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Coordinate descent based agricultural model calibration and optimized input management

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ABSTRACT

Well-calibrated agricultural system model with many parameters is critical for optimized agriculture management and decision making. Here, Root Zone Water Quality Model (RZWQM) was calibrated automatically using Coordinate Descent (CD) algorithm against measured data from a fully irrigated corn field in terms of yield, plant height, leaf area index, evapotranspiration, and soil water content. Fifty-six soil hydraulic and three crop parameters were calibrated. The CD calibrated model was validated against data from adjacent deficit irrigated field. Average R^2 (Coefficient of Determination) measure was found to be 0.77 (against 0.74 for prior works) and average ME (Model Efficiency) was 0.64 (against 0.61 for prior works). Once calibrated, fertilization and irrigation decisions were optimized so that farm profit is maximized. Three global optimization methods, namely, Differential-Evolution, Basin-Hopping, and Particle-Swarm and two local optimization methods, namely, Sequential-Least-Square and Constrained-optimization-by-linear-approximation were implemented. These methods increased the yield by 7% and profit by 10% as compared to what was applied in the field.

1. Introduction

Agricultural food production is key to sustaining the humanity, and precision agricultural is a mechanism to make agriculture efficient by providing site-specific agricultural resource management (e.g., irrigation, fertilization, pest-control, etc.) to be able to avoid over-application and under-utilization, and loss to environment, leading to pollution. Key to precision agriculture is knowing the current 'state' of the production system, namely, the soil, plant, and environmental conditions, and using those states to make site-specific prescription decisions. For instance, within our own group, subsurface in-situ moisture and salinity sensor based on impedance spectroscopy was developed by Pandey et al. (2014). An in-situ electrophoresis based microfluidic nutrient sensor was developed Xu et al. (2017) for detecting NO^{3-} and SO^{4-} in soil solution sample. The microfluidic sensor developed by Ali et al. (2017) senses and quantifies nitrate ions in soil samples. Volatile organic compounds like ethylene and methanol are sensed by fiber optic gas sensor reported by Tabassum et al. (2017a). The sensor developed by Tabassum et al. (2017b) identify gas species like ethylene, methanol, and ammonia in a complex gas mixture. To know the location of sensor buried in soil, received signal strengths from sensor are analyzed using maximum likelihood method by Sahota and Kumar (2016). The collection of these state data enables a high-fidelity calibrated model that then supports optimized decision-making required for the agricultural production system.

Parameter estimation of agriculture system model, also known as model calibration, is the process of finding values for influential model parameters so the model predicted results is reasonably close to observed data. Calibrated agriculture models are used to understand the effect of climate change and farm management decision on agriculture production. There are many statistical measures which quantify the degree of fit between model predicted and observed values. No agriculture model fits perfectly with the data since a model is an approximate abstraction of a complicated natural process and secondly observed data has measurement errors. Calibration works by adjusting the parameters within a range that is physically possible and comparing with the observed data. Model calibration is also required because not all parameters are directly measured. Also, characteristics of a field changes with time and space, so calibration needs to be done at regular time interval even at each spatial location. Calibrating model against

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measured data from field sites would provide a high-fidelity description of the field.

Agriculture system models many underlying processes, e.g., soil moisture/temperature/macro-nutrients/ions/pesticides, plant biomass/roots, soil evaporation and plant evapotranspiration, surface flows, management, and climate (radiation, temperature, pressure, humidity, precipitation, wind, CO_2 level, etc.) information. Some of the agriculture system (crop-soil) models are RZWQM (Root Zone Water Quality Model) (Ahuja et al., 2000), APSIM (Agricultural Production Systems sIMulator) (Keating et al., 2003), and DSSAT (Decision Support System for Agrotechnology Transfer) (Jones et al., 2003). Each process has its corresponding set of mathematical equations relating input and output variables, and involving several parameters. All the agronomic processes are interlinked, and so their governing equations are also coupled. Thus, one needs to study the complete system and estimate parameters of the full system model by fitting to the data.

For a complex agriculture system possessing multiple modules, it has large number of equations and parameters. Accordingly, the measured outputs are also of different types (e.g., plant biomass versus soil moisture level). Given this, finding the right combination of parameter values is a challenging problem as the underlying system is nonlinear and high (order of 100 parameters) dimensional leading to a huge search space. As discussed below in Section 1.1, Root Zone Water Quality Model (RZWQM) has been autocalibrated with PEST using limited numbers of parameters. For instance, Malone et al. (2010) calibrated (around 20 parameters) organic matter transformation coefficients, lateral hydraulic gradient, root growth factor, pore size distribution index and hydraulic conductivity curve slope in RZWQM using PEST by fitting yield and nitrate concentration in drain flow. The problem is further complicated by the fact that two or more different set of parameter values can give the same goodness of fit. In such a case, domain expertise is required to choose a preferred one. The Coordinated Descent based approach, described in later Section, may be useful to calibrate complicated agricultural models with large numbers of parameters such as RZWQM.

Building on the work first reported by Bhar et al. (2018) at the ASABE meeting, in this work, we employ Coordinate Descent algorithm by Wright (2015) to calibrate RZWQM. Coordinate Descent is a popular algorithm in Machine learning community for solving optimization problem with many variables. For instance, Friedman et al. (2007, 2010), Wu and Lange (2008) have used Coordinate Descent variant for L1-penalized regression (lasso) problem where number of variables (of the order thousand) exceeds number of observations. Hsieh et al. (2008) used a Coordinate Descent method for training large linear SVM (Support Vector machine). This is the first application of Coordinated Descent in an agricultural modeling. The data for the calibration and validation is taken form experiment conducted by USDA-Agriculture Research Service in northeastern Colorado in 2010 by Trout (2016). The calibration is done using the data from a fully irrigated field and validation is done using an adjacent deficit irrigated field in the same time period. Its improved accuracy is shown in comparison to a prior tuning performed by a domain expert in (Qi et al., 2016). Once we have the calibrated model, decisions are made as how much fertilizer and irrigation water needs to be applied for maximizing farm profit where profit is defined as simply the selling price of produce minus the cost of fertilization and irrigation.

The yield of a crop depends on the weather, soil properties and crop cultivar, and fertilization and irrigation. Of these, fertilization and irrigation can be controlled by a farmer for a given crop cultivar. The yield increases with the increase in fertilizer and irrigation amounts, but only up to a point. Afterwards, the yield saturates, and in some cases, the yield may decrease because excess fertilizer and water can be harmful to the plants. So, applying more inputs beyond a point might incur costs to a farmer without improving the yield. Excess fertilizer and irrigation adversely affect environment too by way of N pollution through runoff and leaching. In this work, we have used the calibrated RZWQM model to determine the recommendations for fertilizer (Urea Ammonium Nitrate UAN) and irrigation amount which would help maximize the profit per hectare of the farm.

Rest of the paper is organized as follows. We review related works on parameter estimation of agriculture models in Section 1.1, and management of fertilizer and irrigation application guidelines in Section 1.2. We conclude Section 1 by mentioning our motivations for this work. Sections 2.1, 2.2 and 2.3 cover the Materials of this paper, while Sections 2.4 and 2.5 report the Methods: 2.1 describes the agriculture model, Root Zone Water Quality Model (RZWQM) that we calibrate; the automatic calibration procedure, Coordinate Descent Algorithm, is described in Section 2.2; the description of the field dataset with which the model is calibrated and validated is described in Section 2.3; software integration and setup for the calibration of RZWQM using Coordinate Descent is described in Section 2.4; and finally the usage of the calibrated model for finding optimum fertilizer and irrigation application is mentioned in Section 2.5. Results are presented and discussed in Section 3. Section 4 provides Conclusion and future work.

1.1. Related works in agriculture model calibration

One way of parameter estimation is to focus on only a subset of processes at a time. This kind of calibration may be suitable in lab or greenhouse setting. Soil hydraulic parameters in lab are estimated by measuring soil water content and water potential at different time during wetting of soil and evaporation from soil. Hence, they are though accurate are very time consuming and tedious. For instance, in (Tamari et al., 1993), soil hydraulic conductivity is estimated in laboratory by measuring soil water content and water potential head at different time during evaporation of water from soil sample using gamma attenuation and tensiometer. Masrouri et al. (2008) gives a comprehensive review of laboratory methods, their pros and cons, for estimating hydraulic parameters. Around five soil hydraulic parameters are calibrated from the water retention curve obtained by water infiltration and evaporation experiments in lab. The number of parameters in a complete agricultural system model is large (of the order of hundred) though, and so researchers approach the calibration process by generally fixing many of the parameters whose values are available in literature or easily measured to their default values (these parameters are expected to not change), and calibrate only the sensitive parameters as in (Tremblay and Wallach, 2004) where fourteen crop parameters from STICS (Simulateur mulTIdiscipli-naire pour les Cultures Standard) model (Brisson et al., 2003) were calibrated. Calibration can be done manually as done by Saseendran et al. (2010) where in seven crop genetic coefficients were estimated first by calibrating against soil moisture then phenology, biomass, and yield. Qi et al. (2016) calibrated many soil hydraulic parameters manually. Calibration is also done through computer program as done by Xi et al. (2015) to calibrate 6 crop parameters of RZWQM using modified Particle Swarm Optimization, Nolan et al. (2010) and Fang et al. (2010) to calibrate around 15 RZWQM parameters using PEST (Doherty 1994) software. PEST uses gradient based procedure to give local minima. A user of PEST can choose an objective function according to their liking and sometimes the optimized parameters have no real field meaning. Another software package that automates genotype parameters' calibration is GENCALC (Genotype Coefficient Calculator) (Hunt et al., 1993). The coefficients are determined in a sequence with those that relate to phenological aspects being determined first. GENCALC was used by Anothai et al. (2008) to calibrate a model for peanut cultivars. Calibration can also be categorized as offline, i.e., fitting the model to the entire experimental data in one go, or online where model parameter are updated when new data is available. Offline methods are more common. All the calibration methods cited above are offline. Kalman filters (Brown and Hwang, 1992), which is an algorithm that uses noisy observations over time and produces accurate estimate of unknown as time progresses, and their extensions are popular for online estimations. For instance, parameters like recharge rate and transmissivity of ground water flow was estimated by Hendricks and Kinzelbach (2008). In (Gove and Hollinger, 2006), four photosynthesis parameters were estimated through Kalman filter. Linear Kalman filter was used to calibrate RZWQM drainage component by Jiang et al. (2018). Kalman filter requires the process equations, and the error distribution of measurement model to be Gaussian. It is very difficult to use Kalman filter for calibrating more than ten parameters. Such offline or online parameter estimation is also referred to as data assimilation. For offline estimation, standard regression techniques (Seber and Wild, 2003) are used. Also, global optimization techniques like Simulated Annealing (Goffe et al. 1994) and Particle Swarm Optimization (Kennedy, 2011) are used by Mavromatis et al., (2001) and Xi et al. (2015). These population-based techniques need long runtime for large number of unknown variables. Another parameter estimation approach is estimating in sequence a set of parameters, using different types of observations. Ma et al. (2011) while calibrating RZWQM2′s parameter sequentially, the recommended order proposed was: soil water, soil nutrients, plant growth, and lastly, pesticide. A sequential optimization method must keep in mind that a certain observation may depend on several parameters and not just a single parameter. Guillaume et al. (2011) also estimated the parameters sequentially for the STICS model. Bayesian method (Gelman, 2013) is also used for parameter estimation. The method starts with a prior probability distribution of the parameters, and then updates the parameters' distribution using the measurements. As an example, in (Jones et al., 2011), a Bayesian parameter estimation procedure was used to estimate eleven soybean cultivar specific parameters in DSSAT model. Tremblay and Wallach (2004) used ridge regression, in a form corresponding to the Bayesian method, to estimate parameters in STICS model. Bayesian methods requires domain expert to select a prior and requires high computational cost for models with large number of parameters. Table 1–18 on page 57 of (Ma et al., 2011) lists comprehensive references on RZWQM2 calibration, along with the parameters calibrated and the observations used. Readers interested in more in-depth mathematical background for agriculture model calibration can refer the book by Brun et al., (2006).

1.2. Fertilizer and irrigation application guidelines

Fertilizer and irrigation application is crucial for optimum crop growth and farm profit. Optimization for fertilizer and irrigation cannot be done in isolation as fertilizer uptake by crop depends on soil moisture level. Too much water would drain the fertilizer and too little would make root uptake unattainable. Farmers follow general guidelines, some of which are mention in this section.

Optimum fertilizer application amount and timing for maize have been explored by many researchers. In (Blackmer, 1997), rate of N (Nitrogen) needed is given for scenarios when all N is applied pre-plant or before emergence for different cropping scenarios, like continuous corn, corn-soybean rotation, corn-on-manured-soil, etc. Recommendation for farmers who wish to split their N application between pre-plant and in-season are also given. Soil sample tests, to measure plant available N before pre-plant and in-season (when crop is 6 in. tall), also play a role in deciding how much N to apply. Majority of N required by Maize is between V8 (8 leaves on corn) and VT (complete visibility of tassel) growth stages (Hanway, 1966): Adequate N during this period is essential for good yield. One-third of plant N requirements must still be met by uptake during the reproductive period otherwise pollination would be hampered. Also, applying N multiple times, including the time of maximum crop uptake, mitigate the risk of N loss due to heavy rain and subsequent N runoff and leaching.

Irrigation is also critical for farming, especially for places where natural precipitation is not enough for crop growth. Full benefit of N application can be realized when water is also present in correct amount. Too little moisture would prevent N uptake by plant and excess water will take N away from plant roots, increase chances of plant disease, and disturb oxygen balance near roots as shown by Irmak et al. (2008). The needed irrigation amount depends on the growth stage of the plant, weather condition, and soil properties. Grant et al., (1989) and Goyal (2012) has shown that maize is more sensitive to water stress during tasseling, silking, and grain filling stages. According to Kranz et al. (2008), plant demand of water is less in initial growth stage because of small leaf area transpiring less water. Water demand increases linearly and is maximum at Tassel and silking stage. The demand then drops slowly till maturity. Weather conditions like low humidity, high radiation and wind increases evapotranspiration and plant water demand increases. Soil property as well affects how irrigation should be done. For instance, sandy soil requires more frequent water application with less quantity each time because sandy soil possess high hydraulic conductivity. Clay soil allows larger irrigation interval because of higher water holding capacity. Optimal irrigation scheduling is explored by Mbamalu and Yigezu (2016) by considering the instantaneous root depth, soil moisture, leaching and soil moisture depletion rate. Varying treatments based on different soil moisture depletion were applied. For clay soil it was found that 120% of the recommended value of 0.55 soil moisture depletion gave best water use efficiency. Stress happens when soil water is less than 50% of plant available water (Panda et al., 2004; Rhoads and Yonts, 1991). According to Panda et al. 2004, irrigation could be scheduled at 45% maximum allowable depletion of available soil water during non-critical stages of growth of maize in sandy loam soils in order to maximize above ground biomass and water use efficiency.

Motivation and Goal: As seen in related works Section 1.1, most prior works have calibrated around 20 parameters through computer algorithm, a small subset of the total number of parameters in an agricultural model. To attain higher modeling accuracy, in this work, we calibrate RZWQM's 8 soil hydraulic parameters at 7 soil layers (total 56), and additionally 3 crop growth parameters (brining the overall total to 59). To solve this, we employ Coordinate Descent algorithm, shown to be promising in large scale optimization (Nesterov, 2012; Hsieh et al., 2008; Wu and Lange, 2008; Friedman et al., 2007; Friedman et al., 2010). Fertilizer and irrigation prescription are given to farmers as approximate guidelines to increase their yield and profit. The prescription can be further optimized taking into account the state of the field and weather. This motivates to optimize fertilizer and irrigation application by using RZWQM calibrated to the field (at Greeley, CO). From the results section we validate that fertilizer and irrigation application can be improved by 7–10%.

2. Materials and methods

2.1. The model: Root Zone water Quality model (RZWQM)

RZWQM (Ahuja et al., 2000) is an agricultural system simulator developed by USDA (United States Department of Agriculture) scientist. It is a one-dimensional (vertical direction) model of an agriculture production system that simulates one crop at a time and evolves on a daily time step. Some of the core inputs to RZWQM are the crop cultivar and their genetic coefficient, weather or meteorological data like daily radiation, minimum and maximum temperature and precipitation, soil information like hydraulic, physical, chemical and heat properties, management practices like irrigation, fertilizer, tillage, planting and pesticide application. Some of the outputs of RZWQM are soil water, Nitrogen, pesticide, organic matter content, N losses (to runoff, leaching, denitrification), plant N uptake, evapotranspiration, water losses (runoff, seepage, drainage/tile flow),soil temperature, plant height, biomass, yield, leaf area index (LAI), phenology. The model can accommodate up to ten soil horizons. For a more complete list of RZWQM inputs, outputs and parameters, readers are encouraged to refer Ma et al. (2012).

The modules of RZWQM are soil water balance, soil nutrient, equilibrium soil chemistry, potential evapotranspiration, surface energy balance and heat transfer module, pesticide processes module, plant growth and management practices module. The modified Brook-Corey equations (Brooks and Corey, 1964) describe the soil water retention curves in RZWQM. The Green-Ampt equation models infiltration during rainfall or irrigation, and the Richards equation models the soil water redistribution, with plant water uptake and tile drainage as sinks. Estimated plant water uptake is limited by potential transpiration calculated from Shuttleworth-Wallace potential evapotranspiration (PET) module (Shuttleworth and Wallace, 1985). The soil nutrient (Nitrogen) module divides organic N into five pools, i.e., fast, and slow residue pools and fast, intermediate, and slow humus pool. The microbes are divided into three pools, namely, aerobic heterotrophs, autotrophs, and anaerobic heterotrophs. The microbes transfer and decompose matter from different N pools. Each pool has a fixed C:N ratio. The module simulates mineralization, immobilization, urea hydrolysis, nitrification/denitrification, ammonia volatilization and microbial growth as first or zero order reactions. The soil chemistry module simulates the long-term effects of agriculture management on soil pH and salinity. The module includes cations and anions like H^+, Ca^{2+}, Mg^{2+}, Na^+, ${NH_4}^+$, Al^{3+} ,${SO_4}^{2-}$, ${CO_3}^{2-}$, OH^-, ${NO_3}^-$, and Cl^- and simulates dissolution and precipitation of partially soluble salts through solubility equations. Adsorption-desorption of cations in solution and on the soil surface are simulated through ion exchange equations. The convective–dispersive heat equation is solved for heat transfer in soil. The crop growth module simulates above and below ground biomass, yield, leaf area, crop height, phenology, water, and N uptake from soil. Each of these modules' processes are model through coupled differential or difference equations and implemented in Fortran programming language. For more details regarding the model, the readers are encouraged to explore the literatures by Ahuja et al. (2000) and RZWQM team (Hanson et al., 1998). RZWQM has many parameters which must be properly estimated to simulate an agriculture field (Hanson et al. 1999).

2.2. The calibration Algorithm: Coordinate Descent

Coordinate Descent (CD) (Wright, 2015) finds a local optimum of a multivariate objective function by successive optimization along coordinate directions or coordinate hyperplanes. Optimizing of many variables simultaneously is a complex problem. CD breaks a complex problem into smaller simpler problems. In the simplest variant of CD, only one variable is adjusted at a time. But a group of variables can also be adjusted at a time. This variant of CD is known as Block Coordinate Descent (BCD). In the simplest form of CD, the order of choosing the variables for optimization remains fixed from one global iteration to next. But in randomized CD, the order of choosing the variables is random in each global iteration. The pseudo code of different variant of CD are given below. The multivariate objective function is detonated by $f(\boldsymbol{x})$, $\boldsymbol{x}$ is an N-dimensional vector with x_i being the i^{th} component of x,$\boldsymbol{x}^0$ is the initial value and '←' is the assignment operator.

Algorithm 1. (*Simple CD method*).

1. Initialize $\boldsymbol{x} \leftarrow \boldsymbol{x}^0$
2. for i = 1 through N
3. $x_i \leftarrow \underset{\substack{x_i \\ LL_i \le x_i \le UL_i}}{\operatorname{argmin}} f(\boldsymbol{x})$
4. Repeat Steps 2 & 3 until termination condition meet

In the simple Coordinate Descent of Algorithm 1, the objective function is minimized with respect to the N variables, sequentially, in a cycle. In step 3 of Algorithm 1, the i^{th} component of x is varied while other components are fixed. The value of x_i that minimizes $f(x)$ is used to update x_i. The range of variation of x_i can be bounded by lower and upper limits (more generally by a set of constraints). Each component variable can have its own set of constraints. The terminating condition can be that there is no substantial improvement in the objective value in the consecutive cycles. Algorithm 1 is generalized to obtain Algorithm 2 for Block Coordinated Descent.

Algorithm 2. (*Block CD method*).

1. Initialize $\boldsymbol{x} \leftarrow \boldsymbol{x}^0$
2. Create B blocks each with S variables
3. for i = 1 through B
4. $x_i \leftarrow \underset{\substack{x_i \\ LL_i \le x_i \le UL_i}}{\operatorname{argmin}} f(\boldsymbol{x})$
5. Repeat Steps 3 & 4 until termination condition met

In a Block Coordinate Descent method of Algorithm 2, in each cycle instead of searching along a line (a one-dimensional space) as in Algorithm 1, the search is performed along a hyperplane (a multi-dimensional space). Here, B is number of blocks with each block $B_i$can having N_i variables. Here, $\boldsymbol{x}_i$ is a vector whose components are elements of B_i, and the constraints bound the vector of variables from above and below.

In the randomized Coordinate Descent method, the order of the variables optimized is randomly chosen in each cycle. Both Algorithm 1 and 2 above can be randomized. The randomized version of Algorithm 1 is given next in form of Algorithm 3. In the present work, this variant of Coordinate Descent method is used. In the method below, ***Seqn*** is a random sequence of first N natural numbers obtained by the 'jumble' operation. Step 3 iterates N variables according to the order present in *Seqn*.

Algorithm 3. (*Randomized CD method*).

1. Initialize $\boldsymbol{x} \leftarrow \boldsymbol{x}^0$
2. Seqn ← jumble(1,…,N)
3. for i in *Seqn*
4. $x_i \leftarrow \underset{\substack{x_i \\ LL_i \le x_i \le UL_i}}{\operatorname{argmin}} f(\boldsymbol{x})$
5. Repeat steps 2, 3 & 4 until termination condition met

2.3. The field dataset

We used the dataset from a field experiment conducted on USDA-ARS Limited Irrigation Research Farm near Greeley, Colorado by Trout and Bausch (2017) in the year 2010. There multiple time series observations of different types of outputs were recorded. Fig. 1 shows the experimental site in Greeley, CO. Note the different plots for different crops and treatment. We consider only maize with full and deficit irrigation. The same figure also shows the drip irrigation system to apply controlled amount of water to the field. Corn was planted on 12th May 2010 and harvested on 19th Oct 2010. Fertilizer as urea-ammonium-nitrate (UAN) was applied at planting and then applied through irrigation water throughout the growing season. Different irrigation treatments were applied, of which only two are of interest in this work, namely, (i) irrigation treatment to meet 100% of potential crop Evapotranspiration (ET_c) requirements and (ii) to meet 55% of ET_c requirements. Total N applied was 146 kg N ha^{-1} for both treatments. The timing and amount of N applied by Trout and Bausch (2016) was according to recommendation by Davis and Westfall (https://extension.colostate.edu/topic-areas/agriculture/fertilizing-corn-0–538/). For the 100% or full treatment, irrigation was applied every three to seven days based on the estimated amount of crop water used (i.e. actual ET) based

Fig. 1. Aerial view of 16 Hectare of Greeley, Colorado, USDA experimental site (left); Irrigation control, monitoring system and turbine flow meters (middle); Drip irrigation pipes in field (right). Taken from (Trout, 2016).

on a daily reference ET_o, crop coefficient, rainfall, and soil water deficit (Allen et al., 1998).

In this work, the calibration data from fully irrigated plot in the year 2010 was used. The 7 types of outputs that were recorded are given below in bullets. Among these the 4th output below was recorded at 7 different depths. Biomass, Yield and Harvest Index were measured only once at time of harvest.

- plant height,
- evapotranspiration (ET),
- leaf area index (LAI),
- soil water content (SWC) at seven different soil depths,
- biomass,
- yield, and
- harvest index.

ET data was collected daily in the growing season from May through October. Other outputs were recorded approximately on a weekly basis. Soil moisture was measured with neutron moisture meter (CPN-503 Hydroprobe, InstroTek, San Francisco, CA) as shown in left picture of Fig. 2(c). DeKalb brand 52–59 (VT3) maize seed was planted with John Deere Maxiplex planter at 81,000 seeds per Hectare on 12th May 2010 at a 0.76 m interrow spacing. Irrigation applications were measured with turbine flow meters (Badger Recordall Turbo 160 with RTR transmitter). Irrigation application were controlled by and recorded with Campbell Scientific CR1000 data loggers. In Fig. 2(b), Bowen Ratio Energy Balance, BREB, system was used to measure maize evapotranspiration (actual ET). The weather station in Fig. 2(a) measured meteorological values like humidity, wind speed, temperature, etc. Plant height was measured throughout the season with measurement rod to the top of the leaf canopy. Leaf Area Index, LAI, was estimated by measuring the length and width of each leaf on five plants and multiplying the average leaf area (m^2) per plant by the plant population per m^2. Crop canopy ground cover was measured at noon with digital camera from a nadir view six meters above ground surface as seen in Fig. 2(d). Above ground biomass was measured before harvest. 10–15 corn plants were cut 2 cm above ground, ears removed, and remaining stover dried in oven at 60 °C for two days and weighed. Similarly, ears were dried, grain removed from cobs and both components re-dried and weighed. Harvest index was calculated as the ratio of dry grain weight to total above ground biomass. Grain yield was measured by harvesting the ears by hand. Grain moisture content at harvest was measured with a Dickey-John GAC500-XT Moisture Tested. Yield was converted to dry weight by accounting 15.5% moisture content.

2.4. RZWQM calibration using coordinate descent and its software setup

In this work, the third variant of Coordinate Descent method (Algorithm 3) has been used. It was observed while calibrating, that the randomized Coordinate Descent provided better results. In a Block Coordinate Descent, many tunings need to be done like size of blocks and partitioning. Block partitioning has exponential number of choices in the number of variables. Also, two blocks can have overlapping variables. Because of this added complexity, randomized variant of the simple Coordinate Descent algorithm was used in this work.

In our case, calibration of RZWQM was performed by varying the parameters and comparing with the objective function. The variable $\boldsymbol{x}$ mentioned in Algorithm 3 would correspond to the parameters that needs to be calibrated. The objective function, defined next, is such that the error between the model predicted values and field observations are minimized.

The soil hydraulic parameters characterize the water retention curves (relation between water content and potential). The eight hydraulic parameters for each of the 7 layers calibrated are:

Fig. 2. (a) Weather Station, (b) Bowen Ratio Energy Balance meter, (c) Neutron Moisture Meter, and (d) High clearance reflectance tractor taking canopy ground cover image. Taken from (Trout, 2016).

- bubbling pressure,
- pore size distribution index,
- saturated hydraulic conductivity,
- residual water content,
- saturated water content,
- field capacity at 1/3 bar,
- field capacity at 1/10 bar, and
- wilting point.

The model divides the soil depth of 200 cm into seven layers. Each of the seven layers have the above mentioned eight parameters. Apart from these 56 soil parameters, three maize crop parameters were also calibrated. Those are:

- Phylochron interval (development time taken for elongation of successive leaf),
- maximum plant height at maturity, and
- plant biomass at half of maximum height.

Thus, a total of 59 parameters were calibrated in the present work. The objective function is defined to minimize the weighted sum root mean square errors over the different types of field outputs. Also, since the units of different outputs are different, each root mean square error value was multiplied by a normalizing factor. Similar objective function has been used in prior works by Xi et al. (2015) and Xi et al. (2017). The expression for the objective function $f(\boldsymbol{x})$ is as follows.

$$f(\boldsymbol{x}) = \sum_{i=type\ of\ outputs} \gamma_i \cdot \sqrt{\frac{\sum_{j=1}^{No.\ of\ obs.\ of\ type\ i} \{m_i \cdot (o_{ij} - p_{ij})/o_{ij}\}^2}{(No.\ of\ obs.\ of\ type\ i)}} \tag{1}$$

Here γ_i is the normalizing factor defined as the ratio of mean of the measured outputs of type $i = plant\ height$ and the mean of the measured outputs of type i. o_{ij} and p_{ij} are the j^{th} observed versus model predicted values of the data type i. Note p_{ij} is the model-predicted output from the RZWQM model. The different outputs that we used have been listed earlier in this section. The 'intensity' of an error is relative to its actual value, and relative to the maximum value. Therefore, to equalize the weightages among all the errors, each error (o_{ij} - p_{ij}) is normalized by (m_i/o_{ij}), where m_i is the maximum of all the observations of data type i. The expression in (1) above is the objective function *f(x)* mentioned in the previous section. Rewriting (1) in the form of the objective function $f(\boldsymbol{x})$ of Algorithm 3, we obtain:

$$f(\boldsymbol{x}) = \sum_{i=type\ of\ outputs} \gamma_i \cdot \sqrt{\frac{\sum_{j=1}^{No.of\ obs.\ of\ type\ i} \{m_i \cdot (o_{ij} - RZWQM(\boldsymbol{x})_{ij})/o_{ij}\}^2}{(No.\ of\ obs.\ of\ type\ i)}} \tag{2}$$

Here, the optimization variable x is a vector of 59 dimensions that represents the parameters to be calibrated, whereas *RZWQM(x)* is an external call to the RZWQM with model parameters x to simulate the model and provide the predicted outputs p_{ij}. With the objective function defined in eqn. (2), the calibration is done according to Algorithm 3 of the previous section. Tables 1 gives the starting values of the parameters $\boldsymbol{x}^0$ that we chose for our randomized Coordinate Descent algorithm. This initial value of the parameters have been taken from the work by Qi et al. (2016), where the same set of parameters were calibrated manually against the same field data. The upper and lower limit of the range of variation was set to be ± 10% of the starting value. The starting value of the parameters is critical, as otherwise the minimization method might find a local minimum. Hence, an educated initial guess is required, and can be obtained from experts such as Qi et al. (2016).

Table 1b
Starting or initial values of three crop growth parameters for the CD algorithm.

Phylochron interval(deg. day)	Max. height at maturity(m)	Biomass at ½ max. height (gm)
50	2.70	30

The Coordinate Descent algorithm of third variant in Section 2.2 is implemented within the R programming language (Team, 2013). To evaluate the objective function in (2), command line interface of RZWQM is invoked from R code through *system()* function. RZWQM can be run from GUI and through command line as well. In our case though, RZWQM is run through the command line interface. The command is argument to the *system()* function in R. To change the soil parameters, entries in the rzwqm.dat file are changed at the appropriate places. To change the crop growth parameters, the entries in the mzcer040.cul file are changed. Once these files are changed, RZWQM is run by executing RZWQMrelease.exe (located in bin folder of RZWQM installation) in the command line. Many outputs are generated and logged in several output files, but only two files are required in our case. From the COMP2EXP.OUT file, simulated plant height, evapotranspiration, leaf area index, yield, biomass, and harvest index are obtained. Simulated soil water content of seven layers are obtained from LAYER.PLT output file. In this file, the soil water content (SWC) values are given at discrete soil depth. For instance, for layer 1, that ranges from 0 to 15 cm depth in the field experiment, LAYER.PLT gives simulated SWC at six depths, namely, 1, 2, 4, 7, 11, and 15 cm of depth. To simulate the field measured SWC of layer 1, weighted average of these six (at 1, 2, 4, 7, 11 and 15) simulated SWC values is used. Similarly, for the other six soil layers, weighted average of the discrete SWC values is used to simulate SWC. Files, namely, mzcer040.cul, COMP2EXP.OUT and LAYER.PLT are located within the RZWQM scenario, that is equivalent to working directory or workspace in a programming language integrated development environment.

The R program and the RZWQM model are run on the same desktop computer, with the configurations shown in Table 2.

When performing the optimization to determine the model parameters using Coordinate Descent of Algorithm 3, the *optimize()* function of R is used in Step 4. This function internally uses Golden Section search to find the minima. It is observed that two iterations of Coordinate Descent attain the near optimality. The objective value does not improve much after the second iteration.

Table 1a
Starting or initial values of 56 (8 parameters × 7 layers) soil hydraulic parameters for the CD algorithm.

Layer(m)	Bubbling Pressure(m)	Pore size distribution index	Saturated hydraulic cond. (cm/hr)	Residual water content(m^3 m^{-3})	Saturation water content(m^3 m^{-3})	Field capacity at 1/3 bar(m^3 m^{-3})	Field capacity at 1/10 bar(m^3 m^{-3})	Wilting point(m^3 m^{-3})
0.0–0.15	0.35974	0.222	2.0	0.035	0.437	0.280	0.355201	0.140
0.15–0.30	0.43786	0.222	5.0	0.035	0.437	0.291	0.369646	0.145
0.30–0.60	0.35045	0.180	5.0	0.035	0.437	0.303	0.367829	0.170
0.60–0.90	0.26719	0.160	5.0	0.035	0.408	0.283	0.336971	0.170
0.90–1.20	0.25814	0.184	5.0	0.035	0.408	0.267	0.325575	0.150
1.20–1.50	0.24350	0.189	4.0	0.035	0.389	0.251	0.30645	0.140
1.50–2.00	0.26212	0.177	4.0	0.035	0.389	0.261	0.314774	0.150

Table 2
Software system environment configuration.

Operating System	Windows 10, 64 bit
System Model	Dell OptiPlex 9010
Processor	Intel i7 3.4 GHz
Memory	8 GB
RZWQM2 Ver.	3.00.00
R Ver.	3.4
RStudio Ver.	1.0.143

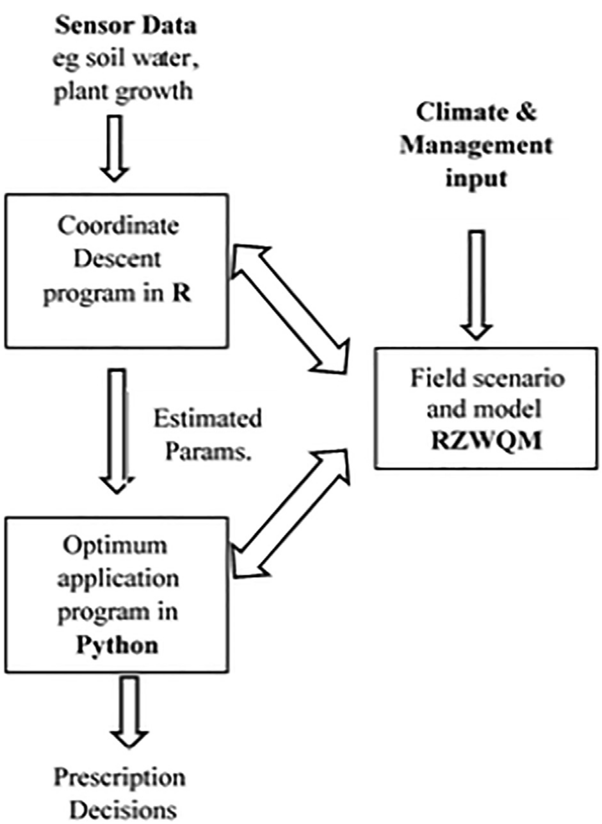

Fig. 3. Overall Software architecture.

The software setup is given in Fig. 3. The outputs from the field like soil water content, LAI and plant height are given to the Coordinate Descent within the R program. The program repeatedly calls RZWQM which is mimicking the field scenario. In each call, the parameters in rzwqm.dat and mzcer040.cul files are modified. These parameter files serve as input to RZWQM. The Coordinate Descent program stops when the weighted root mean square error does not decrease any further.

Two or more different set of parameter values can give the same goodness of fit. A way to resolve this issue is to validate the performance of the calibrated model by comparing model predicted values to a data set in a different scenario. For instance, in our work, we have used fully irrigated treatment data to calibrate the model and deficit irrigated treatment data to validate the model. The deficit irrigated plot was adjacent to the fully irrigated plot so that it can be reasonably assumed that the soil parameters, amount of rainfall, sunlight and fertilizer added in the two cases were very similar (if not the same). The only thing different was the amount of irrigated water.

To measure goodness of calibration and validation, the fit between the observed and the simulated values of output type i was determined using the coefficient of determination (R_i^2) and Nash-Sutcliffe model efficiency (ME_i). They are defined as follows in (3a).

$$R_i^2 = \frac{\left[\sum_{j=1}^{n_i}(O_{ij}-\bar{O}_i)(P_{ij}-\bar{P}_i)\right]^2}{\sum_{j=1}^{n_i}(O_{ij}-\bar{O}_i)^2\sum_{j=1}^{n_i}(P_{ij}-\bar{P}_i)^2} \tag{3a}$$

$$ME_i = 1.0 - \frac{\sum_{j=1}^{n_i}(P_{ij}-O_{ij})^2}{\sum_{j=1}^{n_i}(O_{ij}-\bar{O}_i)^2} \tag{3b}$$

where n_i is number of data pairs or observation of output type i, $\bar{O}_i$ and $\bar{P}_i$ are mean measured and simulation predicted values respectively of output type i, and O_{ij} and P_{ij} are j^{th} measured and predicted values respectively of output type i. R^2 varies from -1 to 1. Closer the R^2 value to 1, the better is the fit. ME varies from negative Infinity to 1. Closer the ME value is to 1, the better is the fit.

Once the parameters are optimized i.e. RZWQM is calibrated to the field and is a representation of the field, the calibrated RZWQM model is used in finding the optimum application of water and fertilizer. This is done by a second phase application of Python program, namely, the 'Optimum application program'. Python was used in second case phase because of availability of many optimization libraries and quick processing time. This program also repeatedly calls RZWQM but now the water and fertilizer inputs are changed in each iteration rather than the model parameters. This phase is explained in next section along with the algorithms used for finding the optimum application.

2.5. Algorithms for optimum fertilization and irrigation

There exists tradeoff between yield and cost of agricultural inputs. This trade-off can be captured using a simple economic cost for the net profit:

$$\text{Profit} = (\text{yield} \times \text{unit price}) - (\text{fertilizer amount} \times \text{fertilization cost} + \text{irrigation amount} \times \text{irrigation cost}) \tag{4}$$

Note, this cost is from a farmer's perspective, which accounts for cost of fertilization, and so it is expected that excess application of it will not be optimal. In case there is a corresponding penalty/tax for N losses, this can be captured explicitly by subtracting the 'amount of N loss' times 'penalty rate for N pollution'. Further, in order to validate and compare with prior work, we resort to field and weather data from the year 2010 at Greeley, Colorado (Trout and Bausch, 2017), and also keep the same application days: We vary the amount of fertilizer and irrigation application at the same days as in the experiment conducted in Trout and Bausch (2017). The corresponding optimization space is significantly large, 18-dimensional: the fertilization was done six times in the growing season, while the irrigation was done twelve times in Trout and Bausch (2017). Also, the nonlinear nature of the governing equations makes the optimization problem further complex.

In order to solve the proposed complex profit optimization problem, three *global optimization* techniques were used and compared, namely, Differential Evolution (DE) (Storn and Price, 1997), Basin Hopping (BH) (Wales and Doye, 1997), and Particle Swarm optimization (PSO) (Kennedy, 2011). Also, two other optimization techniques that may only find a *local optimum*, namely, Sequential Least Square Programming (SLSQP) (Kraft, 1988) and Constrained Optimization By Linear Approximation (COBYLA) (Powell, 1994), were also tried. These methods are numerical, owing to the non-availability of any closed-form solution, yet they explore the solution space efficiently, yielding a near optimum application prescription that maximizes the farm profit of equation (4). All the python implementation of these five techniques are available as Python packages.

DE is a stochastic global optimization method. It is an instance of evolutionary algorithms, such as Genetic Algorithm. DE can be used to optimize functions that are non-differential and non-continuous. It maintains a population of candidate solutions subject to iterations of mutation, recombination and selection. Each population member is characterized by its fitness (profit in this work). For each member, its next generation is constructed. If next generation member has better fitness, then it replaces the parent. The next generation of a member is created from three other randomly chosen members (say x,y and z). The new member is value of x plus scale factor times difference between y and z. The process continues over enough generations to reach convergence close to the global optimal solution. BH too is a stochastic global optimization method. It was first applied in chemistry to find stable molecular configuration with lowest energy. Typically, there are many local optimum molecular configuration. Briefly, the steps of BH are: choose an initial point, compute a local minimum using any local optimization method, apply a random perturbation to the coordinates of the local minimum (perturbation should be sufficiently large to escape from local minima), compute next local minimum, compare the local minima with the previous, and select the better. PSO is a stochastic technique inspired by social behavior of bird flocking in search of food. PSO is initialized with a group of random particles (candidate solutions). It searches for the optimum by updating through iterations. In every iteration each particle's velocity and position is updated by following two best values. First is the position of the best solution the particle itself has achieved so far. Second is the best solution attained so far by any particle in the swarm.

Population based evolutionary algorithms can provide near optimum solution, but they are quite computationally expensive. Keeping this in mind, we also tried two local optimization methods, SLSQP and COBYLA. SLSQP is known to be an efficient computational method to solve general nonlinear programming with equality and inequality constraints. The optimization is done iteratively starting with a vector of initial values. The $(k+1)^{th}$ value is sum of k^{th} value and product of search direction and step length. Both search direction and step length are adapted in every iteration. The search direction is evaluated by a quadratic programming sub problem. The sub problem is formulated as quadratic approximation of the Lagrange function (objective function minus sum of scaled constrained functions) of the constrained optimization problem. COBYLA minimizes objective function subject to constraints. The method works by linearly approximating the objective and constraint function. For a number N of the optimization variables, the approximation is done by a linear interpolation at $N+1$ points. These interpolation points are like the vertices of a simplex. A parameter *Rho* controls the size of the simplex. For each *Rho,* the method finds a good set of variables' values, then it reduces the *Rho* value and simplex size. The method, unlike summing each constraint into a single penalty function, considers each constraint individually when calculating the change to the variables.

For arriving at the optimization results, the price of corn per bushel was taken to be $4 from Johanns (2011). A bushel of shelled corn weighs 56 lbs (South Dakota State Univ. Extension). Neglecting 15% moisture content, a bushel of corn weighs 47.3 lbs (or 21.45 kg) by dry weight. This translates to $0.186 per kg of dry corn cost. This value was used in eq. (4) for the yield price of corn. In the expression for profit, eq. (4), it is supposed that the cost of fertilizer UAN32 is $251/ton according to (DTN Retail Fertilizer Trends). This rate translates to $0.86 kg^{-1} of N that we used in eq. (4) toward fertilization cost. Half of the N in UAN is supplied by Urea. One-fourth N is supplied by nitrate N and the remaining one-fourth N supplied by Ammonia. Irrigation cost comprises of cost of water and cost of pumping water and delivering to crops. We have supposed cost of water and cost of pumping to be both $30 per acre feet based on Farm and Ranch Irrigation Survey (Table 22 and 20) by USDA (NASS, 2008). An acre foot corresponds to 325,851 gallons of water. The unit of amount of irrigation in the expression for profit in (4) is in cm. A cm of irrigation in a hectare of field is 26,417.2 gallons of water. This translates to $4.86/cm as cost of irrigation in Eq. (4).

While running the optimization, the fertilization variables were given an upper bound of 48 kg N ha^{-1} and lower bound of 0.4 kg N ha^{-1}, and the irrigation variables were provided an upper bound of 7 cm and lower bound of 0.1 cm. The optimizers were run with the default settings for their internal parameters. The optimization was run in Python ver3.7 programming language, that has built in packages for the optimization methods used.

Table 3
Goodness of fit comparison of manual vs CD automated calibration using full (100% of ET_c) irrigation data.

	Manual CalibrationQi et al. (2016)		Coordinate Descent	
Output Types *i*	R^2	ME	R^2	ME
Plant Height	0.99	0.97	0.99	0.95
ET	0.83	0.75	0.84	0.78
LAI	0.94	0.92	0.95	0.88
SWC 1	0.40	0.39	0.40	0.33
SWC 2	0.55	0.44	0.58	0.49
SWC 3	0.81	0.76	0.83	0.77
SWC 4	0.87	0.76	0.90	0.81
SWC 5	0.79	0.62	0.83	0.58
SWC 6	0.74	0.72	0.70	0.56
SWC 7	0.66	0.65	0.79	0.78
SWS	0.88	0.88	0.90	0.86
Average	**0.77**	**0.71**	**0.79**	**0.71**

3. Results and discussion

This Section is divided into three Subsection. Section 3.1 has the results and discussion of RZWQM calibration using Coordinate Descent and Section 3.2 has the results and discussion of optimum fertilizer and irrigation application and Section 3.3 has the discussion encompassing more general remarks.

3.1. Results on calibration and validation of RZWQM with field data

Table 3 gives the R^2 and ME values for the manually calibrated parameters by Qi et al. (2016) versus the proposed Coordinate Descent method. The average R^2 values for Coordinate Descent method is better than the manual method. It can be seen that the Coordinate Descent performs similar to manual calibration on ME measure, but it has about 3% improvement on R^2 measure. Plus being automated, *no expert guidance required* for the Coordinated Descent. Calibration is done with data from fully irrigated field. The calibrated parameters' value are given in Tables 4,.

Table 5 gives the validation result of the calibrated parameters. Once the model is calibrated, it is validated on a scenario different from the training or calibrating data. This scenario was the deficit irrigated field of the same year 2010. This field was situated adjacent to the fully irrigated field. The same maize cultivar was grown. Even though the deficit irrigated field was located adjacent to the field whose data was used for calibration, there can be variation in the soil parameters. To account for this minor change in parameters, five parameters of the RZWQM model are again adjusted with deficit irrigation field data. Remaining parameters' value are same as learned from the full irrigation data. The work by Qi et al. (2016) also adjusted those parameters using deficit irrigation data before validating. Table 6 gives the adjusted or calibrated parameters of the five soil hydraulic parameters using the deficit irrigation field data. Again, the calibration was done using Coordinate Descent method. The validation performance in Table 5 shows improvement of about 4 – 5% of R^2 and ME using CD over manual method. In the Coordinate Descent (CD) optimization, the parameters were varied ± 10% from their initial value. Increasing the ranges to ± 20% and ± 30% did not improve the model calibration, while the time required for CD convergence increased.

3.2. Results on optimized fertilization and irrigation using calibrated model

The optimization of fertilization and irrigation application was

Table 4a
Coordinate Descent Calibrated hydraulic parameters' value from full irrigation dataset.

Layer(m)	Bubbling Pressure(m)	Pore size distribution index	Saturated hydraulic cond. (cm/hr)	Residual water content($m^3\ m^{-3}$)	Saturated water content($m^3\ m^{-3}$)	Field capacity at 1/3 bar($m^3\ m^{-3}$)	Field capacity 1/10 bar($m^3\ m^{-3}$)	Wilting point($m^3\ m^{-3}$)
0.0–0.15	0.32071	0.242	1.883	0.0351	0.426	0.310	0.394	0.155
0.15–0.30	0.46879	0.235	5.290	0.0363	0.423	0.323	0.410	0.160
0.30–0.60	0.36785	0.190	4.870	0.0350	0.445	0.336	0.408	0.188
0.60–0.90	0.26074	0.160	5.068	0.0356	0.398	0.315	0.373	0.188
0.90–1.20	0.27825	0.193	5.129	0.0340	0.398	0.296	0.361	0.166
1.20–1.50	0.26704	0.200	4.102	0.0332	0.386	0.278	0.340	0.155
1.50–2.00	0.25529	0.185	4.086	0.0322	0.388	0.289	0.349	0.166

Table 4b
Coordinate Descent Calibrated crop growth parameters' value from full irrigation dataset.

Phylochron interval(deg. day)	Max. height at maturity(m)	Biomass at ½ max. height(g)
52.747	2.76998	26.753

Table 5
Comparison of manual vs CD automated validation using deficit (55% of ET_c) irrigation data.

	Manual Calibration Qi et al. (2016)		Coordinate Descent	
Outputs	R^2	ME	R^2	ME
Plant Height	0.98	0.60	0.98	0.35
ET	0.84	0.73	0.86	0.77
LAI	0.90	0.88	0.91	0.89
SWC 1	0.27	0.26	0.29	0.22
SWC 2	0.52	0.40	0.57	0.54
SWC 3	0.50	0.32	0.58	0.37
SWC 4	0.73	0.60	0.78	0.63
SWC 5	0.90	0.86	0.89	0.84
SWC 6	0.91	0.75	0.94	0.79
SWC 7	0.80	0.54	0.80	0.79
SWS	0.84	0.84	0.87	0.84
Average	**0.74**	**0.61**	**0.77**	**0.64**

Table 6
Coordinate Descent Calibrated parameters' value for deficit irrigation.

Layer(m)	Bubbling Pressure (m)	Pore size distribution index	Field capacity at 1/3 bar($m^3\ m^{-3}$)	Field capacity at 1/10 bar ($m^3\ m^{-3}$)	Wilting point($m^3\ m^{-3}$)
0.0–0.15	0.32999	0.318	0.270	0.367	0.115
0.15–0.30	0.37849	0.275	0.292	0.382	0.136
0.30–0.60	0.33252	0.220	0.307	0.385	0.159
0.60–0.90	0.25905	0.214	0.273	0.344	0.140
0.90–1.20	0.32171	0.207	0.282	0.356	0.144
1.20–1.50	0.37323	0.151	0.319	0.375	0.197
1.50–2.00	0.53577	0.089	0.370	0.413	0.265

performed to compare the profits against the experimental applications in Greeley Colorado by Trout and Bausch (2017), that used UAN32 (Urea Ammonium Nitrate) as N fertilizer. The fertilizer were applied by dissolving through drip irrigation. Irrigation was roughly applied on a weekly basis whereas fertilization was applied according to recommendation by Davis and Westfall (https://extension.colostate.edu/topic-areas/agriculture/fertilizing-corn-0–538/). The results of different optimization methods to maximize the profit are summarized below in Tables 7 and 8, whereas Table 10 lists the profits.

Table 7 gives amount of N applied in kg per hectare for the field experiment at Greeley, CO (Trout and Bausch, 2017), versus the proposed amounts by the different optimization methods we examined.

Table 7
Amount of fertilizer N applied per hectare (kg N ha^{-1}) for different methods in 2010 growing season.

Date	Trout and Bausch (2017)	DE	BH	PSO	SLSQP	COBYLA
5/24/2010	22.4	46.4	22.4	25.2	22.0	30.8
6/23/2010	22.4	20.0	25.6	45.6	22.0	31.6
7/9/2010	22.4	35.2	23.2	48.0	22.0	34.8
7/21/2010	22.4	10.4	18.4	0.4	22.0	18.8
8/3/2010	22.4	4.0	26.4	0.4	22.0	17.2
8/16/2010	33.6	0.4	34.4	0.4	33.2	27.6
Total	**145.6**	**116.4**	**150.4**	**120.0**	**143.2**	**160.8**

Table 8
Amount of irrigation (in cm) applied for different methods in 2010 growing season.

Date	Trout and Bausch (2017)	DE	BH	PSO	SLSQP	COBYLA
6/11/2010	0.63	0.63	1.23	0.1	0.61	1.35
6/23/2010	3.04	2.01	3.44	6.56	3.75	3.69
6/29/2010	3.01	3.25	2.61	4.12	2.94	3.36
7/8/2010	3.07	4.34	3.27	2.13	3.73	3.27
7/16/2010	3.19	1.41	3.78	3.06	3.9	3.0
7/21/2010	3.01	6.64	3.4	3.16	3.72	3.57
7/28/2010	4.22	2.47	4.02	0.1	4.2	3.91
8/3/2010	4.02	3.09	3.82	7.0	4.45	4.19
8/16/2010	3.86	0.63	3.26	0.1	3.88	3.88
8/20/1010	2.51	1.44	2.31	4.09	2.45	2.65
8/25/2010	3.01	4.8	2.81	0.29	3.71	3.03
9/1/2010	3.01	6.56	3.4	7.0	3.27	3.36
Total	**36.58**	**37.27**	**37.35**	**37.71**	**40.61**	**39.26**

Total N applied in the field site at Trout and Bausch (2017) was 145 kg N ha^{-1}. The two better performing evolutionary methods, DE and PSO, applied more N towards the early stages and negligible at later stages. All optimization method except for BH and COBYLA required less N but gave more profit (see Table 10 for profits). The best possible saving in fertilization of about 20% was found by DE.

Table 8 gives the recommended amount of irrigation to be applied at the given dates for the different optimization methods, while the actual amount applied to the field is mentioned in Column labelled Trout and Bausch (2017). The total irrigation prescription given by different methods are slightly greater than field applied of 36.58 cm in Trout and Bausch (2017), with DE offering the smallest increment of 1.8%. Table 9 gives the rainfall amount in 2010 growing season. Fig. 4 consolidates Tables 8 and 9 (irrigation and rainfall) for visualization, with the X-axis marked with the dates and the growth stages.

Table 10 tabulates the yield, total N and irrigation applied in the growing season by different methods, profit, and the number of RZWQM model runs required for all the cases. All the five profit optimization methods gave an increase in yield and profit compared to Trout and Bausch (2017), with best yield increase of 8% offered by PSO, resulting in 10% increase in profit. Therefore, we recommend the

Table 9
Precipitation (cm) between planting and harvest.

Date	Rain	Date	Rain	Date	Rain
5/11/2010	2.01	6/12/2010	2.36	8/3/2010	0.05
5/12/2010	0.79	6/13/2010	0.96	8/4/2010	0.08
5/14/2010	0.15	6/14/2010	0.13	8/9/2010	3.15
5/15/2010	0.15	6/19/2010	0.15	8/13/2010	0.05
5/16/2010	0.33	6/26/2010	0.41	8/16/2010	0.1
5/18/2010	1.35	7/4/2010	1.55	8/19/2010	0.33
5/19/2010	0.05	7/8/2010	0.08	8/23/2010	0.36
5/20/2010	0.02	7/10/2010	0.02	8/25/2010	0.02
5/26/2010	0.08	7/11/2010	0.02	9/23/2010	0.02
5/29/2010	0.02	7/14/2010	0.51	10/1/2010	0.18
6/6/2010	0.2	7/16/2010	0.08	10/12/2010	0.61
6/8/2010	0.08	7/20/2010	0.02	10/16/2010	0.1
6/10/2010	0.1	7/22/2010	0.1		
6/11/2010	3.63	7/30/2010	1.75		

irrigation and fertilizer application strategy generated by the PSO method. We observe that judiciously applying water and fertilizer has the potential to increase profit and yield without requiring significant extra fertilizer and water. Table 10 also gives the number of RZWQM model runs required by each optimization methods. This is indicative of the time required to run an optimization method. Runtime depends on the computer hardware configuration and the optimization algorithm. DE and PSO that gave the better results in terms of profit and yield required larger processing times. In contrast, the local optimizers SLSQP and COBYLA were faster but worse in terms of optimality.

We also calculated the nitrogen and water stress levels at various growth stages under different optimizers, as listed in Table 11. There is no stress initially, and it progressively increases as the crop matures, which is to be expected since the goal is to optimize the profit. At maturity, development ceases, so to maximize the profit less resources get prescribed by different optimization methods.

3.3. Discussion

The 10% increase in profit is promising given that nearly 2/3rd of US farms operate on a margin of less than 10% after accounting for the government subsidies (Hoppe 2014). Fine tuning the default parameter values of the optimization methods could further improve yield and profit. It turns out that each cycle of Coordinate Descent takes nearly 2.5 hrs. This is primarily because at each iteration, the R optimizer needs to make numerous calls to the RZWQM simulator to explore different candidate parameter values. These consume lots of I/O time in passing the data back and forth between the two programs, R and RZWQM, and is unavoidable. To speed-up the overall computations, one could implement the model-simulation and optimization within a same programing language.

Ma et al. (2012) used the PEST parameter estimation tool available in RZWQM to calibrate the same hydraulic parameters in RZWQM and same field dataset as used in this work. The corresponding R^2 and ME values (Table 10 of Ma et al. 2012) are lower than the manual calibration in Qi et al. (2016) which in turn is lower than those from our CD approach (meaning CD is superior to all). It should also be remarked that fitting outputs sequentially (first fit height, then ET and so on), as done by Saseendran et al. (2010), Ma et al.(2011) and Guillaume et al. (2011), performed worse than fitting all the different types of outputs (plant height, ET, LAI, SWC) at the same time using equation (1). Also note that many complex processes (like close interaction of soil organic matter with atmosphere, effect of root growth, variability of radiation, surface residue reactions, etc.) occur near the top/boundary surface that are not fully modeled in RZWQM yet. This explains the relatively poorer fit of soil water content at level 1 (as seen from the relatively lower R^2 and ME values in Table 3 and 5).

4. Conclusion and future work

In this work, an automated, sensor-data driven agricultural model calibration method, involving Coordinated Descent (CD), was proposed for model calibration and calibrated model used for fertilization and irrigation prescription. The method was used successfully to calibrate a total of 59 parameters of a RZWQM model of an agricultural field in Greeley, Colorado (Trout and Bausch, 2017), completely automatically, without needing any expert input. Yet it was able to improve a previously optimized model by a further around 4%. The proposed method can be easily scaled to calibrate more number of parameters if additional types of field measurements become available. The runtime of the method can be significantly improved if the RZWQM model and the calibration program are coded in the same programming platform. This is because the system() calls and file read/write take up extra time. Running of the model too takes time and it is hoped that refactoring the RZWQM model code from legacy programming language like Fortran to Python would improve runtime. This would require porting the two, the RZWQM simulator and the R-based optimizer, in a same platform. Currently, those are coded separately. RZWQM in Fortran and calibration program in R language.

We further used the calibrated model for fertilizer and irrigation prescription through a profit maximization formulation, and performed the nonlinear optimization using three global and two local optimization algorithms, and compared the results with the one used in Trout and Bausch (2017). The optimization variables chosen here were 6 fertilizer and 12 irrigation application days as in Trout and Bausch (2017). The comparison showed about 7% improvement in yield and about10% improvement in profit could be realized when compared to the treatment provided in the experimental data of Trout and Bausch (2017). As with calibration, the time required for the heuristic algorithms performing nonlinear optimization can also significantly be improved by integrating the optimization routine and modeling equations in the same programming platform.

In the current optimization work, the application dates of fertilizer and irrigation were taken be the same as in the experimental setting by Trout and Bausch (2017). Future work can explore how to optimize the extended problem of optimizing both the amounts and the days of applications efficiently. The fertilizer and water prescription optimization can further be made more efficient employing machine learning. Training data would be used based on history of weather versus prescription. The approach would be empirical (as opposed to model-based), but computationally much fast, allowing obtaining an initial estimate, prior to a model-based refinement if needed. Also in this work, the fertilizer and water prescriptions were computed offline. It would be interesting to develop a runtime version where the offline

Table 10
Yield and Profit per Hectare for different optimization methods.

	Trout and Bausch (2017)	DE	BH	PSO	SLSQP	COBYLA
Yield(kg ha^{-1})	9987.1	10732.1	10319.5	10783.7	10325.2	10734.1
Total N applied(kg N ha^{-1})	145.6	116.4	150.4	120.0	143.2	160.8
Total irrigation applied(cm)	36.58	37.27	37.35	37.71	40.61	39.26
Profit($ ha^{-1})	1554.6	1714.2	1608.4	1719.2	1600.0	1666.8
No. of Model Runs	–	4449	31,486	4055	56	233

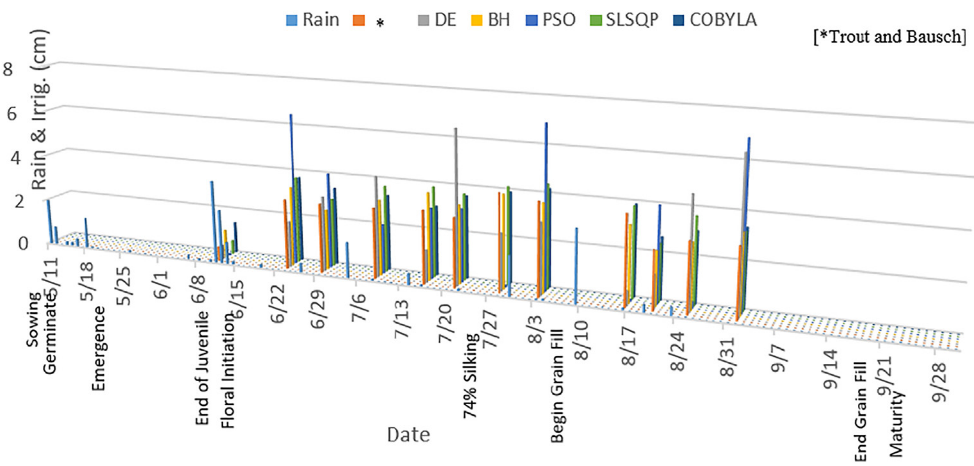

Fig. 4. Rain and applied Irrigation by different methods in cm. (Rainfall after 9/30 not shown to preserve readability).

Table 11
Nitrogen and water Stress (0–1; 0 least stress, 1 most stressed) at various growth stages of maize for different optimization strategy.

		Nitrogen Stress					Water Stress				
Date	Growth Stage	DE	BH	PSO	SLSQP	COBYLA	DE	BH	PSO	SLSQP	COBYLA
5/11	Sowing	0	0	0	0	0	0	0	0	0	0
5/12	Germinate	0	0	0	0	0	0	0	0	0	0
5/22	Emergence	0	0	0	0	0	0	0	0	0	0
6/10	End of Juvenile	0	0	0	0	0	0.1	0.1	0.1	0.1	0.1
6/15	Floral Initiation	0	0	0	0	0	0	0	0	0	0
7/24	75% Silking	0.02	0.04	0.02	0.04	0.03	0	0	0	0	0
8/4	Begin Grain Fill	0.02	0.03	0.02	0.03	0.02	0	0	0	0	0
9/14	End Grain Fill	0.24	0.1	0.23	0.12	0.09	0.02	0.05	0.02	0	0.02
9/17	Maturity	0.6	0.49	0.6	0.52	0.45	0.32	0.59	0.33	0	0.33
10/19	Harvest	0.6	0.49	0.6	0.52	0.45	0.32	0.59	0.33	0	0.33

decisions would be updated as and when new data arrives.

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CRediT authorship contribution statement

Anupam Bhar: Conceptualization, Methodology, Software, Writing - original draft, Investigation, Formal analysis, Visualization. **Ratnesh Kumar:** Project administration, Funding acquisition, Supervision, Writing - review & editing, Validation, Investigation. **Zhiming Qi:** Visualization, Writing - review & editing, Data curation, Validation, Resources. **Robert Malone:** Visualization, Resources, Validation, Writing - review & editing.

Declaration of Competing Interest

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

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