



Machine learning for ecosystem services

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1 Machine learning for ecosystem services

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25 Contributions

24

SW, INA, JML, KJB, SB, BV & FV conceived the paper. SW, DAPH, JMB & INA carried out the South
African case study. JML, SB, AM, CP, SS, GS & FV carried out the Sicilian case study. SW & INA wrote
the manuscript, with comments and revisions from all other authors.

29 Abstract

30 Recent developments in machine learning have expanded data-driven modelling (DDM) capabilities, 31 allowing artificial intelligence to infer the behaviour of a system by computing and exploiting 32 correlations between observed variables within it. Machine learning algorithms may enable the use 33 of increasingly available 'big data' and assist applying ecosystem service models across scales, 34 analysing and predicting the flows of these services to disaggregated beneficiaries. We use the Weka 35 and ARIES software to produce two examples of DDM: firewood use in South Africa and biodiversity 36 value in Sicily, respectively. Our South African example demonstrates that DDM (64-91% accuracy) can 37 identify the areas where firewood use is within the top quartile with comparable accuracy as 38 conventional modelling techniques (54-77% accuracy). The Sicilian example highlights how DDM can 39 be made more accessible to decision makers, who show both capacity and willingness to engage with 40 uncertainty information. Uncertainty estimates, produced as part of the DDM process, allow decision 41 makers to determine what level of uncertainty is acceptable to them and to use their own expertise 42 for potentially contentious decisions. We conclude that DDM has a clear role to play when modelling 43 ecosystem services, helping produce interdisciplinary models and holistic solutions to complex socio-44 ecological issues.

45 **Key words:** ARIES; Artificial Intelligence; Big data; Data driven modelling; Data Science; Machine 46 learning; Mapping; Modelling; Uncertainty, Weka.

47 Introduction

Many scientific disciplines are taking an increasingly integrative approach to planetary problems such 48 49 as global climate change, food security and human migration (Baziliana et al., 2011; Bullock et al., 50 2017). To address such challenges, methods and practices are becoming more reliant on large, interdisciplinary data repositories often collected in cutting-edge ways, for example via citizen 51 52 scientists or automated data collection (Isaac et al., 2014). Recent developments in information 53 technology have expanded modelling capabilities, allowing researchers to maximise the utility of such 54 'big data' (Lokers et al., 2016). Here, we focus on one of these developments: data-driven modelling 55 (DDM). DDM is a type of empirical modelling by which the data about a system are used to create 56 models, which use observed systems' states as inputs for estimating some other system state(s), i.e., 57 outputs (Jordan and Mitchell, 2015; Witten et al., 2016). Thus, DDM is the process of identifying useful 58 patterns in data, a process sometimes previously referred to as knowledge discovery in databases 59 (Fayyad et al., 1996). This process consists of five key steps: 1) understanding the research goal, 2) 60 selecting appropriate data, 3) data cleaning, pre-processing and transformation, 4) data mining 61 (creating a data driven model), and 5) interpretation/evaluation (Fayyad et al., 1996) (Figure 1). A 62 variety of methods for data mining and analysis are available, some of which utilise machine learning algorithms (Witten et al., 2016; Wu et al., 2014) (Figure 1). A machine learning algorithm is a process 63 64 that is used to fit a model to a dataset, through training or learning. The learned model is subsequently 65 used against an independent dataset, in order to determine how well the learned model can 66 generalise against the unseen data, a process called testing (Ghahramani, 2015; Witten et al., 2016). 67 This training-testing process is analogous to the calibration-validation process associated with many 68 process-based models.

69

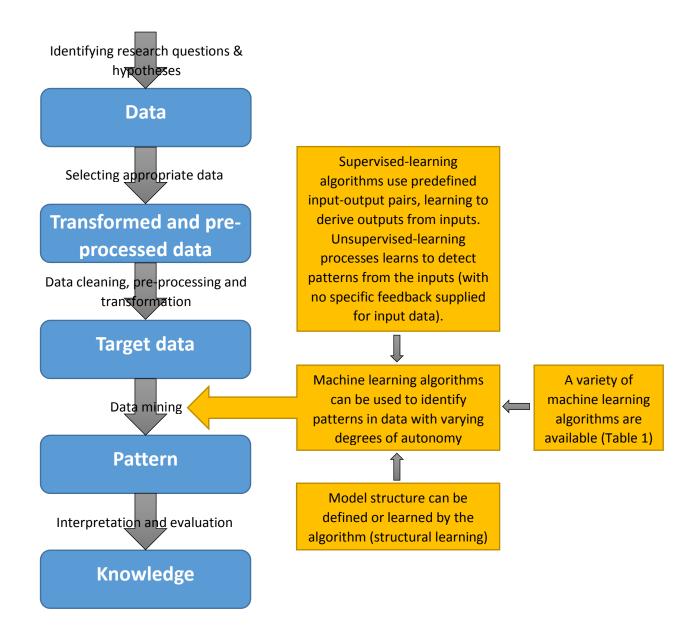


Figure 1 – A schematic outlining how machine learning algorithms (yellow) can contribute to the
 data-driven modelling process (blue) (Fayyad et al., 1996).

73

74 In general, machine learning algorithms can be divided into two main groups (supervised- and 75 unsupervised-learning; Figure 1), separated by the use of explicit feedback in the learning process 76 (Blum and Langley, 1997; Russell and Norvig, 2003; Tarca et al., 2007). Supervised-learning algorithms 77 use predefined input-output pairs and learn how to derive outputs from inputs. The user specifies 78 which variables (i.e., outputs) are considered dependent on others (i.e., inputs), which sometimes 79 indicates causality (Hastie et al., 2009). The machine learning toolbox includes several linear and non-80 linear supervised learners, predicting either numeric outputs (regressors) or nominal outputs 81 (classifiers) (Table 1). An example of supervised machine learning that is familiar to many ecosystem 82 service (ES) scientists is using a general linear model, whereby the user provides a selection of input 83 variables hypothesised to predict values of an output variable and the general linear model learns to 84 reproduce this relationship. The learning process needs to be fine-tuned through a process, as for 85 example in the case of stepwise selection where an algorithm selects the most parsimonious best-fit 86 model (Yamashita et al., 2007). However, note that stepwise functions may also be used in 87 unsupervised learning processes when combined with other methods. Within unsupervised-learning 88 processes, there is no specific feedback supplied for input data and the machine learning algorithm 89 learns to detect patterns from the inputs. In this respect, there are no predefined outputs, only inputs 90 for which the machine learning algorithm determines relationships between them (Mjolsness and 91 DeCoste, 2001). An example unsupervised-learning algorithm, cluster analysis, groups variables based 92 on their closeness to one another, defining the number and composition of groups within the dataset 93 (Mouchet et al., 2014). Within the supervised- and unsupervised-learning categories, there are several 94 different varieties of machine learning algorithms, including: neural networks, decision trees, decision 95 rules and Bayesian networks. Others have described the varieties of machine learning algorithms 96 (Blum and Langley, 1997; Mjolsness and DeCoste, 2001; Russell and Norvig, 2003; Tarca et al., 2007) 97 and so we only provide a brief summary here, leaving out more advanced methods such as 98 reinforcement learning, and deep learning (see Table 1).

99

| 100 | Table 1 – A simplified summary of machine learning algorithms (categorised as supervised and |
|-----|--|
| 101 | unsupervised). |

102

| Category | Task | Common algorithms |
|---------------------------------|----------------------------|-------------------------------|
| Unsupervised learning | Clustering | k-means |
| (learning without feedback | Associations | Apriori |
| from a trainer) | Dimensionality reduction | PCA |
| Supervised learning | Classification (learning a | Bayesian Networks, Decision |
| (learning past | categorical variable) | Trees, Neural Networks |
| actions/decisions with trainer) | Regression (learning a | Linear Regression, Perceptron |
| | continuous variable) | |

103

104 DDM undoubtedly has a role to play when modelling socio-ecological systems and assessing ES. DDM 105 can give useful predictive insight into areas where understanding of the underlying processes is 106 limited. However, as with many statistical methods, DDM requires adequate data availability. The level 107 of data required is determined on a case-by-case basis, depending of the research question being 108 asked. For example, to use machine learning algorithms, data must be able to be divided into training 109 and testing subsets (Smith and Frank, 2016). Machine learning algorithms assume considerable 110 changes in the modelled system have not taken place during the time period covered by the model 111 (Ghahramani, 2015; Jordan and Mitchell, 2015), though machine learning can also be used for 112 identifying change, i.e., detecting concept drift (Gama et al., 2004). Model validation/testing, which has yet to become standard practice within the ES modelling community (Baveye, 2017; Hamel and 113 114 Bryant, 2017), is an integral part of the machine learning process within DDM. This is vital as DDM can 115 result in overfitting, which occurs when the model learns the training data well (i.e., a close fit to the training data), but performs poorly on independent test data (Clark, 2003). 116

117

118 To assess the quality of the learning process, machine learning algorithms use various methods 119 (summarised in Witten et al. (2016)) to ensure that the results are generalizable and avoid overfitting. 120 For example, k-fold cross validation allows for fine-tuning of model performance (Varma and Simon, 121 2006; Wiens et al., 2008). This approach maximises the data availability for model training by dividing 122 the data into k subsets and using k-1 subsets to train the model whilst retaining a subset for 123 independent validation. This process is repeated k times so that all available data have been used for 124 validation exactly once. The results of the k-folds are then combined to produce metrics of quality for the machine learning process, often accompanied with an estimation of the model uncertainty (i.e., 125

126 the cross-validation statistic). Whilst the goodness-of-fit parameter used varies within DDM (e.g., root 127 mean square error is used extensively within regression models, but the standard error is more 128 commonly used in Bayesian machine learning (Cheung and Rensvold, 2002; Uusitalo, 2007)), it 129 provides the user with a transparent estimate of model uncertainty. Whilst estimates of uncertainty 130 are useful, users of DDM should be aware that such models do not represent the underlying processes 131 within socio-ecological systems, but instead capture relationships between variables (Ghahramani, 132 2015). However, for some datasets and model applications (see Discussion for further details), DDM 133 can produce more accurate models than process-based models, as the latter may suffer from an 134 incomplete representation of the socio-ecological processes (Jordan and Mitchell, 2015; Tarca et al., 135 2007). Finally, as with any modelling, DDM depends on the quality of the training and testing datasets 136 used; whilst some extreme cases or outliers might get ignored during DDM, the quality of the 137 information supplied to the machine learning algorithms should be verified beforehand (Galelli et al., 138 2014).

139

140 The aim of this paper is to demonstrate the utility of DDM to the ES community. We present two 141 examples of DDM using Bayesian networks (a supervised learning technique), as implemented in the 142 Waikato Environment for Knowledge Analysis machine learning software (Weka; 143 http://www.cs.waikato.ac.nz/ml/weka/; Frank et al. (2016); Hall et al. (2009)), used both standalone 144 and as part of the Artificial Intelligence for Ecosystem Services (ARIES; 145 http://aries.integratedmodelling.org/; Villa et al. (2014)) modelling platform. We chose Bayesian 146 network methods as uncertainty metrics describing both the model fit and the grid-cell uncertainty 147 can be calculated (Aguilera et al., 2011; Landuyt et al., 2013; Uusitalo, 2007). Our Weka example focusses on firewood use in South Africa, and is comparable to conventional ES models recently 148 149 published by Willcock et al. (in revision). Using ARIES, we model biodiversity value within Sicily, and 150 demonstrate how DDM can make use of volunteered geographical information by incorporating data 151 from Open Street Maps into the machine learning process. In both examples, we highlight how model 152 structure and uncertainty computed in the machine learning process supplement and enhance the 153 value of the results reported to the user.

154

155 Methods

156 For the first example, we used Weka, an open-source library of machine learning algorithms (Frank et al., 2016; Hall et al., 2009), to create a model capable of identifying the upper quartile of sites for 157 158 firewood use in South Africa. We chose this example as: 1) firewood use is of high policy relevance in 159 sub-Saharan Africa (Willcock et al., 2016); 2) robust spatial data on firewood use are available within 160 South Africa and may, for some municipalities, provide a comparable context to other parts of sub-161 Saharan Africa, which are often more vulnerable but data deficient (Hamann et al., 2015); 3) models 162 ranking the relative importance of different sites were rated as useful to support ES decision-making by nearly 90% of experts in sub-Saharan Africa (Willcock et al., 2016); and 4) multiple conventional 163 164 models have recently been run for this ES covering this spatial extent (see Willcock et al. (in revision) 165 for full details).

The firewood use data are freely available (Hamann et al., 2015) and are based on the South African 2011 population census, which provides proportions of households per local municipality using a specific ES (similar data are available for a set of other ES; see <u>www.statssa.gov.za</u> for all 2011 census output). For this paper we used the proportion of households that use collected firewood as a resource for cooking (Hamann et al., 2015). To derive a measure of total resource use, we multiplied the proportion of use by the 2011 official census municipal population size (from <u>www.statssa.gov.za</u>) as: [(% households using a service) x (municipal population size)]. We then divided this value by the area of each local municipality to provide an estimate of firewood use density, ensuring that model inputsare independent of the land area of the local municipality.

175 To utilise Bayesian networks, the decision variable (firewood use density) had to be converted into a 176 categorical (nominal) attribute; note, the categories created during this process are unordered. The 177 goal of this task was to predict the areas in the upper quartile, reflecting demand from decision-178 makers for identification of the most important sites for ES production and, once identified, enabling 179 these areas to be prioritised for sustainable management (Willcock et al., 2016). Thus, the firewood use density data were categorised within the highest 25% (Q4) and the lowest 75% (Q1-Q3) quartiles 180 181 using Weka's Discretize filter to create ranges of equal frequencies (four in our case). Out of the 182 generated quartiles, the three lower ones were merged with the MergeTwoValues filter. To ensure 183 like-for-like comparisons between our DDM and conventional models, we provided the machine 184 learning algorithms with the same user supplied input data used to model firewood within Willcock et 185 al (in revision) (Table 2). Since most Bayesian network inference algorithms can use only categorical 186 data as inputs, the input data were discretised by grouping their values in five bins of equal 187 frequencies. Selecting the number of bins is a design choice and may impact model output (Friedman 188 and Goldszmidt, 1996; Nojavan et al., 2017). As such, the sensitivity of the modelled output to variable 189 bin numbers warrants future investigation, but is beyond the scope of this first-order introduction to 190 machine learning for ES.

191 Table 2 – The municipal-scale inputs into the Weka machine learning algorithms to estimate firewood

use in South Africa. Overfitting is avoided by first training the algorithm on subset of these data and
 then testing against the remaining data.

| Attribute | Description | | |
|--------------------|--|--|--|
| LCAgriculture | The proportion of agricultural land area, derived from GeoTerraImage (2015) | | |
| LCForest | The proportion of forested land area, derived from GeoTerraImage (2015) | | |
| LCGrassland | The proportion of grassland land area, derived from GeoTerraImage (2015) | | |
| LCUrban | The proportion of urban areas, derived from GeoTerralmage (2015) | | |
| LCWater | The proportion of water bodies area, derived from GeoTerralmage (2015) | | |
| COFirewood | The proportion of area on which firewood can be produced (Forest, Woodland, Savanna), derived from GeoTerraImage (2015) | | |
| OProtected | The proportion of protected natural areas, derived from the World Database on Protected Areas (<u>www.protectedplanet.net</u>) | | |
| MOCarbon | Mean amount of carbon stored per hectare, as calculated in Willcock et al. (in revision) | | |
| OGrowthDay | Average number of growing days in the area as driven by the relationship between rainfall and evapotranspiration, as calculated in Willcock et al. (in revision) | | |
| ZScholesA | A metric of the nutrient-supplying capacity of the soil (Scholes, 1998) | | |
| ZScholesB | A metric of the nutrient-supplying capacity of the soil (Scholes, 1998) | | |
| ZScholesD | Scholes (1998) land use correction, as calculated in Willcock et al. (in revision) | | |
| ZSlope | This is the mean slope in the area, based on the global 90-m digital elevation | | |
| | model downloaded from CGIAR-CSI | | |
| | (srtm.csi.cgiar.org/SELECTION/inputCoord.asp). | | |
| Population_density | The municipal population based on the South African 2011 census (<u>www.statssa.gov.za</u>). | | |
| Firewood_density | Observed firewood use for cooking from the South African 2011 census (Hamann et al., 2015). | | |

195 We used the BayesNet implementation of Weka to train our DDM. The machine learning algorithm 196 can construct the Bayesian network using alternative network structures and estimators for finding 197 the conditional probability tables (Chen and Pollino, 2012). In a Bayesian network, conditional 198 probability tables define the probability distribution of output values for every possible combination 199 of input variables (Aguilera et al., 2011; Landuyt et al., 2013). Unlike the use of expert elicitation or 200 Bayesian network training (e.g., Marcot et al. (2006)), the machine learning approach fits the structure 201 of the model, as well as the conditional probabilities, a process also called structural learning (Figure 202 1). In this example, we evaluated 16 alternatives for parameterising the Bayesian network learning 203 (see Appendix 1). We used 10 cross-fold validation (Varma and Simon, 2006; Wiens et al., 2008), 204 repeated 10 times with different seeds, for creating the random folds.

205 ARIES has recently incorporated the Weka machine learning algorithms into its modelling framework, 206 with the aim of enabling use of DDM within the ES community (see Villa et al. (2014) for a description 207 of the ARIES framework). In our second example, we used the ARIES implementation of Weka 208 BayesNet to propagate site-based expert estimates of 'biodiversity value' and so build a map for the 209 entire Sicilian region (Li et al., 2011). Here, biodiversity value does not refer to an economic value, but 210 to a spatially explicit relative ranking. The original biodiversity value observations were the result of assessments made with multiple visits by flora, fauna and soil experts (Figure 2). The same experts 211 212 who had ranked high-value sites were asked to identify sites of low biodiversity value, with the 213 constraint that the low value depended on natural factors and not on human intervention, as datasets 214 combining high and low value observations generally produce more accurate models (Liu et al., 2016). 215 These data were originally interpolated using an inverse distance weighted technique to provide a 216 map of biodiversity value to support policy- and decision-making (Figure 2a), and our DDM attempts 217 to improve on this map. The DDM process involved 20 repetitions, each using 75% of the data to train 218 the model and 25% to validate it. Using ARIES, we instructed the machine learning algorithm to access 219 explanatory variables, indicated by the same experts who provided the estimates used in training as 220 the most likely predictors of biodiversity value (see Appendix 2). The data used by the machine 221 learning process (Appendix 2) included distance to coastline and primary roads metric calculated using 222 citizen science data from Open Street Map (https://www.openstreetmap.org/; Haklay and Weber 223 (2008)). The trained model was then used to build a map of biodiversity value for the entire island, 224 computing the distribution of biodiversity values for all locations not sampled by the experts. The 225 machine learning algorithms used quantitative variables, discretised in 10 equal intervals, for both 226 inputs and outputs (Friedman and Goldszmidt, 1996; Nojavan et al., 2017). The resulting map was 227 subsequently discussed and qualitatively validated by the same experts who collected the data, as 228 well as quantitatively using a confusion matrix accuracy assessment.

229 Results

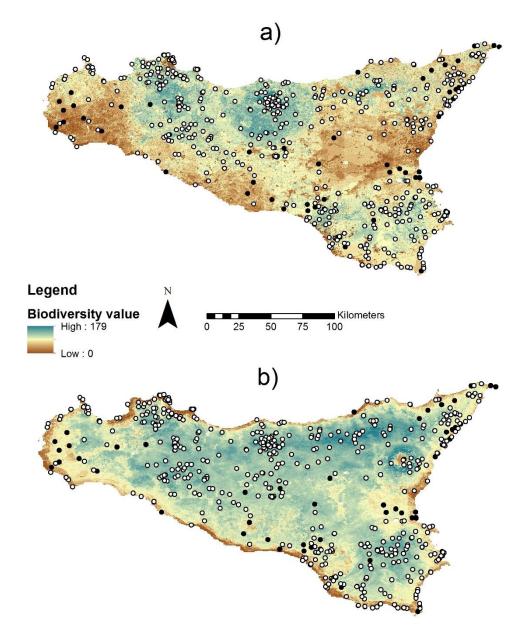
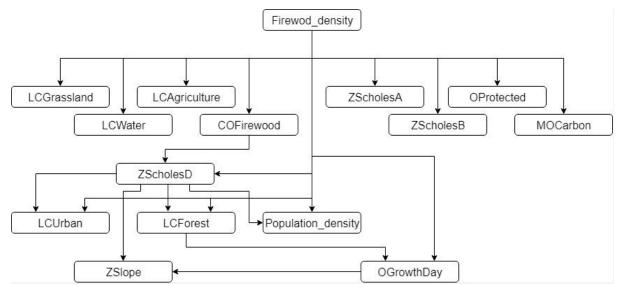
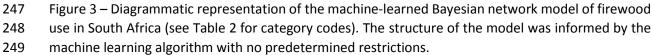


Figure 2 – The relative value of terrestrial biodiversity in Sicily estimated by a) inverse distance
weighted interpolation of observed values and b) Bayesian networks using data-driven modelling.
Both original (white) biodiversity value observations and the additional sites of low biodiversity value
(black) are shown as points.

235 In the first example, the results for all configurations of the DDM created for firewood use in South 236 Africa had a classification accuracy above 80% (see Appendix 1). The model predictions are statistically 237 significant with a confidence level of 0.05 (two tailed) when compared to the ZeroR classifier (a baseline classifier that always predicts the majority class). Using ArcGIS v 10.5.1, we spatially mapped 238 239 the outputs of the most accurate Bayesian network DDM (Figure 3; Figure 4; Appendix 3). The 240 confusion matrix for this model shows that 186 out of the 226 local municipalities were correctly 241 classified (an overall classification accuracy of 82%), and, out of 56 municipalities classified in the 242 upper quartile (Q4), 36 were correct predictions (64% recall [i.e. the percentage of the most important 243 sites for firewood ES correctly identified], comparable with conventional modelling methods evaluated against independent data [Table 3; Willcock et al (in revision)]; Appendix 3). The DDM also 244 245 produces probabilistic outputs for the respective inputs (Appendix 4).





250 For biodiversity value in Sicily, 43% of the testing subsample was correctly classified into 1 of 10 251 biodiversity value categories, with a majority of the incorrectly classified results falling into 252 immediately close numeric ranges (Appendix 5). During a workshop in June 2017, the same Sicilian 253 experts that provided the training set (a team of five including an academic conservationist, an 254 academic ornithologist, an academic botanist and an expert on agricultural biodiversity) qualitatively 255 evaluated the output in non-sampled but well-known regions and deemed it a distinct improvement 256 on previously computed biodiversity value assessments, built through conventional GIS overlapping 257 and interpolation techniques; an assessment that was embraced by other participants from both local 258 governmental and conservation institutions (Figure 2). As the map reflects the human assessment of 259 biodiversity value rather than objective measurements, the consensus of experts and practitioners 260 was deemed equivalent to a satisfactory validation. The confusion matrix (Appendix 5) shows how the 261 majority of misclassifications are between similar value categories. For example, 73% of test data were 262 predicted within one class above or below their actual class, and 84% of test data were correctly 263 classified within two classes above and below their actual class. A Spearman Rho test highlights the 264 significant correlation between the ranked model and validation data categories (Rho: 0.58; p-value < 265 0.001). The root-mean-squared error of the model prediction was also computed and resulted in a 266 value of 0.26 (Hyndman and Koehler, 2006).

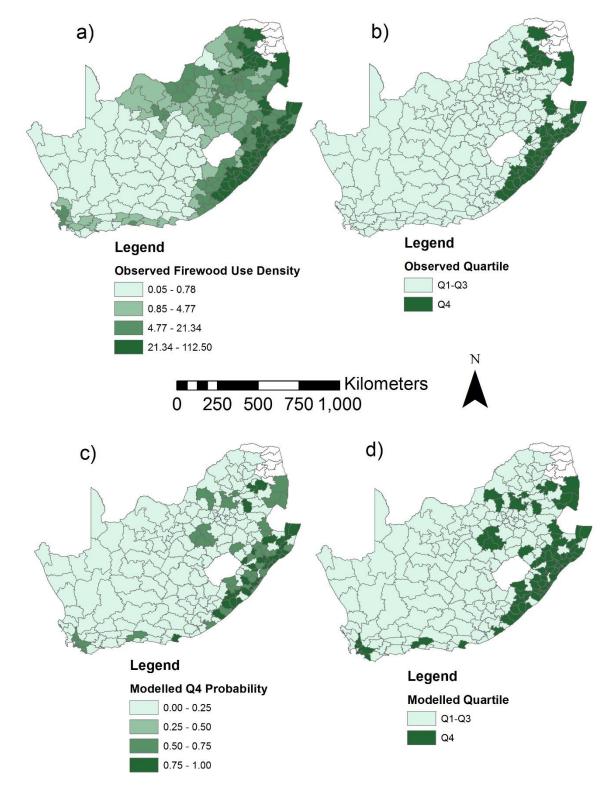


Figure 4 – Observed (a and b) and modelled (c and d) data on firewood use density within South Africa.
 The Weka *BayesNet* DDM process derives a probabilistic output (c) from the observed data (a). The

- modelled output can be categorised into quartiles (Q1-4, with Q4 being the upper quartile; d) and
- 271 compared to the observed data within the same categories (b).
- 272
- 273 Discussion

Lack of credibility, salience and legitimacy are the major reasons for the 'implementation gap' between ES research and its incorporation into policy- and decision-making (Clark et al., 2016; Olander et al., 2017; Wong et al., 2014). A lack of uncertainty information and the inability to run models in data-poor environments and/or under conditions where underlying processes are poorly understood may contribute to the implementation gap. However, DDM can help to address these current shortcomings in ES modelling. Here, we have demonstrated that DDM is feasible within ES science and is capable of providing estimates of uncertainty.

281

282 For our South African case study, the machine learning algorithms were able to produce a modelled 283 output of comparable accuracy to conventional modelling methods when using the same input 284 variables, despite our DDM using data at a much coarser (local municipality) scale (Table 3). Using the 285 spatially attributed uncertainty (i.e., the probability of each local municipality being in Q4), decision-286 makers would be able to set their own level of acceptable uncertainty. In our example, since we have 287 two categorical bins (i.e., Q1-3 and Q4), any local municipality with a modelled Q4 probability over 0.5 288 is assigned to the Q4 category. This assignment threshold can be varied; e.g., it is possible to state that 289 municipalities where modelled Q4 probability is less than 0.25 or greater than 0.75 are likely to be 290 grouped within Q1-3 and Q4 respectively, and to admit that we are less certain for the remaining 291 municipalities. In our example, this would result in a 96% (135 out of 140) categorisation accuracy for 292 Q1-3 and a 91% (30 out of 33) categorisation accuracy for Q4, with 53 local municipalities left 293 uncategorised due to uncertainty.

294

Table 3 – Comparing recall of DDM outputs with conventional models when producing estimates of
 firewood use in South Africa. Outputs from conventional models of varying complexity were validated
 using independent data (see Willcock et al (in revision) for full model descriptions and model
 complexity analysis). DDM outputs were validated using k-fold cross validation (see Methods).

| 200 | |
|-----|--|
| 299 | |

| Model | Model Criteria | Recall for the upper quartile of firewood use (%) |
|---|----------------------------|---|
| Bayesian network within | Assignment threshold = 50% | 64.3 |
| Weka (Frank et al., 2016; Hall et al., 2009) | Assignment threshold = 75% | 90.9 |
| Conventional model A | Gridcell size = 1 km | 75.0 |
| (Complexity score: 2; Willcock et al (in revision))* | Gridcell size = 10 km | 73.2 |
| Conventional model B | Gridcell size = 1 km | 75.0 |
| (Complexity score: 4; Willcock et al (in revision))* | Gridcell size = 10 km | 76.8 |
| Conventional model C | Gridcell size = 1 km | 60.7 |
| (Complexity score: 4; Willcock et al (in revision))* | Gridcell size = 10 km | 60.7 |
| Conventional model D (Complexity score: 36; Willcock et al (in revision))* | Gridcell size = 55.6 km | 76.8 |
| Conventional model A (Complexity score: 31; | Gridcell size = 5 km | 53.6 |

* Models have been anonymised as identification of the best specific model for a particular use is likely to be location specific and may shift as new models are developed (Willcock et al., in revision).

302

303 Thus, using Bayesian networks and machine learning, we are able to convey to decision-makers not 304 only which sites show the highest ES use or value, but also how confident we are in our estimate at 305 each site (Aguilera et al., 2011; Chen and Pollino, 2012; Landuyt et al., 2013). This information allows 306 decision-makers to 1) apply an assignment threshold of their choosing to the modelled output before 307 making a policy- or management-decision, and 2) use their own judgement for potentially contentious 308 decisions, where uncertainty is higher (Olander et al., 2017). For example, whilst it is perhaps obvious 309 that sites where we are highly certain that there is high ES value should be appropriately managed, it 310 is unclear which sites should be the next highest management priority. Given a limited budget, is a 311 medium-ES value site with high certainty more or less worthy of management than a potentially high-312 value site with medium or low certainty? Decision-makers show both capacity and willingness to 313 engage with the uncertainty information should these data be made available (McKenzie et al., 2014; 314 Scholes et al., 2013; Willcock et al., 2016), even when results may indicate high levels of uncertainty. 315 This is illustrated by a Sicilian case study, in which decision-makers, when advised of the relatively low 316 overall classification accuracy (43%), accepted it as predictions were close to their actual value (i.e. 317 73% of test data were predicted within one class above or below their actual class) and were viewed 318 as an improvement on previous estimates (Figure 2). Thus, providing estimates of uncertainty should 319 become standard practice within the ES community (Hamel and Bryant, 2017).

320

321 There are both advantages and disadvantages to using machine learning algorithms for the 'data 322 mining' step of DDM (Fayyad et al., 1996). As highlighted above, machine learning algorithms provide 323 indications of uncertainty that could usefully support decision-making. However, similar uncertainty 324 metrics can also be obtained using conventional modelling (i.e., via the confidence intervals 325 surrounding regressions (Willcock et al., 2014) or Bayesian belief networks (Balbi et al., 2016)). Similar 326 to conventional modelling, the performance of model algorithms substantially depends on the 327 parameters, model structure and algorithm settings applied (Zhang and Wallace, 2015). For example, 328 many machine learning algorithms require categorical data and so potentially an additional step of 329 data processing whereby continuous data are discretised. In our South African case study, we divided 330 firewood use data into five bins but acknowledge that the number of bins may affect model 331 performance and the impact of this warrants further investigation (Friedman and Goldszmidt, 1996; 332 Nojavan et al., 2017; Pradhan et al., 2017). However, a variety of machine learning algorithms are 333 available (Table 1) and not all of them required discretised data (Jordan and Mitchell, 2015; Witten et 334 al., 2016). Furthermore, for our firewood models, we used machine learning to create the model 335 structure. Structural learning can yield better performing models (i.e., all our South African model 336 configurations had a classification accuracy above 80%; Appendix 1) and may highlight relationships 337 that have not yet been theorised (or have previously been discarded) (Gibert et al., 2008; Suominen 338 and Toivanen, 2016). However, the obtained structures (Figure 3) may not be causal and could confuse 339 end-users (Schmidhuber, 2015). Thus, predefined network structures may be preferred for 340 applications where causality is particularly important. Further generalisations useful for ES modellers 341 considering machine learning algorithms include the following: 1) Multi-classification problems may 342 have lower accuracy - as highlighted by comparing our South African (2 category output, 82% 343 accuracy) and Sicilian (10 category output, 43% accuracy) examples – the more categories in the 344 modelled output, the lower the apparent accuracy. Thus, the number of categories in the output 345 should be considered when interpreting the model accuracy metric. For example, a random model 346 with a two category output and a four category output will be accurate 50% and 25% of the time 347 respectively. Thus, a machine-learned model with an accuracy of 40% is poor if the output had two 348 categories, but learned more (and so might be of more use) if a four category output was being 349 considered; 2) Supervised learning can be used when drivers are known – for example, with no a priori 350 assumptions, unsupervised learning could cluster beneficiaries into groups, but these may not match 351 known beneficiary groups (i.e., livelihoods) and so might be difficult to interpret (Schmidhuber, 2015). Supervised learning can be used to align the outputs from machine learning algorithms with decision-352 353 maker specified beneficiary groups; 3) machine learning algorithms are best applied to the past and 354 present, but not the future – Although machine learning algorithms can detect strong relationships, 355 accurately describing past events and providing useful predictions where process-based 356 understanding is lacking (Jean et al., 2016), the relationships identified may not be causally linked and 357 so may not hold when extrapolating across space or time (Mullainathan and Spiess, 2017). Thus, where 358 the process is well understood, DDM is unlikely to be more appropriate than conventional process-359 based models (Jordan and Mitchell, 2015). Understanding the caveats and limitations of machine 360 learning algorithms is important before the algorithms are used for DDM.

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362 A further critique of DDM is that it can appear as a 'black box' in which the machine learning processes 363 are not clear to the user and so they could widen the implementation gap (Clark et al., 2016; Olander et al., 2017; Wong et al., 2014). However, we have demonstrated that utilisation of machine learning 364 365 algorithms can be transparent and replicable. For example, Bayesian networks allow the links between 366 data to be visualised (Figure 3) (Aguilera et al., 2011; Chen and Pollino, 2012; Landuyt et al., 2013). 367 The standalone Weka software is user friendly and requires minimal expertise, and ease of use has 368 been further simplified within the ARIES software as DDM can be run merely by selecting a 369 spatiotemporal modelling context and then using the 'drag-drop' function to start the machine 370 learning process (Villa et al., 2014). Machine learning and machine reasoning (Bottou, 2014) are 371 facilitated within the ARIES system through semantic data annotation, which makes data and models 372 machine readable and allows for automated data selection and acquisition from cloud-hosted 373 resources, as well as automated model building (Villa et al., 2017). To ensure that this complex process 374 remains transparent, the Bayesian network is described using a provenance diagram (Figure S2), 375 characterising the DDM process, i.e., which data and models were selected by ARIES (Figure 1). 376 Furthermore, work has begun to enable the ARIES software to produce automated reports that 377 describe the DDM process and modelling outputs in readily understandable language (see Appendix 378 2 for a preliminary automated report for the ARIES example used in this study). Advances such as this 379 may enable decision-makers to run and interpret ES models with minimal support from scientists, 380 potentially increasing ownership in the modelled results and closing the implementation gap (Olander 381 et al., 2017).

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The DDM process encourages scientists to use as much data as possible to generate the highest quality 383 384 knowledge. Machine learning algorithms provide a tool by which 'big data' can be incorporated into 385 ES assessments (Hampton et al., 2013; Lokers et al., 2016; Richards and Tuncer, 2017). For example, 386 using the ARIES software, we demonstrated how Open Street Map data can be included in the 387 machine learning process (Haklay and Weber, 2008). Whilst future research is needed to determine 388 how much data is actually needed, it is clear that ES scientists must contribute to and make use of 389 large datasets to participate in the information age (Hampton et al., 2013), particularly where data 390 are standardised and made machine-readable (Villa et al., 2017). Using machine learning algorithms 391 to interpret big data may help provide a wide range of ES information across the variety of temporal 392 and spatial scales required by decision-makers (McKenzie et al., 2014; Scholes et al., 2013; Willcock et 393 al., 2016). There has been a recent call-to-arms within the ES modelling community to shift focus from

394 models of biophysical supply towards understanding the beneficiaries of ES and quantifying their 395 demand, access and utilisation of services, as well as the consequences for well-being (Bagstad et al., 396 2014; Poppy et al., 2014). Combining social science theory and data to explain the social-ecological 397 processes of ES co-production, use and well-being consequences will likely result in substantial 398 improvements to ES models (Bagstad et al., 2014; Díaz et al., 2015; Pascual et al., 2017; Suich et al., 399 2015; Willcock et al., in revision). Such social science data are sometimes available at large scales (e.g., via national censuses) but, with some notable exceptions (e.g., Hamann et al. (2016, 2015)), are rarely 400 401 used within ES models (Egoh et al., 2012; Martínez-Harms and Balvanera, 2012; Wong et al., 2014). 402 The process of DDM guides researchers in how to incorporate of big data into ES models, scaling up 403 results from sites to continents (Hampton et al., 2013; Lokers et al., 2016). DDM allows an 404 interdisciplinary approach across a large scale and so may help guide global policy-making, e.g., within 405 the Intergovernmental Science-Policy Platform for Biodiversity and Ecosystem Services (IPBES; 406 www.ipbes.net).

407

408 In conclusion, DDM could be a useful tool to scale up ES models for greater policy- and decision-making 409 relevance. DDM allows for the incorporation of big data, producing interdisciplinary models and 410 holistic solutions to complex socio-ecological issues. It is crucial that the approach and results of 411 machine learning algorithms are conveyed to the user to enhance transparency, including the 412 uncertainty associated with the modelled results. In fact, we hope that the validation of ES models 413 becomes standard practice with the ES community for both process-based and DDM. In the future, 414 automation of the modelling processes may enable users to run ES models with minimal support from 415 scientists, increasing ownership in the final output. Such automation should be accompanied by 416 transparent provenance information and procedures for a computerised system to select context-417 appropriate data and models. Taken together, the advances described here could help to ensure ES 418 research contributes to and inform ongoing policy processes, such as IPBES, as well as national-, 419 subnational-, and local-scale decision making.

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