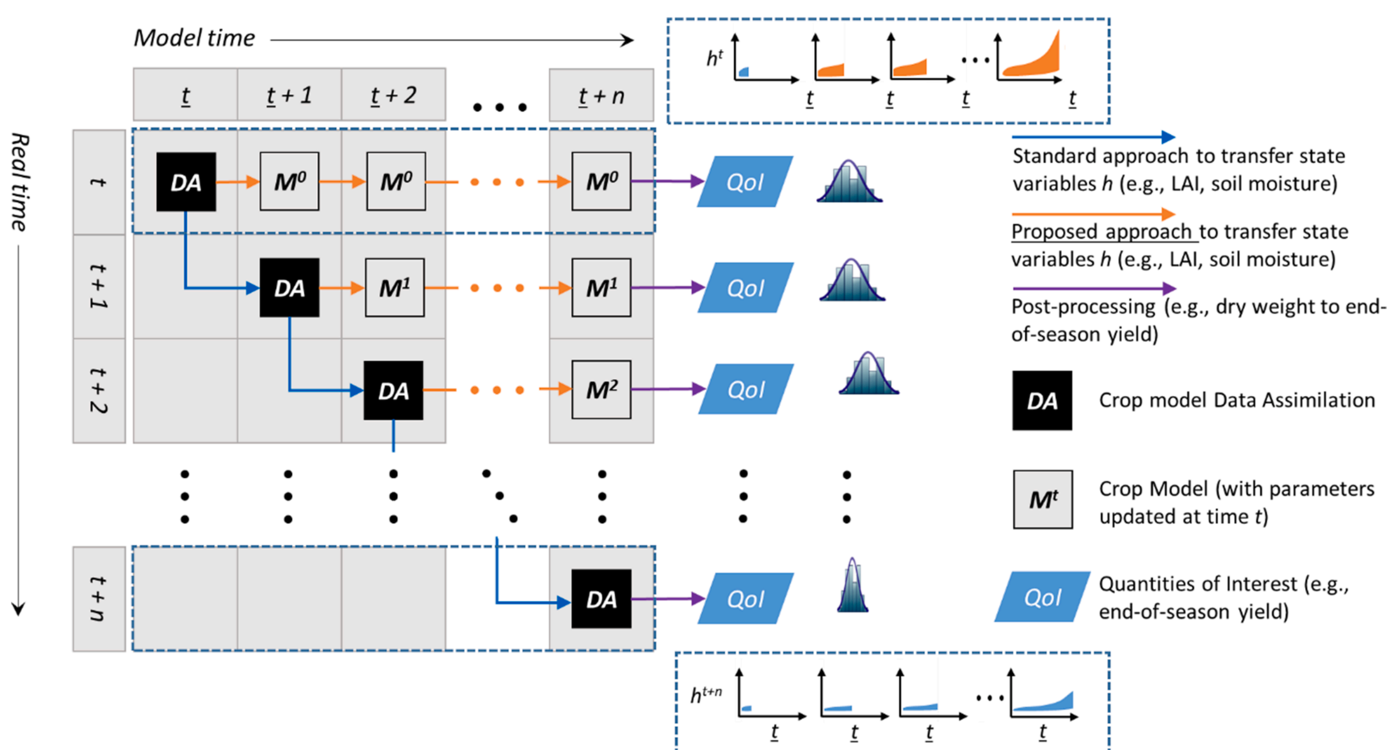

Fig. 1. Schematic representing how a standardapproach to DA differs from what is proposed for crop model DA to provide on-farm decision support. Purple arrows depict the expression of decision-relevant QoI (Section 2.2.1). Orange arrows (combined with purple arrows) depict real-time mapping to QoI throughout the season (top-to-bottom) (Section 2.2.2). The model superscripts (M^0, M^1, …) represent the sequential updating (in real time, t) of static model parameters. The dashed boxes show the progression of a model state variable h (in model time, $\underline{t}$) for two real-time points within the season (h^t and h^{t+n}).

While enhancing reliability is challenging in general terms, several means to enhance reliability exist. A promising means to enhance reliability is increased parameterization dimensionality (e.g., the number of model input variables that are used to express uncertainty). By using increased dimensionality, there exist more receptacles for the information contained in observation data, therefore reducing the potential for states and parameters to take on compensatory roles as part of the inversion process, which can be a key driver of bias and overconfidence (Doherty and Christensen, 2011; Knowling et al., 2019).

However, using increased dimensionality poses challenges due to the additional complexity and flexibility required as part of the DA algorithm as well as the crop model-DA algorithm interface. This likely explains why the majority of crop model DA studies estimate only state variables (e.g., Nearing et al., 2012; Huang et al., 2019). These studies therefore 'fix' uncertain model parameters, sometimes at values obtained from a separate model calibration exercise. Such an approach may result in inappropriate state/parameter compensation. The importance of estimating states and parameters simultaneously (referred to herein as 'joint parameter-state estimation') has been widely recognized (Clark and Vrugt, 2006; Zhang et al., 2017; Markovich et al., 2022). Fig. 2 shows schematically the information flow within the DA process when performing joint parameter-state estimation as opposed to state-only estimation. Hu et al. (2017) showed the superior performance of joint parameter-state estimation compared to state-only estimation in the context of crop model DA.

The need to perform joint parameter-state estimation and use increased parameterization more generally indicates the requirement for a DA software tool that can scale to high dimensions in parameter and state space. The recently developed open-source DA tool developed by Alzraiee et al. (2021) offers a unique opportunity to enable DA in high dimensions in a non-intrusive way. The demonstrated scalability of the tool is expected to be sufficient to facilitate crop model DA for on-farm decision support.

2.3. Guiding principles

The challenges and opportunities identified (corresponding to the three preceding sub-sections) can be used to establish guiding principles for achieving effective crop model DA for on-farm decision support. We consider three guiding principles, corresponding to Sections 2.2.1 to 2.2.3, respectively, as follows (Fig. 3):

1. Employ a model that can express QoI;
2. Map insights from DA to QoI using a flexible and non-intrusive DA tool; and
3. Perform joint estimation of model parameters and states in an attempt to enhance reliability.

We follow these guiding principles in our case study (Section 3), serving to operationalize these principles. The guiding principles are intended to pave a way to address commonly encountered limitations at the intersection of crop modelling, DA and decision support. They are not intended to be exhaustive and deal with all facets of crop model DA. We refer readers to Jin et al. (2018) and Huang et al. (2019) for detailed reviews of crop model DA.

3. Case study application

Here we present a case study application of crop model DA that follows the guiding principles arrived at in Section 2. Our case study concerns a real-world vineyard in South Australia. The following subsections describe the key elements of the case study; namely the vineyard study site, the process-based model representing the study site, the observation data available for assimilation, and the DA procedure adopted.

3.1. Study site

The study site considered is a single 0.64-hectare vineyard block, part of a vineyard located in Loxton (Riverland region, South Australia). The Riverland region experiences a Mediterranean climate. The 2020–2021 growing season is considered herein. Table 1 summarizes key vineyard attributes.

3.2. Process-based model

We adopt VineLOGIC (Walker et al., 2005, 2020a, b, c), a crop model designed specifically to simulate grapevine growth and development. VineLOGIC was selected for its relatively advanced representation of biophysical processes and relationships across the soil-plant-atmosphere continuum, especially those associated with berry development, as well as its ability to simulate the impact of decision levers related to water and canopy management (Knowling et al., 2021). VineLOGIC simulates,

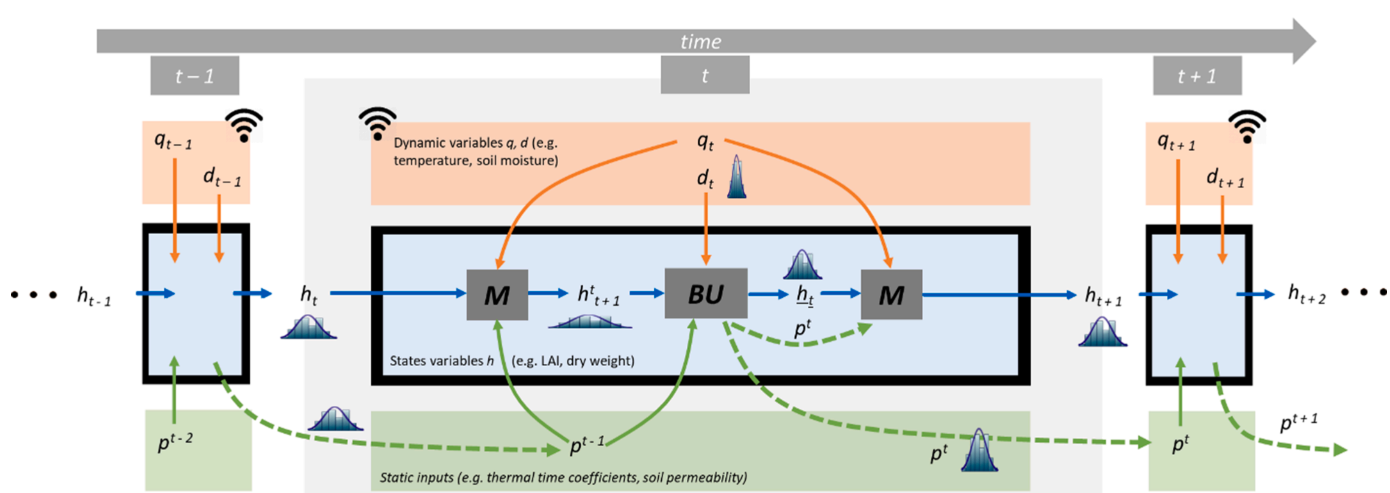

Fig. 2. Schematic representation of the DA process, including the forecast and analysis steps. "M" refers to the forward model and "BU" refers to the Bayesian updating procedure. The flow of information within the crop model DA process is depicted (arrows). The contrast between the typical approach (state-only estimation) and the proposed approach (joint parameter-state estimation) is shown via dashed arrows. Note we add superscript indices for clarity where appropriate. For example, "h^t_{t+1}" represents the prior estimate of the state variable h at time $t+1$ given forcing data up to time t (i.e., forecast without any conditioning), whereas "h_{t+1}" means the best estimate of the state variable h at time $t+1$ (i.e., which will arise from all information available up to time $t+1$).

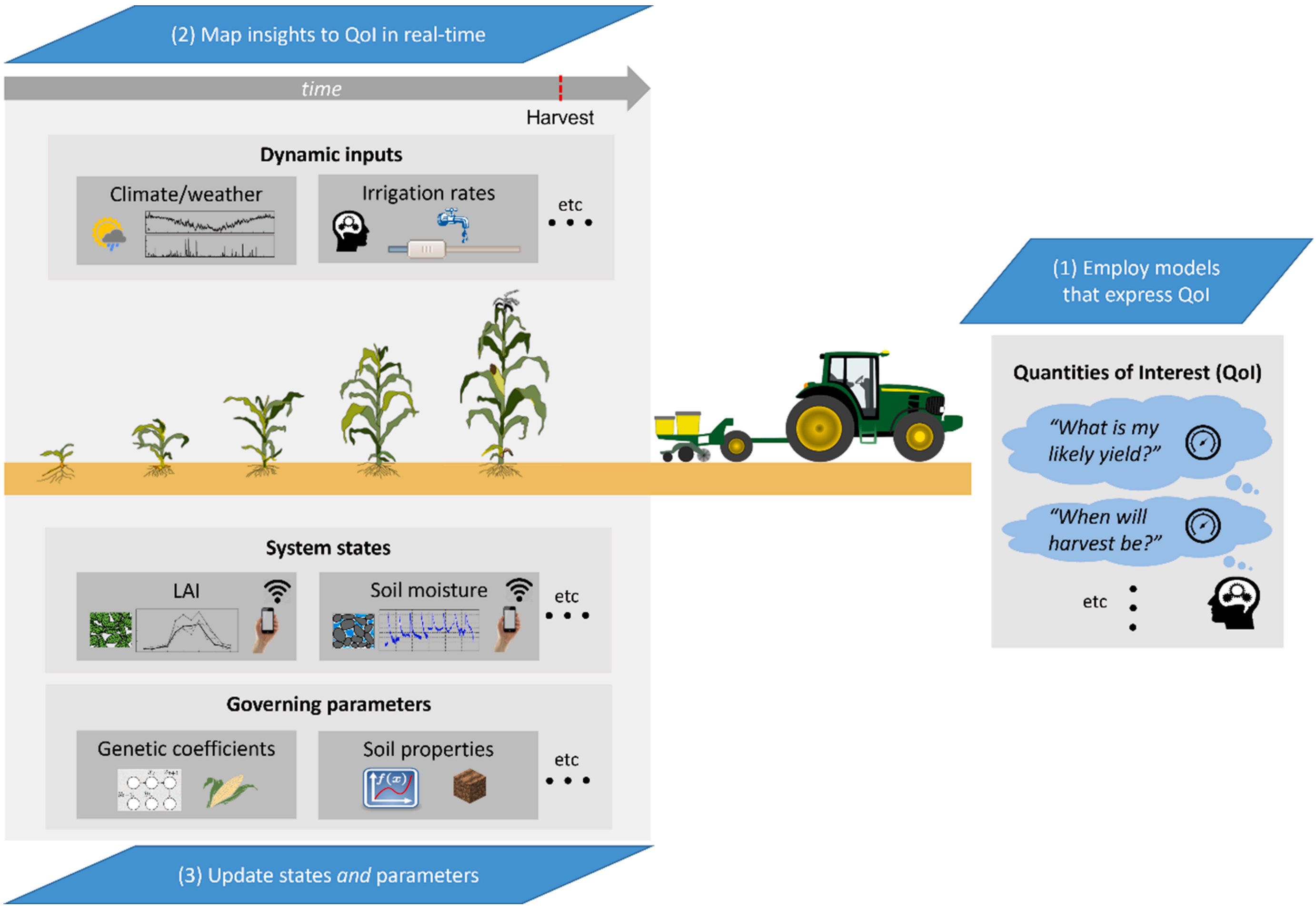

Fig. 3. Schematic representation of how the three guiding principles combine to enable effective crop model DA for improved on-farm decision making.

Table 1
Key attributes of the case study vineyard in the Riverland region (South Australia).

Vineyard attribute	
Wine grape variety	Chardonnay
Rootstock	Ramsey
Trellis system	Vertically separated double cordon permanent arm
Trellis dimensions (height)	Cordon 1: 1230 mm; Cordon 2: 1700 mm
Pruning method	Mechanical, followed by spur pruning
Retained buds per vine	230
Soil type	Sandy loam
Row and vine spacing	3 m (row); 2.4 m (vines)
Irrigation method	Drippers

at a point scale and on a daily basis, the main biophysical processes and relationships governing soil water balance, phenological transition controls, light interception, biomass accumulation (carbon assimilation), and biomass partitioning between different organs (leaf, shoot, fruit and root) as a function of phenological stage. The reader is referred to Walker et al. (2005, 2020a, b, c) for a detailed description of VineLOGIC and its supporting datasets.

3.2.1. Forcing variables

Forcing variables (q in Eq. [1]) requiring specification in VineLOGIC include exogenous climate/weather variables as well as management decision levers. Climate/weather variables are specified on a daily basis, including minimum and maximum temperature, solar radiation and rainfall. VineLOGIC requires climate/weather data not only for the growing season period (2020–2021), but also the preceding growing season to simulate factors affecting fruitfulness that are determined at early stages of the preceding season (Guilpart et al., 2014). Data used to populate climate/weather time series are described in Section 3.3.1.

Management practices represented in VineLOGIC for which forcing variables require specification, include irrigation application and canopy intervention. Given that irrigation data are not available over the period of investigation (Section 3.3.2), we simulate daily irrigation rates as a function of simulated soil moisture deficit and decision levers including percentage of extractable soil water used to initiate irrigation, percentage of soil water deficit to refill, minimum number of days between applications and maximum daily irrigation rate (Edraki et al., 2003), some of which are treated as uncertain (Table 2). Canopy management (e.g., trimming, tipping) is simulated through direct alteration of canopy size via the LAI state variable. Given that the severity of canopy reduction per intervention is unknown (Section 3.3.2), the amount by which LAI is reduced is also treated as an uncertain decision variable (Table 2).

3.2.2. Static parameters

Static parameters (p in Eq. [1]) requiring specification in VineLOGIC include:

- cultivar variables such as thermal time thresholds, potential fertility and genetic coefficients, and for grafted plants, rootstock indices, e.g., vigour index that influences biomass production and sensitivity to stress factors;
- soil hydrology variables such as moisture content at the start of the season, vertical saturated hydraulic conductivity, depth to water table; and

Table 2
Static parameters and forcing variables that are treated as uncertain. Uncertainty associated with climate/weather forcing variables are expressed using scenarios (Section 3.4.1). Parameters and forcing variables not treated as uncertain include those that are directly observable such as trellis dimensions, row and inter-vine spacing, etc. (Table 1).

Parameter	Description (units)	Prior mean value	Range	Supporting reference
Cultivar				
GCoefBerryDW1	Fruit demand coefficient pre-sugar loading period	1.75×10^{-4}	1.4×10^{-4}—2.1×10^{-4}	Walker et al. (2020b)
GcoefBerryDW2	Fruit demand coefficient post-sugar loading period	1.2×10^{-3}	8.0×10^{-4}—1.6×10^{-3}	Walker et al. (2020b)
GcoefCritBrix	Brix to trigger stage 4 of berry development (°Brix)	20.5	17.5—23	Pellegrino et al. (2008); Rogiers et al. (2017)
GcoefSugarDw	Fruit demand coefficient post-sugar loading of berry development	0.7	0.6—0.8	Pellegrino et al. (2008); Rogiers et al. (2017)
P1VV	Thermal time to end vernalization (dormancy) (°C days)	5	4—6	Walker et al. (2020b)
P2BB	Thermal time from vernalization (dormancy) to bud burst (°C days)	265	258—273	Walker et al. (2020b)
P3FF	Thermal time from bud burst to flowering (°C days)	170	163—178	Walker et al. (2020b)
P4HH	Thermal time from fruit set to harvest (°C days)	1500	1490—1510	Walker et al. (2020b)
P5LF	Thermal time from harvest to leaf fall (°C days)	800	793—808	Walker et al. (2020b)
G1BN	Genetic coefficient used to determine number of shoots	1.0	0.9—1.1	Walker et al. (2020b)
PHINT	Used to determine thermal time fraction for leaf growth (°C days)	50	42—58	Pallas et al. (2008); Walker et al. (2020b)
Rootstock				
RstockVigIndex	Rootstock vigour scale factor	9.0	7.8—10.1	Walker et al. (2020b)
RstockAernSens	Rootstock aeration sensitivity	9.0	7.8—10.1	Walker et al. (2020b)
Soil and hydrology				
Ksmx	Surface saturated hydraulic conductivity (cm/s)	1.0	0.5—5.0	Edraki et al. (2003)
Salb	Albedo of bare soil (-)	0.13	0.10—0.15	Van Wijk and Scholte Ubing (1963)
SLLL	Soil water lower limit (cm^3/cm^3)	0.14*	0.13—0.16*	Hubble and Crocker (1941); Maschmedt et al. (2002)
SDUL	Soil water drained upper limit (cm^3/cm^3)	0.33*	0.29—0.36*	Hubble and Crocker (1941); Maschmedt et al. (2002)
SSAT	Soil water saturation (cm^3/cm^3)	0.37*	0.33—0.41*	Hubble and Crocker (1941); Maschmedt et al. (2002)
SRGF	Soil hospitality factor (i.e., factor representing suitability for root growth and development) (-)	0.41*	0.37—0.45*	Skene (1951); Maschmedt et al. (2002)
SSKS	Macroscopic hydraulic conductivity (cm/s)	5.37*	4.84—5.91*	Edraki et al. (2003)
SBDM	Soil bulk density (g/cm^3)	1.51*	1.36—1.67*	Skene (1951); Maschmedt et al. (2002)
InitialSoilWater	Initial soil water condition (cm^3/cm^3)	0.2*	0.18—0.22*	Field estimate
TruDepWt	Depth to water table (m)	2.0	1.8—2.2	Field estimate
Vineyard				
BerryBunch	Berry count per bunch	67	61—74	Walker et al. (2020b)
BudNoVine	Bud count per vine post-winter pruning	230	170—290	Field estimate
BunchNoVine	Bunch count per vine	210	165—265	Field estimate
TrunkCHO	Trunk carbohydrate mass per dry matter (g/kg)	90	79—101	Clingeleffer and Pellegrino (2006)
TrunkDW	Trunk dry mass (kg)	9.0	7.9—10.1	Clingeleffer and Pellegrino (2006)
ParFrac	Potential dry matter production scale factor	0.5	0.47—0.53	Smith and Silva (1969)
PropAccessResv	Proportion of carbohydrate reserves available per day	0.1	0.075—0.125	Godwin et al. (2002)
FruitSinkCoeff	Scale factor for berry development cost (e.g., respiration)	1.25	1.19—1.31	Vivin et al. (2003)
Decision levers				
IrrDayStageCap	Maximum daily irrigation application rate (mm)	6.0	5.0—7.0	
TrimRedLAI	The amount by which to reduce LAI per canopy intervention	1.0	0.75—1.25	
TrimTrigLAI	Threshold LAI to trigger trimming	3.0	2.75—3.25	

* Represents soil profile depth-averaged values.

- vineyard attributes such as row and inter-vine spacing, trellis geometry, post-winter pruning bud number.

Table 2 lists the key inputs—both static parameters and forcing variables—as well as their values and ranges assumed for the case study. Values and bounds were specified in accordance with site specific information and viticultural expert knowledge.

3.2.3. Simulated outputs

Although VineLOGIC simulates many state and flux variables (h in Eq. [1]) associated with energy, water and carbon balances, here we focus specifically on the LAI state variable.

LAI is represented in VineLOGIC as the total leaf area per vine (m^2) divided by the total ground area per vine (in this case, 7.32 m^2). In the model, the daily increment in leaf area at the vine level is determined from primary and secondary leaf growth considering the phyllochron of the main stem, the number of developing laterals and the leaf area expansion, which is assumed to be similar for the two types of axes (mains and laterals) (Godwin et al., 2002; Poni and Giachino, 2000). The individual leaf area growth rate and the number of laterals are negatively impacted by abiotic stresses such as water deficit (e.g., Lebon et al., 2004; 2006; Edwards and Clingeleffer, 2013), temperature and salinity (e.g., Dunlevy et al., 2022). The number of laterals is also regulated by shoot density (Reynolds et al., 1994; Sommer and Goodwin, 2000). The overall vine leaf area increment is also regulated when there is an insufficient pool of carbon at the plant level to meet growth demand (Williams and Matthews, 1990; Pallas et al., 2008).

Mathematically, LAI is given by:

$$LAI_{t+1} = LAI_t + \Delta LAI_{t+1} \quad (3)$$

where ΔLAI_{t+1} is the change in LAI from time t to $t+1$, as given by:

$$\Delta LAI_{t+1} = (\Delta LA_S \times N_S + (\Delta LA_S \times (N_L - 1) \times N_S)) \times S \times A \quad (4)$$

where ΔLA_S is the leaf area increment per main shoot (cm^2/shoot), N_s and N_L are the numbers of main shoots per vine and laterals per main shoot, respectively, S is a carbon limiting scale factor, and A is an area conversion factor (cm^2/vine to m^2/m^2). The leaf area increment per shoot (ΔLA_S) is determined from (i) the number of main leaves, which is calculated as a function of the phyllochron and the cumulated thermal time post-bud burst, and (ii) the individual leaf area, which relies on a potential leaf area and leaf expansion reducing factors including temperature, water deficit and salinity. The number of shoots (N_S) is a function of the number of buds per vine and the percentage of budburst. The number of laterals per shoot (N_L) is a function (i) of the phyllochron of the main stem (lateral production after a specific main stem development rate), (ii) of the density of shoots (progressive reduction of lateral production as the density of shoot number increases), and (iii) of abiotic regulating factors including water deficit and salinity. The carbon limiting scale factor (S) is equal to 1.0 if the available carbohydrate pool (C_A) exceeds total demand of vegetative sinks (D_V), and otherwise equal to C_A/D_V. The reader is referred to Ritchie and Godwin (2000) for more details.

We also evaluate the end-of-season yield Y, which is given by:

$$Y = \int_{FS}^{H} P_i \, DW_i \, F dt \tag{5}$$

where DW_i is the change in total crop dry mass (including fruit, shoot [leaf plus stem] and root) for day i, P_i is the proportion of dry mass partitioned to fruit for day i, F is a dry-to-fresh mass conversion factor (= 4; Garcia de Cortazar-Atauri et al., 2009), FS is the day index at which fruit set is initiated, and H is the day index at which harvest is initiated.

3.3. Observation data

The case study involves a typical observation data stream (LAI) and a typical QoI (yield). We focus on canopy data because these have been effective in informing vineyard evolution and stress conditions, due to its role in determining water relations and gas exchange, and its influence on photosynthetic primary production (Williams and Ayars, 2005; Hall et al., 2011; Bellvert et al., 2014). For these reasons, it is expected that case study findings will be of relevance to the agriculture community.

3.3.1. Climate/weather data

Daily weather data are obtained from a nearby weather station (located approximately 100 m from the vineyard) (Loxton Research Centre Station 024,024; Bureau of Meteorology). Data spanning the current (2020–2021) and preceding growing season (2019–2020) are used for direct assimilation (Section 3.4.1). Data spanning the preceding 10-year period (2009–2018) are also used for the purposes of characterizing plausible future climate/weather conditions (Section 3.4.1).

3.3.2. Management practices

Available data pertaining to vineyard management practices include only the approximate date of canopy intervention. Canopy trimming was carried out on December 2, 2020. The extent of canopy trimming per intervention is somewhat uncertain since canopy data collection was not undertaken before and after these interventions, and as such, we treat the canopy reduction as uncertain (Section 3.2.1).

3.3.3. LAI data

LAI data were obtained at between weekly and fortnightly time intervals (giving rise to a total of 33 observation times) using the non-destructive VitiCanopy system (De Bei et al., 2016). This involved photographing one section of canopy per panel or approximately every 6 m (each image represents up to 1.81 m of linear cordon), with images then being processed through the VitiCanopy system to determine a *plant* area index (PAI) value for each image, which was then averaged to represent the vineyard scale. Photographs were taken along vine rows between stems (trunks) to avoid interference, using a smartphone camera tilted at 30° to capture the whole canopy with the sky as background rather than the row behind it (Fig. 4). Processed images reflect PAI as the entire plant area is captured including the cordon or permanent wood, which becomes occluded by leaves, at which time the value represents LAI. For example, early PAI measures include the permanent wood, which for this site has a mean PAI of 0.3. This value is therefore subtracted from PAI values prior to permanent wood becoming occluded by leaves to give values indicative of LAI. Ground-based image canopy data have been shown to be particularly effective for mapping grapevine canopies across a vineyard (Arno et al., 2013; De Bei et al., 2019; Ouyang et al., 2020).

3.3.4. Field estimate of yield

While the harvest yield for the vineyard patch under investigation was not directly measured, an estimate of final yield per vine is made via destructive sampling of fruit from 10 test grapevine panels, accounting for approximately 18 m of linear cordon in total. Fruit sampling was undertaken on February 20, 2021, immediately prior to the commercial harvest date. As per standard industry practice, this is multiplied by the number of linear metres of cordon per ha and expressed as tonnes per ha.

An average yield estimate of 36 tonnes/ha was obtained from the test panels, with a range of 18 to 41 tonnes/ha amongst individual panels. To express the variance in average yield estimate, the sample standard deviation was calculated to be 2.2 tonnes/ha (standard deviation of population [= 7.0 tonnes/ha] divided by the square root of the number of samples [= 3.2]).

3.4. Data assimilation

We adopt PESTPP-DA (Alzariee et al., 2021). PESTPP-DA enables iterative sequential DA in a non-intrusive (i.e., model-independent) and scalable-to-high-dimensions fashion. PESTPP-DA is flexible in its ability to enable both sequential and batch DA, as well as arbitrary combinations thereof by mixing the EnKF, the Ensemble Kalman Smoother (EnKS) and the Ensemble Smoother (ES).

We use the EnKF (Evensen, 1994; 2003). The EnKF is an ensemble Monte Carlo variant of the Kalman filter. The motivation for ensemble formulations is to tolerate to some extent departure from key assumptions made in the standard Kalman filter—a linear forward model and multi-variate Gaussian distributions. Ensemble formulations also alleviate the prohibitive computational expense that would otherwise be encountered in high dimensional problems. Previous studies have successfully applied the EnKF for crop model DA (e.g., de Wit et al., 2007; Zhao et al., 2013; Zhuo et al., 2019).

Here we use the Multiple Data Assimilation (MDA) solution scheme of Emerick and Reynolds (2012). An ensemble comprising 20 members is used. This is a conservatively large ensemble size given the dimensionality of the solution space (Moore and Doherty, 2005; Knowling et al., 2019) is expected to be low (Section 3.4).

The ‘hotstart’ functionality in PESTPP-DA (White et al., 2020) is adopted. This enables DA in an operational manner, whereby assimilation cycles are initiated as new observation data become available.

3.4.1. Direct updating of climate/weather data

Daily weather data corresponding to the 2019–2020 and 2020–2021 growing seasons are directly updated in the model (Section 3.2.1). This involves, for each day, replacing the ‘background’ climate/weather data, representing prior climate/weather uncertainty, with observed data from Loxton Research Centre weather station. We assume zero variance about these climate/weather observations. Climate/weather data used as ‘background’ conditions represent samples of historical records collected at the same weather station spanning the period 2009–2019.

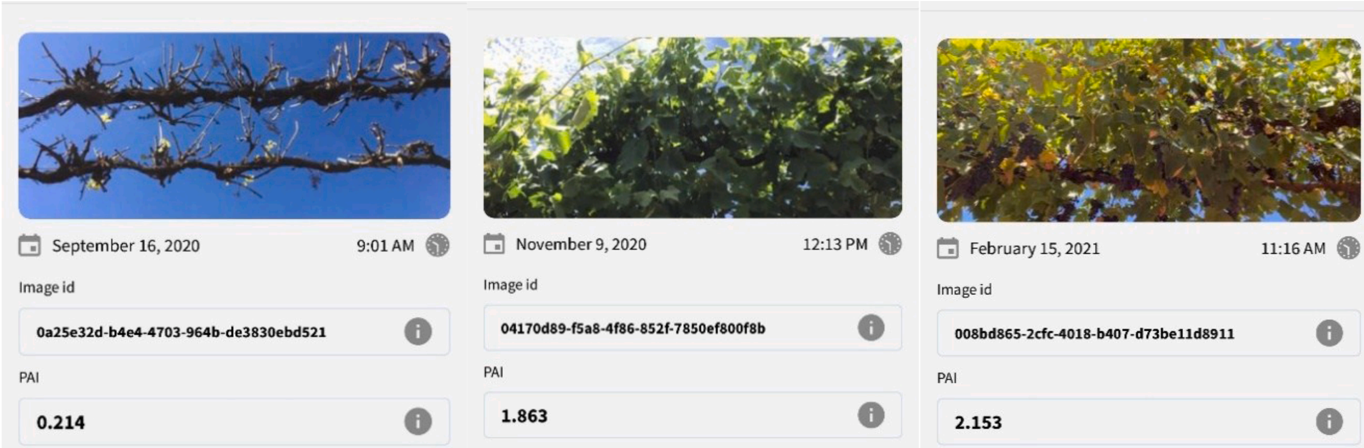

Fig. 4. Sample of images taken by VitiCanopy during growth stage (Coombe, 1995) E-L 4 (bud burst), E-L 26 (flowering complete) and E-L 37 (pre-harvest), and the PAI values interpreted on their bases.

3.4.2. *Assimilation of LAI data through Bayesian updating*

We jointly estimate initial states and static parameters (third guiding principle) by sequentially assimilating observed LAI data (Section 3.2) through Bayesian updating. The standard deviation of uncertainty surrounding each LAI observation used for DA is assumed to be 0.1 m^2/m^2 to account for the effects of factors such as wind.

The DA problem is formulated in such a way that initial states for each assimilation cycle are estimated. That is, we do not estimate final states for each assimilation cycle to be used as starting conditions for the subsequent cycle; instead, following estimation of initial states and parameters for each cycle, the final states are obtained through forward model simulation, helping to maintain physical and conservation relations in the process model. The low computational expense of VineLOGIC that makes possible efficient sequential estimation of initial states for a large number of cycles, while maintaining coherence with the physics embedded in the model (Section 3.2), also allows the opportunity for the entire simulation period to be undertaken for each cycle. This enables quantification of the change in forecasts of end-of-season QoI (first guiding principle) as a function of time as new observations become available (second guiding principle).

All static parameters except those pertaining to directly observable vineyard attributes (e.g., row and vine spacing, trellising) are subject to estimation (Table 2). The initial parameter value is assumed to represent the mean of the prior parameter probability distribution. The upper and lower parameter value limits are assumed to represent 95% confidence limits.

4. Results

4.1. *DA outcomes in terms of LAI*

The outcome of DA is first evaluated in terms of the observed state variable LAI. We specifically evaluate how the LAI forecasts are conditioned as the season progresses.

The ensemble LAI trajectory displays substantial conditioning as more observation data are assimilated (Fig. 5). First consider the situation before the occurrence of bud burst in real time (Figure 5; top panel). Forecasted LAI trajectories display a familiar temporal pattern, with distinct periods of canopy growth, stabilization and senescence, despite considerable uncertainty that surrounds LAI trajectories prior to conditioning on observations. Uncertainty in LAI trajectories during canopy growth appears largely due to that surrounding simulated phenology (e.g., bud burst uncertainty spans 6 weeks). However, LAI uncertainty is dampened to some extent by the effect of canopy intervention (simulated in the model when LAI reaches a threshold; Section 3.2.1), which can be seen in terms of instantaneous reductions in LAI.

Through assimilation of an increasing number of canopy observations (Fig. 5; top to bottom), as well as weather and canopy management data, the variance in LAI forecasts is substantially reduced. The reduction is apparent not only in the short-term, but also throughout the remainder of the growing season. Importantly, the reduction in variance occurs while maintaining familiar canopy growth characteristics. Despite the ensemble LAI trajectories encompassing most LAI observations, due in large part to the flexibility offered by parameter-state estimation (Section 4.3), the model was unable to reproduce some of the 'surprising' LAI observations—those that display a stark change in LAI that perhaps reflect unknown changes to forcing variables such as irrigation rates, which are not captured in the model.

4.2. *DA outcomes in terms of yield*

While assimilation of LAI observations generally led to substantially improved LAI forecasts as expected (Section 4.1), the question remains: "how are forecasts of other unobserved variables, particularly decision-relevant quantities, impacted by DA?" Here we evaluate the forecast of end-of-season yield and how it evolves throughout the growing season as an increasing amount of data are assimilated. This subsection illustrates the first and second guiding principles—expression of and mapping to decision-relevant QoI (Section 2.3).

The yield ensemble displays considerable variability throughout the season (Fig. 6). As expected, the variance of the yield forecast shows a decreasing trend with time as more observations are assimilated, with the ensemble standard deviation reducing from approximately 8 tonnes/ha shortly after bud burst to 2 tonnes/ha during January, approximately two months before harvest. The yield forecast ensemble converges within the range of destructive sampling field estimates of yield. The yield forecast ensemble range is largely consistent with the field estimate not only at the time of harvest but also throughout most of the season. However, the variance in yield late in the season still may be considered conservative, which could be addressed through refinement of prior uncertainty specifications (noting in particular that this study is the first operational decision support application of VineLOGIC), or imposing penalties on yield in accordance with expert and/or grower knowledge into the assimilation procedure.

4.3. *Joint state-parameter estimation*

This subsection illustrates the third guiding principle (Section 2.3). Here we show the outcomes of DA when undertaking state-only estimation in terms of both LAI and end-of-season yield forecasts, drawing

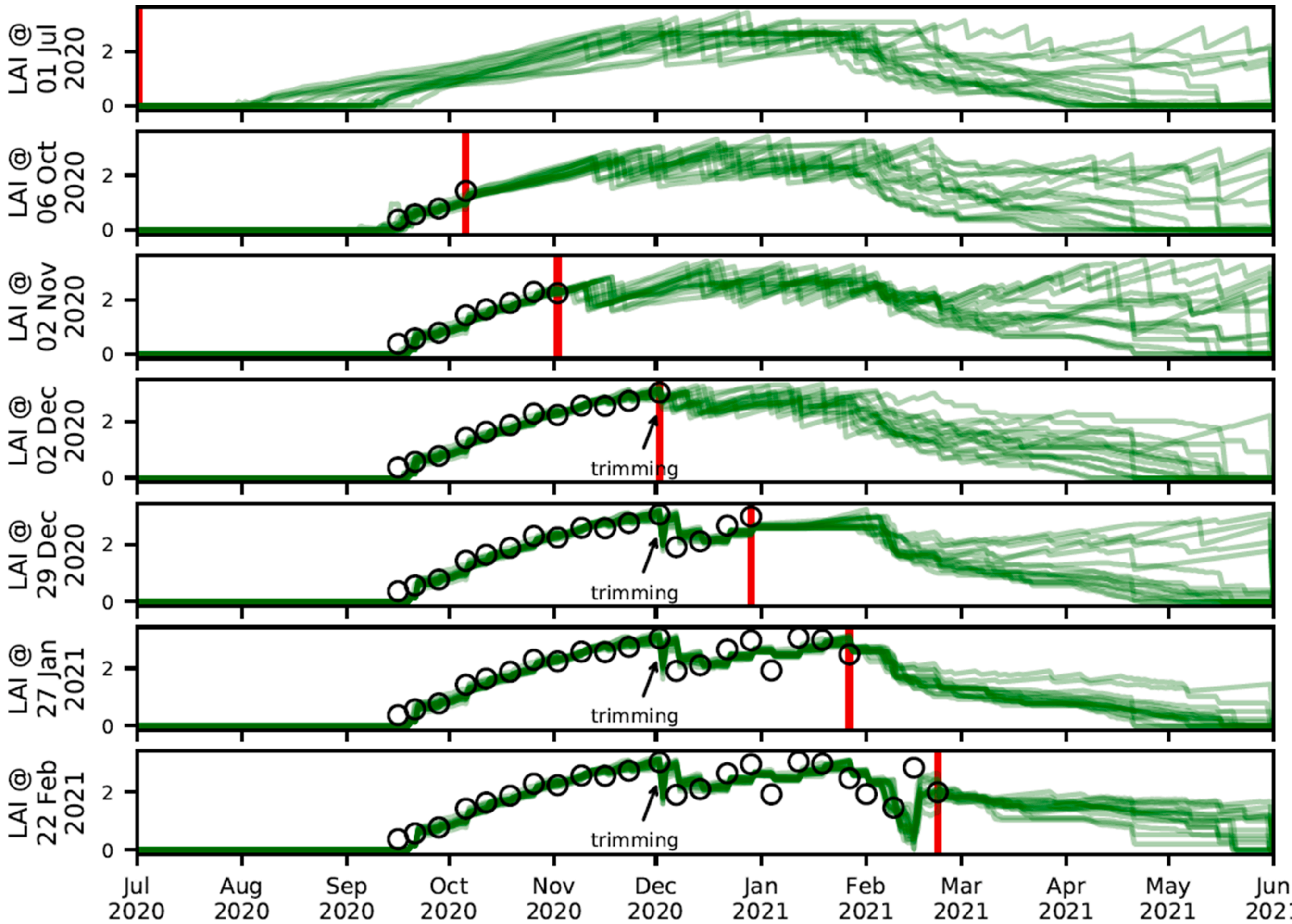

Fig. 5. Ensemble LAI time series at different stages throughout the growing season (depicted by red line). Observed LAI values are depicted by black circles. Canopy intervention events (i.e., trimming) are labelled.

comparisons to the use of joint state-parameter estimation.

Estimation of only state variables is shown to produce significantly smaller variances in LAI (Fig. 7) and in particular end-of-season yield (Fig. 8) compared to the estimation of states and parameters simultaneously (Figs. 5 and 6). The smaller variance associated with LAI trajectories hampers the ability of the forecast ensemble to capture observed LAI behaviour, especially at later stages in the season. For example, there appears to be tension between the ability of the model to fit LAI observations while also respecting that only one trimming event occurred. Forecasts of end-of-season yield exhibit overconfidence, limiting the extent to which yield forecasts can be conditioned as observations become available. The reduced variance in LAI and yield via state-only estimation is attributable to neglecting the uncertainty associated with static parameters that would otherwise be conditioned through the growing season, and may be compounded by relatively low state dimensionality leading to corruption of the DA analysis.

5. Discussion

5.1. Demonstrated benefits of guiding principles

5.1.1. Expression of decision-relevant quantities

The expression of end-of-season QoI is shown to facilitate the communication of DA outcomes in terms that are relevant to a grower or advisor and their decision-making process. For example, in our case study, the assimilation of LAI data as well as climate/weather and canopy intervention data led to a considerable conditioning of the yield forecast made at the beginning of veraison or berry ripening (mid-January) (Fig. 6), representing a particularly important point in time regarding on-farm irrigation decision making (Clingeleffer, 2001, 2010; Pagay and Collins, 2017).

Insights gained from DA are expected to be of greater value to growers or advisors when expressed in terms of forecasts of end-of-season QoI compared to forecasts of observable state variables such as LAI and soil moisture. While improved forecasts of state variables (Fig. 5) may be of interest in that they are familiar and tangible (e.g., canopy size and density can be ‘seen’ in the field), a grower or advisor still faces the challenge to understand what these insights mean in terms of farm outcomes. For example, for a grower to be informed of the status of their crop and its likely yield on the basis of LAI forecasts only, a sound understanding of the complex relationship between LAI and yield is required (Ballesteros et al., 2015). Notably, despite the greater expected ‘value’ of forecasts of QoI, these forecasts may be less conditioned through DA (Section 5.2.1).

The need to adopt crop models that can simulate end-of-season quantities such as yield and their sensitivity to stress factors is not expected to represent a significant barrier to effective crop model DA for decision support. This opportunity reflects that currently available crop models can simulate various end-of-season quantities and their sensitivities (Palosuoa et al., 2011; Knowling et al., 2021). However, crop model adoption in the future is likely to be limited by long-standing and complex socio-technical factors rather than model capability per se (McCown, 2002). It is therefore suggested that particular attention should be focused on better supporting real-world implementation of

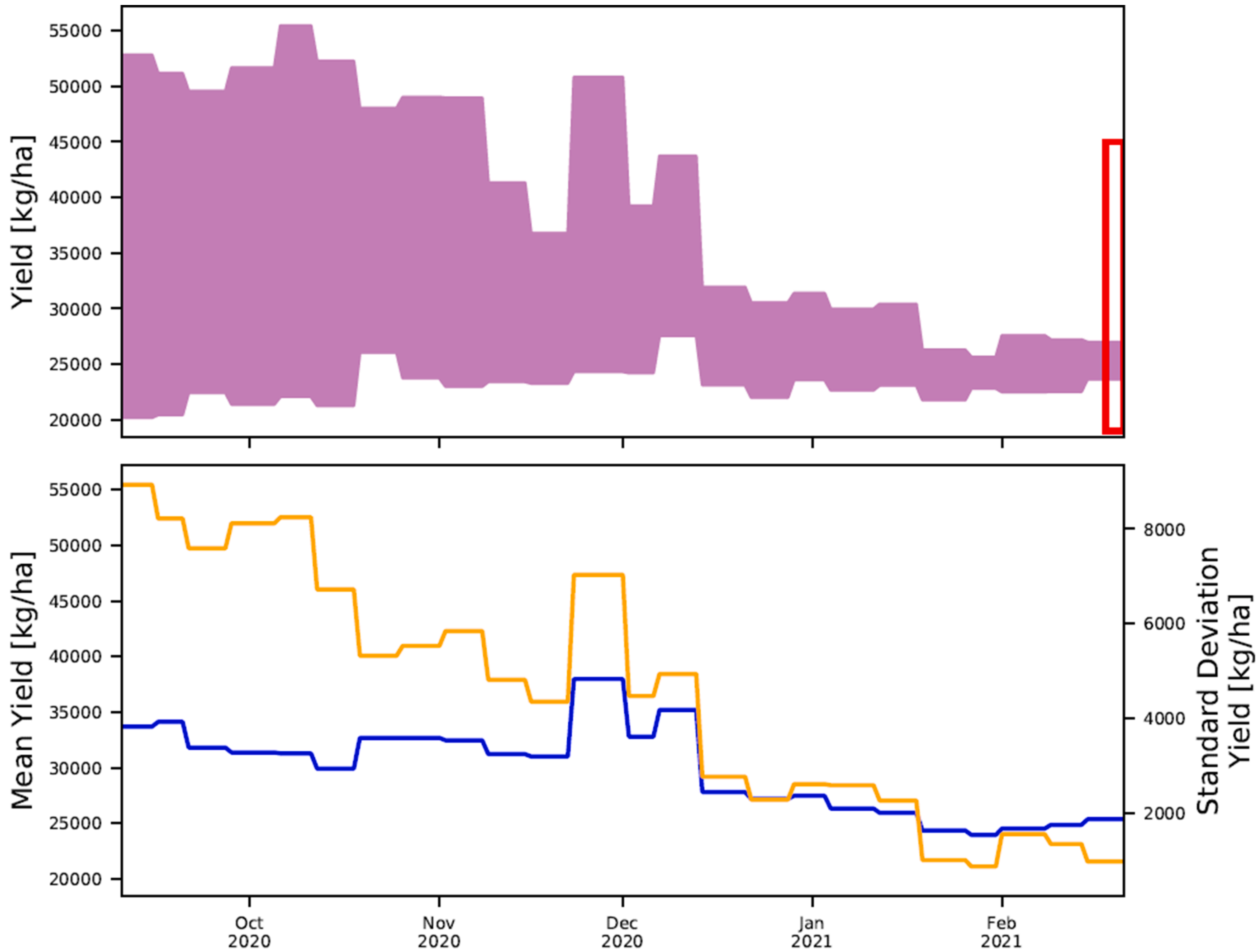

Fig. 6. End-of-season yield ensemble (purple) and mean (blue) and standard deviation (orange) as a function of time. The range of field estimates of yield via destructive sampling is depicted by the red box.

crop models for decision support through, for example, the development of software packages that facilitate the interfacing of crop models and non-intrusive DA algorithms.

5.1.2. Real-time mapping to decision-relevant quantities

Mapping DA outcomes to end-of-season QoI is shown to enable continuously up-to-date insights, building upon what has been learned from previous observations, that are relevant to a grower's decision-making process. For example, in our study, the sequential assimilation of LAI data as well as weather and canopy management data as the season progresses led to gradual conditioning of the yield forecasts, both in terms of the ensemble mean and the ensemble variance (Fig. 6).

The mapping of insights gained through DA to QoI is expected to enhance situational awareness, ultimately empowering growers or their advisors to make better-informed decisions. Enhanced situational awareness may arise from insights regarding how their crop is currently tracking in terms of its likely yield compared to the same time in previous years, for example. Evans et al. (2017) explored how situational awareness translates to informed decision making (Section 5.2.3). For example, in the context of viticulture, enhanced situational awareness may allow for on-farm decisions regarding irrigation strategies to be improved, especially at times such as the beginning of veraison, when berry growth is particularly sensitive to water stress (e.g., Petrie et al., 2004; Greven et al., 2009; Intrigliolo et al., 2016).

Continuous evaluation of DA outcomes in terms of QoI also provides an opportunity to quantitatively compare the effectiveness of different observation data for particular decision contexts in real time, representing a decision-relevant measure of the value of data. Insights from such analyses can be used to guide future data acquisition campaigns. The reader is referred to Section 5.2.2 for more details.

The need for a DA software tool that is non-intrusive (i.e., can interface flexibly with any model, without the need for 'statically linking') to continuously map insights to end-of-season QoI is not expected to serve as a significant barrier to effective crop model DA. This reflects the availability of the recently developed software tool PESTPP-DA (Alzariee et al., 2021). PESTPP-DA—and indeed all the software tools within the PEST++ suite (White et al., 2020)—has potential to facilitate model-based agricultural decision support beyond that demonstrated herein, particularly given its non-intrusiveness, public availability and open-source development environment. It is therefore anticipated that PEST++ can play an important role in accelerating adoption of model-based decision support analyses in agriculture, especially given recent and ongoing software developments to lower the barrier to entry (e.g., White et al., 2021).

5.1.3. Enhancing reliability

Joint parameter-state estimation is shown to provide a means to enhance reliability. For example, the forecast of end-of-season yield is

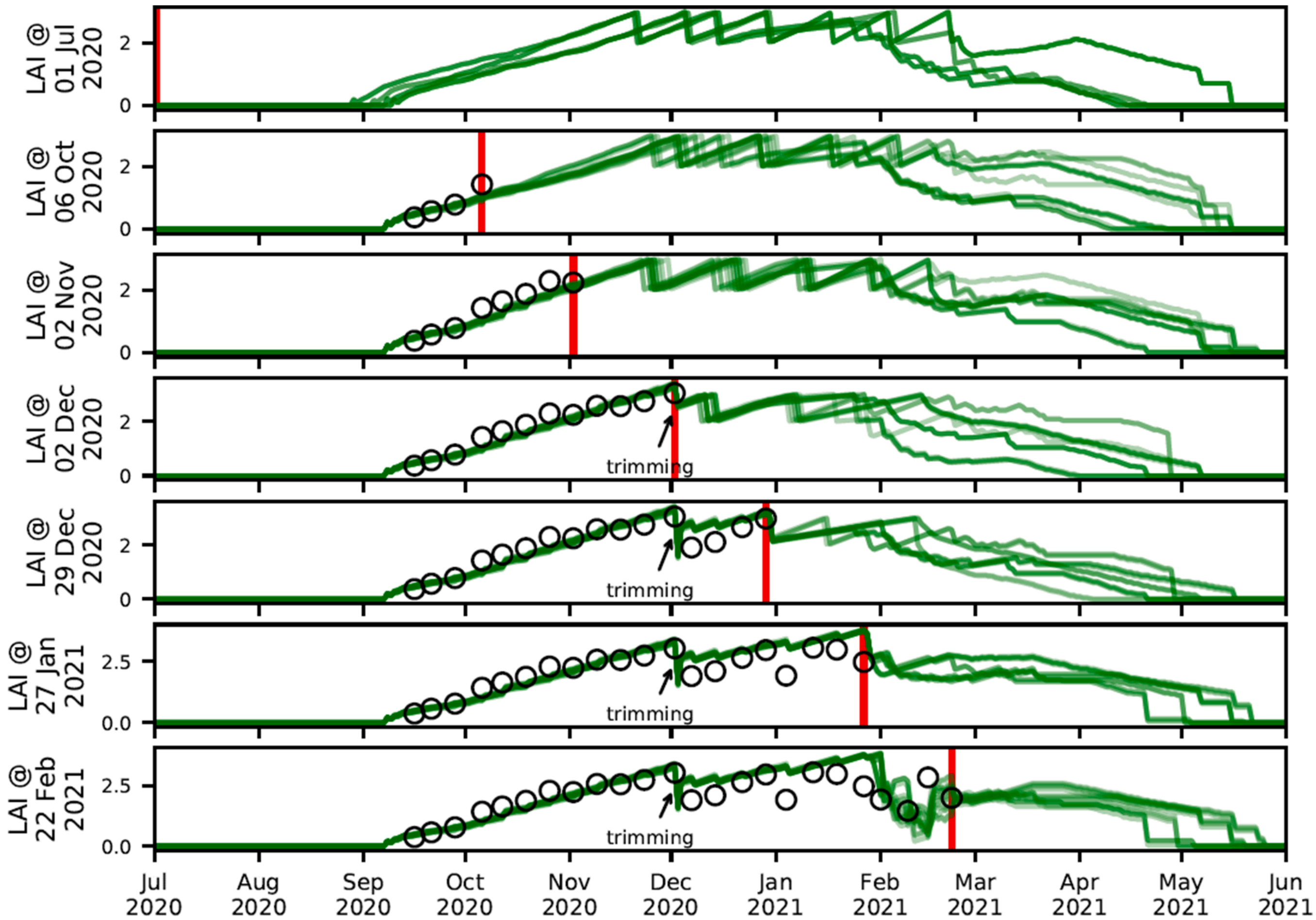

Fig. 7. Ensemble LAI time series when using state-only estimation at different stages throughout the growing season (depicted by red line). Observed LAI values are depicted by black circles. Canopy intervention events (i.e., trimming) are labelled.

more robust when jointly estimating states and parameters as opposed to state-only estimation (Figs. 6 versus 8).

We note that the more 'subtle' conditioning of forecasts of decision-relevant QoI afforded by joint parameter-state estimation, due to the more diffuse flow of information from observations to model states and parameters, may initially be interpreted as counter-productive from a decision-making perspective. However, increased variance may be required to avoid overconfidence, especially in the presence of bias (Cooley and Christensen, 2006; Knowling et al., 2019), and may serve to reduce the likelihood of an undesirable outcome (e.g., low yield) in response to a particular course of management action that was informed by forecasts of QoI.

The higher level of flexibility (or 'degrees of freedom') afforded by joint parameter-state estimation can also serve to accommodate model-data conflict to some extent (Evans and Moshonov, 2006). For example, significant adjustments in LAI states were necessary in addition to sequential parameter estimation to capture factors that are not represented in the model (e.g., unknown changes in irrigation practice). Such an ability to accommodate model structural errors is reduced when estimating states or parameters only (Fig. 7), or when undertaking DA in a batch sense (e.g., via the ensemble smoother; Chen and Oliver, 2013). The ability to accommodate model error in the context of batch and sequential DA is currently under investigation (Markovich et al., 2022).

The need for a DA software tool that can scale to high (parameter and state) dimensions to support joint parameter-state estimation, is not expected to represent a significant barrier to effective crop model DA. This is due to the recent development of PESTPP-DA (Alzraiee et al., 2021). PESTPP-DA has been demonstrated to enable flexibility in DA problem formulation (e.g., batch and sequential, state and/or parameter estimation, different update algorithms) as well as scaling to high dimensions. It is anticipated that PESTPP-DA can support the range of requirements that are likely to be encountered in crop model DA.

5.2. Recommendations for future work

5.2.1. Observation data and QoI specificity

The extent to which DA enables improved forecasts is problem-specific, depending on factors related to the observation data (e.g., number and diversity of observations, data quality), the QoI, and the degree of 'alignment' between them (Moore and Doherty, 2005; Knowling et al., 2020). Such alignment occurs where QoI forecasts and state variables corresponding to observations exhibit similar sensitivity signals with respect to model inputs. For example, in our study, forecasts of yield appear to experience less conditioning compared to LAI forecasts (Figs. 5 and 6). This reflects that the information encapsulated within the LAI observations is, unsurprisingly, more aligned to forecasts of LAI compared to those of yield, and that yield forecasts are sensitive to factors that are not informed by LAI observations. While it is well-known that assimilating observations pertaining to a particular state variable is expected to condition forecasts of that state variable into the future, the extent to which this is true for forecasts of other state variables and QoI is a more interesting and important question to pose (e.g., Linker and Ioslovich, 2017).

Despite that our case study focuses on the assimilation of canopy data from ground-based images (De Bei et al., 2016)—which are particularly effective in mapping grapevine canopies across vineyards (Arno et al.,

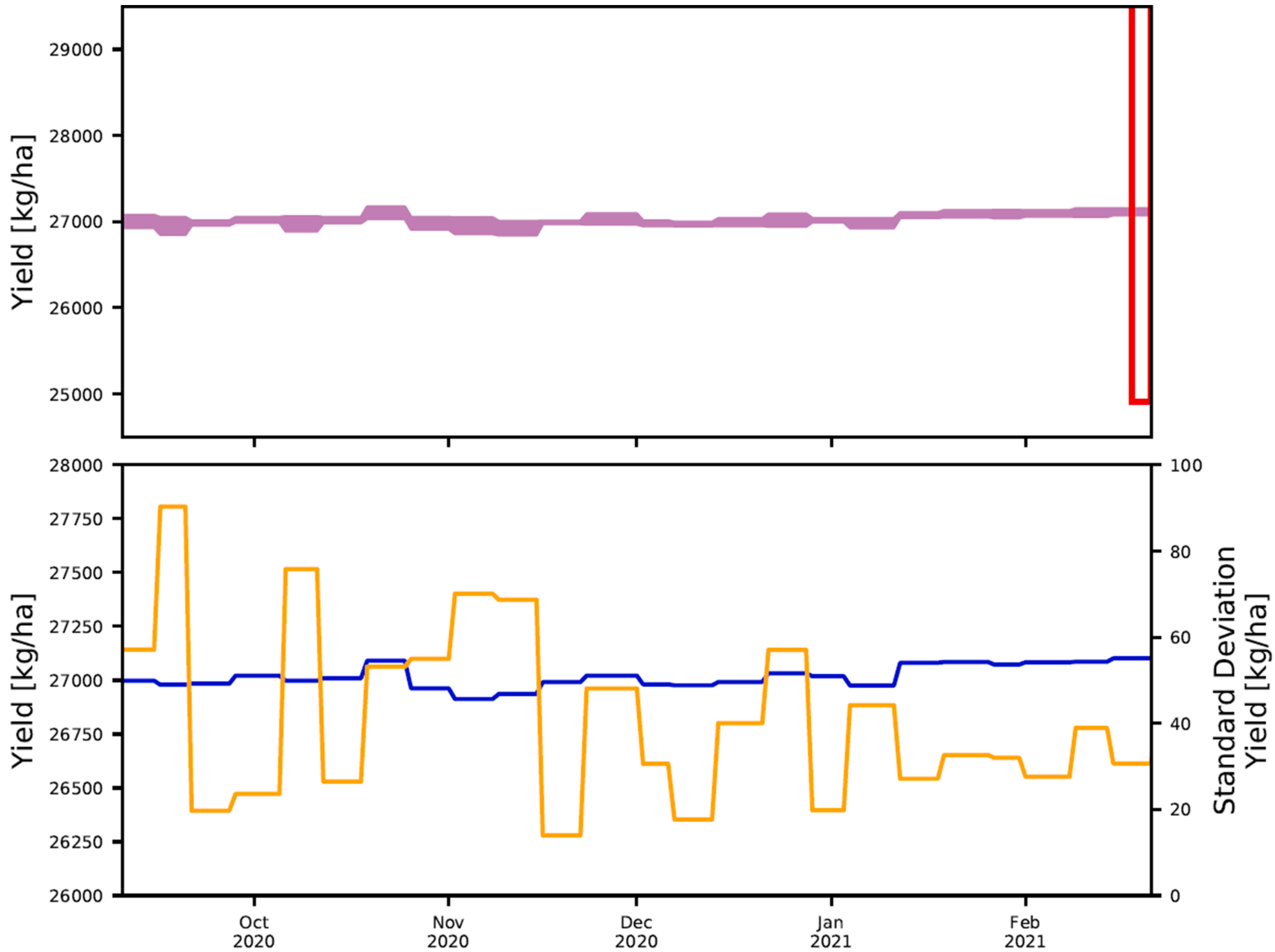

Fig. 8. End-of-season yield ensemble (purple) and mean (blue) and standard deviation (orange) when using state-only estimation as a function of time. The range of field estimates of yield via destructive sampling is depicted by the red box.

2013; De Bei et al., 2019; Ouyang et al., 2020)—the process of DA as well as the guiding principles introduced herein, lend themselves to be extended to assimilate different observation data streams and support different QoI. It is suggested that future studies leverage the generalizability of both DA and the guiding principles to support different agricultural decision-making contexts. Application of crop model DA in different settings will also help elucidate generalizable patterns regarding which observation data are most informative for different QoI (Section 5.2.2).

5.2.2. *Data acquisition guidance*

The guiding principles introduced provide an opportunity to evaluate the 'value' of different observation data in a way that is relevant to a decision maker. Quantifying the value of observation data in terms of their ability to condition forecasts of QoI is gaining popularity in disciplines such as hydrology (e.g., Dausman et al., 2009; Partington et al., 2020). While the value of a particular data stream will be problem-specific (Section 5.2.1), case studies that empirically evaluate the generalizability of a data stream's value amongst different decision contexts may be particularly useful. Moreover, future studies could compare the relative value of different observation 'types' including less traditional data streams such as sap flow rates (e.g., Sus et al., 2014) and phenological observations (e.g., Viskari et al., 2015). Future studies could also evaluate the value of observation timing (e.g., during which growth stage) as well as frequency (e.g., daily, fortnightly). Insights from such analyses could offer guidance regarding "which data to collect?" and "when to collect them?" in a way that considers both the uniqueness and decision-relevance of the information contained within observations.

5.2.3. *Enhanced situational awareness and decision support*

This study serves as a step towards bridging the gap between data and decisions in agriculture. This gap is currently growing due to the greater focus on observation data acquisition compared to translating observation data into information to support decisions, through data processing, modelling etc. (Leonard et al., 2017). The real-time fusion of observation data and prior knowledge embedded in models by practitioners (e.g., advisors) allows for enhanced on-farm situational awareness via a unified, up-to-date depiction of crop status and development. Situational awareness has been achieved through formal DA across a wide range of fields from epidemiology (Li et al., 2020) to space weather (Mehta and Linares, 2018).

Despite enhanced situational awareness, how this creates value for growers and their advisors is complex (Evans et al., 2017) and will vary significantly from individual to individual (Rossi et al., 2014). It is expected that combining situational awareness afforded by DA with a sound understanding of the impact of operational farm decisions such as irrigation amount and timing, will enable improved on-farm decisions. A promising opportunity to further extend the decision support capacity of crop model DA is to leverage the 'cause-and-effect' relationships that are embedded within crop models (Knowling et al., 2023) by simulating different management scenarios within the DA workflow. These relationships may benefit through derivation from participatory modelling approaches (Naulleau et al., 2022).

6. Conclusions

This paper introduces three guiding principles aimed at operationalizing crop model DA for robust on-farm decision support. By applying these principles to a viticulture case study, the potential for crop model data assimilation (DA) to enhance forecasts of decision-relevant quantities is demonstrated. Assimilation of leaf-area index (LAI) data as well as climate/weather and canopy intervention data led to a significant improvement in yield forecasts, with the mean and variance of the forecast ensemble converging towards independent field-based estimates approximately two months before harvest. By mapping DA outcomes to end-of-season quantities in real-time, insights could be gained about when various observations are most informative in terms that are relevant to a decision maker. The case study also highlights the potential of joint parameter-state estimation as a means to avoid forecast overconfidence.

This study serves as an important step towards bridging the gap between data and decisions in agriculture. It demonstrates a vital capability to integrate, in real-time, diverse observation data and predictive models, enabling situational awareness, i.e., a unified depiction of what is happening and what is likely to happen on the farm. This is a prerequisite for digital agriculture to succeed in supporting decisions towards improved farm outcomes.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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