Probabilistic petrophysical reconstruction of Danta's Alpine peatland via electromagnetic induction data

N Zaru¹, S Silvestri², M Assiri³, P Bai⁴, T M Hansen⁵, and Giulio Vignoli^{1,6}

¹DICAAR, University of Cagliari ²Department of Biological, Geological, and Environmental Sciences, University of Bologna ³TESAF, University of Padua ⁴SINOPEC Geophysical Research Institute Co. Ltd ⁵Department of Geoscience, Aarhus University ⁶Near Surface Land and Marine Geology Department, GEUS

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Abstract

Peatlands are fundamental deposits of organic carbon. Thus, their protection is of crucial importance to avoid emissions from their degradation. Peat is a mixture of organic soil that originates from the accumulation of wetland plants under continuous or cyclical anaerobic conditions for long periods. Hence, a precise quantification of peat deposits is extremely important; for that, remote- and proximal-sensing techniques are excellent candidates. Unfortunately, remote-sensing can provide information only on the few shallowest centimeters, whereas peatlands often extend to several meters in depth. In addition, peatlands are usually characterized by difficult (flooded) terrains. So, frequency-domain electromagnetic instruments, as they are compact and contactless, seem to be the ideal solution for the quantitative assessment of the extension and geometry of peatlands. Generally, electromagnetic methods are used to infer the electrical resistivity of the subsurface. In turn, the resistivity distribution can, in principle, be interpreted to infer the morphology of the peatland. Here, to some extent, we show how to shortcut the process and include the expectation and uncertainty regarding the peat resistivity directly into a probabilistic inversion workflow. The present approach allows for retrieving what really matters: the spatial distribution of the probabilistic approach, we compare the outcomes against the more traditional deterministic fully nonlinear (Occam's) inversion and against some boreholes available in the investigated area.

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4	¹ DICAAR, University of Cagliari, Cagliari, Italy.		
5 6	² Department of Biological, Geological, and Environmental Sciences, University of Bologna, Ravenna, Italy.		
7	³ TESAF, University of Padua, Padua, Italy.		
8	⁴ SINOPEC Geophysical Research Institute Co. Ltd., Nanjing, China.		
9	⁵ Department of Geoscience, Aarhus University, Aarhus, Denmark.		
10	⁶ Near Surface Land and Marine Geology Department, GEUS, Aarhus, Denmark.		
11	Corresponding author: Giulio Vignoli (gvignoli@unica.it); ORCID: 0000-0002-3437-5826		
12	Key Points:		
13 14	• Electromagnetic data can be inverted directly for the probability of peat and clay occurrence.		
15 16	• The 3D geometry and volume of Alpine peatlands were determined via a fast, proximal- sensing, geophysical method and verified against boreholes.		
17 18	• Probabilistic approaches to geophysical inversion can incorporate complex prior information and, contextually, assess result uncertainties.		

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20 Abstract

Peatlands are fundamental deposits of organic carbon. Thus, their protection is of crucial 21 importance to avoid emissions from their degradation. Peat is a mixture of organic soil that 22 originates from the accumulation of wetland plants under continuous or cyclical anaerobic 23 conditions for long periods. Hence, a precise quantification of peat deposits is extremely 24 25 important; for that, remote- and proximal-sensing techniques are excellent candidates. Unfortunately, remote-sensing can provide information only on the few shallowest centimeters, 26 whereas peatlands often extend to several meters in depth. In addition, peatlands are usually 27 characterized by difficult (flooded) terrains. So, frequency-domain electromagnetic instruments, 28 29 as they are compact and contactless, seem to be the ideal solution for the quantitative assessment of the extension and geometry of peatlands. Generally, electromagnetic methods are used to infer 30 the electrical resistivity of the subsurface. In turn, the resistivity distribution can, in principle, be 31 interpreted to infer the morphology of the peatland. Here, to some extent, we show how to 32 shortcut the process and include the expectation and uncertainty regarding the peat resistivity 33 directly into a probabilistic inversion workflow. The present approach allows for retrieving what 34 really matters: the spatial distribution of the probability of peat occurrence, rather than the mere 35 electrical resistivity. To evaluate the efficiency and effectiveness of the proposed probabilistic 36 approach, we compare the outcomes against the more traditional deterministic fully nonlinear 37 38 (Occam's) inversion and against some boreholes available in the investigated area.

39 Plain Language Summary

40 Wetlands are carbon pools subtracting carbon dioxide from the atmosphere and accumulating it underground. The processes ongoing in these ecosystems form a dark soil, 41 extremely rich in organic matter, known as "peat". Globally, peatlands are responsible for storing 42 almost as much carbon as the atmosphere. For that reason and to preserve them, it is very 43 important to develop tools capable of mapping peatlands. A good candidate for this goal is a 44 geophysical method based on the diffusion of electromagnetic signals into the ground. How the 45 electromagnetic signals propagate depends on the electrical resistivity of the subsurface. So, by 46 studying those signals, we can think of reconstructing, point-by-point, the electrical resistivity 47 48 variability in the subsurface. Broadly speaking, different resistivities correspond to different sediments. So, in turn, we can use the reconstructed resistivity distribution to map the peat 49 deposits. In this study, we show how to translate directly the electromagnetic signal into the 50 probability of finding peat (rather than in recovering the electrical property of the subsurface). 51 We tested our approach on a dataset collected across an Alpine peatland in Italy and we verified 52 our results against direct investigations and against more traditional ways to interpret the 53 54 geophysical signals.

55 **1 Introduction**

Peatlands are important carbon reservoirs, and some of them are located in mountain 56 57 settings for which efficient and reliable methodologies for the detection of their geometry, bottom morphology, and volumes are still lacking (Silvesti et al., 2019a; Trappe & Kneisel, 58 2019; Pezdir et al., 2021). Here, we explore the use of ground-based frequency-domain 59 electromagnetic induction (FDEM) technology to quantify peat thickness and extension in a bog 60 located in the Italian Dolomites in which peat overlays electrically conductive clay substrate. 61 Electrical resistivity is the main physical property retrieved via the inversion of the FDEM 62 63 measurements (Guillemoteau et al., 2016; Guillemoteau et al., 2019). Unfortunately, per se, this

64 physical property of the investigated medium is of little importance to map peatlands. Instead, a 65 direct estimation of the probability of the occurrence of peat or clay would be preferable. In this 66 paper, such probability is inferred by means of a probabilistic petrophysical inversion of the 67 geophysical measurements (Bosch et al., 2010; Grana et al., 2022a; Guo et al., 2023).

Probably, the first attempts to include petrophysical relationships into probabilistic 68 69 inversion frameworks date back to the beginning of the 21st century, when such schemes were proposed for the uncertainty assessment of the spatial distribution of physical properties in 70 seismic reservoir characterizations (Malinverno & Briggs, 2004; Connolly and Kemper, 2007). 71 Since then, they gained increasing interest over the years (Hansen et al., 2012; Zunino et al., 72 2015). In fact - in addition to directly retrieving the crucial lithological information, rather than 73 merely the physical property - probabilistic petrophysical inversion has the intrinsic advantage of 74 providing an estimation of the uncertainty associated with the results, which is often missing in 75 traditional predictions (e.g., of the electrical resistivity) via deterministic inversions (McLachlan 76 et al., 2021a). Moreover, the proposed probabilistic approach allows for the formalization of 77 quite complex prior information (Bai et al., 2021). This is a further advantage with respect to 78 more standard deterministic schemes in which the ill-posedness of the problem is tackled via the 79 introduction of a regularizing term, which is often capable of formalizing/enforcing (too) simple 80 information/constraints related to the presence of smooth/sharp transitions between different 81 lithologies (Klose et al., 2022; Klose et al., 2023). 82

In the last decades, several ground geophysical methods have been effective in detecting 83 and characterizing peat deposits, both laterally and in-depth. Ground penetrating radar (GPR) has 84 been proven reliable and precise in inferring the deposit thickness (Warner et al., 1990; Comas et 85 al., 2015). Electrical resistivity tomography has also been found successful (Elijah et al., 2012), 86 especially, when used to reconstruct the variations of chargeability associated with the presence 87 of peat (Slater & Reeve, 2002; Comas & Slater, 2004). However, in general, the above-88 mentioned geophysical methodologies can be applied to relatively small areas and are extremely 89 90 difficult to perform in flooded environments like wetlands/peatlands (Zaru et al., 2023). In this respect, FDEM presents several advantages as it does not require any direct coupling with the 91 surface. In fact, several FDEM systems are specifically designed to be operated while mounted 92 on helicopters (Yin & Hodges, 2007; Karshakov et al., 2017) and, probably, soon, on drones 93 94 (Mitsuhata et al., 2022).

95 Due to measurement and modelling errors, and because of the band-limited observations and finite amount of data points (Qiu et al., 2020), retrieving the spatial distribution of electrical 96 resistivity from the FDEM observations requires solving an ill-posed problem (Tarantola, 2005). 97 98 In both deterministic and probabilistic inversion approaches, the ill-posedness is addressed by making use of the available prior information. In the deterministic approaches, such prior 99 information is formalized via the regularization term (Zhdanov, 2002). Traditionally, the L2-100 norm of the spatial gradient of the model parameters is the most common choice for the 101 regularization term (implementing the so-called Occam's inversion – Constable et al., 1987). 102 Hence, in the case of the L2-norm of the gradient, the unique and stable solution of the 103 regularized inversion is selected to be the smoothest possible model that also fits the data within 104 the noise level assumed for the measurements. In fact, the inverse problem is reduced to the 105 minimization of an objective functional consisting of the weighted sum of the regularization term 106 (the regularizer or stabilizer) and the data misfit. The weight between the two terms (generally, 107 indicated with the letter λ and sometimes named Tikhonov's parameter) is selected to ensure 108

adequate matching between observed and calculated responses while minimizing the regularizer

- 110 (Zhdanov et al. 2006). In many cases, the geological targets to reconstruct are expected not to be
- smooth; in such cases, the L2-norm of the model gradient should not be used, and more
- appropriate information (i.e., more consistent with the prior geological expectations) must be included in the objective functional. In this respect, for example, recently, several regularizers
- based on the minimum support of the model are gaining popularity (Vignoli et al., 2015; Rossi et
- al., 2022; Guillemoteau et al., 2022). In the case of the minimum gradient support regularization,
- the inversion algorithm searches for the model with the minimum number of significant
- 117 variations of the physical parameters (and not for the model with the minimum variation). Thus,
- 118 the minimum gradient support favors the retrieval of sharp boundaries between the geological
- 119 structures (Vignoli et al., 2021).

However, the regularization terms need to meet some (mathematical) requirements: not 120 all functional can be regularizers able to transform an ill-posed problem into a conditionally 121 well-posed one (Portniaguine & Zhdanov, 1999). Furthermore, formalizing complex (and 122 realistic) prior information through a set of functionals might be troublesome (if not impossible). 123 In this respect, probabilistic approaches have indubitable advantages: prior information can be 124 described and incorporated into the inversion via the prior distribution, which, in turn, can be 125 defined by its samples (Hansen & Minsley, 2019; Hansen, 2021a). This leads to the possibility of 126 creating the samples in accordance with quite arbitrary expectations about the investigated 127 geology (Bai et al., 2021; Zaru et al., 2023), without the limitations connected to the necessity of 128 formalizing that information in terms of a functional to be minimized. 129

Another crucial advantage of probabilistic approaches consists in their capability to 130 provide an estimation of the result uncertainty in a very natural way. The posterior probability 131 distribution is the solution of probabilistic inverse problems, and it is typically represented as an 132 ensemble of models (realizations of the posterior probability distribution) conditioned on the 133 data. This is different from the solution of deterministic inversions which consists of the unique 134 135 model minimizing the objective functional. Hence, in the probabilistic framework, for example, from the final ensemble of models, the uncertainty of a specific feature can be readily extracted 136 by simply counting the relative occurrence of that feature (Mosegaard & Tarantola, 1995; 137 Mosegaard & Sambridge, 2002; Tarantola, 2005; Minsley, 2011; Høyer et al., 2017; Hansen, 138 139 2021b).

The above-mentioned inversion strategies are generally used to image the geophysical 140 property distribution (in most of the FDEM methods, that is limited to the electrical resistivity of 141 the subsurface). However, the estimation of petrophysical properties - such as porosity, lithology, 142 143 and fluid saturations - can be formulated as an inverse problem. In this case, they are usually referred to as petrophysical inversions (in seismic exploration, they are sometimes also known as 144 rock-physics inversion - e.g., Grana et al., 2022b). In the deterministic frameworks, a physical 145 relationship mapping the rock properties to the geophysical parameters is often necessary 146 (Mastrocicco et al., 2010; Foged et al., 2014; Cao et al., 2023). Instead, in the probabilistic 147 context, like the one used in the present research, the connection between lithology and physical 148 properties is formulated in statistical terms and inherently incorporates the associated 149 uncertainties (here, the uncertainty is not the one characterizing the geophysical measurements, 150 but, rather the one associated with the petrophysical link) (Grana & Della Rossa, 2010; Grana, 151 2016; Grana, 2020; Bai, 2022; Madsen et al., 2023). 152

Thus, in the present work, we test a probabilistic petrophysical inversion on an FDEM dataset originally collected for the characterization of an Alpine peatland. We assess the performance of the proposed inversion scheme at the locations of the several available boreholes

156 (not used to constrain the inversion) and by comparing the obtained results against more

157 traditional deterministic Occam's inversions.

158 2 Materials and Methods

The forward modelling tools used in electromagnetic inverse problems are, nowadays, 159 fully nonlinear and, despite 3D forward options could be available (Cox et al., 2012; Oldenburg 160 et al., 2020), the use of 1D approximations is still the standard in the industry and in the 161 academia (Viezzoli et al., 2008; Ley-Cooper et al., 2015; Dzikunoo et al., 2020; Bai et al. 2020; 162 Hansen & Finlay, 2022). The reason is mainly related to the computational costs of 3D 163 modelling (Guillemoteau et al., 2017; Cai et al., 2022; Kara & Farquharson, 2023). In the present 164 165 research, we make use of the fully non-linear 1D forward modelling discussed, for example, in Elwaseif et al., 2017. Given a sequence of layers with known electrical, homogeneous properties 166 - represented by the model \mathbf{m} - the 1D forward modelling $F(\mathbf{m})$ maps the resistivity (the sole 167 electrical property we are investigating) distribution into the observed FDEM response collected 168 169 at the surface (described by **d**):

170

$$\mathbf{d} = F(\mathbf{m}). \tag{1}$$

The goal of probabilistic formulations is to infer the posterior probability density (PDF) function, $p(\mathbf{m}|\mathbf{d}^{\text{obs}})$, measuring the probability of the model **m** being compatible with the observations \mathbf{d}^{obs} . According to Bayes' theorem, $p(\mathbf{m}|\mathbf{d}^{\text{obs}})$ is proportional to the product of the prior probability density function of the model parameters $p(\mathbf{m})$ and the conditional probability density function $p(\mathbf{d}^{\text{obs}}|\mathbf{m})$. Thus, $p(\mathbf{m}|\mathbf{d}^{\text{obs}}) \propto p(\mathbf{d}^{\text{obs}}|\mathbf{m})p(\mathbf{m})$, with $p(\mathbf{d}^{\text{obs}}|\mathbf{m})$ connecting the measured data and the model parameters. In the specific case of normally distributed noise in the measurements, the conditional probability can be written as

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$$p(\mathbf{d}^{\text{obs}}|\mathbf{m}) = k_{\text{d}} \exp\left(-\frac{1}{2}\left(\mathbf{d}^{\text{obs}} - F(\mathbf{m})\right)^T \mathbf{C}_{\text{d}}^{-1}\left(\mathbf{d}^{\text{obs}} - F(\mathbf{m})\right)\right), \quad (2)$$

where: (i) k_d is simply a normalization factor and (ii) C_d is a matrix taking into account 179 180 the correlated Gaussian data noise. Here, we assume the noise to be uncertain and, consistently, consider diag $(\sigma_d)^{-2} = C_d^{-1}$ in which the *i*-th component of the vector σ_d is the standard 181 deviation of the *i*-th data component. In our specific case, $[\sigma_d]_i$ is the standard deviation of the 182 quadrature component of the ratio between the induced and the primary fields associated with the 183 *i*-th frequency. In fact, during FDEM surveys, the measurements consist of the real and 184 imaginary parts of the ratio between the secondary (interacting with the subsurface) and the 185 primary field (generated by the source). Here, we limit our analysis to the imaginary part (the 186 quadrature component) since it is the one mostly sensitive to the electrical resistivity, whereas 187 the real (in-phase) component is mainly related to the magnetic susceptibility of the investigated 188 medium (Hendrickx et al., 2002). 189

Assuming a Gaussian distribution also for the model parameters, the prior information about the model **m** can be formalized as follows:

192
$$p(\mathbf{m}) = k_m \exp\left(-\frac{1}{2}(\mathbf{m} - \mathbf{m}_0)^T \mathbf{C}_{\mathbf{m}}^{-1}(\mathbf{m} - \mathbf{m}_0)\right), \qquad (3)$$

- 193 with: (i) k_m being another normalization factor and (ii) the Gaussian being centered on 194 the reference model \mathbf{m}_0 .
- 195 When Gaussian distributions are assumed both for the data noise (with Gaussian
- uncertainties described by the covariance operator \mathbf{C}_{d}) and the model parameters (with prior
- 197 information on \mathbf{m} described by the a priori reference model \mathbf{m}_0 with the associated uncertainty
- represented by the covariance operator \mathbf{C}_{m}), the maximization of the probability $p(\mathbf{m}|\mathbf{d}^{obs})$

199 corresponds to the minimization of the regularized inversion objective functional $\left\| \mathbf{C}_{d}^{-\frac{1}{2}} \left(\mathbf{d}^{obs} - \mathbf{C}_{d}^{-\frac{1}{2}} \right) \right\|$

200 $F(\mathbf{m}) \Big\|_{L_2}^2 + \Big\| \mathbf{C}_{\mathbf{m}}^{-\frac{1}{2}}(\mathbf{m} - \mathbf{m}_0) \Big\|_{L_2}^2$. This is a well-known result (e.g., Tarantola & Valette, 1982;

- Tarantola, 1987; Zhdanov, 2002) that bridges the gap between probabilistic and deterministic
- approaches. For example, if the inverse of the model covariance \mathbf{C}_m^{-1} is taken equal to $\lambda^2 \mathbf{L}^T \mathbf{L}$ -
- 203 with the positive scalar λ weighting the relative importance of the regularizer and the data
- 204 misfit, and L being a discrete approximation of the spatial derivative then, the minimization of
- 205 the objective functional implements the standard Occam's inversion (Constable et al. 1987). In
- this specific case, the objective functional $P^{(\lambda)}(\mathbf{m}, \mathbf{d}^{\text{obs}})$ to be minimized during the deterministic inversion is:
- 208

$$P^{(\lambda)}(\mathbf{m}, \mathbf{d}^{\text{obs}}) \propto \left\| \mathbf{C}_{\mathbf{d}}^{-1/2} (\mathbf{d}^{\text{obs}} - F(\mathbf{m})) \right\|_{L_2}^2 + \lambda \| \mathbf{L}(\mathbf{m} - \mathbf{m}_0) \|_{L_2}^2.$$
(4)

On one hand, the strategy we are proposing here relaxes one of these working hypotheses; in particular, in the following, we do not make any assumptions on the Gaussianity of the model parameters distribution $p(\mathbf{m})$ as we consider quite general prior distributions defined via their realizations, which are generated through a geologically informed procedure.

On the other hand, we keep considering the noise contaminating the observed quadrature 213 components to be frequency-by-frequency, and location-by-location, independent, even though it 214 is clearly not (Mitsuhata at al., 2001; Minsley et al., 2012; Liu et al., 2023). Consistently with 215 this assumption, we still approximate $C_d^{-1/2}$ with a diagonal matrix, whereas, for example, with 216 the availability of a 3D FDEM forward modelling, we could have included the noise component 217 attributable to the modeling error associated with the 1D modelling approximation. Bai et al., 218 2021 showed, for the time-domain electromagnetic case (and following the prescriptions in 219 Hansen et al. 2014), how the inclusion of that additional source of data uncertainty into a 220 probabilistic inversion via a more complex (non-diagonal) approximation of C_d can prevent 221 misinterpretations and artifacts even in the case of environments where the 1D approximation 222 seems reasonable (so, even in the case of settings where the assumption of the absence of 223 significant 3D effects contaminating neighboring 1D soundings seems acceptable). This is 224 something to be investigated in future research; in the present manuscript, we simply evaluate 225 the probability associated with a certain model by using uniquely Eq. 2. 226

Moreover, as it will be discussed below, each resistivity component of **m** will be a function of a specific lithology, allowing the assessment of the probability of occurrence of a lithological category rather than the mere prediction of a resistivity value characterizing a discretizing layer.

232 2.1 Generation of the prior models

The prior distribution can be defined via its realizations. In the case under investigation, 233 the hypothesis is that the subsurface consists of a sequence of two lithologies: peat and clay. It is 234 true that, in some cases, peat might overlay more resistive bedrock (Boon et al., 2008; Comas et 235 al., 2015; Kowalczyk et al., 2017), but our assumption is that, anyhow, even in the case of a 236 shallow bedrock, a clay unit is present due to the rock weathering or alluvial/glacial origins 237 (Osman 2018). In addition, we assume that, for each sounding location, the associated model can 238 be composed of three lithological units, with no restrictions concerning their vertical sequence. 239 So, for example, a clay unit comprised between a shallower and a deeper peat layer can, in 240 principle, be allowed. Consequently, each 1D model of the prior distribution is discretized with 241 200 layers with a thickness of 0.1 m, and two interface depths are picked from a uniform 242 distribution with values ranging from 0 to 20 m. This procedure defines the three units. 243 Subsequently, a lithology (either peat or clay) is randomly associated to each of the layers. 244 Therefore, prior sample models - consisting of 200 layers (gathered in 3 lithological units) - are 245 generated. For each layer, it is now possible to match a resistivity value drawn from two 246 distributions describing the ranges of resistivity values expected for each lithology (bar plots in 247 Figure 1a). In order to ensure some additional vertical spatial coherence, the original 200-layer 248 resistivity models are smoothed by means of a 5-layer sliding average filter. In this way, the 249 250 assumption of independence between neighboring layers is loosened up and a vertical spatial correlation between the 1D model parameters is introduced. The rationale behind this choice is 251 that renouncing the high entropy choice generates more geological plausible 1D resistivity 252 profiles. After this model parameters conditioning, , the associated resistivity distributions for the 253 peat and clay units are different from the original ones (solid lines in Figure 1). The 5-layer 254 width for the filter has been chosen by inspecting the effect on the final resistivity vertical 255 profiles: a shorter span would have not satisfactorily reduced the erratic behavior of the original 256 resistivity (thick lines in Figure 1), whereas a filter window larger than 0.5 m would have 257 smeared out the sharp interfaces between the lithologies. 258



Figure 1. Resistivity distributions associated with each lithology. Panel (a) displays, as green 261 bars, the probability density distribution (PDF) of having a peat layer with a specific resistivity, 262 and, as yellow bars, the corresponding PDF for the clay layers. The solid lines show the 263 corresponding distributions after a 5-layer vertical moving average filtering of the samples of the 264 prior. In panel (b), the corresponding cumulative density functions (CDFs) are shown: the solid 265 lines are related to the CDF obtained after the 5-layer vertical filtering and highlight that 266 resistivity values lower than 200 Ω m are almost certainly associated with clay, whereas layers 267 with resistivities higher than 400 Ω m, most likely, are peat. Resistivities around 270 Ω m have 268 the same probability of being clay or peat. 269

270

The resistivity ranges in Figure 1 have been deduced from the examples in the literature. Peat soil has a wide resistivity range spanning from tens to a few hundred Ω m, depending on the

- 273 moisture content, salt concentration, degree of decomposition, and mineral composition
- (Silvestri et al., 2019a; Silvestri et al. 2019b; Valois et al. 2021; Mohamad et al., 2021). Also the
- resistivity of clay sediments may vary significantly depending on the soil conditions (in
- particular, the water content and its salinity) (Samouëlian et al. 2005; Solberg et al. 2014; Cheng
- et al. 2019). However, for the fresh-water-saturated clay expected in the Alpine peatland, low
- resistivity values of the order of a few tens Ωm seem to be reasonable (Binley & Slater, 2020).

Therefore, based on these assumptions concerning the possible lithological stratification 279 and the resistivities associated with such geological units, the samples of the prior distribution 280 can be easily generated. Figure 2 displays two examples of the prior distribution models. It might 281 be worth noticing that three lithological units provide additional flexibility since the case of two 282 effective units (e.g., peat covering clay – Figure 2a) is still a feasible option, but, at the same 283 time, it is also possible to experience a clay substrate with a peat intrusion (Figure 2b). Clearly, a 284 285 very informative prior (e.g., only two units) might be misleading in case of wrong initial assumptions, whereas, to a certain extent, allowing a higher variability in the prior assumptions 286

287 cannot be detrimental (the only drawback is connected to the higher computational time).





290 Figure 2. Samples of the prior distribution. Each prior model consists of 200 layers characterized

by different resistivity values (thin green or orange solid lines) gathered in three lithological units

292 (of either clay or peat). The original 200 resistivities have been subsequently filtered to obtain

293 1D model samples with some vertical correlation (thick blue or red solid lines). The mean 294 resistivity calculated from the filtered values over each lithological unit is shown as a black thin

294 resistivity calculated from the intered values over each inhological unit is shown as a black time 295 straight segment. Panel (a) displays a sample with the following lithological sequence: peat-clay-

clay; consequently, the mean resistivities for the two deepest units are almost indistinguishable

297 (their interface occurs at around 5.5 m depth). Panel (b) illustrates another example of a prior

sample characterized by a peat unit sandwiched between two clay units.

299

Following this strategy, we populated (and defined) the prior ensemble with 10^5 samples. 300 For each of them, the associated FDEM response has been calculated by taking into account the 301 geometry parameters, frequencies, and elevation of the employed sensor. In this respect, the 302 303 measured dataset consists of 153621 soundings collected by using the following 11 frequencies: 1025, 1525, 2875, 5825, 7775, 12775, 15325, 25525, 36225, 63025, 80225 Hz, with the 304 recording device assumed at 1.0 m height from the surface. During the survey, we used a GEM-2 305 (Haoping & Won, 2003) in the horizontal co-planar configuration. This device has a receiver-306 transmitter inter-coil distance of 1.6 m. Performing the standard FDEM processing procedure 307 preliminary to the inversion, we laterally stacked and averaged between adjacent soundings in 308 order to remove the outliers and assess the noise in the data (cf., e.g., Zaru et al., 2023). 309

For every sounding, the response $F(\mathbf{m})$ of each of the prior realizations is evaluated 310 against the observed data \mathbf{d}^{obs} through the Eq. 2. The posterior distribution is then defined by 311 replicas of the models based on their probability. Hence, the probabilistic inversion consists of an 312 independent extended Metropolis algorithm, which is analogous to the standard extended 313 Metropolis algorithm (Mosegaard & Tarantola, 1995; Hansen et al., 2016) with an infinitely long 314 step-length; this is equivalent to state that every new model proposal from the prior distribution 315 is a completely independent realization: indeed, in our specific case, it is precalculated. The 316 proposed inversion scheme is implemented in the SIPPI toolbox (Hansen et al. 2013a; Hansen et 317 al. 2013b). 318

319 **3 Results**

Figure 3 shows the horizontal slices at different depths (namely: 0.5 m, 3.0 m, 5.0 m, 8.0 320 m) of: i) the realization of the posterior distribution with the maximum likelihood (first column 321 322 on the left); ii) the mean model obtained by averaging the realizations of the posterior models (second column from the left); iii) the probability of encountering peat; and iv) the probability of 323 clay occurrence. Clearly, since we are simply assuming two lithological categories (peat and 324 clay), the two probabilities are complementary: the maximum probability of having peat 325 corresponds to the minimum probability of clay. It is fundamental to clarify that across the 326 present paper, for the sake of conciseness, we use the term maximum likelihood model to 327 328 indicate the model of the prior ensemble which is characterized by the highest likelihood; strictly speaking, that is not the actual maximum likelihood model since it relates to the prior 329 distribution. However, in this context, and after this caveat, there should be no room left for 330 331 ambiguities.

From Figure 3, it is evident that peat is mainly present in the northern-central portion of the investigated area and its evolution can be followed from the surface to significant depths (more than 8.0 m). In addition, a shallower peat deposit can be detected in the southern part of the study area. It is worth highlighting the spatial coherence of the result (including the maximum likelihood one) despite each sounding has been inverted separately without introducing any horizontal constraint (again, prior information is provided uniquely via the prior distribution).

In order to verify our result, we compare the probabilistic outcome against the available 339 boreholes and electrical resistivity models obtained by a deterministic inversion. In this respect, 340 Figures 4c-f shows a vertical section extracted from the (pseudo-)3D volume in Figure 3. All the 341 boreholes were drilled aiming at reaching the clay bottom unit (more difficult to penetrate); 342 however, that was not always possible. So, the depth of the boreholes is supposed to be 343 344 shallower or match the top of the clay substrate. For sake of clearness, the names of the boreholes reaching the top of the clay unit contain an asterisk (for example, B26*). From Figures 345 4c-f, it is evident that the geophysical reconstruction can detect quite precisely the morphology 346 of the peat unit as it appears from the boreholes. In particular, that is true for the boreholes B26* 347 and B11, in the middle of the section. On the other hand, a possible explanation for the mismatch 348 with the borehole B31* is that it is actually quite off the profile. In fact, the borehole B31* is 349 approximately 4 meters apart from the profile. It is worth mentioning that the borehole B26* is 350 the most reliable well as, differently from the others, its core has been extracted and analyzed 351 (Poto et al., 2013). Concerning the much shallower B33, that borehole simply confirms that, at 352 that location, the peat substrate is thicker than 2.5 m, and this evidence is compatible with what 353 is inferred from geophysics. On the contrary, accordingly to the borehole B6*, at that location, 354 the top of the clay unit should be found at 1 m depth, whereas the probable peat thickness 355 (Figure 4e) is supposed to be around 4 m. A plausible justification for such a mismatch will 356 require further investigations; however, because of the noticeable lateral consistency of the 357 358 geophysical solution, despite the fact that each individual sounding is inverted separately, it is hard to believe in a systematic artefact in the inversion process. In addition, as it will be 359 discussed in the following, similar conclusions about the B6* location can be drawn also by 360 looking at the alternative deterministic reconstruction (Figure 4b). 361

In general, as it should be, many of the details visible in the maximum likelihood model (Figure 4c) disappear when we check the mean model (Figure 4d) or the peat probability (Figure 4e). This is particularly evident at depth, below the conductive clay, where the model parameters do not have a significant sensitivity with respect to the (noisy) measurements; in other terms, those layers are below the DOI (Depth Of Investigation – e.g. Zhdanov, 2002; Vignoli et al., 2021) and the details retrieved in some specific realizations of the posterior distribution are, indeed, artifacts and are characterized by a low occurrence probability.

When we check the data fitting of the different models in terms of $\chi^2 = (1/N) \|\mathbf{C}_d^{-1/2} (\mathbf{d}^{\text{obs}} - F(\mathbf{m}))\|_{L_2}^2$, in which *N* is the number of data points per sounding (so, in this specific case, N = 11, with 11 being the number of used frequencies), we can see that, not surprisingly, the maximum likelihood model (Figure 4a – red "+" markers) is characterized by responses closer to the observations than the mean model (green "×" markers). Besides, the maximum likelihood model generally fits the data below the optimal threshold $\chi^2=1$. Interestingly, also the mean model, which does not have any physical meaning, sensu stricto, is associated to reasonable χ^2 values.

The maximum likelihood solution is equivalent to an inversion obtained by minimizing 377 the data misfit in which the well-posedness of the inversion is enforced by selecting the solution 378 among the prior models (Zaru et al., 2023) rather than via the regularization term. The impact of 379 the prior information is evident as the maximum likelihood reconstruction is characterized by a 380 significant lateral coherence (i.e., the solution turns out to be stable with respect to perturbations 381 in the data - i.e., moving from one sounding to the adjacent one) without an explicit 382 regularization term, and this while the data misfit is comparable with alternative, "more 383 standard", inversions. In this perspective, it might be worth it to compare our probabilistic 384 outcome with the deterministic Occam's inversion (Figure 4b). In doing that, we used the 385 extremely valuable open-source McLachlan et al., 2021b's implementation: EMagPv, with a 386 parameterization similar to the one used for the probabilistic inversion. Hence, for example, 30 387 layers discretize each 1D model; 30 layers seemed to be a good compromise between using a 388 too-coarse discretization (with the risk of introducing an additional, unwanted, regularization 389 parameter: the number of layers) and the practical impossibility of running 200-layer inversions 390 in a reasonable amount of time. In the deterministic approaches, the calculation of the Jacobian is 391 generally the computational bottleneck of the minimization process (Christiansen et al., 2016); 392 even if, in the present research, we have not profusely investigated this aspect, most likely, 393 within the conjugate gradient minimization utilized, the Jacobian's update makes the cost of the 394 deterministic inversion too high to be able to run it for the entire survey (even with a relatively 395 small number of layers). For this reason, we performed the deterministic inversion uniquely 396 along the section highlighted in Figure 3 and shown in Figure 4b. The starting model for each of 397 the 1D deterministic inversions along the investigated profile is the same, with a decreasing 398 resistivity with depth, ranging from around 500 Ω m at the surface to approximately 100 Ω m at 399 the bottom. The regularization weight, λ (Eq. 4), is set for all soundings equal to 0.07. This 400 uniform value of λ along the entire profile guaranties an optimal mean data fitting ($\gamma^2=1$) 401 across the section (cf. the horizontal blue dotted line in Figure 4a), despite, in principle, it should 402 be adjusted in order to ensure that similar condition being fulfilled sounding-by-sounding and 403 not merely on average. Figure 4b shows the deterministic reconstruction, whereas the associated 404 data fitting levels can be checked in Figure 4a. In a few sounding locations, the deterministic 405 inversion has difficulties in fitting the data to a reasonable level. Possible reasons for that could 406 be related: to local minimization issues of the objective functional, and/or to the inconsistency 407 between the prior information enforced by the stabilizer, which promotes smoothly varying 408 solutions, not really compatible with the geology characterized by quite a sharp peat-clay 409 interface (sometimes occurring at shallow depths). In this perspective, a sounding-by-sounding 410 optimization of the λ value might have been useful even if extremely time and computationally 411 consuming. The deterministic inversion has a data misfit that is largely overlapping with the one 412 413 of maximum likelihood model; still, it is more laterally erratic, while, not surprisingly, favors the retrieval of vertically elongated structures. On this matter, the comparison, for example, of the 414 portion of the sections between B26* and B11 as inferred by the two alternative inversion 415 schemes, demonstrates the impact of the different prior information incorporated in the 416 probabilistic approach and in the deterministic regularization: the complex information 417 formalized via the prior distribution samples allows the retrieval of a spatially consistent 418 419 morphology of the peat unit, whereas this is prevented by the smooth regularization (even in case of similar data fitting). 420

In addition, the good correspondence between the probabilistic result and the
 deterministic reconstruction in the vicinity of borehole B6* questions the reliability of the direct
 measurement of the peat thickness deduced by the drilling.

In terms of inversion performances, the probabilistic inversion basically requires only the 424 forward calculations of the samples of the prior distribution, which can be performed 425 independently and, so, are massively and easily parallelizable. The calculation of the conditional 426 probability of Eq. 2 is, then, straightforward and, in the specific case of the entire Danta's dataset 427 (consisting of around 150000 soundings - a size comparable with an airborne survey; cf., e.g., 428 Viezzoli et al., 2009; Christiansen et al., 2016), with a prior ensemble of 100000 samples, took 429 approximately one hour (on a quite standard laptop equipped with an Intel i7-10750H/2.60GHz). 430 Clearly, on top of that, for a fair comparison, the time used for generating the prior samples and 431 the associated measurements must be considered (for the 100000 samples, on the same laptop, it 432 took around one additional hour). However, it should be stressed that for similar geological 433 settings (and the same configurations of the geophysical instrumentation), the prior models do 434 not need to be recalculated every time and can be generated once and for all. On the other hand, 435 at least with the parameterization we used, the deterministic inversion of the entire Danta's 436 dataset was not feasible (it would have needed weeks of calculation), and, for each of the several 437 2D profiles it was tested on (like in Figure 4), required more than one day. Furthermore, it might 438 439 be relevant to stress that even if populating the prior distribution might be difficult, similar troubles might be encountered with deterministic inversion schemes, not only in the definition of 440 the most appropriate stabilizer, but also in the selection of the optimal regularization weight and 441 in addressing all the issues connected with the optimization of the objective functional 442 (including, e.g., the definition of a suitable starting model). It is worth stressing once more that 443 the high performances characterizing the proposed probabilistic approach relate to the proposal 444 strategy: since all the evaluated models are mutually independent, they can be precalculated in 445 advance (in parallel) (Hansen, 2021a). 446



- 449 Figure 3. Horizontal slices of the inversion results of the FDEM data collected across the Danta
- 450 peatland (Italy). Each row displays, from left to right: i) the resistivity solution with the
- 451 maximum likelihood; ii) the mean model of the samples of the posterior probability; iii) the
- 452 probability of peat; and iv) the probability of clay. Rows (a-d) shows the horizontal slices of
- those models and probabilities, respectively, at depth 0.5 m, 3.0 m, 5.0 m, and 8.0 m. In the
- 454 column 3, on top of the peat probability, the location of the profile in Figure 4 is shown (in
- 455 magenta), together with the position of the related boreholes (green circles).



Figure 4. Inversion results. Panel (b) shows the fully nonlinear deterministic Occam's inversion performed with the software package EMagPy (McLachlan et al. 2021b). Panels (c-f) display the results of the probabilistic petrophysical inversion; in particular, panel (c) shows the

461 maximum likelihood resistivity solution, whereas panel (d) exhibits the resistivity section

obtained by averaging the resistivity samples of the posterior distribution. Panels (e) and (f)
 show respectively the probability of peat and clay occurrences for each of the 200 layers

465 show respectively the probability of peat and cital occurrences for each of the 200 layers 464 discretizing each 1D model. Panel (a) shows the χ^2 value obtained by comparing, against the

464 observed data, the FDEM responses of: i) the deterministic solution (blue dots); ii) the maximum

likelihood model (red crosses); and iii) the mean model (green "×" markers); the horizontal

dotted lines are simply the mean χ^2 value across the section for the three models in panels (b-d).

The parameterization for the two kinds of inversion is different: 200 layers are used for the

469 probabilistic inversion; 30 for the deterministic one.

470

471 4 Discussion

Even if, in presenting the inversion results we referred repeatedly to the mean map 472 (Figure 4d), clearly, the actual probabilistic outcome (the posterior PDF) contains much more 473 information than the mean model and its associated standard deviation. In this respect, it is 474 important to stress, that, also because of the non-linearity of the forward modelling, the resulting 475 PDF might be non-Gaussian. Therefore, the possible multi-modality would make the reduction 476 of the probabilistic result to its mean and standard deviation misleading. In this respect, four 477 sounding locations (Figure 5a) have been selected to show the risk of taking just the mean as an 478 immediately interpretable result; in particular, in Figures 5b-e, the posterior resistivity PDFs 479 associated with those four locations are plotted and compared against the mean resistivity 480 vertical profile (red solid line), together with the corresponding standard deviation band 481 (between the green solid lines). Consistently with the previous caveat, the resistivity PDFs 482 present, at depth (specifically, where the occurrence of clay is more probable), a bi-modal 483 pattern, which, in turn, makes the mean resistivity move between the probability maxima. 484

Hence, panels in Figure 5 confirm once more the importance of a probabilistic approach
as, in this multi-modal situation, also deterministic approaches (e.g., orange dashed line in Figure
5b) could merely provide a local assessment of the uncertainty (based on the Jacobian)
associated with the unique retrieved solution. And, of course, the same risk may take place if we
draw our conclusions merely based on the mean model.

Also, it is worth noticing how the probability of peat occurrence (magenta solid line)
drops rapidly when the gyttja starts to be encountered (on the left side of Figure 5b, the detailed
lithological description of borehole B26* can be found).

In Figure 5, the vertical resistivity profile corresponding to the maximum likelihood solution (black solid line) is also plotted for each of the picked sounding locations. The maximum likelihood solutions are those (within the prior ensemble) better fitting the data, not the most probable. Indeed, the maximum likelihood model is the maximizer of the conditional probability density function, $p(\mathbf{d}^{\text{obs}}|\mathbf{m})$, in Eq. 2, and not of the posterior PDF, $p(\mathbf{m}|\mathbf{d}^{\text{obs}})$. In the presented framework, since the prior is defined uniquely via its samples and there is no closed form for it, the calculation of the most probable model is not possible.

Despite the maximum likelihood model being simply the model better fitting the observations, in the present scheme, to some extent, it is still a regularized solution as the prescriptions infused by the prior distribution impose a non-arbitrary final model. As mentioned before, this is clear, for example, from Figure 4c: even though neighboring soundings

- 504 (characterized by similar measurements) are independently inverted, the corresponding results
- are similar (demonstrating a continuity of the models with respect to the data). And this is
- 506 particularly remarkable because no lateral constraints have been enforced. In other
- 507 circumstances, it might be useful to constrain the inversion also horizontally. An extension of the
- present scheme capable of considering the expected lateral continuity might consist of adding a
- term taking into account the probability of a 1D model being different from some reference
- 510 model (possibly, the reference model can result from the previously considered adjacent 1D
- sounding inversion). Similar attempts are described, for example, in Ardid et al. 2021 and Zaru
- 512 et al. 2023.



Figure 5. Comparison of individual soundings. Panel (a) shows the locations of the

515 selected FDEM soundings and the position of the borehole B26*. Panels (b-e) display the 516 electrical resistivity PDFs as a function of depth for each of the four selected locations

electrical resistivity PDFs as a function of depth for each of the four selected locations
 (respectively associated with soundings no. 26805, 50000, 100000, and 150000); for each of the

selected soundings, the posterior PDF is compared against the corresponding mean model

resistivity (solid red line) and the relative standard deviation limits (the band between the solid

520 green lines), and, for completeness, also with the maximum likelihood model (black solid line)

and the peat probability (solid magenta line, whose x-axis is shown on the top of each panel). For

the sounding 26805, the deterministic inversion is also available and, consistently, is plotted in

523 panel (b) as a dashed orange line. Sounding 26805 was selected since it is the closest to the 524 borehole B26* whose stratigraphy is known and appears alongside panel (b).

525

526 **5 Conclusions**

We presented a workflow for the probabilistic petrophysical 1D inversion of FDEM 527 528 measurements and tested it on a dataset consisting of 11 frequencies collected throughout an Alpine peatland in northern Italy. The retrieved posterior distribution has been analyzed in terms 529 of maximum likelihood and mean models, and via the associated peat (and clay) occurrence 530 probability. It turned out that the peat probability can effectively reconstruct the geometry of the 531 peat layer and satisfactorily match the additional ancillary pieces of evidence about the 532 investigated site. In particular, the probabilistic results have been compared against the available 533 boreholes and their capability was confirmed at least for the deepest (and most reliable) direct 534 investigations. Furthermore, the probabilistic scheme was also verified against the most standard 535 deterministic Occam's inversion implemented in a very well-known open-source software 536 package. The deterministic and the probabilistic inversion show remarkable differences due to 537 the different prior information formalized in the two schemes (smooth vertical constraints in the 538 deterministic inversion; three lithological units with specific resistivity ranges in the probabilistic 539 approach). We also highlight that the adopted probabilistic approach can be extremely efficient 540 paving the way to quasi-real-time inversion in the field and on-the-fly optimization of the survey 541 plans. 542

543 Future developments should involve the assessment of the modelling error and the inclusion of

such an inevitable source of uncertainty into the inversion scheme as has already been done for

the time-domain counterpart (Bai et al., 2021).

546

547 Data Availability Statement

The FDEM data inverted in this study, together with the associated uncertainties, are available at

549 <u>https://zenodo.org/records/10155293</u> (Vignoli & Zaru, 2023). The code used to generate the

forward responses can be retrieved from <u>https://github.com/elwaseif/FEMIC-Code</u> (Elwaseif et

- al., 2017b), whereas the probabilistic inversion scheme is implemented in the SIPPI toolbox
- (Hansen et al. 2013a; Hansen et al. 2013b), available at <u>https://github.com/cultpenguin/sippi</u>
- (Hansen et al., 2013c). For the deterministic inversion, we used the software package EMagPy

554 (McLachlan et al. 2021a), which can be downloaded from here:

555 <u>https://github.com/hkexgroup/emagpy</u> (McLachlan et al. 2021b).

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