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Why make inverse modeling and which methods to use in agriculture? A review

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ABSTRACT

Inverse modeling (IM) is a valuable tool in agriculture for estimating model parameters that aid in decision-making. It is particularly useful when parameters cannot be directly measured or easily estimated due to logistical constraints in agricultural settings. Unlike other estimation methods, IM combines a mechanistic model with observations of its outputs to derive the parameters of interest, allowing for the integration of various sources of knowledge. The availability of numerous data sources, such as remote sensing and crowdsourcing, with high spatial and temporal resolution, has expanded the potential of IM in agriculture. Practitioners can now incorporate the spatial and temporal footprint of observational data into parameter estimation. However, common IM techniques currently applied in agriculture often struggle to account for effectively spatial and temporal variability. Relevant IM methods that address these challenges are usually isolated within specific developer and user communities and are not well known within the agricultural community. There is a lack of comprehensive reviews focusing on IM methods suitable for handling spatial and temporal data in agriculture. In parallel, the process of conducting IM in agriculture remains under-formalized. Typically, specific IM methods are chosen for specific combinations of models and types of observational data, but the rationale behind their selection is rarely explained in publications. The relationship between IM methods, models, and observational data is unclear, making it overwhelming for new practitioners to choose an appropriate method. This complex problem, along with the diversity of IM methods, has yet to be adequately addressed while taking into account the specificities of agricultural applications. To address these challenges, this review aims to provide a structured classification of IM methods based on the practical needs of new practitioners in agriculture. It examines a wide range of inversion methods applied in agriculture-related domains and covers four key topics: i) the essential elements and general process of IM, ii) the main families of IM methods in agriculture and their characteristics, iii) the circumstances in which practitioners prefer using IM over other approaches, and their motivations, and iv) practical guidance on choosing a method family based on operational criteria. The review aims to help readers develop a clear understanding of the practice of inverse modeling, gain insights into the diversity of IM methods, and make informed choices when selecting a method family for their agricultural applications.

1. Introduction

Inverse modeling (IM) is used in a wide range of applications domains such as crop and soil modeling (Cousin et al., 2022), groundwater modeling (Irsa and Zhang, 2012), atmospheric modeling (Hrad et al., 2021) or environmental modeling (Lu et al., 2013). IM is considered as a powerful approach for estimating unknown parameters of mechanistic models based on observations of their output as well as the models themselves (Milledge et al., 2012). By utilizing both: a mechanistic model and observational data, IM is often used to estimate model parameters that correspond to useful information which are hard and tedious to measure due to logistical constraints (e.g. soil hydraulic properties (Pinheiro et al., 2019)), or conceptual variables (e.g. leaf structural parameters introduced in PROSPECT (Jacquemoud and Baret,

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1990)). In agriculture, IM has gained recognition to estimate parameters for decision support (e.g. for crop water management (Araya et al., (2013), Kumar et al. (2022)), and/or to calibrate mechanistic models (e.g. crop model STICS (Wallach et al., 2011)). Depending on the application, the variables estimated in agriculture by using IM are highly diverse, including the estimation of plant available water capacity (Morgan et al., (2003), Jiang et al. (2008), Florin et al. (2010), Todoroff et al. (2010), Campos et al. (2016), Gaudin et al. (2017), Dewaele et al. (2017), He et al. (2021), He et al. (2022)), soil water holding capacity (Sreelash et al., 2017), plant growth traits (e.g. Leaf Area Index (LAI)) (González-Sanpedro et al., (2008), Dzotsi et al. (2015), Xu et al. (2019), Wan et al. (2021), Wang et al. (2022)), plant root water uptake (Wang et al., 2021), evapotranspiration (Angaleeswari and Ravikumar, 2019), soil hydraulic properties (Ritter et al., (2003), Verbist et al. (2009), Montzka et al. (2011), Charoenhirunyingyos et al. (2011), Dokoohaki et al. (2018), Gabriel et al. (2019), Fernández-Gálvez et al. (2021)), soil moisture (Del Frate et al., (2003), Ghorbanian et al. (2019), Liang et al. (2021)), soil organic content and associated parameters (Kwon and Hudson (2010), Gurung et al. (2020)), plant nutrient level (e.g. Leaf Chlorophyll Content) (Houborg and Boegh (2008), Camino et al. (2018), Chaabouni et al. (2021), Antonucci et al. (2023)), or aquaculture system properties (Jamu and Piedrahita, 2002). This diversity highlights the potential of IM in agriculture, as the approach allows accounting for both general process-based simulation and specific observational data, providing a cost-effective way to estimate unknown quantities, especially when data availability is low.

One of the main limitations of IM is that it is only possible when observations of output variables of the system are available. For many years, this limitation slowed the development of IM in agriculture because observations were difficult or expensive to obtain but in the last years, new sources of observations have emerged in agriculture. Indeed, new satellite constellations offering better temporal (Chintala et al., 2022) and spatial (Cheng et al., 2020) resolutions, open-access databases focusing on soil (Quiros et al., 2009) or vegetation (Mylonas et al., 2022), point-cloud-based data like LiDAR (Akwensi et al., 2023), or projects of crowdsourcing collecting substantial number of ground observations (Minet et al., (2017), Pichon et al. (2022)) are reaching maturity. This availability of observations with better spatial and temporal resolutions increased the potential of applying IM in agriculture. However, certain data sources are prone to errors in measurement or obtention (e.g. low-cost sensors (Satoh and Kakiuchi, 2021), observations made by farmers (Pichon et al., 2022) etc.). It is also important to note that not all accessible data directly correspond to the observations of mechanistic models: the exact coincidence between what a sensor measures and what a model simulates is rare (Zhang et al., 2021), which introduces extra uncertainty in inverse modeling. As a result, it is crucial to take into account uncertainty when making inverse modeling (Iizumi et al., 2009). Uncertainty information is however, often overlooked in agricultural IM applications (Uusitalo et al., 2015).

In parallel, IM techniques that are commonly applied in agriculture often struggle to account for temporal and/or spatial variability (Cousin et al., 2022). Nonetheless, agricultural stakeholders regularly face dynamic systems related to plant growth and/or nutrient assimilation, which also manifest spatial variability (Kerry and Oliver, 2008). Relevant approaches do exist in other scientific domains (Hendricks Franssen et al., (2009), Montzka et al. (2012)), but they seem to be little known in agriculture. Furthermore, the methodological choices made on inverse modeling and their justification related to the specificities of agricultural applications are rarely formalized and explained in the literature. Authors seldom explain or justify why they applied inverse modeling, instead of other more straightforward approaches, like direct measurements or statistical modeling. Indeed, most model parameters have physical meanings hence can be directly evaluated (e.g. soil critical humidity (Cousin et al., 2022)). While another approach that builds statistical models can predict a searched parameter with other explanatory variables, which is a common practice in agriculture (Song et al., 2023). Additionally, the process of conducting IM in agriculture also remains under-formalized. Typically, specific IM methods are chosen for specific combinations of models and types of observational data, but it has been observed that the rationale behind their selection (if it exists) is rarely explained in publications. The relationship between IM methods, models, and observational data remains unclear, posing challenges for new IM practitioners to choose an appropriate inversion method.

This review aims to fill these gaps by offering a comprehensive and structured classification of IM methods commonly used in agriculture. It covers a broad range of inversion methods employed in agriculture-related domains and focuses on four key topics. Firstly, it explores the fundamental elements required for conducting IM and provides a general overview of various IM approaches (section 1.1). Secondly, it categorizes the main families of IM methods used in agriculture, and examines their unique characteristics (section 1.2). Thirdly, it investigates the circumstances in which practitioners prefer IM to other approaches for deriving model parameters. The review highlights not only the motivations of practitioners, but also the operational benefits of preferring IM approach to other approaches when it deals to provide estimations (section 2). Lastly, based on the literatures, it offers practical guidance for selecting an appropriate IM approach based on practitioners' specific situations, and emphasizes potential pitfalls to consider throughout the process (section 3).

2. What is inverse modeling and which are available methods for agricultural applications?

2.1. Definitions

2.1.1. Forward modeling

Forward modeling and inverse modeling are paired concepts. Forward modeling (or just modeling) refers to actions to build process-based models from modeler's understanding of a natural or artificial system in agriculture (Wallach et al., 2014a). The objective of a process-based model (or mechanistic model) is to predict the future or unobserved behavior of a system of interest, like the environmental or biological processes. A simplified description of the main elements of a process-based model is given in Fig. 1.

A process-based model consists of, on the one hand, i) mathematical formulas and ii) parameters, which both describe how the system of interest works and are supposed to be strictly invariant; on the other hand, iii) explanatory variables describing external conditions that may impact the system. These latter can be independent (e.g. soil-depth) or dependent (e.g. weather data) on time. A process-based model can be either static or dynamic. Static models are independent on time, while dynamic models predict the temporal evolution of a system, by iteratively updating a set of state variables at each time step. The system modeled by a process-based model can either be dimensionless (i.e. aspatial models), or occupy a certain depth/surface/volume in space (i.e. spatial models). A spatial model requires parameters and explanatory variables to be specified at each simulated location. The computer program which accounts for all elements of a process-based model forms a numerical model. Model simulation is the process in which a numerical model generates outputs, or predictions. A process-based model can be represented in a simple form by Equation (1).

$$\widehat{\boldsymbol{Y}} = \boldsymbol{f}(\boldsymbol{u}, \boldsymbol{\theta}) \tag{1}$$

where $\widehat{\boldsymbol{Y}}$ is the vector of model predictions (i.e. model outputs), f is the function including mathematical formulas describing the studied sys-

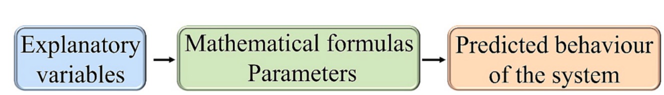

Fig. 1. A simplified view of the main elements of a process-based model.

tem, u is the vector of explanatory variables and θ is the vector of parameters (u, θ are model inputs). Depending on whether the $\boldsymbol{f}$ is static or dynamic, aspatial or spatial, $\widehat{Y}$ could be predictions that are independent or dependent on time ($\widehat{Y}_t$) and location ($\widehat{Y}_s$).

The difference between $\widehat{Y}$ and actual observed behavior of a studied system (observations: $\boldsymbol{Y}$) is the model residual ($\boldsymbol{\varepsilon}$). The presence of $\boldsymbol{\varepsilon}$ is generally inevitable, due to the uncertainties associated to the model structure, model inputs, and observations. The relationship between $\widehat{Y}$ and $\boldsymbol{Y}$ can be described by Equation (2).

$$\boldsymbol{Y} = \widehat{\boldsymbol{Y}} + \boldsymbol{\varepsilon} = \boldsymbol{f}(\boldsymbol{u}, \boldsymbol{\theta}) + \boldsymbol{\varepsilon} \tag{2}$$

2.1.2. Inverse modeling

Inverse modeling corresponds to the inverse principle of forward modeling (Fig. 2). Inspired from the definition of inverse problem (Nakamura and Potthast, 2015), inverse modeling can be described as a process which infers the "causes" that lead a certain system to produce certain behaviors (i.e. "effects"), by using observations on those behaviors and knowledge on that system (Hendricks Franssen et al., (2009), Zhou et al. (2014), Ghorbanidehno et al. (2020), Zhao and Luo (2021)). Hence, inverse modeling is not a singular method, but an ensemble of approaches which allow to retrieve unknown model parameters, and/or (initial) state variables, and/or explanatory variables, by using observations ($\boldsymbol{Y}$) and a process-based model f. For simplification, the unknown quantities mentioned above will be referred together as the estimated parameters, or $\boldsymbol{\theta}^*$ in the following text, with two specifications noted as $\boldsymbol{\theta}_t^*$ and $\boldsymbol{\theta}_s^*$, respectively for $\boldsymbol{\theta}^*$ in dynamic and spatial models. Correspondently, observations used to retrieve $\boldsymbol{\theta}_t^*$ and $\boldsymbol{\theta}_s^*$ are noted as $\boldsymbol{Y}_t$ and $\boldsymbol{Y}_s$.

In the literature related to agriculture, two types of inverse modeling approaches satisfy the definition given above, hence are used to estimate $\boldsymbol{\theta}^*$. The first type treats the forward model as a black box (Wallach et al., (2011), Lamsal et al. (2017)). This latter provides simulations which are essential for inversion. The fundamental idea behind this first type of methods is to reduce the incoherence ($\boldsymbol{\varepsilon}$) between model simulations and real-life observations ($\boldsymbol{\varepsilon}$) using various techniques. This type of inversion methods is referred to as simulation-based methods in this review.

The second type of methods focuses on expressing $\boldsymbol{\theta}^*$ with an inverse model that incorporates observations (Román et al., 2011). The latter can be the explicit mathematical inverse function of the f , or an approximate solution based on some simplifications/reformulations. The key point of the second type of methods is to build an inverse model, then to use observations to directly calculate the estimated parameter. These methods are referred to as model-based methods.

Depending on the specific problem to deal with, both types of methods can be found in agriculture. Sometimes they can even be used in a combinational way (Campos et al., (2016), Farthing et al. (2017)). However, such applications remain rare, and this review will focus on the most general approaches.

2.2. Available methods of inverse modeling in domains of agriculture

In the search for relevant literature to ensure a global coverage on inverse modeling applications in agriculture, the search strategy involved the use of specific keywords, including "inverse modeling", "(model) inversion (methods)", "inverse method/problem/model", "parameter identification/retrieval/optimization", "model/parameter calibration", "optimization", "Bayesian calibration", "PROSAIL", "RTM", and "remote sensing + crop model". The search encompassed a broad spectrum of agricultural science-related journals (e.g. Agriculture Water Management, Computers and Electronics in Agriculture, European Journal of Agronomy, Smart Agricultural Technology and etc.). Additionally, papers from journals in the fields of hydrology and remote sensing were included (e.g. Journal of Hydrology, Advances in Water Resources, Geoderma, Remote Sensing of Environment, Comptes Rendus Geoscience, International Journal of Applied Earth Observations and Geoinformation, ISPRS Journal of Photogrammetry and Remote Sensing and etc.). In total, 76 scientific papers were regarded as examples of inverse modeling in agriculture, hence were used for extracting the main approaches of model inversion. Among them, 25 papers focused on retrieving soil hydraulic properties (e.g. field capacity, permanent wilting point etc.) and/or soil/plant available water capacity, 25 papers aimed at estimating plant growth traits and/or nutrient levels (e.g. LAI, leaf chlorophyll content), 13 papers strived for obtaining flow properties of a groundwater system (e.g. hydraulic transmissivity, conductivity etc.), 7 papers focused on retrieving soil moisture, while other papers (n = 6) searched various parameters in crop modeling, like soil organic matters, or canopy parameters.

Seven families of inverse modeling methods were identified: i) Frequentist Parameter Estimation (section 1.2.1), ii) Bayesian Parameter Estimation (section 1.2.2), iii) Sequential Filters (section 1.2.3), iv) Geostatistical Inversion (section 1.2.4), v) Explicit Inversion, vi) Approximate Inversion, and vii) Hybrid Inversion (section 1.2.5). The classical usage of regressions, decision trees, neural networks, or other Machine/Deep Learning models for predicting searched parameters using explanatory variables, was not considered as inverse modeling approaches in this review, if no process-based model was used to train those models. However, readers can find further discussion on this topic in section Perspective 4.2.2.

Frequentist and Bayesian Parameter Estimation are firstly presented, because they represent the majority of existing agricultural applications. Afterwards, the other families of method will be introduced. It should be acknowledged that the proposed organization aims at highlighting general differences between families of methods, and it is not intended to be exhaustive. For identifying more specific inversion algorithms, readers may consult the work of Zhou et al. (2014), Rajabi et al. (2018), Verrelst et al. (2019), and Ghorbanidehno et al. (2020).

2.2.1. Frequentist parameter estimation (FPE)

To date, Frequentist Parameter Estimation is the most applied family of methods of inverse modeling in agriculture, as it has been applied on a wide range of agricultural models (e.g. crop models (Zhang et al., 2011), canopy models (Wigneron et al., 1993), disease models (Jørgensen, 2000), irrigation models (Dari et al., 2022) etc.) by using a generalizable optimization procedure. FPE methods are simulation-based inversion techniques. They rely on the estimation of the disagreement between simulated and observed model outputs through an objective function. The latter is minimized by searching the best possible vector of $\boldsymbol{\theta}^*$ values. The challenge lies on assuring that the searching algorithm will converge to an optimum solution of estimated parameters that is physically sound. The process can be considered as similar to a classical model calibration process (Wallach et al., 2014b).

Illustrated by Fig. 3, the general optimization procedure consists of three common actions which are carried out iteratively:

(i) Parameterization of the forward model. Firstly, parameters which are not the goal of inversion, noted as $\boldsymbol{\theta}^-$, must be specified with appropriate values and be fixed during upcoming steps. Secondly, a vector of $\boldsymbol{\theta}^*$ values (noted as $\boldsymbol{\theta}^*{}_i$) selected from the parameter space of $\boldsymbol{\theta}^*$ is input into the forward model with the $\boldsymbol{\theta}^-$.

(ii) Simulation of the forward model. The forward model generates a set of predictions, $\widehat{\boldsymbol{Y}}_i$, using $\boldsymbol{\theta}^-$ and $\boldsymbol{\theta}^*{}_i$.

(iii) Evaluation of the selected $\boldsymbol{\theta}^*{}_i$. An objective function $\boldsymbol{O}(\widehat{\boldsymbol{Y}}_i, \boldsymbol{Y})$ assembles model predictions and actual observations, hence quantifies

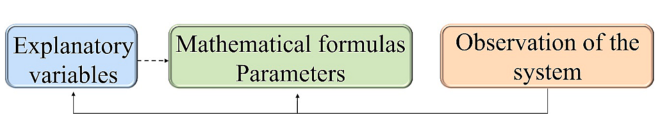

Fig. 2. A simplified view of the objective of inverse modeling.

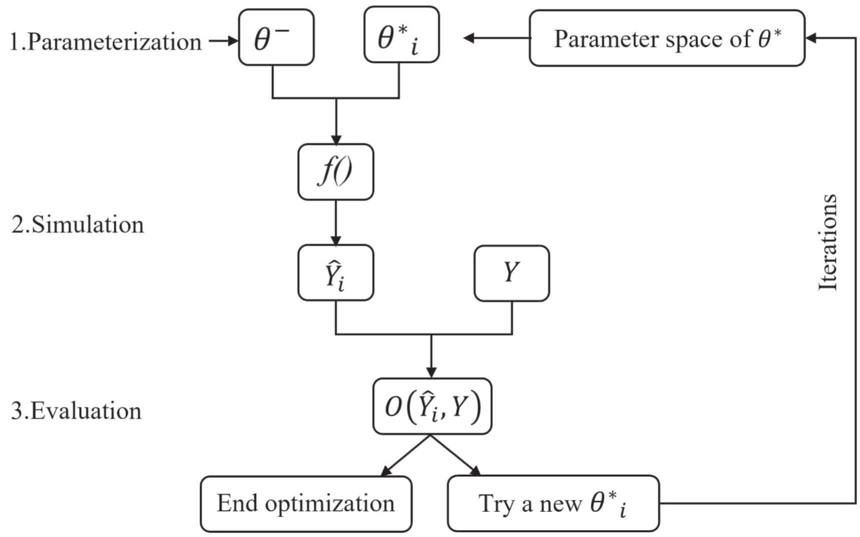

Fig. 3. The general optimization procedure in Frequentist Parameter Estimation.

$\boldsymbol{\varepsilon}_i$. The outcome is evaluated under a pre-defined criterion, which determines whether a new vector of $\boldsymbol{\theta}^*$ values will be drawn, and step (i) will be repeated. The criterion must allow the optimum solution $\boldsymbol{\theta}^*{}_{opt}$ to satisfy Equation (3).

$$\boldsymbol{min}\{\boldsymbol{O}(\widehat{\boldsymbol{Y}}_{opt}, \boldsymbol{Y})\}$$

$$\widehat{\boldsymbol{Y}}_{opt} = \boldsymbol{f}(\boldsymbol{\theta}^-, \boldsymbol{\theta}^*{}_{opt}) \tag{3}$$

Although the objective of the FPE approach is to optimize $\boldsymbol{\theta}^*$, the choice of $\boldsymbol{\theta}^-$ is critical. A realistic parameterization is indispensable for getting accurate values of $\boldsymbol{\theta}^*$, while the opposite can ruin the estimation due to the compensation effect (Wallach et al., 2014b) (i.e. because the retained estimated parameters' values can be selected to reduce the prediction errors only because of wrongly chosen $\boldsymbol{\theta}^-$). The parameterization can be improved through bibliographic research, in-field measurements, or preliminary model calibration (Alkassem et al., 2022).

The number of iterations depend a lot on the chosen optimization algorithm and the searching criteria provided by practitioners. Numerous optimization algorithms are open-sourced (e.g. gradient-based, sampling-based algorithms) (Chaabouni et al., 2021). Agricultural communities commonly use black-box optimizers (e.g. PEST (Doherty, 2015)) or metaheuristic algorithms (César Trejo Zúñiga et al., 2014) like the Genetic Algorithm (Ferreiro et al., (2016), Wallach et al., (2014c), Ghorbanian et al. (2019)). The search of $\boldsymbol{\theta}^*{}_{opt}$ can be facilitated by wisely setting initial values and boundary conditions. The objective function can account for multiple types of observations and take different forms for satisfying specific application context (Sreelash et al., (2012), Mahévas et al. (2019)).

2.2.2. Bayesian parameter estimation (BPE)

Bayesian Parameter Estimation methods are model calibration methods which are carried out under the probabilistic framework (Wallach et al., 2014c). In agriculture, BPE methods have become popular since two decades thanks to the growth of computational power (Makowski et al., 2002). Similar to the FPE approach, their applications can be found in various domains (e.g. hydrology (Lu et al., 2013), crop science (Gao et al., (2021), Hjelkrem et al. (2021))). The BPE methods consider $\boldsymbol{\theta}^*$ as random variables, which can take different values under certain associated probability according to a Probability Density Function (PDF). The objective is to obtain $\boldsymbol{\theta}^*$ posterior PDFs by optimally accounting for prior knowledge and observations. The use of probabilistic distributions permits also to describe possible interactions between estimated parameters (Wang et al., 2022).

BPE algorithms are based on Bayes theorem (Equation (4):

$$P(\theta^*|\boldsymbol{Y}) \propto P(\boldsymbol{Y}|\theta^*)^* P(\theta^*) \tag{4}$$

Where $P(\theta^*)$ is the PDF that reflects the prior belief of θ^* (i.e. prior), $P(\boldsymbol{Y}|\theta^*)$ stands for the function of likelihood of observing observations given each value of θ^*, and $P(\theta^*|\boldsymbol{Y})$ represents the PDF of θ^* updated from the prior using observations (i.e. posterior), $\propto$ means "is proportional to".

In general, the exact mathematical expression of $P(\theta^*|\boldsymbol{Y})$ cannot be obtained analytically (Lizumi et al., 2009). Consequently, the BPE approach usually strives for representing the posterior PDF with samples, whose general procedure is illustrated in Fig. 4. The individual prior PDF of each estimated parameter in θ^* must be defined at first (step 1). Each estimated parameter is usually assumed to be independent from the others, so the joint prior PDF of θ^* can be computed as product of individual PDFs (step 2). Then, a possible combination of $\boldsymbol{\theta}^*{}_i$ is sampled from the joint prior PDF, and input into the forward model. This latter is used as a black-box to generate simulations (i.e. which makes the BPE approach a simulation-based inversion method) (step 3). A likelihood function that quantifies the plausibility of $\boldsymbol{\theta}^*{}_i$ given observations is computed, producing $P(Y|\theta^*)$ (step 4). Depending on the algorithm, certain calculations are made to decide whether the $\boldsymbol{\theta}^*{}_i$ is accepted based on information from previous steps (step 5). Steps between step 3 and 5 are repeated to obtain a set of accepted $\boldsymbol{\theta}^*{}_i$, which represents the joint posterior PDF of θ^*. At last, the individual posterior PDF of each estimated parameter can be obtained by using the set of accepted values (i.e. samples).

Typically, samples are combinations of possible estimated parameter values, and the high-density zones of the posterior PDF consist of values that are the most present among samples. Popular sampling algorithms are based on the Markov Chain Monte Carlo (MCMC) (Lu et al., 2013), Hamiltonian Monte Carlo (Neal, 2011), or the Sampling-Importance-Resampling (SIR) (Gurung et al., 2020). They approximate the posterior PDF from a large number of model simulations. Some methods don't search the entire posterior PDF, but only extract useful information of it, such as Generalized Likelihood Uncertainty Estimation (GLUE) (Sreelash et al., 2017), Look Up Table (LUT) (González-Sanpedro et al., 2008), or Maximum-A-Posteriori (MAP) oriented optimization (Hippenstiel, 2017). These methods focus on searching the statistical mode of the posterior PDF, which can be interpreted as the most probable value of the estimated parameter.

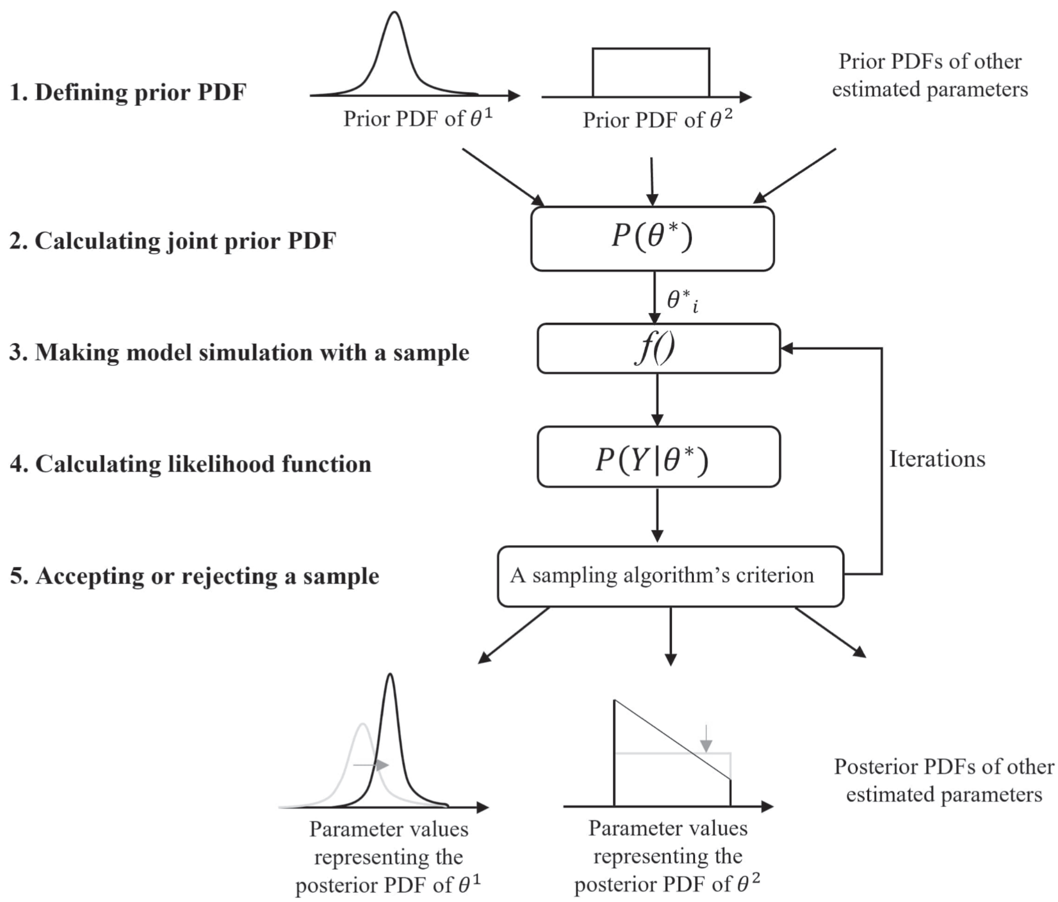

Fig. 4. The general procedure of Bayesian Parameter Estimation.

Prior information can impact greatly the BPE outcome. Wallach et al., (2014c) showed that a BPE method using very flat prior PDF generates results close to those estimated by a FPE method. While excessively narrow priors can bring in too much impact on posterior PDF, making observations under-considered (Rajabi et al., 2020). It is common to put effort in preliminary literature research to obtain prior PDFs of $\boldsymbol{\theta}^*$ (Gimson and Uliasz, 2003). In agricultural applications, parameters often have some clear physical meanings, hence expert or background knowledge are also common sources of prior information (Zhang et al., 2021). In-field experiments can also be conducted to construct priors of estimated parameters (Sreelash et al., 2017).

2.2.3. Sequential filters (SF)

Sequential Filters are algorithms originally developed for estimating state variables which have been mostly used in the Data Assimilation community (Montzka et al., (2012), Jiang et al. (2014)). However, the SF approach can focus especially on estimating model parameters. They are considered as a family of simulation-based inverse modeling methods, because the approach also relies on simulations of a forward model. The SF approach makes use of high temporal resolution data streams ($\boldsymbol{Y}_t$) like satellite imagery or soil sensor data, to estimate $\boldsymbol{\theta}_t^*$ in dynamic models (e.g. crop models (Huang et al., 2019), or hydrological models (Montzka et al., (2011), Chaudhuri et al. (2018))). SF methods can demonstrate how $\boldsymbol{\theta}_t^*$ may evolve in time by estimating it each time when a new observation becomes available (Liu et al., 2020).

The signature feature of SF methods consists in a duo-model formalism, which is composed by a process model and an observational model. A process model is a numerical object that is globally coherent with what is described by Equation (1), which generates simulations ($\widehat{\boldsymbol{Y}}_t$). In the classical context where SF approach is applied, this model tends to be a set of equations representing the evolution of state variables. However, static model parameters can also be included in $\widehat{\boldsymbol{Y}}_t$, by applying a Gaussian random-walk model to propagate their values from one time step to the next one (Zhang et al., 2021). The observational model, for its part, links what the process model simulates (i.e. $\widehat{\boldsymbol{Y}}_t$) to what are actually observed (i.e. $\boldsymbol{Y}_t$). A simple linear model (Y = X) can be used (Zhang et al., 2021), but a more complex mechanistic model (e.g. PROSAIL) can equally be employed (Machwitz et al., 2014). This duo-model structure allows separately accounting for the uncertainty in model simulations and observational data.

The inversion in SF methods consists of using the duo-model system through two steps: i) the forecast step: making a forecast of $\widehat{\boldsymbol{Y}}_t$ using the process model that is used as a black-box; ii) analysis step: transforming $\widehat{\boldsymbol{Y}}_t$ using the observational model and inputting the transformed forecast together with $\boldsymbol{Y}_t$ into a mathematical structure (e.g. a likelihood function) to generate useful information that allows updating the forecast (which includes $\boldsymbol{\theta}_t^*$) in the previous step. The forecast and analysis step are carried out recursively, which means that the result from analysis step will be used in the next forecast step, whose output will then be updated again in the following analysis step.

The update in analysis step can be done in two different ways. On the one hand, the explicit mathematical expressions representing estimated parameters' PDF can be formulated under the Gaussian assumption (i.e. the computation of the Kalman Gain in Extended Kalman Filter (Terejanu, 2009) or Ensemble Kalman Filter (Evensen, 2003)). On the other hand, sampling and resampling techniques (e.g. Particle Filter (Gen Nakamura, 2015)) can be used to approximate $\boldsymbol{\theta}_t^*$ distribution using samples of estimated parameters values. These methods do not require the Gaussian assumption on $\boldsymbol{\theta}_t^*$'s PDF, but takes more time in computation.

2.2.4. Geostatistical inversion (GI)

Geostatistical inversion methods are mainly applied in hydrology or other scientific domains focusing on large scale phenomena (Gómez-Hernández et al., 2003). They allow to produce a spatial map of $\boldsymbol{\theta}_s{}^*$ under a certain discretization scheme. The main motivation behind the approach is that conventional geostatistical tools (e.g. ordinary kriging) produce too smooth estimates at unsampled locations, so the GI approach was developed to introduce local adjustments to improve estimation by conditioning them on observations of a forward model output (Franssen et al., 1999). A typical example can be the estimation of hydraulic conductivities over an entire field by inverting a water flow model (i.e. Richards' equation) from multiple groundwater pressure measurements (Franssen and Gómez-Hernández, 2002).

Hendricks Franssen et al. (2009) pointed out that most GI methods can be summarized into three steps: i) define and parameterize a forward model so that black-box simulations can be made, ii) generate some initial guesses of $\boldsymbol{\theta}_s{}^*$ while preserving their spatial variability using geostatistical tools, using ordinary kriging (Cressie, 1990) or a certain zoning algorithm (Hendricks Franssen et al., 2009) (i.e. obtain a smooth estimation), iii) using $\boldsymbol{\theta}_s{}^*$ to make model simulations, and adjust iteratively their values in order to minimize an objective function that quantifies the difference between not only simulations ($\widehat{\boldsymbol{Y}}_s$) and observations ($\boldsymbol{Y}_s$), but also the adjusted and initial guess of spatially discretized parameters (i.e. in order to adjust locally the smooth estimation so that they better fit to observations).

The second step highlights that the GI approach usually requires some observed $\boldsymbol{\theta}_s{}^*$ before making inversion, which allows to make appropriate geostatistical analysis (Kitanidis, 1995). Indeed, the GI approach does not invent the spatial structure of a parameter, but only preserve it from available data or knowledge. What the GI approach estimates, are parameter values at unsampled locations.

The third step makes the GI approach inherently similar to the Frequentist Parameter Estimation approach: they both make optimization under certain constrains. However, the GI approach is used to estimate a much larger number of estimated parameters (i.e. typically over 10^2). Actually, the number of $\boldsymbol{\theta}_s{}^*$ is always greater than the number of available observations in GI applications (Miller et al., 2020). This implied multiple possibilities of $\boldsymbol{\theta}_s{}^*$ exist given a set of observational data, thus the estimation uncertainty should be accounted for. For instance, the Self-Calibrating method produces multiple equally-likely inversion outcomes (Gómez-Hernández et al., 2003); specific methods can also be formulated in a Bayesian fashion (Woodbury and Ulrych, 2000).

2.2.5. Explicit Inversion (EI), Approximate Inversion (AI), and Hybrid Inversion (HI)

Three families of model-based inversion methods are presented in this section. The Explicit Inversion (EI) and Approximate Inversion (AI) both aim at building an analytical inverse model of $\boldsymbol{\theta}^*$, so that it can be directly calculated using $\boldsymbol{Y}$. While the Hybrid Inversion (HI) relies partially on model simulations.

The EI approach aims at obtaining an explicit mathematical inverse function of $\boldsymbol{f}$: $\boldsymbol{f}^{-1}(\boldsymbol{Y})$, when the forward model processes an invertible mathematical structure. Few applications of this approach were found in agriculture, potentially because agricultural models are generally complex and involve several modeling modules (Wallach et al., 2014a). Some examples can be found in groundwater studies, where the studied physical process is governed by a set of partial differential equations, and spatially discretized flow properties (i.e. $\boldsymbol{\theta}_s{}^*$) like transmissivity or conductivity are searched (William (1986), Irsa and Zhang (2012)). The EI approach consists of solving the partial differential equation under certain discretization scheme (Neuman, 1973). Nonetheless, this represents a very specific application, hence cannot be generalized in other domains in agriculture.

Consequently, the AI approach builds an analytical inverse model $\boldsymbol{g}(\boldsymbol{Y})$ when $\boldsymbol{f}^{-1}(\boldsymbol{Y})$ is difficult or impossible to obtain. The approach relies on certain physical consistency within the studied system (e.g. the conservation of mass), as well as certain specific conditions imposed by modelers. The inverse model $\boldsymbol{g}(\boldsymbol{Y})$ may require less parameters, given that it is usually obtained by simplifying the studied process, or isolating it from a more complicated process. Even though, each reformulation is very specific to the model of interest. As a result, a generalized description of AI methodology can hardly be made. However, AI applications can be found more commonly among agricultural communities. Some representative examples can be cited: Gaudin et al. (2017) built an inverse model to represent Total Transpirable Soil Water by reformulating a simple soil water balance model. They expressed the vine transpiration rate using two different equations that are validated only under a specific climatic condition, which was coherent to the period and region of study; Boonstra et al. (1996) built a surrogate model to retrieve seasonal groundwater recharge using water level observations, by discretizing the studied area and inverting a soil water transport model in each discretized zone; Angaleeswari and Ravikumar (2019) built an inverse model to estimate evapotranspiration by reformulating the original process-based model: HYDRUS-1D.

Instead of building an inverse model analytically, the HI approach obtains an inverse model numerically through a learning process. Applications exist frequently in the Earth Observation community, where several θ^* are searched (Wang et al., (2022), Announce et al. (2023)). In Precision Agriculture, Florin et al. (2010) also built an inverse model using Neural Network model. The numerical models are trained using synthetic datasets generated by simulations made by a process-based model, and a large number of combinations of θ^* which are considered as realistic (Fig. 5 - Training step). Then, the trained numerical model is used to predict θ^* with actual observations (Fig. 5 - Prediction step). This approach relies on an inverse model to derive estimated parameters, but that model is trained numerically using process-based model simulations. The HI approach combines the physical advantage of a process-based model, and the computational efficiency of a numerical model (Verrelst et al., 2019). In agriculture, this approach has been used to estimate leaf chlorophyll content (Preidl and Doktor, 2011), LAI (Banskota et al., 2013), or forest structural properties (Homolova et al., 2016).

2.2.6. A decision tree for the classification of methods

The seven families of methods mentioned previously can be organized in a tree form (Fig. 6). Simulation-based and model-based inverse modeling methods are distinguished by the first node (Node 1). Among simulation-based methods, some of them are developed specifically for accounting for the temporal and/or spatial variability of estimated parameters (Node 2). However, when $\boldsymbol{\theta}^*$ are independent on time or location, either frequentist or probabilistic methods can be used (Node 3). On the contrary, the SF approach allows to consider temporal variability and the GI allows to consider spatial variability, for obtaining $\boldsymbol{\theta}_t{}^*$ or $\boldsymbol{\theta}_s{}^*$ (Node 4). As for model-based methods, only the EI approach searches an explicit mathematical inverse function of the forward model (Node 5). While the AI approach builds the inverse model under certain approximations, and the HI approach realizes that task numerically (Node 6). This simple classification covers a large range of inverse modeling applications related to agriculture. It should be noted that boundaries between these classes can be fuzzy sometimes, due to the actual diversity of tools which is constantly increasing.

3. Which are the motivations of making inverse modeling in agriculture?

Despite of the diversity of inversion methods presented in section 1, there are some common motivations which incite practitioners to choose

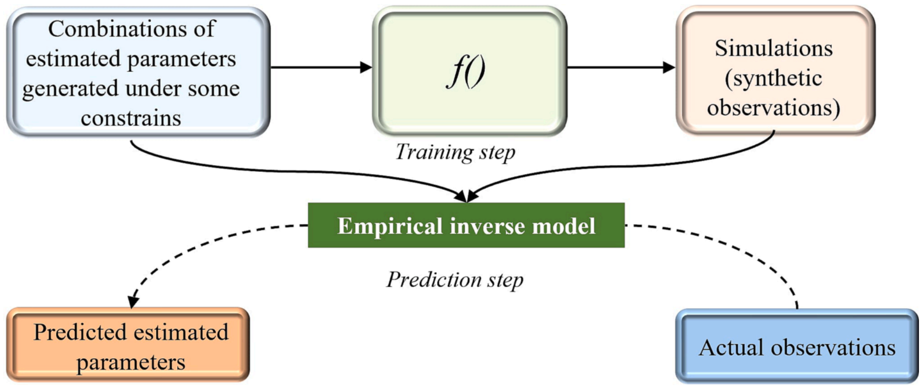

Fig. 5. An illustration for the mechanism of Hybrid Inversion.

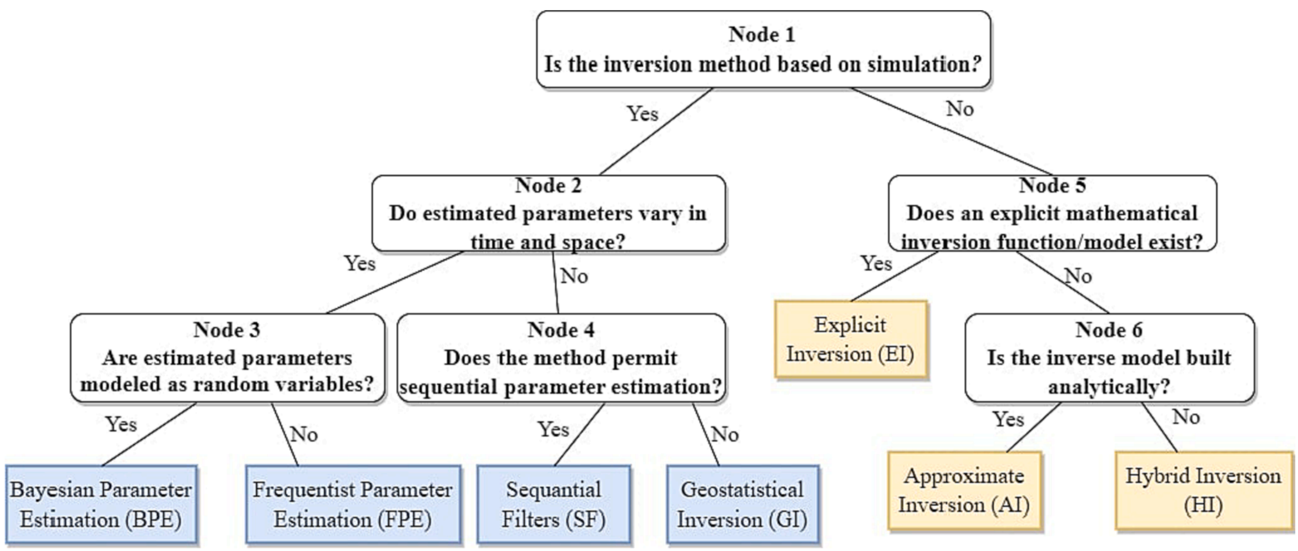

Fig. 6. A classification of seven families of inverse modeling methods.

inverse modeling over other methods to derive parameters in agriculture. Two types of motivations can be distinguished: the first type refers to the situations where other ways allowing to obtain parameter estimation have certain drawbacks (section 2.1), while the second type of motivations are related to the possibility to transmit the spatial/ temporal footprint of certain observational data to estimated parameters by making use of an existing mechanistic model (section 2.2). In the end of this section, a graphical presentation is proposed to summarize these motivations (section 2.3).

3.1. Inverse modeling is more advantageous than alternatives

Making inverse modeling is not the only way by which model parameters can be estimated. At least two alternative methods exist: i) directly measuring $\boldsymbol{\theta}^*$, and ii) estimating them using statistical models. However, these approaches are prone to certain common constrains in agriculture, which makes inverse modeling becomes a more advantageous solution.

3.1.1. More advantageous than direct measurements

Direct measurements depend on specific instruments and protocols to evaluate the unknown quantities of interest from the field/laboratory level (e.g. Nitrogen content (Li et al., 2008), soil hydraulic properties (Angulo-Jaramillo et al., 2000)). However, some common limitations of this approach can be identified.

First of all, certain quantities are inherently inaccessible to direct measurements. This is the case of historical parameters, because they cannot be directly observed anymore (e.g. historical soil hydraulic properties (William, 1986)). Given the principle of inverse modeling, it is unnecessary that estimated parameters must be directly observable. For instance, in the work of Kwon and Hudson (2010), a simulation-based inversion method was used to retrieve historical soil carbon content: a mechanistic model generates simulations ($\widehat{\boldsymbol{Y}}_d$) that start back from the past towards the "future", which are then compared with actual historical observations of the model outputs ($\boldsymbol{Y}_d$).

In some models, some parameters are conceptual, and may be difficult to access or inaccessible (e.g. leaf structure parameter in the radiative transfer model PROSPECT (Jacquemoud and Baret, 1990)). Yet these parameters are essential for making accurate model simulation (Jacquemoud et al., 2009). Given that there is no direct measurement protocol for purely conceptual quantities, naturally, their values can only be obtained through an inverse modeling procedure, usually referred to as model calibration. The BPE approach is especially useful in this case, as certain prior knowledge on a conceptual parameter is often provided by the modelers or other model users (Wigneron et al., 1993), which can be formulated as the prior in the Bayesian framework.

Meanwhile, many parameters in models used in agriculture can actually be directly measured. However, the necessary cost in time/ money is highly significant. For instance, the Soil Available Water Capacity (SAWC) is one of the most important model parameters in soil water balance and crop modeling (Cousin et al., 2022). The conventional protocols for quantifying this parameter are complicated and time-consuming, consisting in soil excavation and a series of laboratory analysis, while also taking into account possible soil heterogeneity (Bouthier et al., 2022). For obtaining SAWC, inverse modeling is a more cost-effective solution when relevant observational data are available, like soil moisture data (Pan et al., 2021). In some other cases, certain outputs of mechanistic models in agriculture are already monitored regularly, like soil organic carbon (Kwon and Hudson, 2010) or plant biomass (César Trejo Zúñiga et al., 2014), hence are available as observations ($\boldsymbol{Y}_{(d)}$) for model inversion.

Last but not the least, most of direct measurements are point-based in space and time, which is inherently restrictive. For instance, traditional single-point measurements in groundwater studies (e.g. the measurement of hydraulic conductivities) cannot easily be used to extrapolate the whole spatial distribution of $\boldsymbol{\theta}^*$ of the studied area (Liang et al., 2021). This limitation greatly highlights the strength of inverse modeling, as a following section will discuss (section 2.2): IM allows obtaining model parameters at the same spatial/temporal scale as those of the observational data.

3.1.2. More advantageous than statistical modeling

Statistical modeling aims at predicting the estimated parameter using a set of explanatory variables with a mathematical structure generated by an algorithm (Kuhn and Johnson, 2013). Typical examples are various Machine/Deep Learning models, which have been applied for estimating model parameters like contaminant concentration (He et al., 2021), or soil moisture (Del Frate et al., 2003), and various vegetation biophysical variables (Bacour et al., 2006). An estimated parameter becomes the output of a statistical model, which uses explanatory variables as inputs. Nevertheless, this approach is prone to some significant drawbacks for applications in agriculture.

Firstly, no statistical model can be built without training data. The latter is a dataset containing combinations of observed explanatory variables and observations of the targeted parameter, which allows algorithms to learn the empirical relationship between them. Consequently, the performance of a statistical model is closely related to the amount of training data (Atzberger et al., (2015), Fu et al. (2023)). Richetti et al. (2023) explored the minimum data size for machine learning and deep learning algorithms to predict crop yield, and showed that at least 234 samples must be acquired in their situation. A similar amount of data was also found in the work of Ren et al. (2022). Therefore, training a robust statistical model for agricultural applications should require at least an almost identical training data size, although the actual size depends largely on the specific relationship between the searched parameter and explanatory variables, hence the level of uncertainty in training data. Moreover, it is often essential to include contrasting combinations in training dataset, so that the statistical model can learn from a diversity of situations (Carrera, 2005). This raises the cost of assembling training data, usually requiring intensive and/or continuous data acquisition. In contrast with the statistical modeling approach, inverse modeling does not need existing observations of an estimated parameter for model training. They can operate well with very parsimonious datasets (Dzotsi et al., (2015), Song et al. (2016)), while using easily accessible data like satellite imagery as observational data ($\boldsymbol{Y}_{(d)}$) (Wang et al., 2021).

Another limitation of statistical modeling consists in its strong dependency to the training dataset, making statistical models poorly suitable for their generalization to a wide range of situations (crop x environment x management) (González-Sanpedro et al., (2008), Kayad et al. (2022)). Concretely speaking, a statistical model which predicts well one situation may perform badly in another case (Zhang et al., 2021). An example can be pedotransfer functions for estimating soil hydraulic properties, which are often site-specific (Vereecken et al., 1990). This dependency to training data raises some great challenges in using statistical models in agriculture, because of the highly diverse situations. Consequently, Wan et al. (2021) and Verrelst et al. (2019) suggested that the physically-based inverse modeling approach is a more generic alternative for estimating quantities of interest. Instead of depending on one single source of information such as training data used for statistical modeling, IM results are generated by using multiple sources of information: process-based equations in the mechanistic model (allowing estimated parameters to generate meaningful simulations), observational data (allowing to quantify the adequacy of chosen $\boldsymbol{\theta}^*$), as well as human knowledge and expertise on $\boldsymbol{\theta}^*$ (allowing to set up prior knowledge on the latter).

Lastly, applications of multiple-responses empirical models are actually very rare in agriculture (Xu et al., 2019). In most of cases, one statistical model is mainly trained for predicting one model parameter. On the contrary, a large number of examples have shown that multiple parameters can be estimated by simulation-based inverse modeling methods (Gurung et al., (2020), Antonucci et al. (2023)). These methods can generate an overall “fitness score” that summarizes the adequacy of all estimated parameters using a cost function or a likelihood function (Charoenhirunyingyos et al., 2011). The parameter estimation problem is then transformed into a multi-dimensional optimization or sampling problem (Hendricks Franssen et al., 2009). This format of estimating parameters is particularly adequate in agriculture, where complex interactions between environment (soil, climate), plant, and management (on soil, plant) are expected.

3.2. Inverse modeling allows to use spatial/temporal footprint of observational data in conjunction with a mechanistic model

Inverse modeling provides a natural way to derive $\boldsymbol{\theta}^*$ at the same location/time where observations were made (Iizumi et al., 2009). Historically, observational data in agriculture were rather sparse in space and time, but this situation is changing as the accessibility of high spatial/temporal resolution data is increasing, thanks to the development of airborne and/or spaceborne sensors and communication technologies. As a result, searching $\boldsymbol{\theta}_s^*$ and/or $\boldsymbol{\theta}_t^*$ is becoming a popular practice in agriculture.

Firstly, the spatial variability is essential for applications in precision agriculture. A high data coverage rate of certain model parameters (e.g. SAWC) over an area of interest (e.g. a field) is essential for planning tactical operations (Pasquel et al., 2022). However, there has been few applications of inverse modeling focusing on the field-scale, implying that such operation is still developing. Instead, Liang et al. (2021) retrieved the soil moisture content at a watershed-scale, using the Water Cloud Model (WCM) and data from Sentinel-1 and Sentinel-2. Similarly, González-Sanpedro et al. (2008) retrieved the LAI also in a large area (51 km × 38 km), using the PROSPECT-SAIL model and two types of Landsat optical data. In both examples, inverse modeling provided a way to obtain $\boldsymbol{\theta}_s^*$ at the pixel level, while linking multiple sources of information (i.e. several types of observational data, and human knowledge) to the estimated parameter through a mechanistic model. This is unique for inverse modeling, in comparison with other spatial mapping methods like Digital Soil Mapping (Arrouays et al., 2021). On the top of that, as mentioned in section 1.2.4, the Geostatistical Inversion (GI) approach also allows to consider a known spatial structure during model inversion.

Secondly, some quantities of interest naturally evolve within a growing season, like the LAI or the leaf chlorophyll content (Darvishzadeh et al., 2008), whose temporal variability must be accounted for in a model. Yet, historically, $\boldsymbol{\theta}_t^*$ can only be estimated at several dates where observations were available (Si et al., (2012), Duan et al. (2014)). Thanks to the high frequency of observational data provided by various sensing techniques, temporal evolution of these quantities can be derived by inverting a mechanistic model. For instance, Yang et al. (2021) estimated LAI and chlorophyll content of various land surface (including cropland and forest) using Sentinel-3 time series at a daily time-step. Darvishzadeh et al. (2019) retrieved LAI using Sentinel-2 and RapidEye data, whose satellite revisiting intervals are both inferior than a week. For other θ^* which are supposed to be invariant in time, Sequential Filter methods permit estimating them using time series repeatedly, while accounting for the associated uncertainties. This practice is enabled by certain specific inverse modeling methods (i.e. the SF approach), which were originally developed for handling continuous but noisy time series of observations (Liu et al., 2020). For instance, Montzka et al. (2011) estimated soil hydraulic properties for a 1D mechanistic soil water model, by applying a Particle Filter algorithm. The estimation was realized at over one hundred time steps, always coupled with a confidence interval. Similarly, Zhang et al. (2021) inverted the AquaCrop-OS model with an improved Particle Filter to estimate winter wheat canopy parameters at 23 dates using UAV images, while representing the estimated parameters as distributions.

To summarize, the popularization of high spatial and temporal resolution observational data greatly raises the potential opportunity for stakeholder to get informed about θ_s^* and θ_t^*. While IM offers a robust toolset for making use of those data and other types of information. However, both types of data can magnify significantly the computational cost (Ghorbanidehno et al., 2020), and particular inverse modeling techniques need to be adopted (i.e. the GI approach, the SF approach, the model-based inversion methods).

3.3. A graphical summary of different motivations

Fig. 7 summarizes the motivations mentioned previously to make IM in agriculture. Above all, inverse modeling is the only way to obtain model parameters which are no longer accessible, or too difficult to be directly measured. When both relevant observational data and a forward model are available, inverse modeling can reduce the cost in making measurements, or in collecting data for model training. The estimation provided by inverse modeling receives automatically the spatial/temporal footprint of observational data, while showing a high potential of employing high resolution data. Lastly, unlike statistical modeling methods which highly depend on training data, the process of inverse modeling always incorporates information from a mechanistic model, some observational data, as well as the knowledge of practitioners. This characteristic makes inverse modeling a generalizable solution towards parameter estimation, for diverse and contrasting situations in agriculture which are related to pedo-climate conditions, type of cultures, human interventions etc.

4. How to choose a family of inverse modeling methods?

In spite of various advantages that inverse modeling can provide for agricultural applications (section 2), no standard procedure for choosing a specific method exists (Seidel et al., 2018). Moreover, regarding the diversity of methods (section 1), practitioners cannot make decisions by purely depending on mathematical/algorithmic characteristics of those methods, because operational constraints exist. These later are seldom formally discussed by authors, but they represent actual reasons for which certain IM methods are chosen over others in practice. Consequently, merely distinguishing methods from a technical perspective is insufficient. The objective of this section is to identify operational criteria that guide practitioners to choose a family of inversion method, while clarifying the reasoning of choice.

From the literature, the choice of inverse modeling technique is mainly based on two types of criteria. They are: i) the resources-oriented criteria, which are related to the specific resources available in a project (e.g. type of forward model, computational budget, level of personal skill…), and ii) the goal-oriented criteria, which are associated to the properties of the inversion result that practitioners expect to receive (e.g. single-value result, distributions of estimated parameters…). Section 3.1 will firstly focus on two main resources-oriented criteria. Section 3.2 will present four goal-oriented criteria, helping practitioners to refine their choice. Lastly, based on this knowledge, section 3.3 will propose an illustrated decision procedure for method selection.

4.1. Resources-oriented selection criteria

Making inverse modeling is a process where a forward model, observational data, and human knowledge all intervene. These three factors form a unique set of resources of a given project. Certain families of method can only be carried out when adequate resources are available. From the literature, two resources-oriented criteria that directly influence the choice of method can be drawn.

4.1.1. Possibility to obtain and use an analytical inverse model

The first resources-oriented criterion is whether it is possible to

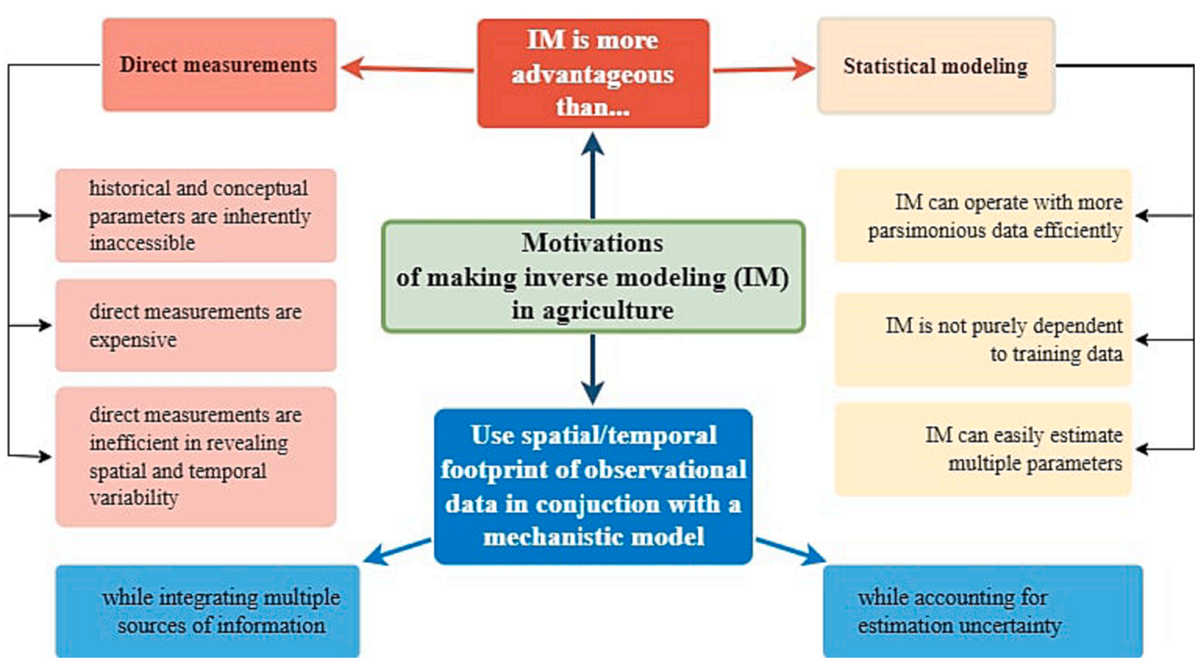

Fig. 7. A graphical summary of different motivations to apply inverse modeling.

produce and use an analytical inverse model. It is important to examine whether it is possible to obtain and use an analytical inverse model, because when satisfied, practitioners can benefit from fast inversion thanks to model-based inversion methods (AI and EI). They allow to obtain θ^* without making model simulation (Neuman (1973), Brouwer et al. (2008)). Using these methods, errors of inversion result will only depend on the inverse model and observational data, while avoiding other sources of uncertainties like the model simulation, the optimization etc. (Irsa and Zhang, 2012).

Nevertheless, the quality of inversion based versus model-based methods will depend largely on how the original forward model can be reformulated, and under which hypotheses. The lack of relevant expertise on agronomic/environmental processes of interest can also impede the implementation of model-based inversion methods.

In agriculture, the key resource is often expert skills: practitioners need to have a deep understanding on the forward model of interest, as well as the mathematical skills to reformulate it (i.e. Approximate Inversion (section 1.2.5)). Such operation allows linking equations that describe different environmental processes together, by using several agronomic relationships and/or bringing in some assumptions specific to the project (Gaudin et al., 2017).

When the forward model has a simple structure, the Explicit Inversion approach can be used to build an analytical inverse model (section 1.2.5). This type of forward model is common in hydrology, where the forward model is often a partial differential equation (Sagar, 1975), but is much less common in agriculture because forward models are often composed by a bunch of equations involving complex soil–plant-atmosphere interactions (Kwon and Hudson, 2010).

According to the final form of an analytical inverse model, one must also verify if relevant observational data are available in order to employ that model (William, 1986). However, as an inverse model is usually conceived for using a certain type of observation that is operationally accessible (Wang et al., 2021), practitioners can focus mainly on the first two points mentioned previously (i.e. expert skills and a suitable model).

4.1.2. Sufficient computational budget

The second important resource is computational budget of a project. Direct factors influencing the budget of a project can be related to hardware (e.g. power of computer), and/or practitioners' skills (e.g. in launching parallel/cloud computing, choosing efficient algorithms) (Combal et al., (2003), Renard (2007), Ghorbanidehno et al. (2020)). It is difficult though to quantify the exact amount of computational budget, which is generalizable to all projects. Therefore, this section describes the factors that influence the computational cost instead.

On the one hand, high computational cost can be caused by the forward model of interest, when its simulation is computationally heavy (Ghorbanidehno et al., 2020). For instance, certain radiative transfer models (RTP) (e.g. DART (Gastellu-Etchegorry et al., 2004), SCOPE (Tol et al., 2009)) are highly computational demanding. Similar mechanistic models exist also in other domains in agriculture, but the review cannot list all of them, because authors seldom precise the amount of time needed for model simulation. Anyhow, a rule of thumb is that the time for model simulation is positively correlated to the realism, hence the complexity of the model (Verrelst et al., 2019). In any case, almost all simulation-based inversion methods are inefficient to invert computationally demanding models, because these methods require to run the expensive simulation many times (Verrelst et al., 2019).

On the other hand, when a forward model contains a large number of estimated parameters (Miller et al., 2020), computational cost is significantly elevated due to the "curse of dimensionality" (Bengtsson et al., 2008). Mahévas et al. (2019) underlined certain complex models were hardly computationally invertible (e.g. $> 10^3\ \theta^*$).

However, common agricultural projects seldom aim at estimating that many parameters simultaneously. In the survey conducted by Seidel et al. (2018), 99 % of respondents (among 211 users of crop models) searched less than 50 model parameters in their projects. Even when inverting complex models like STICS (Brisson et al., 2003) or APSIM (Holzworth et al., 2014) which contain hundreds of parameters, practitioners are usually capable of fixing most of model parameters thanks to existing work and expertise (Alkassem et al., 2022). This allows them focusing only on estimating a limited number of parameters (Wallach et al., 2011). Moreover, practitioners tend to estimate parameters through several stages, which reduces the computational cost per stage (Seidel et al., 2018).

Additionally, a high number of estimated parameters is often observed when the parameter is spatially distributed (θ_s^*). While agricultural applications are often specific to a local environment, thus the utility of estimating large θ_s^* over an extensive area is relatively low (Bandaru et al., 2022). Nonetheless, with the increasing use of high spatial resolution data in the digital agriculture era (Kayad et al., 2022) (section 2.2), the same vector of θ^*, even just consisting in a few model parameters, can be searched at a large number of locations (i.e. per-pixel inversion (González-Sanpedro et al., (2008), Machwitz et al. (2014)). This may greatly raise potential computational cost. However, this potential obstacle has seldom been mentioned by authors.

To summary, the computational cost of a project is related to the forward model simulation, as well as to the number of estimated parameters. When the cost is too high, the interest of all simulation-based inversion methods becomes limited. In this case, the Hybrid Method (HI) can be a better solution, because both methods isolate the truly computation demanding task from the process of inversion *per se* (section 1.2.5) (Verrelst et al., (2019), Schiefer et al. (2021)). The two other model-based inversion methods may also be adequate, but they require validated previous resources-oriented criterion (section 3.1.1).

4.2. Goal-oriented selection criteria

Goal-oriented selection criteria enable method selection, because they are the main reasons for which various methods were originally developed: to solve specific inverse modeling tasks given specific combinations of model, observations, and human knowledge. Nonetheless, these goals were seldom highlighted by authors, who tended to focus on algorithm implementation. In this section, certain common goals, representing interests in agriculture, are presented for selecting simulation-based methods discussed in section 1.2.

4.2.1. Obtaining a single best solution

The single best solution is the most probable vector of estimated parameters given all available information acquired by practitioners. In agriculture, as in many other sectors, this goal is frequently searched (Ritter et al., (2003), Angaleeswari and Ravikumar (2019), Fernández-Gálvez et al. (2021)), because a single inversion outcome is an ideal format for making model prediction and decision making (Dubrule, 2018). Nonetheless, although it is appealing as an operational goal, it is possible that the single best solution does not exist, or cannot be found with available data (He et al., 2017). It is also possible that various parameter vectors are equally probable (i.e. equifinality (Hendricks Franssen et al. (2008), Gan et al. (2014)).

As some model inversion methods seek a single best solution and others do not (section 1.2), the existence of this single best solution is therefore an important criterion to consider when choosing a model inversion method. In the literature, authors generally carry out sensitivity analysis before making inverse modeling in order to filter out $\boldsymbol{\theta}^*$ which are not sensitive enough to observational data, because this operation allows reducing the chance of equifinality (Zhang et al. (2021), Alkassem et al. (2022)). A more robust way is to conduct parameter identifiability analysis (Rothenberg (1971), Coudron et al. (2021), Zhang et al. (2022)) and stability analysis (Hupet et al., 2005). These practices aim at evaluating whether practitioners have enough information, or information that are suitable enough, to obtain a unique vector of estimated parameters. That requires reviewing observational data, forward model, as well as estimated parameters (Guillaume et al., 2019).

When the single best solution is likely to be found, the Frequentist Parameter Estimation (FPE, section 1.2.1) approach can naturally achieve this goal, because the objective of the approach is to retain one set of $\boldsymbol{\theta}^*$ which minimizes an objective function (Ghorbanian et al., (2019), Wan et al., (2021), Dari et al., (2022)). However, other families of methods also allow practitioners to extract a single best solution, by, for example, calculating the statistical mode from a probabilistic distribution (Song et al., 2016). These laters usually require more external knowledge (e.g. Bayesian statistics, Data Assimilation skills), hence more complicated to undertake than the FPE approach (section 1.2.2, section 1.2.3).

4.2.2. Exploring the probabilistic distributions of estimated parameters

When no single best solution is possible, authors often use probabilistic density functions (PDF) to account for uncertainty in model parameter estimation (Hansen et al., (2016), Dubrule (2018)). It is common to this approach when inverting crop models like STICS because of the complex interactions between parameters (Alkassem et al., (2022), Sreelash et al. (2017)). It is also worth noting that, in the agricultural context, many parameters are inherently uncertain because they are influenced by several environmental factors that cannot be exactly quantified (e.g. plant available water capacity (Morgan et al., 2003)). In this context, some authors also use PDF to describe these parameters (Cousin et al., 2022).

In this case, the family of Bayesian Parameter Estimation (BPE) methods are interesting approaches because they permit to reveal the probabilistic form of PDF of estimated parameters using samples (Dzotsi et al., (2015), Gao et al. (2021)) (section 1.2.2). These methods require a basic understanding on Bayesian statistics (Wallach et al., 2014c) and prior information on estimated parameters. Some authors also use Sequential Filters (SF) methods to estimate θ^*'s PDF (Rajabi et al., 2018). In particular, the duo-model formalism in SF approach is used to better quantify uncertainties (Lu et al., 2022) by integrating, in a separated way, knowledge about errors both related to model simulation and to observations (see section 1.2.3). However, SF method are especially suitable for treating continuous observational data (Montzka et al., 2012).

Finally, when using the BPE approach, practitioners should pay attention to the uncertainty quantification (Uusitalo et al., 2015) for priors and for observation errors, whose importance is often undervalued (Linde et al., 2017). Graphically speaking, they should define how narrow a PDF is. This information translates the level of confidence that practitioners attribute to a probabilistic distribution, which should be as realistic as possible (O'Hagan, 2006). Inadequate uncertainty quantification can lead to unwanted results. For instance, a prior with a high level of confidence, which is mathematically very certain, is more difficult to be updated by observations, especially the noisy ones (Hansen et al., (2016), Liu et al. (2020)).

4.2.3. Timely updating model parameters

In agriculture, it is a common situation where observational data are collected gradually over time (e.g. soil moisture (Montzka et al., 2011), Leaf Area Index (LAI) (Dewaele et al., 2017)). This may force practitioners to wait for a long time before having enough data for obtaining robust inversion results. As a consequence, it has been an interesting practice to timely update model parameters using the most recent information (Huang et al., 2019).

The Sequential Filter (SF) approach provides an adequate framework where practitioners can obtain timely updated estimations of $\boldsymbol{\theta}^*$ (Jin et al., 2018). This approach adjusts model parameters, eventually biased at the beginning, to produce simulations matching better with newly received observations (Zhang et al., 2021). Thanks to the recurrent nature of the duo-model formalism, updated parameters can be used during upcoming model simulation, which will be again compared with new observations in order to generate potential corrections on parameters. The SF approach also provides a relevant way to account for different sources of uncertainties in inversion (Vrugt et al., 2008).

Remote sensing data are often used for this type of update thanks to their high temporal resolution (Reichle, 2008). The duo-model formalism of SF approach is especially useful when using these data, because the observational model (section 1.2.3) can unify the spatial scale of model simulations and sensed information (Montzka et al., 2012). Moreover, it is possible that the observational model can be used to link estimated parameters, which are usually related to plants or soil, to spectral information contained in remote sensing data, by using a mechanistic RTM (e.g. PROSAIL) as observation operator (Machwitz et al., 2014).

Nevertheless, a continuous observational data stream is indispensable to achieve this goal, and SF approach works mostly for dynamic models (or a workflow which contains a dynamic model) (Nakamura and Potthast, 2015). Due to the duo-model formalism, practitioners must be able to quantify uncertainties related to model simulations and observations (section 1.2.3). For practitioners in agriculture, employing SF approach can demand external knowledge on estimation theory, hence is more complex to realize (Montzka et al., (2012), Dewaele et al. (2017)). Moreover, certain SF algorithms are based on certain important assumptions, like the linear structure of the process model and observational model, as well as the Gaussian distribution of estimated parameters (Jin et al., 2018). Consequently, these hypotheses must be prudently verified before choosing a SF method.

4.2.4. Integrating geostatistical knowledge on estimated parameters

In agriculture, geostatistical techniques (e.g. semi-variogram analysis, interpolation) have been widely used for estimating agronomic variables in unsampled locations (Oliver and Webster, 2014). Ancillary data have also been used to represent the spatial variability of certain model parameters (e.g. crop heterogeneity highlighted by a remote sensed vegetative index appears to illustrate soil available water capacity heterogeneity (Cousin et al., 2022)). This geostatistic-based knowledge may provide precious prior information on $\boldsymbol{\theta}_s^*$ for inverse modeling. Geostatistical Inversion (GI) approach is based on that type of knowledge, which can be used to generate a prior spatial map of an estimated parameter. The approach focuses on bringing in local adjustments on that prior spatial map, by considering observational data. Therefore, inversion outcome ends up as a "compromise" between geostatistical knowledge and coherence between observed and simulated model outputs (section 1.2.4).

However, GI applications have been mostly developed in hydrology (Franssen and Gómez-Hernández (2002), Gómez-Hernández et al. (2003)), but few in domains where crop models' parameters are searched (e.g. precision agriculture). Nevertheless, the potential of combining geostatistics and inverse modeling for better estimating $\boldsymbol{\theta}_s^*$ in production is raising, thanks to increasing availability of high spatial resolution data (e.g. remote sensing). Agriculture stakeholders are also getting more interested in practicing tactical field management (Pasquel et al., 2022) in order to save budget and/or resources, which requires characterizing their fields with a higher spatial resolution.

Nowadays, still remaining an active research topic, the transfer of GI methods from hydrology to precision agriculture has not achieved a mature stage. There have not been specific papers that mentioned preliminaries and/or risks of applying the GI approach, for example, with crop models. The research is on-going, for instance, Pasquel et al. (2022) showed it is important to use adequate performance metrics to compare downscaled model simulations and observations, which is an essential step during inverse modeling.

4.3. The proposed procedure of method selection

This section summarizes the six selection criteria discussed previously by proposing a procedure of selection (Fig. 8). When available

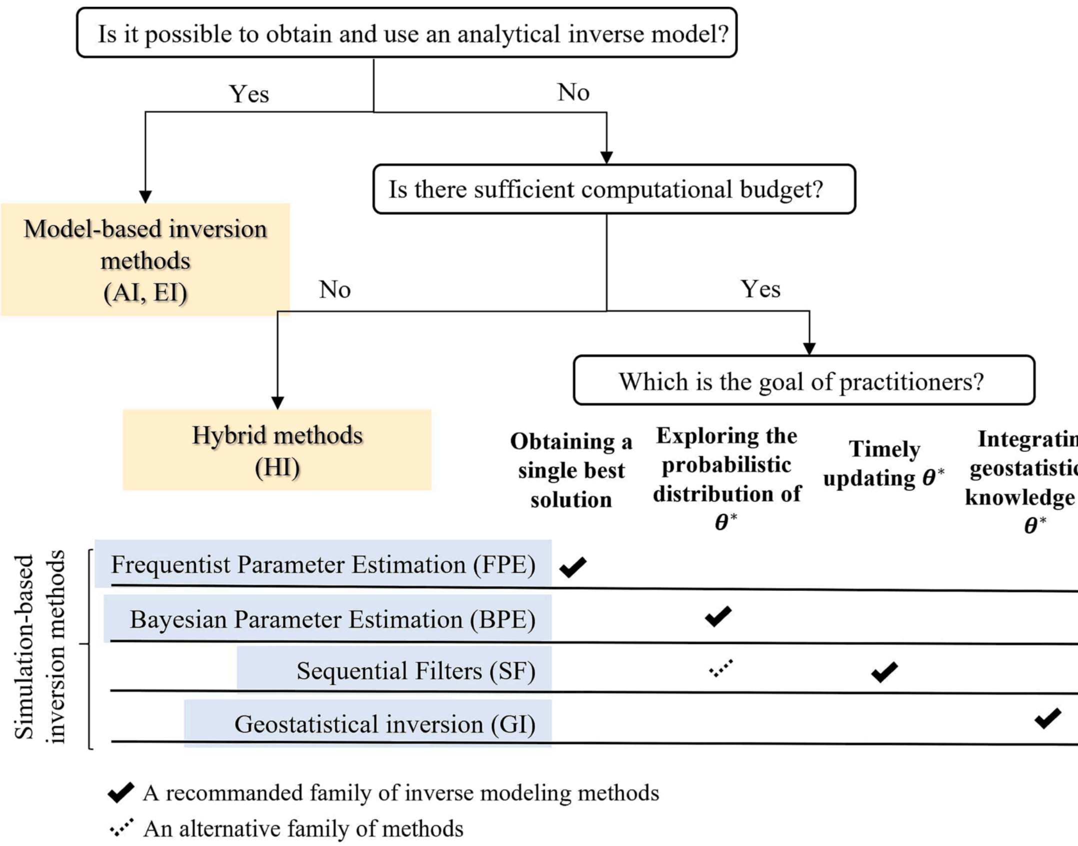

Fig. 8. The proposed procedure to select a family of inverse modeling methods in practice.

resources permit, model-based approaches (AI and EI) are recommended. Otherwise, practitioners should evaluate whether they have a computational budget large enough to cover the expected computational cost. This information can help them to choose between model-based (hybrid) approach and simulation-based methods. Using these two resources-oriented criteria, practitioners should be able to either make a choice, or restrict candidate methods within those which are simulation-based.

In the latter case, practitioners may consider the four goal-oriented criteria to complete the method selection. When a single best solution is searched, the FPE approach was put forward for its simplicity. On the contrary, if practitioners judge it is essential to account for uncertainties of model parameters, the BPE approach can be considered as the best choice, unless they would like to update their estimations in time. Indeed, SF methods are more suitable for using sequential observational data and dynamic models, which makes them the most suitable solution when practitioners want to improve dynamic model predictions, for example, using satellite data. Lastly, when practitioners have already acquired certain geostatistical knowledge on θ_s^* and wish to integrate it during inverse modeling, applying a GI approach is recommended.

5. Discussion

5.1. Summary of the review

The recent emergence of new data sources in agriculture offers new opportunities and raises new questions for the use of inverse modeling for decision support in agriculture. Based on this fact, this paper proposed a global overview of existing IM approaches. It firstly focused on defining the common characteristic of inverse modeling (section 1.1.2). IM aims to estimate the parameters (often difficult to measure) that have brought a system to its current state, based on observations made of the system and knowledge on how it works. Therefore, the review proposed a comprehensive classification comprising seven classes of methods (section 1.2).

However, the review might be the first to formally present IM as an ensemble of approaches that consists of both simulation-based and model-based approaches. Such overview may highlight certain discrepancies in how methods are labeled traditionally as ‘inverse modeling’ in the literature. For instance, model-based methods (Gaudin et al., (2017), Liang et al., (2021), He et al. (2022)), despite fulfilling the definition given in section 1.1.2, are often not considered as IM. While certain simulation-based methods (e.g. Frequentist Parameter Estimation (Verbist et al., (2009), Kwon and Hudson (2010), Charoenhirunyingyos et al. (2011), Rajabi et al. (2018), Chelil et al. (2022)) are excessively used to represent the entire practice of model inversion. This may prevent some practitioners from choosing the most appropriate approach. The definition of IM presented in section 1.1.2 could be linked to more general application cases, and be more specific to problematics in agriculture, like data scarcity or limited computational constraints. Readers should be informed that model-based methods are viable alternatives for achieving inversion, when simulation cannot be done or can only be done with a high computational cost. Likewise, the review did not exclude the possibility of using sequential filters for readers who are interested in accounting for temporal variability in the parameters they seek, as these filters are, in essence, data assimilation methods. The review suggested that by employing filters, practitioners can make IM, even though data assimilation is not equal to inverse modeling.

In the literature, when model inversion is used, the reasons why the authors chose this approach rather than direct measurement or statistical modeling are rarely explained nor justified. The review aimed at tackling this issue by formalizing the rationale behind choosing inverse modeling over alternative methodologies (section 2). It also stressed the importance of sharing this information and suggested that authors should systematically explain their decision-making process in their papers.

Finally, the review proposed a procedure for authors to help them choose the family of IM method that best suits their objectives. The review emphasized the need for careful selection of inversion methods, taking into account available resources and practitioners' goals (section 3). However, it was noted that such considerations have not been adequately addressed in publications in agriculture. The review recommended estimating the computational cost of a project (section 3.1.2), although precise quantitative criteria were challenging to identify in existing publications. Therefore, authors were strongly encouraged to provide detailed information about computational materials used and time spent on inverse modeling in their future work (Jégo et al., (2012), Ferrant et al. (2016)).

The review did not delve into technical implementation details of the presented methods. While certain operational risks were mentioned in section 3, specific resolutions were not provided. Consequently, after method selection, the task of implementing inverse modeling remains challenging, susceptible to equifinality and uncertainties.

The review did not specify the research according to various crop types, because different culture systems have specific operational constrains for inverse modeling. For instance, when estimating plant available water capacity, annual crops (e.g. wheat, maize) must be treated differently compared with perennial plants, like trees or grapevines, because the rooting depth of the latters is usually difficult to evaluate (Archer and Saayman, (2018), Algayer et al. (2020)). Besides, the diversity and complexity of process-based models can vary greatly according to crops, which also impacts the choice of inversion method. Hence, specifying IM applications even just only for the main types of crops can increase considerably the level of complexity of the paper.

Moreover, the review did not use any quantitative metrics to describe the performance of inversion. The choice was meant to keep the review general and comprehensive, because the performance of inversion depends on not only the specific combination of process-based model and observational data, but also the data availability and computational details of each project. For instance, Sreelash et al. (2017) showed inversion errors of soil hydraulic properties can vary from 5 to 20 % depending on agro-environmental situations; location can also be an important factor when inverting a large-scale rice model (Iizumi et al., 2009); many studies showed that the accuracy of soil hydraulic properties derived from inverse modeling depends largely on specific soil depth (Ritter et al., 2003) and soil type (Montzka et al., 2011). Therefore, identifying a general method of comparison goes beyond the scope of this review. However, readers can find reviews which focus on the more specific problems while commenting on the quality of inversion, by viewing the work of Cousin et al. (2022) on estimating Available Water Capacity, Wan et al. (2021) on inverse modeling with different RTM models, Hendricks Franssen et al. (2009) on various methods for inverting a spatial model.

5.2. Perspectives to improve inverse modeling in agriculture

The analysis of existing IM methods, their classification and the identification of practitioners' motivations have led to the identification of several scientific avenues to be explored.

5.2.1. Bridging observations and simulations while accounting for uncertainties

The availability of observational data plays a pivotal role in driving the adoption of inverse modeling applications (section 1.1.2). Kayad et al. (2022) demonstrated that the amount of stored data of a 22-ha farm in Italy (i.e. digitization footprint) may double by 2025. Recent advancements in remote sensing, such as Sentinel (Chintala et al., 2022) and Planet (Cheng et al., 2020), sensor technologies like connected sensors (Paul et al., 2022), and novel data acquisition strategies like crowd sourcing (Minet et al., 2017), offer promising opportunities for the expansion of inverse modeling in the agricultural domain. Nevertheless, it is important to note that not all accessible data directly correspond to the observations of mechanistic models. It is rare that a sensor exists to measure exactly the same variable as the one estimated by a model. Given the rapid evolution of sensor technologies, it is hard to update timely mechanistic models to obtain outputs that can be directly compared with observed data. Consequently, more and more authors are developing statistical models to define specific relationship between available data and outputs of mechanistic models (González-Sanpedro et al., (2008), Campos et al. (2016), Gao et al. (2022)). In other words, observed data are used as inputs of statistical models that predict model outputs for IM.

However, introducing statistical models as an intermediate step in this process is adding uncertainties on top of the intrinsic measurement uncertainties associated with observational data. It is especially the case when the observational data themselves are prone to imprecision, like crowdsourced data (Pichon et al., 2023) or low cost wireless sensor network data (Vandôme et al., 2023). To address this issue, specific algorithms like Quantile Regression Forest (Meinshausen, 2017) or Bayesian Network models (Xu et al., 2019) seem to be interesting approaches to train statistical models in a way that realistically provides uncertainty information. This prediction of uncertainty has also to be accounted for in model inversion. The Sequential Filter (SF) approach may provide a relevant framework for integrating a statistical model and its associated uncertainty in IM. The duo-model formalism appears to be interesting to use a statistical model as the observational model, which is coupled with a mechanistic model that plays the role of the process model (section 1.2.3). It is worth noting that despite its interest, SF approach is still rarely used in agriculture, possibly due to its technical complexity. Additionally, many SF algorithms were originally developed assuming Gaussian errors. This hypothesis may not be appropriate for various agricultural scenarios involving bounded agronomic quantities (e.g. strictly positive or negative values, like Predawn Leaf Water Potential (Deloire et al., 2020)). Moreover, the performance of statistical models connecting observed data and model outputs may exhibit temporal or spatial variations, resulting in prediction uncertainty depending on time or location (Qu et al., 2021). These difficulties have not yet been formally addressed for agricultural applications. From a more general point of view, future research should explore approaches for considering different levels of confidence on the information used in IM, while considering their certitude and reliability.

5.2.2. Combining inverse and statistical modeling

The potential of statistical models in directly predicting model parameters (section 2.1) is widely recognized (Khan et al., (2022), Akhter and Sofi (2022), Song et al. (2023)), driven by the increasing availability of data and the development of powerful learning algorithms (Wang et al., 2021). In comparison, inverse modeling does show some limitations. For instance, mechanistic models often require numerous parameterizations, which are in practice difficult to realize, and can hinder accurate inverse modeling. Moreover, for obtaining parameters at a high spatial resolution, simulation-based methods may be computationally demanding. Although being more efficient, statistical models are weak in generalization, especially when applied to complex agricultural systems (section 2.1.2). Hence, there is a growing interest in combining statistical modeling and inverse modeling, aiming at leveraging the advantages of both approaches and achieving a cost-effective synergy.

One potential approach would be to use statistical models to generate prior estimations of the parameters of interest (i.e. similar to Geostatistical Inversion (GI)), enabling the inverse modeling algorithm to identify better solutions more efficiently. As an example, Cousin et al. (2022) proposed to integrate inverse modeling with Digital Soil Mapping for estimating available water capacity for spatial inverse modeling, but this proposal has not yet been formally tested by any authors. Moreover, it is important to optimize the amount and the type of training data for each specific problem. However, these topics go beyond the scope of this review.

Hybrid Inversion (HI) also represents a potential approach for combining the strength of inverse and statistical modeling, enabling cost-effective inverse modeling (section 1.2.5). This approach has mainly been used for inverting Radiative Transfer Models (Verrelst et al., 2019). Some authors have explored the approach in crop modeling (Florin et al. (2011), He et al. (2022)), but its potential benefits have not been strongly demonstrated yet. However, training a robust numerical inverse model can contribute greatly in model inversion at a large spatial scale, while reducing the effort on parameterization. Learning algorithms that aim to predict multiple variables of interest should receive considerable attention, as their application in agriculture remains relatively uncommon.

5.2.3. Improving spatial inversion for agricultural applications

Mechanistic models are generally designed at a given spatial scale (e.g. plant, field, etc.) but observation data may be available at a different spatial footprint. In this case, upscaling or downscaling of the model is needed to perform inverse modeling. Pasquel et al. (2022) have clearly described this phenomenon and the associated challenges of changing the spatial scale for forward modelling but the question is still not formally addressed for model inversion.

In the context of precision agriculture (Khan et al., 2023), it is essential to account for as properly as possible the within field variability, so practitioners require model parameters for the entire area (Mancipe-Castro and Gutiérrez-Carvajal, 2022). Nonetheless, existing studies have revealed that spatial inversion often leads to high estimation errors (Jégo et al., (2015), Dai et al. (2022)), highlighting the lack of reliability in current inversion methods (e.g. through Frequentist Parameter Estimation).

One of the main challenges is the parameterization of mechanistic models that requires gathering an extensive amount of data. One possible solution to overcome this limitation would be replacing the original mechanistic model by a more parsimonious numerical emulator through model emulation (Blanc (2017), Johnston et al. (2023)). The approach builds an emulator that aims at reproducing the same outputs comparing to a mechanistic model given certain inputs (O'Hagan (2006), Cui et al. (2018)). However, it is unclear whether complex relationships between model inputs and outputs can be accurately simulated using an emulator. Further research in this direction is needed. Another approach might be to reduce the charge of parameterization by simplifying the spatial pattern of the searched parameter. The objective is to discretize the field of interest into zones that regroup similar parameter values, while maximizing the variability between them by considering ancillary data and human knowledge. Performing inverse modeling at a zonal level, instead of at a pixel level, can prevent excessive parameterization and save computational resources. The resulting outcome may also be easier to utilize under limitations imposed by current machinery. However, determining relevant zoning criteria and the appropriate number of zones remains a challenge. This challenge was explored in the context of precision agriculture (Jiang et al., 2018), but impacts of zoning on spatial inversion remain an active research topic (Pasquel et al., 2022). Montzka et al. (2012) have discussed methodologies for treating multi-scale data. Future research should focus on introducing ancillary spatial data with various spatial resolutions in IM projects, and selecting adequate spatial scale and remote sensing techniques that answer the best modelers' practical concerns.

Finally, and more generally, it is important to acknowledge that most of the papers on spatial model inversion are using what Pasquel et al. (2022) called spatialized models. The considered models are point-based models and they are simply run at different locations. Very few authors have used what Pasquel et al. (2022) called spatial models (Yang et al., 2021), which intrinsically simulate the interaction between modeled components in space. Given the importance of the spatial structure of information in agricultural phenomena and for decision-making, the exploration of approaches allowing this type of models to be inverted appears to be an important focus for future research.

CRediT authorship contribution statement

Yulin Zhang: Formal analysis, Investigation, Writing – original draft. **Léo Pichon:** Conceptualization, Writing – review & editing. **Sébastien Roux:** Resources, Validation. **Anne Pellegrino:** Resources, Validation. **Thierry Simonneau:** Supervision. **Bruno Tisseyre:** Conceptualization, Supervision, Writing – review & editing.

Declaration of competing interest

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Data availability

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