Improving data quality to build a robust distribution model for Architeuthis dux

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8 Abstract

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The giant squid (Architeuthis) has been reported since even before the 16th century, and has recently been observed live in its habitat for the first time. Among the species belonging to this genus, Architeuthis dux has received special attention from biologists. The distribution of this species is poorly understood, as most of our information stems from stranded animals or stomach remains. Predicting the habitat and distribution of this species, and more in general of difficult to observe species, is important from a biological conservation perspective. In this paper, we present an approach to estimate the potential distribution of A. dux at global scale, with relative high resolution (1-degree). Our approach relies on a complex preparation phase, which improves the reliability of presence, absence and environmental data correlated to the species habitat. We compare our distribution with those produced by state-of-the-art approaches (MaxEnt and AquaMaps), and use an expert-drawn map as reference. We demonstrate that our model projec-

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tion is in agreement with the expert's map and is also compliant with several biological assessments of the species habitat and with recent observations. Furthermore, we show that our approach can be generalized as a paradigm that is applicable to other rare species.

• Keywords: Ecological Niche Modelling, AquaMaps, Neural Networks, rare

¹⁰ species, Maximum Entropy

11 1. Introduction

12 In recent years, niche models that estimate species distribution have become widely used in conservation biology (Guisan and Zimmermann, 2000). 13 Rare species are examples where the prediction of suitable habitats is paramount 14 to support fisheries management policies and conservation strategies (Pearce 15 and Boyce, 2006; Márcia Barbosa et al., 2003). Defined by Cao et al. (Cao 16 et al., 1998) as species that occur at lower frequency or in low number in a 17 sample of certain size, rare species have a key role in affecting biodiversity 18 richness and by consequence they are indicators of degradation for aquatic 19 ecosystems (Lyons et al., 1995; Cao et al., 1998). In this context, predictive 20 models can considerably support the qualitative and quantitative criteria 21 used to assign a "status" to a species (IUCN Species Survival Commission 22 and Natural Resources. Species Survival, 2001), by providing accurate, ap-23 plicable and reliable spatial predictions to species population monitoring and 24 sampling (Guisan et al., 2006). As discussed in many studies, the method-25 ological progresses of Species Distribution Models (SDMs) allow nowadays to 26

apply robust techniques to rare and endangered species (Guisan and Thuiller, 27 2005; Ferrier, 2002; Gibson et al., 2007; Razgour et al., 2011; Ovaskainen and 28 Soininen, 2011; Rebelo and Jones, 2010; Wisz et al., 2008; Lomba et al., 2010). 29 Here, we propose a procedure to generate a niche model for a species 30 of the giant squid family (Architeuthis dux), based on both presence and 31 estimated absence locations. Our aim is to produce a map that is more 32 accurate with respect to the ones that can be produced by commonly used 33 models. Although giant squids have recently received special attention, little 34 has been published regarding the population demographics and the ecology 35 of these rare species. Most of the records refer to dead stranded animals, 36 individuals captured alive by nets or from the remains found in the stomach 37 of marine mammals (Clarke, 2006). When modelling the distribution of 38 these species, high quality data are crucial but very scarce. This problem 39 is especially important for rare species prediction, where models training is 40 highly dependent on data quality. 41

Given this context, our study investigates a combination of presence only and presence/absences techniques to identify potentially suitable areas for *A. dux* subsistence. We also expect the results to help defining guidelines for use of SDMs for rare species.

We illustrate our approach using data from authoritative sources of observation records. Furthermore, we use an expert system to produce absence locations. In order to ensure high quality for the environmental variables associated to presence information, we use the Maximum Entropy (MaxEnt)

model (Phillips et al., 2006; Berger, 1996) as a filter to select the variables 50 that are important to define the potential habitat of the species. These are 51 the variables that are mostly correlated to the species observations, among 52 those we selected from reference studies. When possible, we make environ-53 mental variables values range from 450 to 1000 m, encompassing the deep 54 ocean waters usually inhabited by A.dux (Guerra et al., 2010). Finally, we 55 train an Artificial Neural Network on these datasets and compare the results 56 with (i) a presence-only method, (ii) an expert system and (iii) an expert 57 drawn map. 58

The paper is organized as follows: Section 2 reports the effort made to model or understand the potential habitat of rare species, and in particular of A. dux. Section 3 reports the details of our method and its expandability as a general approach to rare species modelling. Section 4 reports the results of both a qualitative and a quantitative comparison with other distribution maps for A. dux. Section 5 discusses the results and Section 6 draws the conclusions.

66 2. Overview

This Section is divided into two subsections. The first reports the current understanding of the distribution of *Architeuthis dux*. The second describes the niche modelling approaches that have been applied or that can be applied to rare species.

71 2.1. Species overview

The Architeuthis genus has been recorded since before the 16th century 72 (Guerra et al., 2011), and has recently been observed live in its natural habi-73 tat for the first time (Kubodera and Mori, 2005). Literature studies have 74 recognized up to five species of this genus (Robson, 1933), although Nesis 75 (Nesis, 1987) and Aldrich (Aldrich, 1991) suggested them to be identified as 76 Architeuthis dux. Most of the records refer to stranded animals or stomach 77 remains, and are located in the North Atlantic (e.g. Norway), in the North-78 East Atlantic (off northern Spain), in the South Atlantic (e.g. Namibia and 79 South Africa) and in the South-West Pacific, around New Zealand and Tas-80 mania (Gonzalez et al., 2000; Clarke, 2006; Förch, 1998; Guerra et al., 2004; 81 Bolstad and O'Shea, 2004; Guerra et al., 2004). Most of these animals have 82 been classified as A. dux (Cherel, 2003; Clarke, 2006; Bolstad and O'Shea, 83 2004; Guerra et al., 2010; Clarke, 2006; Nesis, 2003; Aldrich, 1991), but many 84 more refer to the genus level (Architeuthis spp.) without further specifica-85 tion (Lordan et al., 1998; Gonzalez et al., 2000; Ré et al., 1998; Arfelli et al., 86 1991; Kubodera and Mori, 2005; Roeleveld and Lipinski, 1991). In 2003, 87 Nesis (Nesis, 2003) published the distribution of Architeuthis dux by corre-88 lating latitudinal zones and zoogeographic provinces in the pelagic realm. 89 The identified zonality mainly reflects the general oceanic circulation, and 90 no temperature data was used for the selection of the latitudinal zones. The 91 author identified rate of speciation among the Cephalopoda taxon caused by 92 climatic and orogenic isolation and bi-subtropical species of Architeuthis dux 93

⁹⁴ in the North Atlantic, the South Pacific and the Southern Ocean. In this
⁹⁵ paper, we take the map of Nesis as a reference to assess the performance of
⁹⁶ our models.

Several authors have suggested that *Architeuthis* is an epipelagic/mesopelagic 97 species, living in correspondence with continental slopes, submarine channels 98 or canyons (Roeleveld and Lipinski, 1991; Kubodera and Mori, 2005). Guerra 99 et al. (Guerra et al., 2011) examined the relationship between the number 100 of recorded specimens and some of the main characteristics of the observa-101 tion areas. The authors report the close association of giant squids with 102 sperm whales sights (Clarke and Pascoe, 1997). They indicate correlation of 103 Architeuthis spp. sighting with places presenting high primary production 104 and close to shallow fishing grounds. They also report low incidence of genus 105 sighting, in locations where deep channels or canyons are not present (Guerra 106 et al., 2004). On the basis of the distribution of the strandings, Robson (Rob-107 son, 1933) noticed that Architeuthis is adapted to temperate waters of about 108 10 °C. This biological information is in agreement with later studies, that 109 correlate the giant squid presence with the increase of the temperature in 110 some locations (Brix, 1983; Guerra et al., 2004). 111

In this paper, we demonstrate that our results are in agreement with most of these considerations.

114 2.2. Modelling approaches

SDMs produce species distributions at global or local scale, by relating 115 species occurrence records with a set of environmental parameters. Many 116 methods are available (Pearson, 2012), some using only presence records and 117 others using both presence and absence records (Ready et al., 2010; Coro 118 et al., 2013b; Guisan and Zimmermann, 2000; Hirzel and Le Lay, 2008). 119 Niche models usually report either the potential or the actual distribution of 120 a species (Elith and Leathwick, 2009; Pearson, 2012). In the case of the po-121 tential distribution, the model searches for locations with a suitable habitat, 122 rather than detecting locations where the species is really present (actual 123 distribution). 124

Presence-absence methods have been recognized to be the best in produc-125 ing the potential niche of a species, especially for wide-ranging and tolerant 126 species when the quality of the data is high (Elith and Leathwick, 2009; 127 Brotons et al., 2004). Nevertheless, scarcity of data is a common issue when 128 modelling rare species: few records are present in biodiversity databases, and 129 often scarce in both quality and geospatial reliability (Engler et al., 2004). 130 Providing reliable presence and absence data, enhances the performance of 131 niche models (Guisan and Zimmermann, 2000). However, the identification 132 of absences should be carefully addressed, since they bear strong imprints 133 of biotic interactions, dispersal constraints and disturbances (Pulliam, 2000; 134 Gibson et al., 2007; Hirzel and Le Lay, 2008; Cianfrani et al., 2010). 135

¹³⁶ In this paper, we use different approaches to model the potential distri-

bution of A. dux. We take the AquaMaps expert system as reference for the 137 comparison. The AquaMaps algorithms (Kaschner et al., 2006, 2008) are 138 presence-only models that include scientific expert knowledge into species 139 habitats modelling (Ready et al., 2010). The AquaMaps algorithms include 140 two models: AquaMaps Suitable and AquaMaps Native, addressing the po-141 tential and the actual distribution of a species respectively. Expert knowl-142 edge is used in modelling species-habitat relations at global scale with 0.5° 143 resolution, relying on the following environmental variables: depth, salinity, 144 temperature, primary production, distance from land and sea ice concentra-145 tion (Corsi et al., 2000). AquaMaps combines mechanistic assumptions and 146 automatic procedures for habitat parameters and species values estimations, 147 making the modelling approach usually reliable, but less accurate when ex-148 pert knowledge at global scale is missing. In the experiment for this paper, we 149 used AquaMaps Native to produce absence locations and AquaMaps Suitable 150 as reference to assess the performance of the other models. 151

One largely used presence-only technique is Maximum Entropy (MaxEnt) 152 (Phillips et al., 2006; Phillips and Dudik, 2008). The general idea of MaxEnt 153 is to approximate a probability density function, defined on an environmental 154 features vectorial space, ensuring that this function is compliant with the 155 mean values at the presence locations, and that the entropy of the probability 156 distribution is maximum (Elith et al., 2011). The algorithm relies on unbiased 157 samples, so effort in collecting a set of high quality presence records is critical 158 to avoid estimation errors (Elith and Leathwick, 2009). We used MaxEnt as 159

a reference model to assess the performance of our approach. On the other
hand, MaxEnt is a fundamental part of our approach, because we used it to
help a presence-absence model by providing features that are important to
assess habitat suitability. We give more details about our MaxEnt usage in
Section 3.3.

Among the many presence/absence models, Artificial Neural Networks 165 (ANNs) have demonstrated to gain good performance with respect to other 166 approaches, especially for rare species (Pearson et al., 2002; Coro et al., 167 2013b). ANNs try to automatically simulate the probability of occurrence of 168 a species, given certain environmental conditions. They learn on the basis of 169 the environmental characteristics of positive and negative examples. We used 170 ANNs to combine the outputs of our presence/absence data production and 171 of the environmental features filtering phase. In Section 3.5 we give details 172 about our usage of ANNs. 173

174 3. Method

In this Section we describe the technology which supported the experiments, and we also report our procedures for data preparation and environmental features selection. Furthermore, we explain our presence/absence approach to model the distribution of A.dux and its relevance for other rare species.

180 3.1. Technology and tools

Preparing an experimental setup to model the distribution of a rare 181 species requires expertise in several disciplines. The model requires highly 182 reliable presence records. The environmental features describing the ecolog-183 ical niche of the species should be of high quality and with the appropriate 184 spatial resolution (Kamino et al., 2012; Elith and Leathwick, 2009). Since 185 environmental features are distributed as geospatial datasets, their projec-186 tions should be perfectly aligned in order to correctly retrieve correspondent 187 values. During the training phase, different models need to be tested and 188 reapplied to avoid problems of local minimum of the fitting curve (Bishop, 189 1995) and if several models are combined, the output of a model must agree 190 with the input of the next. 191

We overcame these issues of high quality environmental features sets 192 and their alignment by using an e-Infrastructure for biodiversity conserva-193 tion (D4science) (Candela et al., 2009). D4Science supplies several mod-194 els as-a-service. The model compatibility is guaranteed by specialized e-195 Infrastructure services. Furthermore, D4Science uses Cloud computing to 196 speed processing up (Coro et al., 2013b; Candela et al., 2013). D4Science 197 provides automatic alignment and comparison of geospatial datasets (Coro. 198 2014), by re-projecting environmental features into a common coordinates 199 system. 200

D4Science hosts a large variety of environmental features at global scale, with resolution varying from 0.01 degrees to 1 degree (Castelli et al., 2013). D4Science also allows retrieving species presence information from heterogeneous biodiversity data collections (e.g. OBIS (Berghe et al., 2010), GBIF (Edwards et al., 2000) and the Catalog of Life (Wilson, 2003)), under the same format (Candela et al., 2014). Information is attached to each presence record, to indicate the ownership of the observation, its source (e.g. human observation, specimen etc.) and possibly if the record underwent expert review.

210 3.2. Occurrence data preparation

We used a presence-absence modelling approach, to find correlation be-211 tween the presence records of Architeuthis dux and a multidimensional space 212 made up of environmental features. We decided to use high quality presence 213 points and reliable absence locations as input to our models, according to 214 the indications reported in Section 2.2. Using the D4Science web services 215 (Candela et al., 2014), we retrieved human observations for A. dux from 216 authoritative sources. We came up with 11 records from OBIS and 1 from 217 GBIF. The records are reported in Table 1, along with the name of the sub-218 collection hosting each record. The records had indication about the experts 219 that identified the species. Most points belong to the area around the Gulf 220 of Mexico and one is in North-West Atlantic. The point from GBIF is in 221 agreement with the records from OBIS, thus we decided to use it. We lim-222 ited the records to the ones for A. dux only. In the context of improving 223 data quality, we did not include the other Architeuthis species. 224

It is notable that both OBIS and GBIF contain few of the recent live 225 observations of Architeuthis dux. In particular, the observations from Ceph-226 Base in Table 1 are the only direct observations, whereas the records from 227 the Smithsonian Institute and the Florida Museum of Natural History come 228 from specimens that have been found in the stomach of sperm whales or 229 floating on the sea surface. The other observation records are reliable esti-230 mates from the Biodiversity of the Gulf of Mexico Database, derived from 231 literary studies or unregistered observations that have been later validated 232 by experts. The points in Table 1 are associated to the species presence in 233 a depth range between 700 and 475 meters. In our SDM, we used a large 234 resolution of 1° and this softens errors due to the usage of non-exact presence 235 locations. Thus we decided to employ all the points in Table 1 in our model. 236 On the other hand, we used recent live observations of A. dux, not included 237 in OBIS and GBIF, to validate our model (see Section 4.1). 238

Data retrieved using D4Science follow the Darwin Core format (Wieczorek et al., 2012) and can be provided as input to the D4Science models directly. All models accept the same format of input data of presence records, which makes the data preparation phase faster.

243 3.3. Environmental data selection

The environmental characteristics in our model refer to geospatially explicit chemical and physical measurements. During its training session, our model learns from positive and negative examples that are based only on environmental features. In the subsequent projection session, a real value from
0 to 1 is associated to several locations to assess their habitat suitability. A
well performing model is one having good projection on the locations of the
training set and, at the same time, not suffering of overfitting issues on the
training values (Bishop, 1995).

Environmental features selection requires attention (see Section 2.2) to 252 ensure they are not highly correlated: adding a feature that is dependent on 253 previous ones would not bring more information to the model, but it could 254 add noise during the training session. Furthermore, the spatial resolution 255 should fit the precision of the projection: a model that has to produce a map 256 with resolution 0.5 degrees, should rely on environmental information with 257 the same resolution. This allows not using values coming from rescaling pro-258 cesses or kriging that would add uncertainty to the measurements. Global 259 scale maps also contain estimated values, but these have been produced by 260 experts. Thus, we recommend using the native resolution of the environ-261 mental datasets in global scale modelling. Furthermore, the reliability of the 262 data is crucial. This depends on the data provider, as some providers require 263 the dataset to pass a data quality process in order to be published (e.g. My-264 Ocean (Bahurel et al., 2010) and the World Ocean Atlas (Locarnini et al., 265 2006)). 266

Features selection methods analyse the features space. Several approaches try to reduce the dimensions of this space, for example by recovering the most independent features or combining them into new features (Jolliffe, 270 2005; MacLeod, 2010). In our approach, instead, we wanted to reduce the 271 dimension of the number of features to use, but at the same time we wanted to 272 take the correlation between presence points and random points (background 273 points) into account. To such aim, we used the MaxEnt model as a features 274 filter.

We collected environmental features that could a priori influence the 275 habitat suitability for A. dux, according to the studies we have reported in 276 Section 2.1. We chose the parameters reported in Table 2, averaged on 277 annual values. Based on the depth range of our presence points and on 278 indications from literature (Guerra et al., 2010), we took parameters values 279 in the following ranges: (i) in the entire water column, (ii) averaged between 280 450 and 1000 meters, (iii) at surface level. In particular, we used the 450-1000 281 m range when the data provider reported information at several depth ranges. 282 Table 2 indicates the ranges we used for each parameter. The parameters 283 layers come with different projections and reference systems, but the MaxEnt 284 implementation on D4Science automatically accounts for making the layers 285 projections and reference systems uniform, before training the models. In 286 our experiments, the layers from MyOcean and the World Ocean Atlas were 287 available in the e-Infrastructure as GIS layers, while we provided the others 288 as external datasets, in one of the accepted D4Science input formats (Coro, 289 2014). 290

During the training phase, MaxEnt minimizes the relative entropy of the features at the presence locations, with respect to the features of random

points (Phillips et al., 2006). Presence points are taken as constraints during 293 this minimization. The model uses a linear combination of the features, where 294 the coefficients of the combination are adapted to reflect the "importance" of 295 each variable in predicting the distribution of the species. After the training 296 phase, MaxEnt also reports these coefficients. We relied on these to select 297 the features that provided the most information about the species' habitat 298 preferences, from the point of view of a machine learning model. In other 299 words, we used MaxEnt to filter out the features that could bring noise or that 300 did not bring more information to a model for A. dux. We set a non-strict 301 cut-off threshold, taking all the features that had coefficients values higher 302 than the 5% of the maximum coefficient value. In the end, MaxEnt produced 303 the following list of features from the ones in Table 2, ranked according to 304 a decreasing importance: (i) mole concentration of Silicate, (ii) depth, (iii) 305 maximum temperature in the water column, (iv) ph, (v) mole concentration 306 of Nitrate, (vi) range of temperature in the water column, (vii) distance from 307 land, (viii) mass concentration of Chlorophyll. 308

309 3.4. Absence points

In order to improve data quality, we searched for a method to produce robust absence locations. Several methods exist to estimate absence locations (Pearson, 2012), but we avoided introducing biases by using other machine learning models. One approach that proved to be effective, is to use an expert system to generate absence locations (Coro et al., 2013b,a). Expert systems

combine automatic processing with expert indications and can be used to 315 simulate expert opinion. Thus, we used AquaMaps Native (see Section 2.2) 316 to retrieve absence areas by looking at locations having probability lower than 317 0.2 but higher than 0. Setting the threshold over zero, selects areas having 318 low values for several environmental envelopes. This approach simulates 319 locations where an expert asserts that the habitat is particularly unsuited 320 for the species. Furthermore, these locations are reported at a relatively 321 high resolution of 0.5 degrees at global scale. From the AquaMaps Native 322 distribution, we extracted absence scattered locations, because this allows 323 having a wider range of environmental characteristics for low probability 324 locations. We took only absences that were two degrees distant at least. In 325 another work (Coro et al., 2013a), we demonstrated that this method results 326 in better performance than using concentrated absence records. 327

In order to balance the number of presence and absence records, we limited the absence locations to 25 points, slightly more than two times the presence points. These points gave us a wide range of absence environmental features and, at the same time, limited possible over-prediction tendency by niche models. Figure 1 reports the AquaMaps Native distribution for Architeuthis dux, and the presence/absence dataset resulting from our selection.

334 3.5. Modelling

In order to produce distribution maps for *Architeuthis dux*, we used both MaxEnt and Artificial Neural Networks. As input data, we used the presence dataset described in Section 3.2, the pseudo-absences extracted from AquaMaps (see Section 3.4) and the filtered environmental features described in Section 3.3. We assumed that this input was of sufficient quality to ensure the reliability of the models.

We used the MaxEnt model as benchmark to evaluate the performance 341 of an Artificial Neural Network. Our aim was to compare a state-of-the-art 342 model (MaxEnt) that has been yet used to model rare species (Wisz et al., 343 2008; Elith et al., 2011; Phillips and Dudik, 2008), with a new approach using 344 MaxEnt only to filter out noisy environmental features. In our experiment, 345 we used the MaxEnt implementation of D4Science (Coro, 2014), which is 346 based on the one by the Phillips et al. (Phillips et al., 2006). We trained 347 the model at global scale, with 1-degree of resolution, since this was the 348 highest degree available for our layers and we wanted to avoid resampling. 349 Consequently, also the projection of the model had a 1-degree resolution. 350 We assumed a 0.5 value for the default species prevalence parameter and 351 executed 1000 learning iterations. We performed several training sessions 352 to ensure that the model consistently converged to the same parameters 353 estimation. 354

In order to evaluate the performance of MaxEnt in distinguishing between absences and presences in the training dataset, we referred to the AUC curve of the model. This indicates the probability threshold to assert a location is suitable to a species. We found that this probability threshold was 0.03 for our model. Thus, we assumed that all probabilities above this threshold identified a location viable for A. dux to a certain degree. The resulting distribution map is displayed in Figure 2.

Artificial Neural Networks, in particular Feed Forward Neural Networks 362 (FFNNs) (Bebis and Georgiopoulos, 1994), have proven good performance 363 in niche modelling and have been applied to model the distribution of rare 364 species (Pearson, 2012; Coro et al., 2013b). Furthermore, with respect to al-365 ternative models, they have proven to perform better when the quality of the 366 data is high (Coro et al., 2013b). The aim of an FFNN is to build a hierarchi-367 cal multi-layered network, made up of interconnected nodes, which simulates 368 a complex function. The complexity of the function depends on the number 369 of layers and neurons in the network. During a training session, the weights 370 of the network connections are adapted to produce expected values on the 371 training dataset. In our case, the training set consisted of the environmental 372 features at presence and absence locations, where features were extracted 373 at 1-degree resolution. The FFNN performance depends only on the values 374 assumed by the features on the training set, differently from MaxEnt. For 375 presences, the expected value was set to 1 and for absences it was set to 376 0. In order to define the optimal number of layers and neurons per layer 377 to use in the network, we adopted a *growing* strategy (Bishop, 1995). We 378 added neurons and layers as far as the error with respect to the training set 379 decreased after a training session (up to a certain threshold). The threshold 380 was empirically set to 0.01 in order to avoid overfitting. We executed the 381 Network training session 10 times for each topology and eventually took the 382

one with the best learning result, i.e. with the lowest mean error with respect 383 to the training points. This process ended in two Networks achieving good 384 learning capacity: one having two layers, with 10 neurons in the first layer 385 and 2 in the second, the other having two layers too, with 100 neurons in 386 the first layer and 2 in the second. We will refer to the first as the "simple 387 topology FFNN" and to the second as the "complex topology FFNN". One 388 characteristic of the second FFNN is that the learning process is more stable, 389 i.e. it usually ends in the same distance from the training set. On the other 390 hand, using simpler topologies is better especially to avoid overfitting issues. 391 Indeed, in Section 4 we demonstrate that the simpler topology gains overall 392 better performance. In the same way we did for MaxEnt, we calculated that 393 for the FFNNs the best threshold to filter out too low habitat suitability was 394 0.1. Figure 3 reports the maps associated to the two FFNN topologies when 395 we projected the models at global scale, with 1-degree resolution. 396

397 3.6. Applicability to other species

Our approach can be generalized and applied to rare species and to datalimited scenarios that satisfy certain conditions. The main steps and the conditions of this generalized process are the following:

- 1. Retrieve high quality presence locations by relying on the metadata of
 the records,
- 2. Select a number of environmental characteristics correlated to the species
 presence,

- 3. Use MaxEnt to filter the environmental characteristics that are really
 important with respect to the presence points,
- 407 4. Use expert knowledge or an expert system to detect absence locations.
 408 Select absence locations as widespread as possible,
- 5. Train a Feed Forward Neural Network on presence and absence locations and select the best learning topology,

6. Project the FFNN at global scale, using the a resolution equal to the maximum in the environmental features,

413 7. Train a MaxEnt model as comparison system.

414 4. Results

In this Section we describe the qualitative and quantitative approaches we used to compare the trained models with existing literature data. First, we report a "qualitative" comparison on coarse presence locations reported in literature for *Architeuthis dux* and *Architeuthis* spp. In order to investigate the differences between the models in detail, we also report the results of a quantitative comparison, with respect to a map drawn by an expert (Nesis, 2003).

422 4.1. Qualitative evaluation

We used Architeuthis dux and Architeuthis spp. records reported by different authors (Kjennerud, 1958; Aldrich, 1991; Arfelli et al., 1991; Roeleveld and Lipinski, 1991; Lordan et al., 1998; Ré et al., 1998; Gonzalez et al., 2000;

Cherel, 2003; Kubodera and Mori, 2005; Clarke, 2006; Guerra et al., 2010) 426 in a qualitative analysis of the models performance. The list of reference 427 areas resulting from this analysis is reported in Table 3. Architeuthis dux 428 was identified in six areas, while the other eight locations refer to the generic 429 Architeuthis spp. We compared our models on these areas, reporting 1 when 430 there was at least one location having non-zero probability and 0 otherwise. 431 Since our models produce potential niche estimations, we also added the 432 AquaMaps Suitable model to the comparison, which is depicted in Figure 4. 433 In this scenario, the performance of the FFNNs is the same, because they 434 predict habitat suitability in almost all the areas where A. dux was recorded, 435 and in six of the eight areas where only the genus was reported. Differences 436 between the behaviours of the two FFNNs are in Kerguelen Islands and off 437 the bay of Biscay. It seems that MaxEnt performs slightly better than the 438 FFNNs and AquaMaps, because it matches several areas for both A. dux and 439 A. spp. On the other hand, in many locations the probabilities indicated by 440 the model are low. 441

When we set a probability threshold to filter out values lower than 0.8, the maps highlight only the places with high habitat suitability. In this case, the results of the assessments by the models are reported in Table 4. We notice that the FFNN with the simple topology and AquaMaps Suitable still present high performance. In particular, the FFNN predicts species presence in Newfoundland, Norway Sea, South America, South-Eastern Africa and in the Mediterranean Sea. Conversely, the AquaMaps Suitable model covers

the Eastern-North Atlantic, the Kerguelen Islands, the New Zealand coasts 449 and the Tasman Sea. Using this probability threshold, the complex topology 450 FFNN and the MaxEnt model predict very few suitable areas, especially 451 for Architeuthis spp. This means that, overall, the FFNN with the simple 452 topology is more stable and reliable. One evident difference between the 453 FFNNs and the AquaMaps model is that, according to AquaMaps, the species 454 is not present in open ocean but only prefers coastal areas. In order to explore 455 more such difference, we used a quantitative discrepancy analysis. 456

457 4.2. Quantitative evaluation

In order to quantitatively compare the similarity between the maps, we 458 used also a distribution map drawn by an expert, which is depicted in Figure 459 5. Nesis (Nesis, 2003) mapped the distribution of Architeuthis dux relying 460 on his knowledge about the species: he identified three main areas corre-461 sponding to the species presence, i.e. North Atlantic Ocean, North Pacific 462 Ocean and Southern Ocean. In order to make a numeric comparison, we 463 georeferenced this map using QGIS (Quantum GIS, 2011) and obtained a 464 polygonal representation of the distribution. We assigned probability 1 to 465 the regions indicated in the map and forced a 0 value to absence areas that 466 did not contain locations reported in the qualitative analysis, i.e. the Ara-467 bian Sea, the Indian Ocean and the South Atlantic Ocean. The map by Nesis 468 does not have high precision, thus we did not expect a full agreement by the 469 models, but it gives a common field for an overall comparison of the maps. 470

⁴⁷¹ We assumed that the map closest to this was the most reliable.

In order to quantitatively measure the distance between the maps, we 472 used the maps comparison process described in (Coro et al., 2014). This 473 process performs a point-to-point comparison between two maps at a given 474 resolution and calculates indicators of their similarity. Among the measure-475 ments produced by this process, we concentrated on "accuracy", i.e. the 476 ratio of locations where the probabilities by two models give the same value, 477 according to a certain tolerance threshold. We used several tolerance thresh-478 olds to vary the strictness with respect to presence and absence locations. A 479 threshold of 0.3, means that two probability values for a certain location are 480 considered as having the same value if they differ less than 0.3. We performed 48: this point-to-point comparison at 1-degree resolution. 482

Table 5 reports the performance using several thresholds: 0.8, 0.5 and 483 0.3. Furthermore, we made three comparisons with the map of Nesis using 484 presence-only, absence-only and presence-absence polygons separately. In 485 this way we observed that, even if one model can be in good agreement with 486 either presences or absences, it can be in lower agreement with respect to 487 both. The FFNN with the simple topology has lower agreement with absence 488 locations, but overall is the closest to the expert drawn map, according to 489 all the probability thresholds. 490

⁴⁹¹ 5. Discussion

The results demonstrate that, according to a qualitative analysis, the 492 simple topology FFNN gives the most promising results. In this scenario, the 493 AquaMaps Suitable model is indeed the most stable. On the other hand, if 494 we move to a quantitative evaluation with respect to an expert-drawn map, 495 we better understand the differences between AquaMaps and the FFNN. 496 AquaMaps presents few points in open ocean, because the model assigns more 497 weight to the proximity of land, while the expert's map indicates many of 498 these points as suitable locations. This discrepancy is reflected in the overall 499 better similarity between the expert's map and the FFNN map. MaxEnt 500 gains good performance too, but it overestimates absence locations, thus the 501 overall accuracy is lower than the FFNN one. 502

FFNN identifies suitable habitat for Architeuthis dux in the Northern and 503 Eastern Atlantic Ocean (i.e around Newfoundland and in the Norway Sea). 504 This agrees with literature studies that indicate Newfoundland as the original 505 centre of dispersal for the European population of A. dux (Robson, 1933). 506 Our model also agrees with other studies (Roeleveld and Lipinski, 1991; 507 Kubodera and Mori, 2005) reporting records in the North Atlantic Ocean 508 (Sweeney and Roper, 2001) and predicts habitat suitability in correspondence 509 of continental slopes, canyons and abyssal plains. 510

The FFNN is the model that better resembles the expert's map, but more information is needed to ensure its reliability: there are some discrepancy locations, like the South Africa coasts, that need further investigation. The

highest discrepancy with respect to the expert's map is in the South-West 514 coast of South Africa, in the Indian Ocean and in North Australia. This 515 discrepancy could be explained by the fact that the FFNN predicts potential 516 habitat, while the expert indicates the known (actual) habitat. On the other 517 hand, there are studies supporting the indications by the FFNN map: Archi-518 teuthis specimens were captured in South-West Pacific Ocean, and around 519 Australian coasts, especially off the West coasts (Jackson, 1991; Sweeney and 520 Roper, 2001). As for the Indian Ocean, several studies report the presence of 521 Architeuthis near the Reunion Island, the Mauritius Islands and generally in 522 the South-Western Indian Ocean (Sweeney and Roper, 2001; Guerra et al., 523 2011; Cherel, 2003; Mikhalev et al., 1981). In some Indian survey works, it 524 is reported that Architeuthis species are present off the west coasts of India 525 (Silas, 1968, 1985). 526

Some scientists stress out that different species of *Architeuthis* cannot have overlapping populations (Roeleveld and Lipinski, 1991). Although it has been suggested that the West coast of South Africa is a "natural" habitat for *Architeuthis*, no certified record of *A. dux* has been reported yet.

In summary, even if we cannot demonstrate the effectiveness of the FFNN model in this case, we can state that there are good hints about its better reliability with respect to AquaMaps and MaxEnt. This effect is due to the abstraction power of this presence/absence model (Coro et al., 2013b), and also to the data preparation phase of our approach.

536 6. Conclusions

In this paper, we have described a method to predict the distribution 537 of Architeuthis dux at global scale. We have used a presence-only model to 538 identify important environmental features possibly extracted at Architeuthis 539 depth ranges indicated by other studies, we have generated absence locations 540 using an expert system and we have retrieved presence records from two au-54: thoritative data sources. By means of a presence/absence model based on an 542 Artificial Neural Network, we have produced a potential habitat distribution 543 for A. dux having reasonably good reliability. This distribution is the one 544 that is most in agreement with the opinion of an expert. Common traits in 545 the expert's map and in the Neural Network map are visible, e.g. there is a 546 common strip of absences from Brazil to the coasts of Guinea-Sierra Leone. 547 Agreement between the maps in other regions is lower (e.g. in the Indian 548 Ocean), but overall the simple topology FFNN is the best model compared 549 to the maps produced with AquaMaps Suitable and MaxEnt. As discussed 550 in Section 5, the Neural Network map correctly predicts some known species 551 habitat and depicts the potential (not the actual) distribution of the species. 552 It covers locations where the species was observed, but that were not included 553 in the training set, and it neglects other locations where the observations 554 probably did not refer strictly to A. dux. 555

In summary, maximising the reliability of presence, absence and environmental parameters gives good estimate of the distribution of *A. dux*. This maximisation determines reliable patterns of occurrence related to environ⁵⁵⁹ mental gradients, as also supported by other studies (Segurado and Araujo, ⁵⁶⁰ 2004; Franklin, 2010). A large scale distribution for *A. dux* can also help ⁵⁶¹ understanding the role of this species on a broader geographic perspective ⁵⁶² (Lordan et al., 2001).

The work reported in this paper builds on our previous experience on 563 modelling the distribution of the Coelacanth (Coro et al., 2013b). In our 564 previous work, we used a model combining a Neural Network with absence 565 information produced from AquaMaps. The model was trained using only ob-566 servation records near Madagascar and the same environmental parameters 567 used by AquaMaps. The approach was promising, because it predicted habi-568 tat suitability in some locations in Indonesia were a variant of the Coelacanth 569 has been really observed. In this paper we have enhanced this model, because 570 we (i) use other environmental parameters, (ii) select the most influential pa-571 rameters and (iii) suggest a method to compare the results with other maps 572 and understand complementarity. Furthermore, we have explained how our 573 approach can be generalized and extended to other rare species. 574

Generally speaking, the presented work can be useful in species conservation. In fact, model-based approaches for rare species that count on data quality have proved to be valuable when used in population management and conservation strategies (Austin, 2007). In particular, many conservation projects need a complete description of species' geographical distributions, and modelling techniques (e.g. MaxEnt, Artificial Neural Networks and AquaMaps) have already proved to reliably support this activity (Ficetola et al., 2007; Ward, 2007; Hijmans and Graham, 2006; Fitzpatrick et al.,
2008; Thorn et al., 2009; Wollan et al., 2008; Echarri et al., 2009; Cordellier
and Pfenninger, 2009). The produced maps can be also used in fisheries,
because producing a potential distribution for a rare species like the giant
squid can help locating vulnerable marine ecosystems (Auster et al., 2010;
Stevens et al., 2000; Tittensor et al., 2009; Stevens et al., 2000).

The D4Science e-Infrastructure enabled the prediction of the distribution of *A. dux* with powerful modelling resources, automated data retrieval and results sharing. Furthermore, the experiment is fully reproducible. This experiment demonstrates how e-Infrastructures can support species distribution modelling of rare species.

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Data collection	Collection code	Last update	Locality	Lat.	Long.
OBIS	USNM	11/05/2010	Gulf of Mexico	26.98	-90.37
OBIS	HRI	11/12/2009	WSW Gulf of Mexico	22.45	-97.31
OBIS	HRI	11/12/2009	ESE Gulf of Mexico	23.04	-82.93
OBIS	HRI	11/12/2009	NNW Gulf of Mexico	27.69	-91.75
OBIS	HRI	11/12/2009	NNE Gulf of Mexico	29.47	-87.17
OBIS	HRI	11/12/2009	SSE Gulf of Mexico	23.64	-89.18
OBIS	HRI	11/12/2009	ENE Gulf of Mexico	26.91	-84.71
OBIS	HRI	11/12/2009	WNW Gulf of Mexico	26.96	-96.08
OBIS	HRI	11/12/2009	SSW Gulf of Mexico	19.24	-93.51
OBIS	343	n/a	South Carolina coast	31	-76
OBIS	343	n/a	Newfoundland	48.16	-49.33
GBIF	FLMNH	n/a	Florida coast	27.26	-80.01

Table 1: Occurrence records from the OBIS and GBIF data collections. The collection codes refer to the OBIS and GBIF codes for the following sub-collections: Biodiversity of the Gulf of Mexico Database (HRI), Invertebrate Zooology Collections (Smithsonian Institute, USNM), CephBase (343), Florida Museum of Natural History (FLMNH).

Parameter	Spatial Resolution	Unit of Measure	Provider
Minimum tanan ang tung	resolution	Wiedsure	
(in the meter column)	1°	K	World Ocean Atlas
(In the water column)			
(in the meter column)	1°	K	World Ocean Atlas
(In the water column)			
(in the water column)	1°	K	World Ocean Atlas
(In the water column)			
$\left(1000 \text{ m}\right)$	1°	-	World Ocean Atlas
(avg 450-1000 m)			
	0.083°	-	Bio-Oracle
(avg in the water column)			
Mass concentration	0 50	/ . 3	МО
of Uniorophyll	0.5	$m g/m^3$	MyOcean
(avg 450-1000 m)			
Mole concentration	0 50	1/9	
of Nitrate	0.5^{-1}	$\mod m^3$	MyOcean
(avg 450-1000 m)			
Dissolved	10	/1	
Oxygen	1°	m g/l	World Ocean Atlas
(avg 450-1000 m)			
Mole concentration			
of Phosphate	1°	$\mu \text{ mol/l}$	World Ocean Atlas
(avg 450-1000 m)			
Mole concentration	_		
of Silicate	1°	$\mu \text{ mol/l}$	World Ocean Atlas
(avg 450-1000 m)			
Wind stress	0.25°	Pa	MvOcean
(surface level)	0.20	10	Miy O O O U U I
Depth	0 14°		Marine Geoscience
$(\max in a 0.14^{\circ} \text{ sqr. cell})$	0.11		
Distance from land	0.5°	m	AquaMaps
(centre of a 0.5° sqr. cell)	0.0	110	riquamaps

Table 2: Complete list of environmental characteristics related to the *Architeuthis dux* distribution we used in our features selection phase. The datasets come from several and heterogeneous sources: MyOcean (Bahurel et al., 2010), World Ocean Atlas (Locarnini et al., 2006), Bio-Oracle (Tyberghein et al., 2012), Marine Geoscience website (IEDA, 2014) and the AquaMaps website (The AquaMaps Consortium, 2014).

	Species or	FFNN	FFNN		AquaMaps
Areas	Genus	(100-2)	(10-2)	MaxEnt	Suitable
KERGUELEN ISLANDS	A.dux	1	0	0	1
NEW ZEALAND-TASMAN SEA	A.dux	Ţ	1	F-1	Ļ
BAY OF BISCAY	A.dux	0	, - 1	1	Ļ
NORTH-EAST ATLANTIC	A.dux	0	0	1	Ļ
NEWFOUNDLAND	A.dux	Ļ	, - 1	F-1	0
NORWEGIAN SEA	A.dux	Ļ	, - 1	1	Ţ
IRELAND COASTS	Architeuthis spp.	Ļ	, _ 1	1	Ţ,
PATAGONIA	Architeuthis spp.	1	, _ 	1	0
BRAZIL	Architeuthis spp.	1	, _ 1	1	1
JAPAN	Architeuthis spp.	Ļ	, - 1	F-1	1
SOUTH AFRICA-ORANGE RIVER	Architeuthis spp.	0	0	0	0
SOUTH AFRICA-TABLE BAY	Architeuthis spp.	0	0	0	0
SOUTH AFRICA-DURBAN	Architeuthis spp.	1	, _ 	1	Ţ
FUENGIROLA BEACH-MEDITERRANEAN SEA	Architeuthis spp.	1	1	1	<u></u> 1
ACCURACY		71.4%	71.4%	78.6%	71.4%

Table 3: Comparison between the predictions of Architeuthis dux presence on indicative presence areas. The second column
indicates if the species was reported at genus or species level. FFNN (x-y) indicates a Feed-Forward Artificial Neural Network
having 2 layers, with x neurons in the first layer and y neurons in the second. Values equal to 1 indicate that the models report
sensibly non-zero values in that area.

	Species or	FFN	ZZFZ		AquaMaps
Areas	Genus	(100-2)	(10-2)	MaxEnt	Suitable
KERGUELEN ISLANDS	A.dux	0	0	0	
NEW ZEALAND-TASMAN SEA	A.dux	0	0	0	
BAY OF BISCAY	A.dux	0	0	0	
NORTH-EAST ATLANTIC	A.dux	0	0	0	1
NEWFOUNDLAND	A.dux	0	, _ 1	0	0
NORWEGIAN SEA	A.dux	0	, _ 1	1	1
IRELAND COASTS	Architeuthis spp.	0	0	0	1
PATAGONIA	Architeuthis spp.	0	, _ 	0	0
BRAZIL	Architeuthis spp.	0	, _ 	0	1
JAPAN	Architeuthis spp.	Ļ	, _ 1	0	
SOUTH AFRICA-ORANGE RIVER	Architeuthis spp.	0	0	0	0
SOUTH AFRICA-TABLE BAY	Architeuthis spp.	0	0	0	0
SOUTH AFRICA-DURBAN	Architeuthis spp.	0	, _ 	0	1
FUENGIROLA BEACH-MEDITERRANEAN SEA	Architeuthis spp.	0	1	-	1
ACCURACY		7.1%	50%	14.3%	71.4%

Table 4: Comparison between the predictions of *Architeuthis dux* presence on indicative presence areas, when the probability threshold for sensibly non-zero values is set to 0.8. The second column indicates if the species was reported at genus or species level. FFNN (x-y) indicates a Feed-Forward Artificial Neural Network having 2 layers, with x neurons in the first layer and y neurons in the second. Values equal to 1 indicate that the models report sensibly non-zero values in that area.

Accuracy with res	sp. to Ne	sis (Nesis	s, 2003).		
	Compa	rison thr	esholds		
	0.8	0.5	0.3		
Presences and Absences					
FFNN (10-2)	42.83%	30.56%	26.81%		
MaxEnt	21.68%	18.36%	17.65%		
AquaMaps Suitable	22.01%	20.19%	18.83%		
FFNN (100-2)	29.85%	20.56%	16.3%		
Pre	esences-or	nly			
FFNN (10-2)	44.42%	31.42%	27.81%		
MaxEnt	4.72%	0.78%	0.19%		
AquaMaps Suitable	5.35%	3.95%	2.61%		
FFNN (100-2)	17.91%	9.24%	6.42%		
Absences-only					
FFNN (10-2) 38.27% 29.53% 25.09%					
MaxEnt 100% 100% 99.21%					
AquaMaps Suitable	99.46%	95.78%	94.35%		
FFNN (100-2)	87.77%	75.55%	64.5%		

Table 5: Accuracy of a point-to-point maps comparison process at 1-degree resolution (Coro et al., 2014), using presence and absence locations indicated by Nesis (Nesis, 2003). The performance is reported also on presence and absence locations separately.



Figure 1: a. The AquaMaps Native distribution for *Architeuthis dux*. Darker colours refer to higher probability locations. b. The presences/absence points resulting from our process. Darker colours refer to presence locations.



Figure 2: Distribution of A. dux produced with the MaxEnt model, trained using our filtered environmental features.



Figure 3: Distribution of A. dux produced by two Artificial Feed Forward Neural Networks: (a) with 2 layers, containing 10 neurons in the first layer and 2 in the second; (b) with 2 layers, containing 100 neurons in the first layer and 2 in the second.



Figure 4: Distribution of A. dux produced with the AquaMaps Suitable model (Kaschner et al., 2008).



Figure 5: Distribution of A. dux reported by Nesis (2003).