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MoisturEC: A New R Program for Moisture Content Estimation from Electrical Conductivity Data

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Abstract

Noninvasive geophysical estimation of soil moisture has potential to improve understanding of flow in the unsaturated zone for problems involving agricultural management, aquifer recharge, and optimization of landfill design and operations. In principle, several geophysical techniques (e.g., electrical resistivity, electromagnetic induction, and nuclear magnetic resonance) offer insight into soil moisture, but data-analysis tools are needed to “translate” geophysical results into estimates of soil moisture, consistent with (1) the uncertainty of this translation and (2) direct measurements of moisture. Although geostatistical frameworks exist for this purpose, straightforward and user-friendly tools are required to fully capitalize on the potential of geophysical information for soil-moisture estimation. Here, we present MoisturEC, a simple R program with a graphical user interface to convert measurements or images of electrical conductivity (EC) to soil moisture. Input includes EC values, point moisture estimates, and definition of either Archie parameters (based on experimental or literature values) or empirical data of moisture vs. EC. The program produces two- and three-dimensional images of moisture based on available EC and direct measurements of moisture, interpolating between measurement locations using a Tikhonov regularization approach.

Introduction

Geophysical inference of soil moisture is a longstanding problem in hydrogeophysics, with seminal papers

going back several decades (LaBrecque et al. 1992; Sheets and Hendrickx 1995) and a petrophysical basis going back further (e.g., Archie 1942). Whereas conventional measurements of moisture (e.g., time-domain reflectometry, tensiometer, and neutron probe) are invasive and provide only local information at sparse locations, geophysical mapping of soil moisture can provide information noninvasively and over large areas; thus, geophysics offers potential to inform water management for agriculture, aquifer recharge, and landfill operations. A number of geophysical methods have sensitivity to soil moisture, including direct-current electrical resistivity, electromagnetic induction (EMI), nuclear magnetic resonance, ground penetrating radar, seismic, and time-lapse gravity. Here, we focus on the use of electrical conductivity (EC) as a proxy for moisture content (MC). EC can be measured using electrical or EMI methods, which allow for one-, two- or three-dimensional (1D, 2D, or 3D) surveys. We present a new R program, MoisturEC, to facilitate the “translation” of EC to moisture content, fill in gaps

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between measurement locations, and integrate geophysical measurements with direct measurements of EC at sparse locations. Although the petrophysical principles for this translation are well established (Archie 1942; LaBrecque et al. 1992; Binley et al. 2006; Cassiani et al. 2006), the potential of geophysical mapping of MC has not been fully realized for lack of straightforward software tools.

Background

Geophysical Estimation of Electrical Conductivity

Several geophysical methods can be used to estimate EC. Electrical resistivity imaging (ERI) is a technique whereby electrical current is injected into the ground and electrical potential is measured at various points, providing data in the form of apparent resistivities. The measured apparent resistivities can be associated with an approximate position in the subsurface if an electrically homogeneous medium is assumed, which may be a valid assumption for local measurements with small electrode spacings (e.g., Adamchuk et al. 2004; Corwin and Lesch 2005). However, it is often desirable to estimate subsurface EC distributions in electrically heterogeneous conditions where installation of sufficient number local sensors is impractical. In this case, the goal is to estimate EC values based on a limited number of data, which presents a nonlinear problem that requires a nonlinear inversion to solve. EMI operates by inducing eddy currents in conductive bodies that in turn generate magnetic fields that are sensed by a receiving coil. Similar to ERI, the raw data from EMI instruments can only be used to approximate the position of apparent conductivity values within the ground under the assumption that the measurement volume is electrically homogeneous. To provide the EC distribution of the subsurface in electrically heterogeneous conditions, EMI data must undergo an inversion that takes into account electrical heterogeneity.

The nonlinear inversion of ERI or EMI data works by simulating or forward modeling data over conductivity models that are updated through an iterative process until some convergence criterion is achieved—generally by finding a model that fits observed data to the accuracy of the estimated data error. To avoid unrealistic solutions, an additional smoothing constraint is usually enforced in the inversion; this is termed regularization (Tikhonov and Arsenin 1977). Resulting estimates of conductivity are typically smooth in space, decay in resolution with distance from the measurement point, and are subject to imaging artifacts. Given the uncertainty introduced through inversion, it is often appropriate to treat geophysical data as “soft” or even qualitative information (e.g., McKenna and Poeter 1995). Despite these caveats, electrical geophysical methods provide a means for approximating EC distributions in the subsurface at spatial scales (i.e., essentially continuous information over a 3D volume on the scale of meters to kilometers), which are not possible with other instrumentation.

Electrical Conductivity and Moisture Content in the Unsaturated Zone: Archie's Law

Seldom are users of electrical geophysical results interested in EC information alone. In our case, we are interested in using EC information to estimate MC. Archie (1942) established a link between the bulk conductivity of soil, σ_b , and physical properties of the soil:

$$\sigma_b = \sigma_{el} = (\phi_{int})^m S^n \sigma_w, \quad (1)$$

where σ_{el} represents the flow of current through ions in the pore fluid, ϕ_{int} is the interconnected porosity, S is the saturation, σ_w is the conductivity of the pore fluid, m is the “cementation” factor that relates to pore geometry, and n is an exponent describing the variation of conductivity with water saturation. This model considers only current transport through ions in the pore fluid, and neglects current flow pathways along the electrical double layer of mineral surfaces and through the mineral grains themselves. While the latter is likely not a major contribution to the bulk conductivity response for nonmetallic soils, the former (surface conduction) may be important when considerable fractions of negatively charged minerals are present (Friedman 2005), such as in soils with high clay content. Rearranging Archie's Law (Equation 1) to estimate MC, θ , noting that $S = \theta/\phi$, gives:

$$\theta = \phi \left(\frac{\sigma_b}{(\phi_{int})^m \sigma_w} \right)^{1/n}, \quad (2)$$

where ϕ is the total porosity.

Software Implementation

MoisturEC is designed to combine EC information with point moisture data in a joint updating procedure to provide estimates of moisture that capitalize on the spatial coverage of the geophysical data with the accuracy of point sensor information (see flowchart in Figure 1). The software is written in R (R Core Team 2017) and uses the Matrix (Bates and Maechler 2017) and pracma (Borchers 2017) packages for matrix calculations. The primary interface is a graphical user interface (GUI) made with the shiny package (Chang et al. 2017; Figure 2). Mouseover help text is available in the GUI using the shinyBS package (Bailey 2015) and javascript operations are made possible through the shinyjs package (Attali 2017). Plotting is handled using the viridis (Garnier 2017) ggplot2 (Wickham 2009) and plotly (Sievert et al., 2017) packages.

Inputs and Key Parameters

Figure 2a shows input files and parameters for MoisturEC. Data input consists of point moisture and EC data. Point moisture data are estimates of MC at defined locations within the study area, whereas EC data are electrical conductivities. Both point moisture and EC information are uploaded via Comma Separated Values (.CSV) files containing coordinate information, data values, and percent error in five columns, where EC

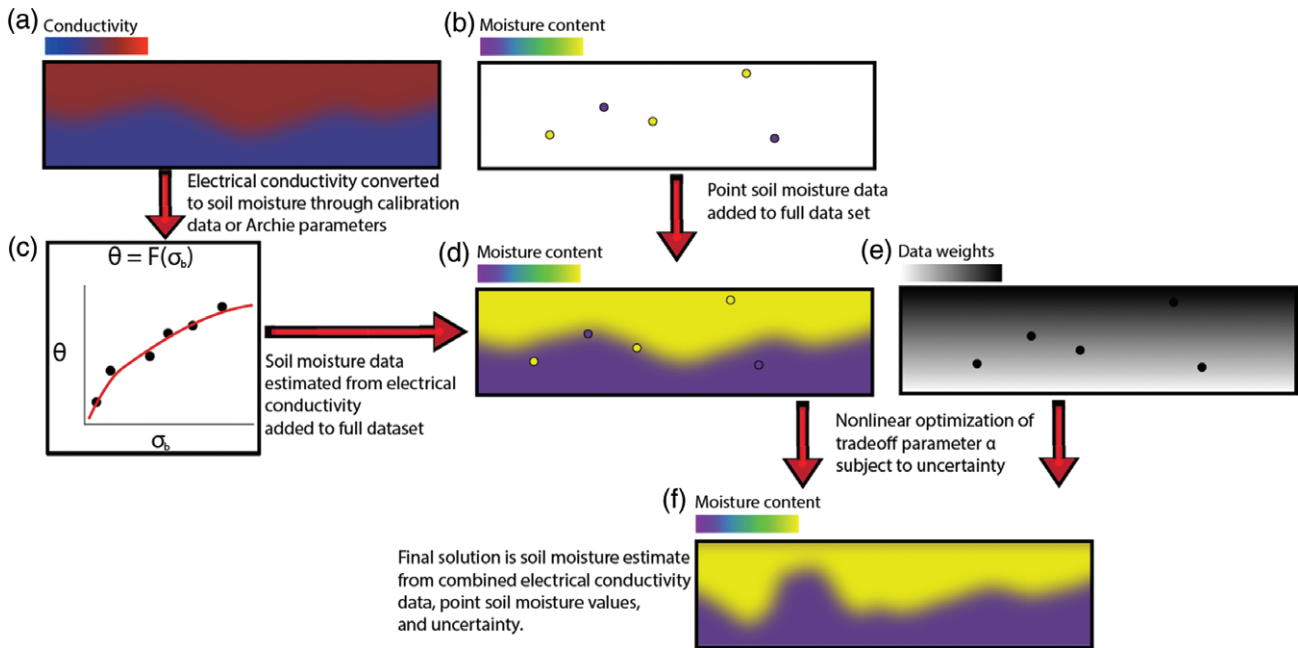


Figure 1. MoisturEC flowchart: (a) Electrical conductivity data and (b) moisture content values are input to the program. (c) A petrophysical transform function converts electrical conductivity data to (d) moisture. (e) Data are weighted based on user inputs and an optional resolution matrix. (f) The final moisture estimate uses all data and errors to estimate an optimal tradeoff between data fit and smoothing.

data are in S/m and volumetric water content (VWC) are fractional values. Note that in the case of EC data, the true error in EC values is both a function of the original data errors as well as those introduced through inversion. Therefore, an optional input of resolution, calculated for example, from the diagonal elements of a resolution matrix, can also be input to MoisturEC. The values of resolution should range from 0 to 1 and are used to scale the data errors (e). For example, a value of σ_b of 1 S/m with a data error of 10% that corresponds to a resolution value of 0.5, the error in σ_b is scaled as $0.1/0.5 = 0.2$ S/m. This error, along with errors in the other Archie parameters specified by the user, is carried through the estimation by the standard rules of error propagation (Farrance and Frenkel 2012).

Petrophysical Transform: EC to MC

In practice, detailed information on most of the parameters in Equation 2 is limited or absent, and it is often necessary to assume a fixed value or a range of values for these parameters. A simpler approach can be used if a relationship between θ and σ_b has been established, as through a wetting experiment in the laboratory using a soil sample from the site of interest. In this case, we can group terms such that:

$$x = \left(\frac{\phi}{(\phi_{\text{int}})^m \sigma_w} \right)^{1/n}$$

and therefore,

$$\theta = x \sigma_b^{1/n} \quad (3)$$

which is the power-law relation that can be solved for through log transformation of the variables:

$$\ln(\theta) = \ln(x) + \frac{\ln(\sigma_b)}{n}. \quad (4)$$

By default, MoisturEC uses Archie parameters and their associated uncertainties to convert EC to MC by Equation 2. Upon user upload of a .CSV calibration file containing σ_b and θ values, MoisturEC estimates the parameters x and n in Equation 4 through a linear regression, which are then used to estimate moisture from EC data. A third option allows the user to perform Equation 4 regression using actual point moisture data and the nearest EC values.

Model Parameterization: Grid Definition

Options exist to define the number of grid nodes in the x , y , and z directions (parameters n_x , n_y , and n_z). Alternatively, a grid is automatically defined in MoisturEC given a maximum number of grid nodes (maxgrid). In this case, the grid spacing in x , y , and z is determined by either bounds defined by the user or by the extent of the data (x_{min} , x_{max} , y_{min} , y_{max} , z_{min} , and z_{max}).

Data Inversion

MC at grid nodes, $\mathbf{m}$, are estimated through a linear solution of the equation:

$$\left[\mathbf{J}^T \mathbf{C}_D^{-1} \mathbf{J} + \alpha \mathbf{D}^T \mathbf{D} \right] \mathbf{m} = \mathbf{J}^T \mathbf{C}_D^{-1} \mathbf{d}, \quad (5)$$

MoisturEC

Inputs Outputs Console Messages

Data files

EC Data File ?

Browse... mEC_soft_small.csv
Upload complete

Moisture Data File ?

Browse... mEC_hard_small.csv
Upload complete

Resolution Data File (optional) ?

Browse... mEC_R_small.csv
Upload complete

Calibration Data File (optional) ?

Browse... mec_calib.csv
Upload complete

use data use Archie's Law

Grid Parameters

maxgrid: 1000

nx: NA ny: NA nz: NA

xmin: NA xmax: NA

ymin: NA ymax: NA

zmin: NA zmax: NA

Archie parameters

σ_w	$\delta\sigma_w$
0.5	0
ϕ	$\delta\phi$
0.3	0
ϕ_{int}	$\delta\phi_{int}$
0.2	0
m	δm
2	0
n	δn
2	0

Inversion

calculate moisture

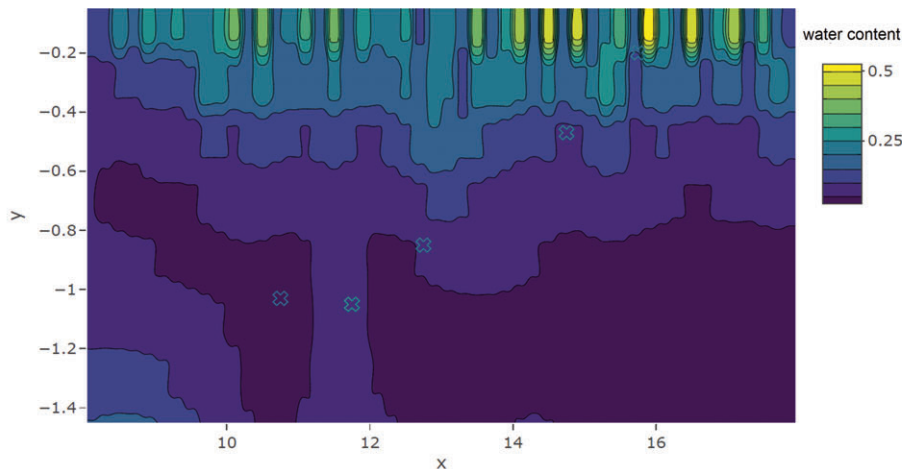


Figure 2. MoisturEC GUI showing (a) input file upload, grid parameters, Archie (petrophysical) parameters and (b) plot of the input data—EC data form the background contour plot while point moisture data are shown as crosses.

where $\mathbf{d}$ are the data (combined point moisture and EC-derived estimates of MC), $\mathbf{J}$ is the Jacobian matrix (in this case $\mathbf{J}$ consists of ones in the rows and columns that correspond to the nearest grid point where data are available; elsewhere zero), $\mathbf{C}_D$ is the diagonal covariance matrix that consists of the measurement error variances $\mathbf{e}$ (and $\mathbf{C}_D^{-1}$ are the data weights), $\mathbf{D}$ is the regularization matrix consisting of a first derivative finite-difference filter between adjacent model elements, and α is the tradeoff term that controls the balance between regularization criteria and data misfit. Larger values for α promote an

increasingly flat solution. In MoisturEC, selection of an appropriate α value is established through an automated method, described in the next section. Although the choice of $\mathbf{D}$ is commonly subjective, the use of the first-derivative here maximizes flatness, as opposed to, for example, the second derivative, which maximizes smoothness. Flatness criteria ensure non-negative results if the data are non-negative, whereas smoothness does not and instead allow results outside the bounds of the data. In the context of moisture estimation, our choice of $\mathbf{D}$ helps to ensure physically plausible results.

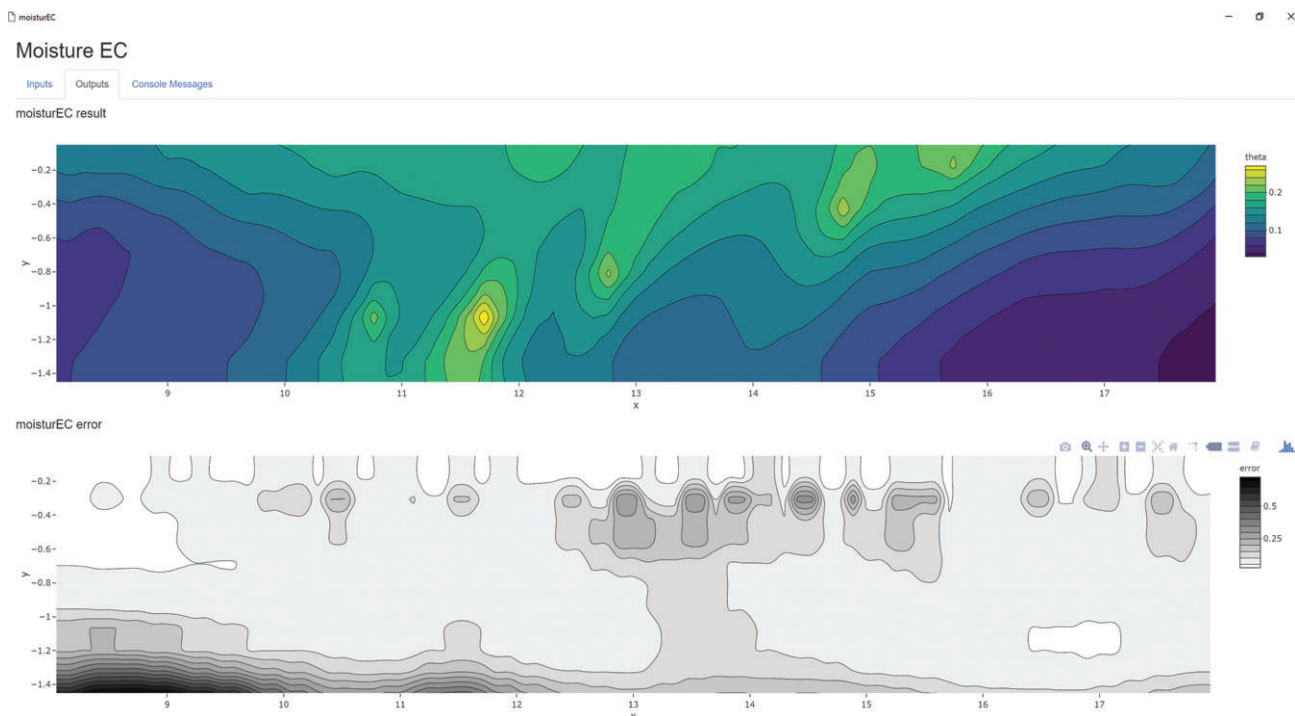


Figure 3. MoisturEC GUI 2D moisture estimate and propagated error, expressed in terms of moisture content.

Optimization of the Tradeoff Parameter α

An initial estimate of $\alpha = 1$ is used in MoisturEC, indicating equal weight given to honoring data values and flatness between model nodes. The solution seeks an optimum value for α by repeatedly solving Equation 5 for $\mathbf{m}$; simulated data values $\hat{\mathbf{d}}$ are generated by selecting the value from the closest model cell. A value for α is achieved through a golden-section search and successive parabolic interpolation (**optimize** function in R) to minimize an objective function, Φ :

$$\Phi = (\chi^2 - 1)^2 \quad (6)$$

which is informed by a chi-squared statistic, χ^2 :

$$\chi^2 = \sqrt{\frac{\sum_{i=1}^{n_{\text{data}}} \left[\frac{(d_i - \hat{d}_i)^2}{e_i^2} \right]}{n_{\text{data}}}}, \quad (7)$$

where e_i values are the propagated errors for each EC-derived and point moisture measurement. Thus, a solution is achieved when data misfit values are in the order of the data errors.

Outputs

Final moisture estimates from MoisturEC are displayed as either 2D or 3D plot (Figure 3). Additionally, moisture estimates are output as text files as well as visualization toolkit (.VTK) files for use with the Paraview visualization software (for more information on this file format, see Schroeder et al. 2006). Point moisture data, EC data, and uncertainty are also output as .VTK files to aid visualization.

Examples

Example 1: 3D Moisture Bulb Model

A block of soil (20 m $\times$ 19 m $\times$ 10 m) was modeled having a background soil moisture of 0.071 and a wet zone with a soil moisture of 0.22 (Figure 4a). These values were converted to bulk EC through Archie's law assuming the following soil properties: $\sigma_w = 2$ S/m, $\varphi = 0.3$, $\varphi_{\text{int}} = 0.3$, $m = 2$, and $n = 2$. Horizontal coplanar frequency domain EMI data were simulated using the 1D forward modeling functions available in frequency-domain electromagnetic inversion code (FEMIC, Elwaseif et al. 2016) for seven frequencies ranging from 1530 to 93,090 Hz. Data were generated assuming a 1-m instrument elevation over a 1-m grid on the surface of the soil block. Gaussian errors of 5% were added to the resulting quadrature values.

To generate EC data for MoisturEC, quadrature data were inverted for EC in EM1DFM (Farquharson et al. 2003) assuming a fixed α tradeoff (Farquharson and Oldenburg 2000), data errors of 5%, and using a 20-layer, 10-m deep model. Point moisture data were taken from the true moisture values at 12 equally spaced points in and out of the wet zone and adding Gaussian errors of 1%.

Results from the 3D Moisture Bulb Model

The results of the MoisturEC inversion of the 3D synthetic experiment are shown in Figure 4, plotted in Paraview (Ayachit 2015) from the .VTK file output of MoisturEC. While data from EMI provide spatial coverage of the moisture bulb shown in Figure 4a, results from this inversion show limited resolution of the feature with depth (Figure 4b). Additional uncertainty

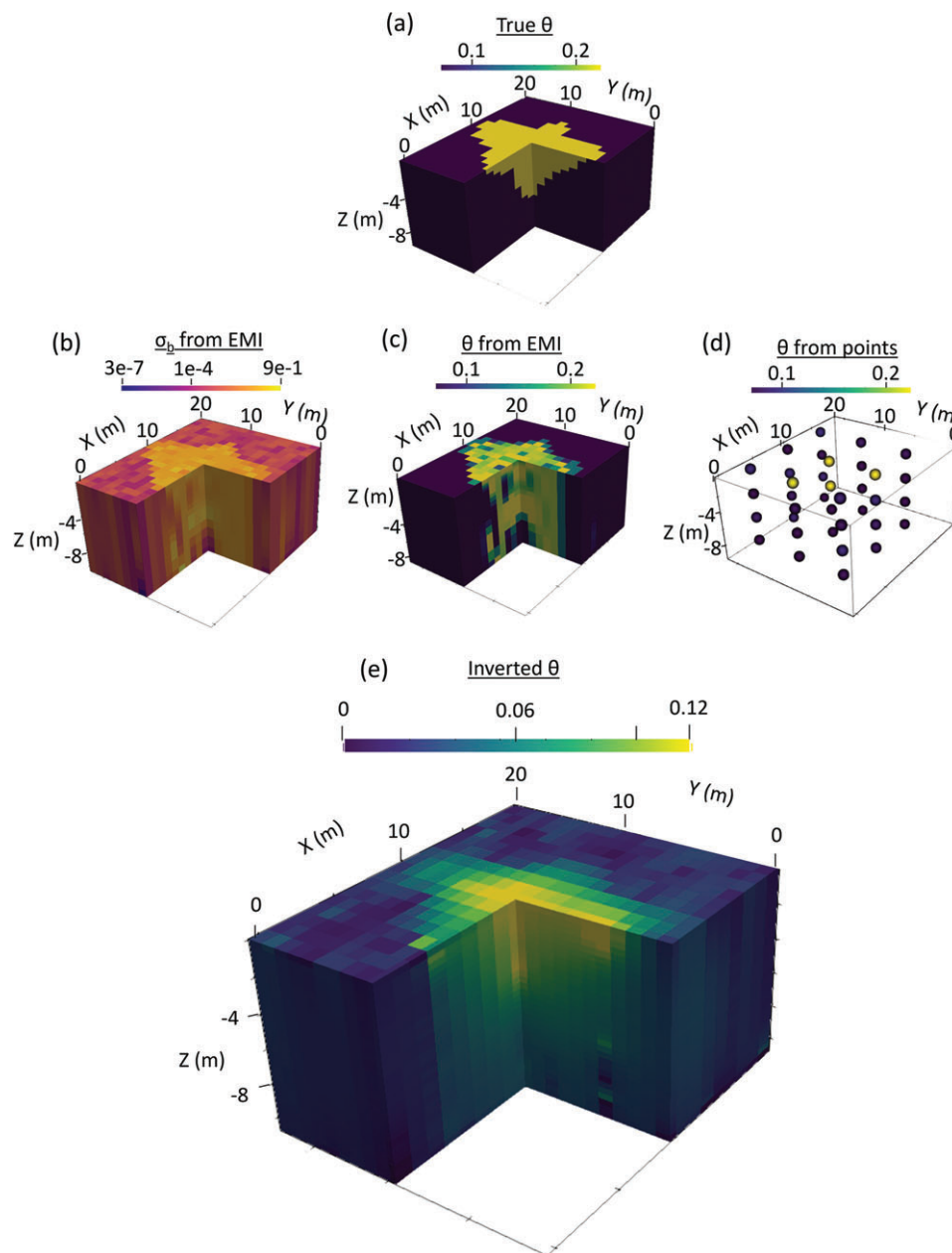


Figure 4. Synthetic 3D example: (a) true moisture model; (b) inverted electromagnetic induction data collected over true moisture model; (c) moisture estimate based on electrical conductivity using an Archie parameterization; (d) point moisture data locations and values; (e) resulting moisture estimate from MoisturEC.

is introduced from conversion of the EC feature to MC (Figure 4c). Moisture estimates at selected locations (Figure 4d) provide reliable information on moisture, but do not give adequate spatial coverage to define the wet feature. MoisturEC combines these two datasets into a common framework to estimate moisture that honors the respective uncertainty in each of the methods, and produces the result shown in Figure 4e. While the moisture feature is blurred compared to that shown in Figure 4a, there is a noticeable improvement in the delineation of the boundary of the feature compared to estimates from EC alone (Figure 4c), and improved spatial resolution compared to point moisture information (Figure 4d).

Example 2: 2D Irrigation Experiment

To demonstrate the use of MoisturEC using field data, we present data from an irrigation experiment that took place during June 2017. The site consists of a small apple orchard in Coventry, Connecticut. Soil survey data from SoilWeb (Soil Survey Staff 2017) classifies the area as belonging to the Woodbridge series; a moderately drained fine sand/loamy soil with rock fragments ranging from 0 to 35%. Although quantitative analysis of soil cores was not performed for this study, this description matches qualitative attributes of the soil gathered from the surface and boreholes at the site. The series description further indicates a depth to densic materials at 0.5 to 1.0 m. This is consistent with our inability to drill much

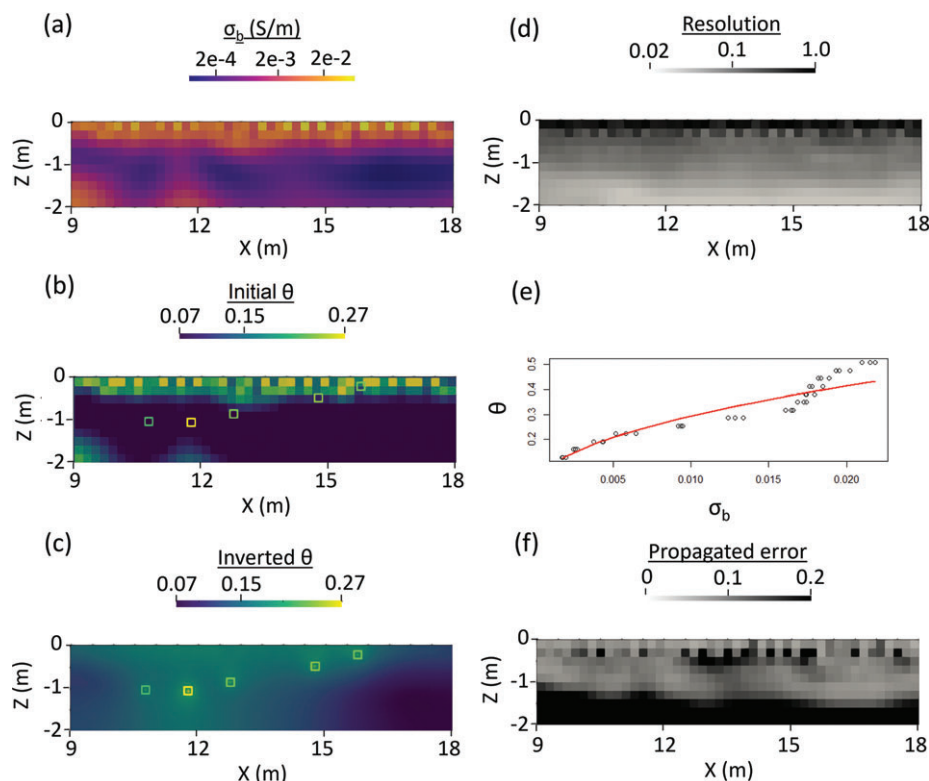


Figure 5. Field 2D example: (a) electrical conductivity estimates from inversion of electrical resistivity data; (b) initial moisture estimates from electrical conductivity data computed through petrophysical transformation combined overlain with in situ point moisture data (shown as colored squares); (c) resulting MoisturEC moisture estimate; (d) resolution matrix used to scale data weights; (e) petrophysical transform function computed through laboratory calibration; (f) propagated uncertainty in the moisture estimates.

below 1.0 m while installing borehole instrumentation. Separately collected passive seismic measurements indicated a bedrock interface at approximately 5 m depth.

Briefly, the experiment consisted of 5TE soil-moisture probes (Decagon Devices, Pullman, WA) connected to an EM50 logger (Decagon Devices) and installed at five different locations at 0.20-, 0.47-, 0.85-, 1.03-, and 1.05-m depths). Prior to data collection, the probes were calibrated using the homogenous soil method, wherein surface soil samples were gathered and mixed, allowed to dry, then gradually wetted to provide a raw instrument reading vs. water content calibration curve. Details of this procedure can be found in (Starr and Paltineanu 2002). The probes were installed by attaching them to plastic poles and inserting the tips of the probes into the bottom of power-augered holes that were backfilled and allowed to settle for 1 week after installation. The probes were located along a linear transect with 1-m spacing between them. The 5TE probes collected data at 2-min intervals and were calibrated prior to the experiment. The area was allowed to dry then subjected to watering by a sprinkler for approximately 2 days. Dipole-dipole and Wenner electrical resistivity measurements were collected four times during the experiment using a 56 electrode SuperSting R8 (AGI Instruments, Austin, TX) at 0.5-m electrode spacing along a line above the soil moisture (5TE) probes.

We present an example using MoisturEC to estimate soil moisture for the electrical resistivity dataset collected 12 h after infiltration began. Point moisture data consist of the average soil moisture probe values measured during each electrical resistivity data collection (approximately 1 h). Estimated uncertainty from these probes is 1% given a custom calibration.

EC data consist of the inverted electrical resistivity data (Figure 5a). Electrical resistivity data were inverted using R2 (Andrew Binley, Lancaster University) assuming a 5% data error assessed through reciprocal measurements gathered during collection. A resolution matrix was computed during the inversion, and the diagonal elements (Figure 5d) were used in weighting the estimated EC to produce moisture estimates in MoisturEC (Figure 5c).

To form the relationship between soil moisture and EC at this site, an additional experiment was performed. Soil was collected from the site and oven dried for 2 days at 160 °C. A known volume of the soil was then taken, weighed, and placed in a test box (size = 0.22 m × 0.04 m × 0.03 m) outfitted with electrodes to measure the resistivity of the sample. A known volume of water was then added to the soil sample and weight and EC were recorded. This process was repeated until the sample reached saturation. The EC and soil moisture values from this experiment were recorded to a .CSV file for input to MoisturEC.

We note that oven drying, mixing, and repacking before calibration measurements may disrupt soil structure and introduce some uncertainty into this calibration. Nevertheless, we felt this method was appropriate to sample the full range of VWC values starting from a minimum VWC.

Results from the 2D Irrigation Experiment

The empirical calibration function used to convert EC data to MC is shown in Figure 5e. This relationship was applied to the inverted EC data shown in Figure 5a to produce moisture estimates shown in Figure 5b. Moisture information from the moisture probes at the time of the resistivity measurement is shown as colored squares in Figure 5b as well. It is evident that there is not a strong agreement between the point moisture and EC data below 0.5 m depth as shown in Figure 5b, potentially due to limited resolution of the resistivity method at these depths. The diagonal of the resolution matrix (Figure 5d) was therefore used to modify the weights of the EC-derived moisture values, effectively decreasing the weight given to model elements distant from the electrodes. The final moisture estimate produced by MoisturEC (Figure 5c) is therefore quite blurred, as the tradeoff parameter α is larger than 1, favoring smoothing over data fit in the final solution. This final solution reconciles the disagreement between point moisture and EC estimates of MC and reflects the relative errors estimated for each data input. The high degree of certainty in the point moisture estimates (input as errors of 1%) has the effect of giving these values dominance in the final result over the EC-derived moisture estimates in the same regions. Where point moisture information is absent, the EC-derived moisture values dictate the result. Finally, an image of the estimated uncertainty in MC is shown in Figure 5f, reflecting uncertainty propagated from both measurements.

Conclusions

Geophysical methods have enormous potential to improve the mapping of soil moisture and thereby enhance hydrologic investigations in support of agriculture, aquifer management, and landfill operations. Here, we presented MoisturEC, a straightforward computer program written in R, for integrating electrical or electromagnetic measurements of EC and direct measurements of MC, using petrophysics and regularization-based interpolation. The program operates in 2D or 3D, weighting geophysical data relative to direct information based on measurement errors while minimizing the roughness of the moisture field, quantified by a first derivative spatial filter. The code supports several options for conversion of EC to moisture, including the use of Archie's Law and an empirical power-law relation. These approaches assume relations described by homogenous parameters, which may limit the utility of MoisturEC in highly heterogeneous settings, where, for example, porosity or cementation exponent may vary substantially in space. The code and example datasets are

available from <https://water.usgs.gov/ogw/bgas/moisturec>, Terry and Day-Lewis (2018), and Terry et al. (2017).

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Authors' Note

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