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End–to–end modelling for an ecosystem approach to fisheries in the Northern Humboldt Current Ecosystem

Modélisation “end–to–end” pour une approche écosystémique des pêches dans le Nord courant de Humboldt

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Abstract

This work represents an original contribution to the methodology for ecosystem models' development as well as the first attempt of an end-to-end (E2E) model of the Northern Humboldt Current Ecosystem (NHCE). The main purpose of the developed model is to build a tool for ecosystem-based management and decision making, reason why the credibility of the model is essential, and this can be assessed through confrontation to data. Additionally, the NHCE exhibits a high climatic and oceanographic variability at several scales, the major source of interannual variability being the interruption of the upwelling seasonality by the El Niño Southern Oscillation, which has direct effects on larval survival and fish recruitment success. Fishing activity can also be highly variable, depending on the abundance and accessibility of the main fishery resources. This context brings the two main methodological questions addressed in this thesis, through the development of an end-to-end model coupling the high trophic level model OSMOSE to the hydrodynamics and biogeochemical model ROMS-PISCES: i) how to calibrate ecosystem models using time series data and ii) how to incorporate the impact of the interannual variability of the environment and fishing.

First, this thesis highlights some issues related to the confrontation of complex ecosystem models to data and proposes a methodology for a sequential multi-phases calibration of ecosystem models. We propose two criteria to classify the parameters of a model: the model dependency and the time variability of the parameters. Then, these criteria along with the availability of approximate initial estimates are used as decision rules to determine which parameters need to be estimated, and their precedence order in the sequential calibration process. Additionally, a new Evolutionary Algorithm designed for the calibration of stochastic models (e.g Individual Based Model) and optimized for maximum likelihood estimation has been developed and applied to the calibration of the OSMOSE model to time series data.

The environmental variability is explicit in the model: the ROMS-PISCES model forces the OSMOSE model and drives potential bottom-up effects up the foodweb through plankton and fish trophic interactions, as well as through changes in the spatial distribution of fish. The latter effect was taken into account using presence/absence species distribution models which are traditionally assessed through a confusion matrix and the statistical metrics associated to it. However, when considering the prediction of the habitat against time, the variability in the spatial distribution of the habitat can be summarized and validated using the emerging patterns from the shape of the spatial distributions. We modeled the potential habitat of the main species of the Humboldt Current Ecosystem using several sources of information (fisheries, scientific surveys and satellite monitoring of vessels) jointly with environmental data from remote sensing and in situ observations, from 1992 to 2008. The potential habitat was predicted over the study period with monthly resolution, and the model was validated using quantitative and qualitative information of the system using a pattern oriented approach.

The final ROMS-PISCES-OSMOSE E2E ecosystem model for the NHCE was calibrated using our evolutionary algorithm and a likelihood approach to fit monthly time series data of landings, abundance indices and catch at length distributions from 1992 to 2008. To conclude, some potential applications of the model for fishery management are presented and their limitations and perspectives discussed.

Résumé

Ce travail représente une contribution originale à la méthodologie pour le développement de modèles écosystémiques ainsi qu'une première tentative d'une modélisation end-to-end (E2E) del'écosystème du Courant de Humboldt Nord (NHCE: Northern Humboldt Current Ecosystem). L'objectif principal du modèle développé dans cette thèse est de construire un outil de gestion écosystémique et d'aide à la décision ; raison pour laquelle la crédibilité du modèle est essentielle, laquelle peut-être établie par confrontation aux données. En outre, le NHCE présente une grande variabilité climatique et océanographique à différentes échelles, la source principale de variation inter-annuelle étant l'interruption du cycle d'upwelling saisonnier par l'Oscillation Australe du phénomène El Niño (ENSO: El Nino Southern Oscillation)qui a un effet direct sur la survie larvaire et le succès de recrutement des poissons. La pêche peut aussi être fortement variable, en fonction de l'abondance et de l'accessibilité des principales ressources halieutiques. Ce contexte amène deux questions méthodologiques principales que nous explorons dans cette thèse à travers le développement d'un modèle E2E qui couple le modèle OSMOSE, pour la partie haut niveau trophique, au modèle ROMS-PISCES, pour les parties hydrodynamique et biogéochimie:(i) Comment calibrer un modèle écosystémique à partir de séries temporelles de données ? (ii) Comment inclure l'impact de la variabilité inter-annuelle de l'environnement et de la pêche ?

En premier lieu, cette thèse met en évidence plusieurs problèmes liés à la confrontation de modèles écosystémiques complexes aux données et propose une méthodologie pour une calibration séquentielle en plusieurs phases des modèles écosystémiques. Nous proposons deux critères pour classer les paramètres d'un modèle: la dépendance au modèle et la variabilité temporelle des paramètres. A partir de ces critères, et en tenant compte de l'existence d'estimations initiales, on énonce des règles qui permettent de déterminer quels paramètres doivent être estimés, et dans quel ordre, dans le processus de calibration séquentiel. De plus, un nouvel Algorithme Évolutionnaire, conçu pour la calibration de modèles stochastiques (tels les modèles individu-centré) et optimisé pour l'estimation du maximum de vraisem-

blance, a été développé et utilisé pour la calibration du modèle OSMOSE avec des séries temporelles de données.

La variabilité environnementale est explicite dans le modèle: le modèle ROMS-PISCES force le modèle OSMOSE et propage les effets bottom-up potentiels dans le réseau trophique à travers les interactions trophiques entre plancton et poisson d'une part, et les changements dans la distribution spatiale du poisson d'autre part. Cette dynamique spatiale des poissons est prise en compte par l'utilisation de modèles de distribution des espèces de type présence/absence, qui sont en général évaluésgrâce à une matrice de confusion et les indicateurs statistiques qui lui sont associés. Toutefois, quand on considère la prédiction d'un habitat au cours du temps, la variabilité de la distribution spatiale des habitats peut être résumée de manière complémentaire et validée en utilisant les patrons émergents de la forme des distributions spatiales. Nous avons modélisé l'habitat potentiel des principales espèces du NHCE en utilisant plusieurs sources d'information (pêches commerciales, campagnes scientifiques et suivi satellite des navires de pêche) conjointement aux données environnementales issues d'observations satellites et in-situ, de 1992 à 2008. L'habitat potentiel est estimé sur cette période d'étude avec une résolution mensuelle, et le modèle est validé à partir d'informations quantitatives et qualitatives du système, en utilisant une approche pattern-oriented.

Le modèle écosystémique E2E ROMS-PISCES-OSMOSE pour le NHCE est calibré en utilisant notre algorithme évolutionnaire et une approche par maximum de vraisemblance pour ajuster des séries temporelles mensuelles de données de débarquements, d'abondances et de captures par classes de taille de 1992 à 2008. En conclusion, quelques applications potentielles du modèle pour la gestion des pêches sont présentées et nous discutons leurs limitations et les perspectives.

Resumen

Este trabajo representa una contribución original a la metodología para el desarrollo de modelos ecosistémicos así como el primer intento de desarrollar un modelo de extremo a extremo (E2E, *end-to-end*) para el Norte del Ecosistema de la Corriente de Humboldt (NECH). El principal propósito del modelo desarrollado es construir una herramienta para el manejo ecosistémico y la toma de decisiones, razón por la cual la credibilidad del modelo es esencial, y ésta puede ser evaluada mediante la confrontación con datos. Adicionalmente, el NECH muestra una alta variabilidad climática y oceanográfica a diversas escalas, siendo la mayor fuente de variabilidad interanual la interrupción de la estacionalidad del afloramiento por El Niño-Oscilación Sur, que tiene efectos directos en la sobrevivencia larval y el éxito del reclutamiento de peces. La actividad pesquera también puede ser altamente variable, dependiendo de la abundancia y accesibilidad de los principales recursos pesqueros. Este contexto genera las dos principales preguntas metodológicas abordadas en esta tesis, a través del desarrollo de un modelo de extremo a extremo por el acoplamiento del modelo de nivel trófico alto OSMOSE y el modelo hidrodinámico y biogeoquímico ROMS-PISCES: i) cómo calibrar modelos ecosistémicos usando series de tiempo y ii) como incorporar el impacto de la variabilidad interanual del ambiente y la pesca.

Primero, esta tesis resalta algunos problemas relacionados a la confrontación de modelos ecosistémicos complejos con datos, y propone una metodología para la calibración secuencial de modelos ecosistémicos. Proponemos dos criterios para la clasificación de parámetros de un modelo: la dependencia al modelo y la variabilidad temporal de los parámetros. Luego, estos criterio en conjunto con la disponibilidad de valores iniciales aproximados para los parámetros son usados como reglas de decisión para determinar qué parámetros necesitan ser estimados y su orden de precedencia en el proceso de calibración secuencial. Adicionalmente, un nuevo algoritmo evolutivo diseñado para la calibración de modelos estocásticos (e.g. Modelos Basados en Individuos) y optimizado para la estimación por máxima verosimilitud ha sido desarrollado y aplicado a la calibración del modelo OSMOSE con datos de series temporales.

La variabilidad ambiental es explícita en el modelo: ROMS-PISCES forza al modelo OSMOSE y dirige los potencial efectos *bottom-up* a la red trófica a través de las interacciones entre el plankton y los peces, así como a través de los cambios en la distribución espacial de los peces. Esto último fue tomado en cuenta usando modelos de distribución de especies que son tradiacionalmente evaluados a través de una matriz de confusión y las métricas estadísticas asociadas a esta. Sin embargo, cuando se considera la predicción del habitat en el tiempo, la variabilidad espacial de la distribución espacial puede ser resumida y validada usando los patrones emergentes de la forma de la distribución espacial. Nosotros modeladmos el habitat potencial de las principales especies del NECH usando varias fuentes de información (pesquerías, cruceros científicos y seguimiento satelital de los barcos) conjuntamente con datos ambientales de sensoramiento remoto y observaciones *in situ*, desde 1992 a 2008. El habitat potencial fue predicho con resolución mensual, y el modelo fue validado usando información cuantitativa y cualitativa del sistema usando un enfoque orientado a patrones.

El modelo de extremo a extremo ROMS-PISCES-OSMOSE para el NECH fue calibrado usando nuestro algoritmo evolutivo y un enfoque de máxima verosimilitud para ajustar datos de series de tiempo de desembarques, índices de abundancia y capturas por longitud y edad de 1992 a 2008. Para concluir, algunas aplicaciones potenciales del modelo al manejo pesquero son presentadas y sus limitaciones y perspectivas discutidas.

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Contents

Abstract

End–to–end modelling for an ecosystem approach to fisheries in the Northern Humboldt Current Ecosystem

Introduction

Fishing is central to the livelihood and food security of 200 million people, especially in developing countries, with one of five people depending on fish as the primary source of proteins (UN 2004). On the other hand, it is now widely recognized that fishing not only affects exploited species but the entire ecosystem in which they are embedded, highlighting the need for an ecosystem-based fisheries management (EBFM). By signing the Nagoya Strategic Plan of the Convention on Biological Diversity in October 2014, 50 nations and the European Union have committed to implement EBFM by 2020 (Aichi Biodiversity Target 6).However, the implementation of EBFM is still at its infancy worldwide. To be effective, EBFM not only requires a thorough understanding of the impact of fishing on ecosystem functioning and of the ecological processes involved, but also quantitative tools such as ecosystem models to provide useful information and predictions in support of management decision. Several marine ecosystem models have been implemented around the world (e.g., Ecopath with Ecosim, Atlantis, OSMOSE, etc.) and have the potential to be important tools for achieving EBFM goals as they incorporate species interactions and environmental forcing. Yet, the use of ecosystems models as decision making tools would only be possible if they are rigorously confronted to data by means of accurate and robust parameter estimation methods and algorithms (Bartell 2003). However, parameter estimation has been considered one of the two weakest points in ecological modeling as well as the ability of models to properly reflect the dynamic properties of the ecosystems (Jorgensen and Fath 2011).

The Humboldt Current Ecosystem (HCE) is one of the four major Eastern Boundary Upwelling Systems of the Earth (with Canary, Benguela and California). It produces more fish per unit area than any other region in the world, and accounts for up to 10% of the global fish catches (Chavez et al. 2008). The HCE has supported, on a long term basis, a fish production 20 times bigger than Canary or Benguela (Bakun and Broad 2003). The HCE extends from 4°S (northern Peru) to 40°S (central Chile), and its environmental variability is one of the highest in the world (Chavez et. al 2008), exhibiting a climatic and oceanographic variability at several scales (e.g. seasonal, interannual and decadal), the major source of interannual variability being the interruption of the upwelling seasonality by the El Nino Southern Oscillation ENSO (Alheit and Ñiquen 2004) which has direct effects on larval survival and fish recruitment success (Ñiquen and Bouchon 2004). Additionally, fishing activity can also be highly variable, depending on the variability in the abundance and accessibility of the main fishery resources like the Peruvian anchoveta (*Engraulis ringens*). Thus, it is particularly crucial to better understand the impact of environmental variability and fishing on the most exploited small pelagic species, namely sardines and anchovies, because they are essential resources for the fishers and for the marine top predators of the HCE. The impacts of environmental variability may be propagated upwards through the food web by a progressive disruption in the phenological synchrony of species at adjacent trophic levels (Cury et al. 2008). In this context, understanding and quantifying the impacts of natural environmental variability on small pelagic fisheries and top predators requires integrated studies covering multiple trophic levels.

In order to better understand the top-down effects of fishing and the bottom-up effects of natural climate variability and climate change on on the HCE, the objective of the thesis was to develop an integrated and multidisciplinary end-to-end (E2E) model of the HCE, including the explicit dynamics of the physical environment, the primary and secondary production, as well as the exploited fish communities. We conceived this E2E model so as to be possibly used in future as a tool for EBFM, adapted to the assessment and management of exploited fish populations, and allowing to better disentangle climate-driven from fishing impacts in the HCE. Therefore, we put emphasis in developing methods to rigorously confront the E2E model to observed data and increase its credibility.

The HCE E2E modeling first required to select and couple different component models together. To represent the High Trophic Level (HTL) community, we applied the spatially explicit individual-based model OSMOSE (Shin and Cury 2001, 2004) as the assumed opportunism in species interactions makes it relevant to use in a changing environment. Once the OSMOSE model properly structured and parameterized to the HCE , we coupled OSMOSE to an existing application of the ROMS-PISCES hydrodynamic and biogeochemical model (Aumont et al. 2003,Echevin et al. 2012) for representing explicitly the seasonal and interannual forcing from the Low Trophic Level (LTL) community and the physical environment. The resulting ROMS-PISCES-OSMOSE E2E model includes 13 species or functional groups: microphytoplankton, diatoms, microzooplankton, mesozooplankton, macrozooplankton, anchovy (*Engraulis ringens*), sardine (*Sardinops sagax*), jack mackerel

(*Trachurus murphyi*), horse mackerel (*Scomber japonicus*), hake (*Merluccius gayi*), munida (*Pleurocondes monodon*), jumbo squid (*Dosidicus gigas*) and mesopelagic fish. The difficulty of the thesis work was due to the combination of the strong technical issues related to the development of the E2E model, along with the conceptual representation of the entire HCE with inherent simplifications required on the selection and formulation of key processes. The former includes the necessity of using robust procedures for parameter estimation for a full calibration of the model, and the latter to find a good way to represent the interactions between the species and their environment.

The OSMOSE model is a multispecies and Individual-based model (IBM) which focuses on fish species and HTL species in general, including invertebrate ones (Shin and Cury 2001, 2004). This model assumes size-based opportunistic predation that is conditioned by spatial co-occurrence and size adequacy between a predator and its prey. It represents fish individuals grouped in schools, which are characterized by their body size, weight, age, taxonomy and geographical location, and which undergo different processes over their life cycle (growth, explicit predation, natural and starvation mortalities, fishing mortality, reproduction and migration). In output, a variety of size-based and species-based ecological indicators can be simulated and confronted to in situ data (surveys and catch data) at different levels of aggregation.

Physical processes in the HCE have been modeled with the ROMS (Regional Oceanic Modeling System, Shchepetkin and McWilliams 2003 and 2005 for more details), which simulated the climatological and interannual variation of temperature, salinity and currents off Peru (Penven et al. 2005, Colas et al. 2008). The outputs of ROMS have been used to force the PISCES (Pelagic Interaction Scheme for Carbon and Ecosystem Studies) biogeochemical model (Aumont et al. 2003). This model currently includes several components such as nutrients, phytoplankton, zooplankton and detritus (Aumont et al. 2003). The ROMS-PISCES model used as the LTL model in this thesis has been applied to the HCE with a spatial resolution of 1/6° and includes 2 size classes of phytoplankton, 2 size classes of zooplankton and 2 size classes of detritus, colimitations of phytoplankton growth by nitrate, phosphate, silicate and iron, and the oxygen cycle. The seasonal chlorophyll a variations in the HCE have been reproduced accurately using the ROMS-PISCES model (Echevin et al. 2008).

The key coupling process used to link OSMOSE and ROMS-PISCES models is the predation process. The ROMS-PISCES model is used as a prey field for the OSMOSE model (concentration of nitrogen/carbon converted into wet biomass). Additionally, a significant contribution of the present thesis is to render explicit the

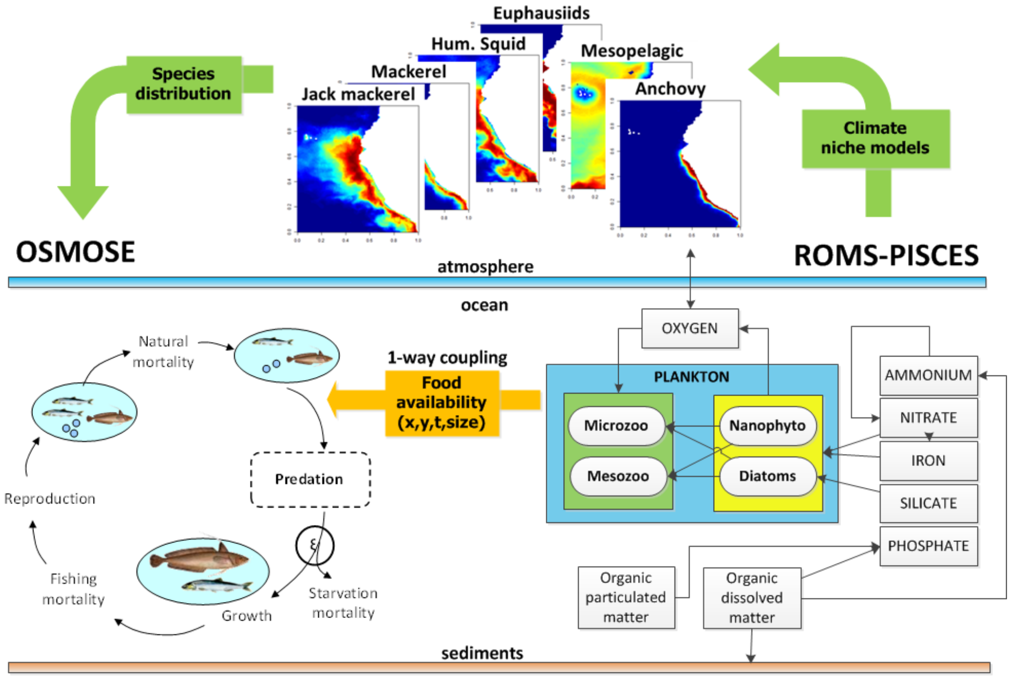
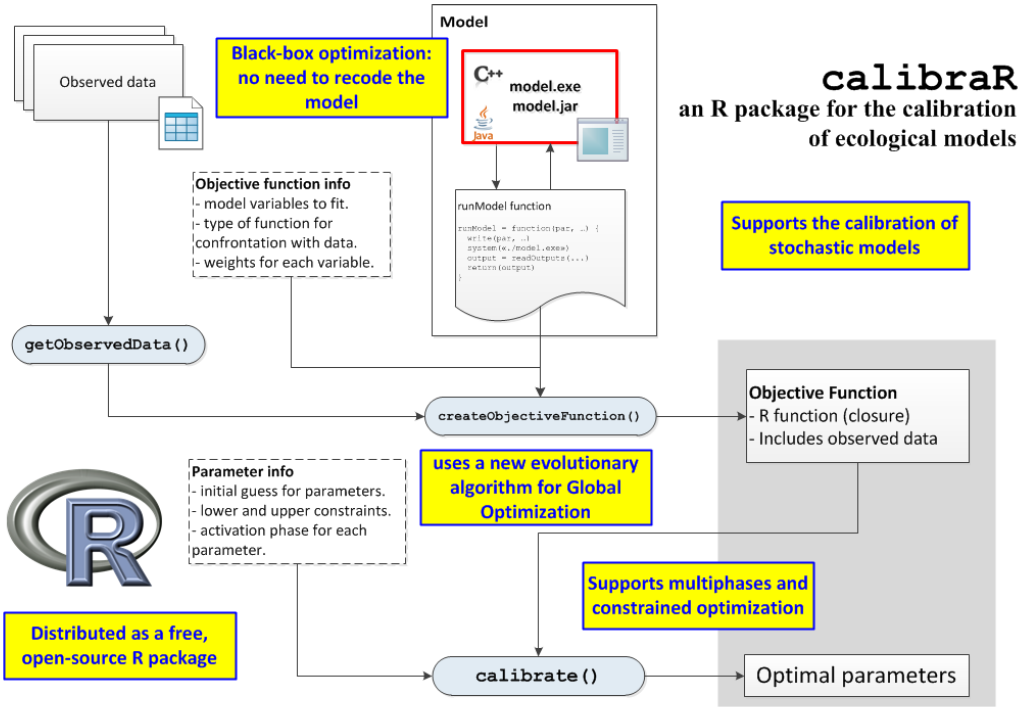


Figure 0.1: Schematic representation of the key processes linking OSMOSE and ROMS-PISCES.

link between fish habitats and the physical environment. Some of the outputs of the ROMS-PISCES model were used (e.g. plankton density, temperature, salinity, oxygen) to predict the spatial distribution of the species modelled in OSMOSE, by building climate niche models. The predictions of the statistical models were then incorporated into the OSMOSE model for each species. A schematic representation of the coupling of OSMOSE and ROMS-PISCES is shown in Figure 0.1.

Once the different pieces of the E2E model were assembled, an essential step consisted in calibrating the model using time series of data, and to do this rigorously, a specific algorithm had to be developed for the specific case of stochastic individual-based models (IBM). We significantly improved the convergence rate of a previous version of an evolutionary algorithm (Duboz et al. 2010) dedicated to OSMOSE calibration and we made the algorithm compatible with well-documented objective functions. In many respects, the calibration of ecosystem models such as OSMOSE is a complex task. In particular, the dynamics represented in ecosystem models allow species-specific parameters to have an impact on one another through ecological interactions, which results in highly correlated parameters, while additionally, critical information and observations on non-commercial species can be missing or poor. Furthermore, the high number of parameters and the long duration of the simulations can be an obstacle to calibrate a model. These diverse reasons hampered the development of flexible and generic enough calibration algorithms and methodologies for ecosystem models, and only sparse documentation has been produced on fitting complex models (Bolker et al. 2013). There are some dedicated tools for non-linear parameter estimation, AD Model Builder (ADMB, Fournier et al. 2012) being one of the most robust and fast (Bolker et al. 2013). Among other advantages, ADMB provides support for calibration in multiple phases (Nash and Walker-Smith 1987), which can be of great interest for the calibration of complex ecosystem models. It also provides support for constraining optimization, which can be helpful for regularizing hard optimization problems (Bolker et al. 2013). However, the model and the objective function itself need to be coded in C++ (using the ADMB scripting), which can be an obstacle for calibrating complex models already implemented in other languages (e.g. Java, Fortran). In addition, as ADMB is based on automatic differentiation, which allows to provide accurate estimates of derivatives (Griewank and Corliss 1992), the tool is not suited for stochastic models for which derivatives cannot be computed, like Individual Based Models (IBM). Parameter estimation methods have been developed for stochastic non-linear models for which the probability of state transitions or the master equation can be written (Ionides et al. 2006, Newman et al. 2009, Ross et al. 2009, Walker et al. 2006). However, many IBMs can only be simulated numerically and are too complex for mathematical analysis and explicit parameter estimation (Black and McKane 2012), resulting in more attention being given to the exploration of model behavior than to a rigorous confrontation with data. As alternative methods, meta-heuristic algorithms have been developed (Cropper and Anderson 2004, Poovathingal and Gunawan 2010, Duboz et at. 2010, Tashkova et al. 2012, Travers-Trolet et al. 2013), and have in some cases shown better performance than derivative-based optimization methods (Tashkova et al. 2012). However, the scientific community lacks generic and flexible enough tools for the calibration of different types of ecological models with different degrees of complexity. In this respect, a major part of this thesis has been dedicated to the conceptual and technical development of calibrar, an R package (R Development Core Team 2014) for the calibration of complex models, in particular stochastic ones. The main features of this software are shown in Figure 2.

Given that the calibration of complex ecosystem models requires a lot of data and potentially involves a high number of parameters to estimate, common practice in the field has been to i) reduce the number of parameters to estimate by using estimates provided by other models (Marzloff et al. 2009, Lehuta et al. 2010) or available for similar species or ecosystems (Bundy 2005, Ruiz and Wolff 2011), ii) use other models outputs as data to calibrate the model (Mackinson and Daskalov 2007), or



```
runModel = function(par, ..) {
  write(par, ..)
  system(«./model.exe»)
  output = readOutputs(...)
  return(output)
}
```

Figure 0.2: Diagram representing the functioning of the calibrar package. The grey area groups the outputs produced for the package (the objective function and the optimal parameters of the model). Rectangles with broken border lines show user inputs which are needed to configure the calibration. Rounded rectangles show main package functions.

both (Shannon et al. 2003, Guénette et al. 2008, Friska et al. 2011, Travers-Trolet et al. 2013). These different strategies allow to calibrate complex models while attempting to synthesize the maximum of available information. However, as the parameters or outputs used rely on different model assumptions, they may lead to the fitting of artificial parameter values or to inconsistent behavior of the model by trying to reproduce other models' dynamics. Additionally, ecosystem models can require more information to be built, information which may not normally be available (e.g distribution maps for all species). This lack of information is particularly true for non-commercial species or when information required is outside the Economic Exclusive Zone of the countries involved. This situation can limit the development of ecosystem models to areas rich in data. Additional issues can however be raised even in data-rich situations, since the reconstruction of valid spatial information to drive the models is not straightforward.

All these challenges were addressed in this thesis, with the objective to build an end-to-end (E2E) model of the HCE in order to investigate the impacts of environmental variability and fishing scenarios on the management of fishery resources. In the process, the HCE proved to be an ideal model case study to address these issues, as it is a well-studied ecosystem with long time-series of data for species at multiple trophic levels. The main outcomes of this thesis are presented in three chapters and some general conclusions and perspectives are finally drawn to pave the way for future work.

In Chapter 1, we describe the development of an end-to-end model of the Northern Humboldt Current Ecosystem, by coupling ROMS-PISCES and OSMOSE models. We particularly deal with the incorporation of the impact of the interannual variability of the environment and fishing as part of the process of constructing our E2E model. One of the main interannual forcing in OSMOSE is the spatial distribution of fish and other modelled species that we incorporated by building ecological niche models. These models were used to produce monthly maps of spatial distribution for all the species included in our model. For the validation of these niche models, typically based on the classification or regression of binary presence/absence data against several environmental or geographical variables, the confusion matrix and the statistical metrics associated to it are normally used. However, when considering the prediction of the habitat against time, the variability in the spatial distribution of the habitat can be summarized and validated using the emerging patterns from the shape of this distribution. To illustrate this approach, we used jack mackerel (*Trachurus murphyi*) spatial distribution results. The potential habitat was predicted over the study period with monthly resolution, and the model was validated using quantitative and qualitative information of the system compared with i) one dimensional profiles inside the scientific survey area (latitudinal and off-shore distributions) and, ii) time series of the center of gravity of the spatial distribution, modes, quantiles and extremes of the profiles (Manuscript 1: Oliveros et al. in prep).

In Chapter 2 we present an optimization method that we developed for the calibration of stochastic models, OSMOSE in particular (Manuscript 2: Oliveros and Shin, in review). The calibration algorithm is an Evolutionary Strategy (Beyer and Schwefel 2002) and its implementation as well the tools related to the calibration have been implemented in a package, `calibrar`, written in R (R Development Core Team 2014). The `calibrar` package is designed for the optimization of "black-box" functions (Jones et al. 1998), where analytical information about the function to be optimized and the model source code are assumed to be unavailable or impractical to modify (Rios and Sahinidis 2013). Our approach is hence "non-intrusive", making the model interact with the optimizer, i.e. the `calibrar` package, in two ways: i) receiving a set of parameters to run, and ii) providing the model outputs to be confronted with the observed data. `calibrar`also helps in the construction of the objective function to be optimized in order to estimate model parameters (Figure 0.2).

In Chapter 3 we propose an approach to deal with the calibration of ecosystem models, and we illustrate it with the end-to-end (E2E) ecosystem model ROMS-PISCES-OSMOSE of the Northern Humboldt Current Ecosystem. Here, we highlight some issues related to the confrontation of complex ecosystem models to data and propose a methodology for a sequential multi-phases calibration of ecosystem models (Manuscript 3: Oliveros et al. in review). We first discuss two criteria to classify the parameters of a model: the model dependency and the time variability of the parameters. Then, these criteria and the availability of approximate initial estimates are used as decision rules to determine which parameters need to be estimated, and their precedence order in the sequential calibration process. The `calibrar`R package and a likelihood approach are used to fit monthly time series data of landings, abundance indices and catch at length distributions from 1992 to 2008.

Finally, we conclude with some perspectives brought out by our work, and particularly on how ecosystem models can be used in the context of the Ecosystem Approach to Fisheries to complement the assessment and recommendations based on single-species models for fishery management.

References

Alheit J., Ñiquen M., 2004. Regime shifts in the Humboldt Current ecosystem. Progress in Oceanography 60:201–222.

Aumont, O. E. Maier-Reimer, S. Blain and P. Monfray. 2003. An ecosystem model of the global ocean including Fe, Si, P colimitations. Global Biogeochemical Cycles, (17) 1060.

Bakun, A. and K. Broad., 2003. Environmental loopholes and fish population dynamics: comparative pattern recognition with focus on El Niño effects in the Pacific. Fisheries Oceanography. 12(4/5):458-473.

Beyer, H.-G. and Schwefel, H.-P., 2002. Evolution strategies: a comprehensive introduction, Natural Computing 1:3-52.

Black, A.J. andMcKane, A.J., 2012. Stochastic formulation of ecological models and their applications. Trend in Ecology and Evolution 27(6):337-345. DOI: http://dx.doi.org/10.1016/j.tree.2012.01.014

Bartell S.M., 2003. Effective use of ecological modeling in management: The toolkit concept. In Dale V (editor).Ecological modeling for resource management, Springer Verlag.

Bolker B.M., Gardner B., Maunder M., Berg C.W. , Brooks M., Comita L., Crone E., Cubaynes S., Davies T., de Valpine P., Ford J., Gimenez O., Kéry M., Kim E.J., Lennert-Cody C., Magnusson A., Martell S., Nash J., Nielsen A., Regetz J., Skaug H., Zipkin E., 2013. Strategies for fitting nonlinear ecological models in R, AD Model Builder, and BUGS. Methods in Ecology and Evolution 4: 501–512.

Bundy A., 2005. Structure and functioning of the eastern Scotian Shelf ecosystem before and after the collapse of ground fish stocks in the early 1990s. Canadian Journal of Fisheries And Aquatic Sciences 62:1453-1473.

Chavez F. P., A. Bertrand, R. Guevara-Carrasco, P. Soler and J. Csirke. 2008. The northern Humboldt Current System: Brief history, present status and a view towards the future. Progress in Oceanography 79:95-105.

Colas F., X. Capet, J.C. McWilliams and A. Shchepetkin. 2008. 1997-1998 El Niño off Peru: A numerical study. Progress in Oceanography 79:138-155.

Cropper, W.P. Jr. and Anderson, P.J., 2004. Population dynamics of a tropical palm: use of a genetic algorithm for inverse parameter estimation. Ecological Modelling 177: 119–127.

Cury PM, Shin Y-J, Planque B, Durant JM, Fromentin J-M, Kramer-Schadt S, Stenseth NC, Travers M and Grimm V (2008) Ecosystem oceanography for global change in fisheries. Trends in Ecology and Evolution 23:338-346

Duboz, R., Versmisse, D., Travers, M., Ramat, E. and Shin, Y.-J., 2010. Application of an evolutionary algorithm to the inverse parameter estimation of an individual-based model. Ecological Modelling 221(5):840-849.

Echevin V., O. Aumont, J. Ledesma, G. Flores. 2008. The seasonal cycle of surface chlorophyll in the Peruvian upwelling system: A modelling study. Progress in Oceanography 79:167-176.

Echevin V., Goubanova K., Dewitte B., Belmadani A., 2012. Sensitivity of the Humboldt Current system to global warming: a downscaling experiment of the IPSL-CM4 model, Climate Dynamics. doi:10.1007/s00382-011-1085-2.

Fournier D.A., Skaug H.J., Ancheta J., Ianelli J., Magnusson A., Maunder M.N., Nielsen A., Sibert J., 2012. AD Model Builder: using automatic differentiation for statistical inference of highly parameterized complex nonlinear models. Optimization Methods and Software, 27:2, 233-249, DOI: 10.1080/10556788.2011.597854.

Friska M.G., Miller T.J., Latour R.J., Martell S.J.D., 2011. Assessing biomass gains from marsh restoration in Delaware Bay using Ecopath with Ecosim. Ecological Modelling 222:190–200.

Garcia, S.M.; Zerbi, A.; Aliaume, C.; Do Chi, T.; Lasserre, G. 2003. The ecosystem approach to fisheries. Issues, terminology, principles, institutional foundations, implementation and outlook. FAO Fisheries Technical Paper. No. 443. Rome, FAO. 71 p.

Griewank, A. and Corliss, G.F., 1992. Automatic Differentiation of Algorithms: Theory, Implementation, and Application. SIAM, Philadelphia, PA, USA.

Guénette S., Christensen V., Pauly D., 2008. Trophic modelling of the Peruvian upwelling ecosystem: Towards reconciliation of multiple datasets. Progress in Oceanography 79: 326–335.

Ionides, E. L., Breto, C. and King, A.A., 2006. Inference for nonlinear dynamical systems. PNAS 103(49): 18438–18443.

Jones, G. (1998) Genetic and evolutionary algorithms. In Encyclopedia of Computational Chemistry (Schleyer, P .v.R. et al., eds), pp. 1127–1136, John Wiley & Sons.

Jorgensen S.E. and FathB.D., 2011. Fundamentals of Ecological Modelling: Applications in Environmental Management and Research. Fourth Edition. Elsevier. 350pp.

Lehuta S., Petitgas P., Mahévas S., Huret M., Vermard Y., Uriarte A., Record N.R., 2013. Selection and validation of a complex fishery model using an uncertainty hierarchy. Fisheries Research 143:57– 66.

Mackinson S., and Daskalov G., 2007. An ecosystem model of the North Sea for use in research supporting the ecosystem approach to fisheries management: description and parameterisation [online]. (CEFAS, Lowestoft.) Available from www.cefas.co.uk/publications/techrep/tech142.pdf.

Marzloff M., Shin Y.-J., Tam J., Travers M., Bertrand A., 2009. Trophic structure of the Peruvian marine ecosystem in 2000–2006: Insights on the effects of management scenarios for the hake fishery using the IBM trophic model Osmose. Journal of Marine Systems 75: 290-304.

Nash J.C. and Walker-Smith M., 1987. Nonlinear Parameter Estimation: an Integrated System in BASIC. Marcel Dekker, New York. 493pp.

Newman, K.B., Fernández, C., Thomas, L. and Buckland, S.T., 2009. Monte Carlo Inference for State–Space Models of Wild Animal Populations. Biometrics 65, 572–583.

Ñiquen M., Bouchon M., Ulloa D., Medina A., 2013. Analysis of the Jack mackerel Trachurus murphyi fishery in Peru. Rev. Peru. Biol. 20(1):097-106.

Penven, P., V. Echevin, J. Pasapera, F. Colas, J. Tam. 2005. Average circulation, seasonal cycle, and mesoscale dynamics of the Peru Current System: A modeling approach. J. Geophys. Res., Vol. 110, No. C10, C1002110.1029/2005JC002945.

Poovathingal, S.K andGunawan, R., 2010. Global parameter estimation methods for stochastic biochemical systems, BMC Bioinformatics 11:414.

R Core Team (2014) R: A language and environment for statistical computing. R Foundation for Statistical Computing, Vienna, Austria. URL http://www.R-project.org/.

Rios, L.M. & Sahinidis, N.V. (2013) Derivative-free optimization: a review of algorithms and comparison of software implementations. Journal of Global Optimization 56:1247–1293.

Ross, J.V., Pagendam, D.E. andPollet P.K., 2009. On parameter estimation in population models II: Multi-dimensional processes and transient dynamics. Theoretical Population Biology 75: 123132.

Ruiz D.J, Wolff M., 2011. The Bolivar Channel Ecosystem of the Galapagos Marine Reserve: Energy flow structure and role of keystone groups. Journal of Sea Research 66 123–134.

Shannon L.J., Moloney C.L., Jarre A., Field J.G., 2003. Trophic flows in the southern Benguela during the 1980s and 1990s. Journal of Marine Systems 39:83 – 116.

Shchepetkin, A. F., and J. C. McWilliams, 2003. A method for computing horizontal pressure-gradient force in an ocean model with a nonaligned vertical coordinate, J. Geophys. Res.,108 (C3), 3090, doi:10.1029/2001JC001047.

Shchepetkin, A. F., and J. C. McWilliams, 2005. The regional oceanic modeling system (ROMS): A split-explicit, free-surface, topography-following-coordinate oceanic model, Ocean Modell., 9 , 347–404.

Shin Y.-J., P. Cury. 2001. Exploring fish community dynamics through size-dependent trophic interactions using a spatialized individual-based model. Aquatic Living Resources, 14(2): 65-80.

Shin Y.-J., P. Cury, 2004. Using an individual-based model of fish assemblages to study the response of size spectra to changes in fishing. Canadian Journal of Fisheries and Aquatic Sciences, 61: 414-431.

Tashkova, K., Silc, J., Atanasova, N. andDzeroski, S., 2012. Parameter estimation in a nonlinear dynamic model of an aquatic ecosystem with meta-heuristic optimization. Ecological Modelling 226: 36– 61.

Travers-Trolet, M., Shin, Y.-J. and Field, J.G., 2013. An end-to-end coupled model ROMS-N2P2Z2D2-OSMOSE of the southern Benguelafoodweb: parameterisation, calibration and pattern-oriented validation, African Journal of Marine Science, 36:1, 11-29, DOI:10.2989/1814232X.2014.883326

United Nations. 2004. Overfishing: a threat to marine biodiversity. “Ten Stories the World Should Know More About.” http://www.un.org/events/tenstories/

Walker, D.M., Pérez-Barbería, F.J. and Marion, G., 2006. Stochastic modelling of ecological processes using hybrid Gibbs samplers. Ecological Modelling 198:40-52.

Chapter 1

Incorporating the impact of the interannual variability of the environment

The Humboldt Current Ecosystem (HCE) is characterized by a high environmental variability, influencing the distribution and abundance of the main fish stocks. The objective of this thesis was to develop an integrated and multidisciplinary end-to-end (E2E) model of the Northern HCE, including the explicit dynamics of the physical environment, the primary and secondary production, as well as the exploited fish communities. For this purpose, the OSMOSE model was selected to represent the High Trophic Level (HTL) community and an existing application of the ROMS-PISCES hydrodynamic and biogeochemical model for the HCE (Echevin et al. 2012) was selected to represent explicitly the seasonal and interannual forcing from the Low Trophic Level (LTL) community and the physical environment. The interannual effect of fishing was introduced in the OSMOSE model as time series of fishing mortality, which were estimated during the calibration process in order to properly fit the landings data. In the first section of this chapter we start by describing the OSMOSE component model that we had to fully parameterize to represent the dynamics of the HTL community of the NHCE, then briefly describe the ROMS-PISCES model available for the HCE and how its outputs were used to force the OSMOSE model, while in the last section we show how we constructed and validated the spatial maps of the distribution of the modeled species, also used to force OSMOSE. The impact of the interannual variability of fishing and how it is modeled are described in chapter 3.

1.1 Modeling the HTL dynamics: OSMOSE

In OSMOSE, the basic unit of simulation is the “school”, a group of individuals of the same species sharing the same properties and history in terms of spatial position, length and age. The state of each school in the system can be described by a vector $S = (s, x, y, N, L, A)$, where s is the species the school belongs to, (x, y) is the position of the school (longitude, latitude), N is the number of individuals in the school (abundance), L is the body length of the individuals and A is its age. At any time, the state of the system can be described by the state of all living schools ($N > 0$). There are three main processes controlling the dynamic of a school: mortality, somatic growth and spatial movement. The core of the first two processes relies in very simple survival and growth assumptions:

$$
\begin{aligned}
N(t+1) &= e^{-Z}N(t) && (1.1)\\
L(t+1) &= L(t) + G && (1.2)
\end{aligned}
$$

In OSMOSE, the total mortality (Z) and growth in length (G) during a time step are functions of the state of the school itself and that of all other schools in a defined neighbourhood given by the discretization of the spatial domain. This means growth and mortality are function of the state of all schools which are present in the same cell of the grid at the same time. In the OSMOSE version considered in this work, the functions defining mortality and growth are deterministic, while the main source of stochasticity is in the movement process.

After one time step, each school can move to an adjacent cell of the grid or remain in the same position in a uniform random way. Additionally, the model is forced by species-specific spatial distribution maps. At any time, each school can be assigned to a unique map, while this map can change during the simulation according to age or time-specific criteria (e.g. seasonal maps, different maps for adults or juveniles). When a change in the map for a school occurs, the school is relocated randomly in the new map according to its spatial probability distribution (which can be uniform in the simplest case).

Taken this into account, growth and mortality in OSMOSE depend stochastically on the complex interactions between several schools of different species. Mortality and growth both depend on the predation process which is length based in OSMOSE. For each species, a school can feed on prey within a limited range of sizes, parameterized by the minimum and maximum ratio between predator and prey sizes. This rule allows each school to "select" which other schools it can feed on, considering only the length of the individuals and the co–occurrence in the same cell, so that for most modeled species in the pelagic column, no a priori species-specific trophic relationship is assumed. As a result, the diets, trophic levels and predation mortalities are derived quantities from the model and the size-based predation assumption, and produced as outputs of OSMOSE.

A key parameter linking predation with growth and mortality is the critical predation efficiency threshold ξ_{max}, defined as the threshold corresponding to maintenance needs of a fish, and beyond which the food ration can be dedicated to fish growth (Shin and Cury 2001, Shin et al. 2004). This parameter allows correcting the actual growth (no growth below ξ_{max}) in the mean length of the school, and adding a starvation mortality M_ξ to the total mortality when predation efficiency is below ξ_{max} (Shin and Cury 2001).

The size of the fish is modeled by a linear relationship below a critical age or length (fast growth at initial stages, and for which von Bertalanffy growth parameters are usually not well estimated), and beyond that age/size threshold is modeled using the von Bertalanffy model. The actual growth rate (difference in size between two time steps) is calculated on the basis of the von Bertalanffy growth model but taking into account a deviation depending on the predation efficiency at each time step, according to Shin and Cury (2001).

The total mortality for a school is calculated taking into account the food ration needed by co-occurring predator schools (predation mortality), the fishing mortality, the starvation mortality and an additional mortality component M_0 representing the mortality due to other processes which are not fully explicit in the model (e.g. due to other predators). The total mortality and its components for each school in the same cell of the grid are solved simultaneously for all species.

An additional important process leading to the renewal of the population is the reproduction process. Here, the total spawner biomass of each species (aggregated over all schools given a size or age of maturity and sex ratio) leads to an egg production (age 0 abundance). While the recruitment level emerges from the different sources of mortality applied at the subsequent time steps, the initial total egg production is assumed proportional to the spawner biomass, the potential relative fecundity (number of eggs per gram of mature female by unit of time) being the factor of proportionality. These eggs are distributed in a number of new schools proportional to the area of distribution of the species and the expected average biomass of the population for the modeled period. This means that for species with bigger distribution areas, abundance, or both, more new age-0 schools are introduced in the model at each time step. The initial state of the new schools is given by: (i) abundance: the number of eggs after the distribution of the total egg production among all the new schools, (ii) length: the assumed size of the egg for the species, (iii) position: randomly distributed within the age-0 map for the species, and (iv) age 0.

The dynamics of the low trophic level (LTL) species is not explicit in the model, reason why plankton fields (provided by observations or biogeochemical models) are used as forcing variables, representing additional food for planktivorous species or for the smaller species and size classes in OSMOSE. The LTL biomass is available to predation in the same way school biomass is in OSMOSE.

The constants, state variables, parameters, forcings, initial conditions and main derived quantities used in the OSMOSE model are described in Tables 1.1 and 1.2.

Table 1.1: Description of main quantities used in the OSMOSE model (1).

	Symbol	Units	Remarks
1. Constants			
Number of low trophic level groups	N_P		Species or functional groups from LTL model.
Number of species modeled	N_S		Species or functional groups modeled in OSMOSE.
Number of age-0 schools	n^s	year^{-1}	Number of new schools per year for species s.
Number of simulation steps per year	N	year^{-1}	
Number of simulation years	T	year	
2. State variables			
Number of schools alive	$n^{\#}$		Schools with positive abundance.
Species	S		$s = 1, \ldots, N_S$
Spatial position	(x, y)	degrees	Position in latitude and longitude.
Abundance of the school	N	ind	Number of individuals
Average length of individuals of a school	L	cm	
Age of individuals of a school	A	year	
State of a school	S		$S = (s, x, y, N, L, A)$
3. Forcing variables			
Biomass of plankton from LTL	$B_p(t, x, y)$	tonnes/km^2	$p = 1, \ldots, N_P$
Probability of presence in the habitat	$P_s(t, x, y, a)$		$s = 1, \ldots, N_S$
4. Parameters			
Critical predation efficiency	ξ_{max}		
Maximum starvation mortality	$M^s_{\xi,max}$	year^{-1}	
Life history parameters	Φ_s		$\Phi_s = (A_{max}, k, L_\infty, t_0, A_{thr}, a, b, l_{egg}, w_{egg}, p_f, L_{50})$, vB equation, length–weight
Predation size ratios	$\rho_{s,min}(a, l)$ $\rho_{s,max}(a, l)$		$s = 1, \ldots, N_S$
Base natural mortality	$M_s(t, x, y, a, l)$	year^{-1}	
Fishing mortality	$F(s, t, x, y, a, l)$	year^{-1}	
Plankton accessibilities	$\alpha_{p,s}(t)$		Fraction of plankton group p accessible to predators species s
Predation accessibilities	$\alpha_{s,r}(t)$		Fraction of species group s accessible to predators species r
Fecundity	$\varphi^s(t)$	eggs/tonne/year	
Larval mortality	$\lambda^s(t)$	month^{-1}	
Inmigration biomass flux	$\psi^s(t)$	tonnes	
Average length of migratory schools	L	cm	
Age of migratory schools	A	years	

Table 1.2: Description of main quantities used in the OSMOSE model (2).

	Symbol	Units	Remarks
5. Derived quantities			
Spatial distribution of abundance	$N_s(t,x,y)$	ind/km^2	$s = 1, \ldots, N_S$
Spatial distribution of biomass	$B_s(t,x,y)$	tonnes/km^2	
Total abundance of the population	$N_s(t)$	ind	
Total biomass of the population	$B_s(t)$	tonnes	
Catch-at-age	$C_s(t,a)$	ind	
Catch-at-length	$C_s(t,l)$		
Yield	$Y_s(t,x,y)$	tonnes/km^2	
Total yield	$Y_s(t)$	tonnes	
Predation mortality	$P_{s,r}(t,x,y)$	year^{-1}	Prey $s = 1, \ldots, N_S$
Starvation mortality	$M_\xi(s,t,x,y)$		Predator $r = 1, \ldots, N_S$
Total mortality	$Z(s,t,x,y)$		
Trophic level	$TL(s,t,x,y,l)$		
6. Initial conditions			
Total biomass	B_0^s	tonnes	
School states	$S_0^i = (s,x,y,l,a)$		$i = 1, \ldots, n_0^\#$.

1.2 Interannual forcing of the plankton: ROMS–PISCES

ROMS (Regional Oceanic Modeling System, Shchepetkin and McWilliams 2005) is a free surface ocean model that solves the primitive equations of oceandynamics. Widely used by the scientific community in a diverse range of applications in the world (Haidvogel et al 2000, Peliz et al 2003, Di Lorenzo 2003, Dinniman et al. 2003, Budgell 2005, Warner et al. 2005a, 2005b, Wilkin et al. 2005), it has been especially designed to produce realistic simulations of the dynamics of regional systems.

The PISCES (Pelagic Interaction Scheme for Carbon and Ecosystem Studies) biogeochemical model simulates marine biological productivity and describes biogeochemical cycles of carbon and major nutrients in the ocean (Aumont and Bopp 2006). PISCES assumes that phytoplankton growth depends on external concentration of nutrients and that the main nutrients in the medium follow the Redfield ratio (C:N:P $\sim$ 106:16:1) (Redfield et al 1963). PISCES has 24 state variables, among which are nutrients (Phosphorus, Nitrogen, Silica and Iron), dissolved oxygen, two kinds of detritus (large and small), two classes of zooplankton (microzooplankton and mesozooplankton) and two kinds of phytoplankton (nanophytoplankton and diatoms). Diatoms differ from nanophytoplankton in their requirements in silicates, an increased consumption of iron and higher levels of saturation due to its larger size (Echevin et al. 2008).

1.2.1 ROMS–PISCES model setup

In Peru, there have been several modeling studies of climatological variability (Penven et al. 2005, Montes et al. 2010) and the effects of El Niño 1997-1998 (Colas et al. 2008).

However, the simulations used in this thesis are the first that investigate a period over 15 years (1992-2008) in an area corresponding to the Southeast Pacific delimited between 100º and 70º W and 10º N to 40º S, covering a larger area to the north than the HCE to reproduce more accurately the equatorial circulation, because changes in the dynamics of equatorial currents (surface and subsurface) would influence directly the dynamics (Montes et al. 2010), richness, oxygenation and productivity (Espinoza-Morriberón 2012) of the waters off Peru. In the present study the PISCES model is coupled to the physical model ROMS, following the approach of Gruber et al. (2006), who coupled ROMS to a simpler biogeochemical model than PISCES. The spatial resolution is 1/6º with 32 sigma vertical levels (which follow the topography of the ocean floor). Atmospheric forcings were constructed from: i) binding of climatological SCOW data (Risien and Chelton 2008) with NCEP anomalies (`www.ncep.noaa.gov`) for wind fields and, ii) binding of COADS climatology data (Da Silva et al. 1994) with NCEP anomalies for the heat fluxes and air temperatures. For boundary conditions the outputs of the global simulation of the ORCA2-PISCES physical-biogeochemical coupled model (Aumont and Bopp 2006) were used, and they were forced with NCEP data. For more information about the construction of simulation forcings and boundaries, the reader can refer to Echevin et al. (2012), Cambon et al. (2013) and the webpage of the project “Peru Ecosystem Projection Scenarios (PEPS)” (`www.locean-ipsl.upmc.fr/PEPS`).

1.2.2 Coupling ROMS–PISCES with the OSMOSE model

The results of this ROMS-PISCES simulation were validated through its ability to represent the climatological and interannual variability from 1992 to 2008 (Romero et al. submitted, Espinoza et al. submitted) of the main physical variables corresponding to the South East Pacific ocean region (temperature, salinity, currents and sea level),the distribution of surface water masses, the depth of the oxygen minimum zone (OMZ), as well as concentrations of nutrients and surface chlorophyll-a.

The concentration fields of the four groups of plankton modeled in PISCES (nanophytoplankton, diatoms, microzooplankton and mesozooplankton) are used as prey fields forcing the OSMOSE model, where planktivorous fish can have access to the plankton according to the size-based predation rules implemented in the model.

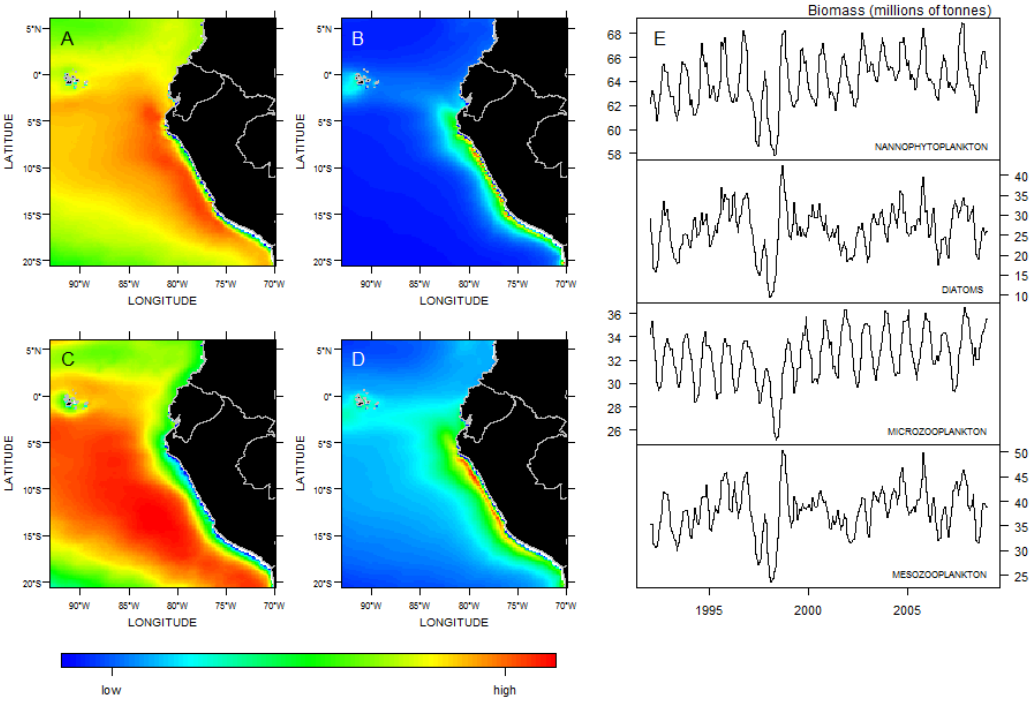


Figure 1.1: Summary of the LTL biomass simulated by ROMS-PISCES model used as forcing for OSMOSE. Average spatial distribution for nanophytoplankton (A), diatoms (B), microzooplankton (C) and mesozooplankton (D) (red is high, blue is low, following the light visible spectrum). Simulated temporal dynamics of thetotal biomass (millions of tonnes) of the four plankton groups (E) is also shown.

Additionally, the depth of the oxygen minimum zone is used as a predictor of the spatial distribution of all the modeled species as described in the next section.

1.3 Modelling the variability in fish habitat distribution

In order to model the interannual variability in the distribution of the species included in the NHCE OSMOSE model, several GAM models were constructed. A more detailed description of the model building and validation for Jack mackerel is presented here, highlighting some of the issues we found when constructing time series of maps. The results for other species are shown thereafter.

1.3.1 Pattern-oriented validation of habitat distribution models

The following manuscript is in preparation for submission as a short communication to the ICES Journal of Marine Science.

Pattern-oriented validation of habitat distribution models: application to the spatial distribution of Jack mackerel in the Humboldt Current Ecosystem

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Abstract

Most modeling methods for habitat distribution models rely on the classification or regression of binary presence/absence data against several environmental or geographical variables, such that the suitability of the model can be assessed through a confusion matrix and the statistical metrics associated to it. However, when considering the prediction of the habitat against time, the variability in the spatial distribution of the habitat can be summarized and validated using the emerging patterns from the shape of this distribution. We modeled the potential habitat of Jack mackerel (*Trachurus murphyi*) off Peru, using several sources of information for fish (fisheries, scientific surveys, satellite monitoring of vessels) jointly with environmental data from remote sensing, *in situ* observations and models, from 1992 to 2008. The potential habitat was predicted over the study period with monthly resolution, and the model was validated using quantitative and qualitative information of the system compared with i) one dimensional profiles inside the scientific survey area (latitudinal and off-shore distributions) and, ii) time series of the modes and extremes of the profiles. We conclude that a good model in terms of classification can predict poorly some particular spatial patterns, and validation based on the predictions of spatial patterns has to be carried out, especially when these are important for management applications.

1. Introduction

Species distribution modelling (SDM) has become a central tool in applied research in biogeography and its use is widespread across disciplines (Araujo and Guisan 2006), particularly to make inference about changes in species distributions under different climate scenarios (e.g., Beaumont et al. 2005, Wiens et al. 2009, Beaugrand et al. 2013) and to produce distribution maps which can be used to force the spatial dynamics of other models (Drexler and Ainsworth 2013). In this context, it is important to ensure that SDMs are able to properly predict the most important spatial patterns, particularly the ones which can have a significant effect in other models.

SDMs are commonly classification or regression models of binary presence/absence data against several environmental or geographical variables, such that the suitability of the model can be assessed through a confusion matrix and the statistical metrics associated to it. However, the evaluation of SDMs in terms of their ability to predict presences and absences, is not enough to ensure the model is able to predict consistent spatial patterns. When considering the prediction of the habitat against time, the variability in the spatial distribution can be summarized and validated using the emerging patterns given by the shape of this distribution, and the quality of the model to be used for the prediction of spatial patternsshould be assessed considering its skills for the prediction of such patterns and not only its power for the classification of presences and absences.

In this work, we evaluate whether a good model in terms of classification can successfully predict some particular spatial patterns. We illustrate this with a SDM for Jack mackerel off Peru, where the predicted spatial distribution against time is expected to be used to force the dynamics of an application of the OSMOSE ecosystem model (Shin and Cury 2001, 2004) to the Humboldt Current Ecosystem. For this particular ecosystem model application, it is particularly important that the off-shore distribution can be properly predicted since it will have a potential impact on other species in the ecosystem, particularly the coastal ones (e.g. anchovy), and can lead to a misspecification of the resulting trophic interactions.

2. Material and methods

2.1. Data

Jack mackerel distribution.

Georeferenced estimates of presence and absence for Jack mackerel were obtained from three sources: i) hydroacoustic surveys conducted by IMARPE (Gutierrez et. al 2000; IMARPE 2010), ii) artisanal and industrial Peruvian Jack mackerel fleet fishing points recorded by IMARPE, iii) published literature of Jack mackerel distribution off Chile in order to cover a broad range of environmental tolerance (Barria P et al. 2001, Martinez and Böhm 2005, Martinez et al. 2009, IFOP 1994, 1996, 1997, 1998, 1999, 2001, 2007a, 2007b, 2008a, 2008b, 2009, IIPOR 1995, 2003, 2001). Monthly data between 1992 and 2008 was selected.

Environmental variables

Environmental variables available for the study area were Sea Surface Temperature (SST), Sea Surface Salinity (SSS), water masses (WM), oxycline depth (OD) and chlorophyll (CHL). These variables were obtained from *in situ* and remote sensing databases and a published ROMS-PISCES model of the region (Echevin et al. 2012).

In situ data

Oxycline depth: Obtained from hydroacoustic surveys (IMARPE), monthly prospections (IMARPE) and international database WOD09 (Garcia et al. 2010). Data were transformed into a 2°x2° grid between 0°S-20°S and 90°W-70°W. Each square of the grid was interpolated in time using Singular Spectrum Analysis (SSA) (Kondrashov and Ghil 2006). Then, interpolation in space was done using Laplace interpolation implemented in Ferret (NOAA 2013).

Surface chlorophyll: Obtained from IMARPE's scientific surveys database. These data were not interpolated because the plankton biological dynamics is very complex and assumptions for spatial interpolation may not hold.

Remote Sensing Data

Sea Surface Temperature: Data from Pathfinder and MODIS satellites were used, both at 4km resolution, and covering the period from 1985 to 2008 (monthly data). These data were validated for Peru by Demarcq and Dagorne (2011). Laplace interpolation was carried out to solve cloud coverage problems.

Surface water masses: These were calculated using SST (from Pathfinder and Modis) and SSS (SODA) and interpolated to 1/12° of resolution. Water masses are identified using a T-S diagram, as described by Romero et al. (submitted) using the classifications of Zuta and Guillen (1970), Moron (2000) and Swartzman et al. (2008).

Surface chlorophyll: Data from SeaWIFS (Behrenfeld and Falkowski 1997) at 9km resolution between 1997 to 2008 were corrected applying an empirical relationship validated for Peru by Quispe et al. (2010).

Model outputs

Sea Surface salinity: Climatic global model SODA (with data assimilation) has been validated for the Peruvian area (Czeschel et al. 2011) and we selected the temporal period from 1985 to 2008 (monthly data) to be consistent withtime series from Remote Sensing data. For the coastal areas we interpolated the data using cubic splines as implemented in ROMStools (Penven et al. 2008) for a final regular resolution of 9km.

Additionally, we used model outputs from ROMS-PISCES (Aumont and Bopp 2006) at 1/9° of resolution, in an area corresponding to the Southeast Pacific delimited between 100° and 70° W and 10°N to 40° S, from 1992 to 2008 (Echevin et al. 2012). ROMS (Regional Oceanic Modeling System) is a free surface ocean model that solves the primitive equations of ocean dynamics, and is widely used by the scientific community in a diverse range of applications in the World (Haidvogel et al 2000, Marchesiello et al 2003, Peliz et al 2003, Di Lorenzo 2003, Dinniman et al. 2003, Budgell 2005, Warner et al. 2005, Wilkin et al. 2005). PISCES (Pelagic Interaction Scheme for Carbon and Ecosystem Studies) biogeochemical model simulates marine biological productivity and describes biogeochemical cycles of carbon and major nutrients in the ocean (Aumont & Bopp 2006). Validation of ROMS and PISCES model outputs is reported in Romero et al. (submitted) and Espinoza et al. (submitted), respectively.

2.2 Spatial Distribution Models

We used GAM (Generalized Additive Models) niche-based models to predict the spatial distribution of Jack mackerel, which have been widely used for SDM (Guisan et al. 2002) and particularly to build distribution maps to be used in ecosystem models (Drexler and Ainsworth 2013). Twelve different models were tested differing in i) the degree of smoothing allowed in the spline functions used in the GAM (controlling the flexibility of the non-linear relationships to capture the relationship between the environmental predictors and the response variable), ii) a logarithmic transformation for chlorophyll-a to facilitate the modeling of the potential quick response of Jack mackerel distribution to chl-a and iii) the inclusion or not of the depth of the ocean floor as a predictor. The details of all the models implemented are shown in Table 1.

Table 1. Variables used for all the models presented. The environmental variables used were Sea Surface Temperature (sst), Concentration of chlorophyll-a in the surface, Sea Surface

Salinity (sss), depth of the oxycline of 1 mL/L (OD), Depth of the sea floor (Depth) and Water mass type (WM). The value indicated is the degree of smoothing allowed to the splines in the GAM. When 'log' is presented, the logarithmic transformation of the variable was used.

Model	sst	chl-a	sss	OD	Depth	WM
l0	2	log, 2	2	2	-	factor
l1	3	log, 3	3	3	-	factor
l2	4	log, 4	4	4	-	factor
p0	2	log, 2	2	2	2	factor
p1	3	log, 3	3	3	3	factor
p2	4	log, 4	4	4	4	factor
f0	2	2	2	2	-	factor
f1	3	3	3	3	-	factor
f2	4	4	4	4	-	factor
g0	2	2	2	2	2	factor
g1	3	3	3	3	3	factor
g2	4	4	4	4	4	factor

The data was split into two sets: the training period (1992-2003) used to fit the model and the validation period (2004-2008) used to test the prediction skill of the models. Cross-validation was used in the training period, fitting the model each time with 70% of the data, leaving the remaining 30% for a validation to test the robustness of the fitting process.

2.3 Validation

For the validation, the last 5 years of information were used (2004-2008). The purpose was to test the prediction skill of the model, since many applications of SDMs have implied their use to predict future scenarios. We used two metrics based on the classification ability of the models: i) the Area under the curve (AUC) of the Receiver Operating Characteristic (ROC) curve, ranging from 0 to 1, 0.5 meaning the model is not better than a random classifier and 1 the model is perfectly accurate, less than 0.6 corresponding to a very poor agreement, 0.6-0.7 poor, 0.7-0.8 fair, 0.8-0.9 good and 0.9 or more excellent (Thuiller et al. 2010); and ii) the Cohen's Kappa coefficient, a statistical measure of concordance, between 0 and 1, which takes into account the agreement occurring by chance, 0.2 or less being considered a very poor agreement, 0.2-0.4 poor, 0.4-0.55 fair, 0.55-0.7 good, 0.7-0.85 very good and 0.85 or more excellent (Metzger et al. 2005). Both measures are widely used to test the quality of SDMs (e.g. Thuiller et al. 2006, Araujo et al. 2005, Aguirre-Gutierrez et al. 2013).

Additionally, we calculated one dimensional profiles (off-shore and latitudinal distributions), emerging from the predictions of the different models. These profiles were calculated inside the scientific survey area for every survey in order to compare the predicted profiles with the observed survey ones. With these profiles for every survey, time series of the modes and extremes of the profiles (5% and 95% percentiles) were calculated. The mean squared error (MSE) was computed for these time series and used as a metric of the quality of the prediction of the spatial patterns by the models.

3. Results and discussion

The results for the twelve models tested show that, using the AUC and Cohen's Kappa statistics, all the models are classified as being excellent or very good within the training period and the validation data for the same time, but an important decrease in performance is observed in the independent validation period for all models (Table 2). Most models changed from excellent/very good to a poor fit, the model p2 decreasing from excellent/very good to just fair, but being consistently better than the other models tested according to these indicators. These highlight the point that SDMs should be used carefully in prediction of future scenarios. Using the MSE for the time series of spatial indicators (Table 3), an important increase in the error is observed for the validation period. Considering that the validation period is just 5 years after the training period, more efforts will be needed to use these spatial statistical models in forecast mode. The model p2 has the best score in 2 of the 6 spatial indicators calculated for the validation period using the MSE (Table 3). The results suggest that p2 is the best at predicting the mode and the 5% percentile of the off-shore distribution of Jack mackerel, which is an important pattern to reproduce for the purpose of accounting for the spatial overlap between coastal and oceanic species. For the other indicators, there is not a consistently better model.

The observed and predicted modes of the off-shore distribution of Jack mackerel showed a good agreement for most of the surveys but with important outliers within the training and validation period (Figure 1), being these the ones contributing the most to the MSE. The errors for the predictions of the modes of the off-shore distribution increase for the predictive validation period (Figure 2). However, some of the points in the training period show errors bigger than most of the points of the validation period, indicating profiles which are not predicted properly. Analyzing all the observed profiles for each survey against the different predictions of the models show that the quality of the predictions range from almost perfect (Figure 3: Aug 1997, Mar

1998) to very poor (e.g. Oct 2003 in the training period and Feb 2006 and Jul 2007 in the predictive validation period). Considering that one important application of the SDM is to better understand the spatial and trophic interactions between species in the Humboldt Current Ecosystem, the error in the predictions like in August 1998, indicating a more coastal Jack mackerel, could have important impacts in determining the predation relationships with other species, mainly the dominant anchovy, knowing in particular that 1998 was an El Niño year where anchovy could also experience an increased starvation mortality (Ñiquen and Bouchon 2004). On the other hand, the error in predictions for Oct 2008 where Jack mackerel is supposed to have a more oceanic distribution can lead to an underestimation of its trophic interactions with coastal species.

Table 2. Performance of the models for Jack mackerel presence/absence classification. AUC and Cohen's kappa for the training data (T, 1992-2003), validation data (V, 1992-2003) and predictive validation (PV, 2004-2008) periods are shown.

		l0	l1	l2	p0	p1	p2	f0	f1	f2	g0	g1	g2
AUC	T	0.931	0.943	0.951	0.935	0.946	0.953	0.93	0.938	0.946	0.934	0.942	0.949
	V	0.93	0.943	0.951	0.934	0.946	0.952	0.93	0.937	0.945	0.933	0.941	0.948
	PV	0.719	0.756	0.766	0.757	0.788	0.793	0.72	0.724	0.73	0.751	0.761	0.763
Kappa	T	0.696	0.728	0.762	0.698	0.748	0.776	0.7	0.725	0.75	0.707	0.741	0.771
	V	0.693	0.729	0.764	0.696	0.75	0.777	0.695	0.722	0.747	0.704	0.739	0.767
	PV	0.319	0.363	0.357	0.332	0.391	0.405	0.335	0.336	0.331	0.322	0.362	0.356

Table 3. Performance of the models for Jack mackerel distribution. Several indicators of performance measured by the MSE for the training (T, 1992-2003) and predictive validation (PV, 2004-2008) periods are shown.

		l0	l1	l2	p0	p1	p2	f0	f1	f2	g0	g1	g2
dc.mode	T	452.5	351.3	287.5	1443	202.3	287.5	425.9	319.4	197	255.5	175.7	117.1
dc.mode	PV	3100	3114	2311	2464	2727	1993	3211	3377	3308	2533	2796	2450
dc.p05	T	205	137	107.6	110	84.88	82.54	234.1	206	128.8	131.4	105.6	91.46
dc.p05	PV	712.3	671.1	659.7	680.6	622.3	564.5	693.6	734.8	730.9	675.6	711.3	674.4
dc.p95	T	2822	1737	597.3	689.1	531	528.1	1516	8909	5319	584.7	3529	1036
dc.p95	PV	4846	4837	4892	4507	3619	4366	3131	4366	5237	3119	4063	4266
lat.mode	T	7.86	8.09	5.46	3.66	5	6.52	6.49	7.97	9.42	3.9	4.58	6.67
lat.mode	PV	8.87	8.27	8.07	7.75	7.35	9.75	9.56	9.17	8.71	8.81	8.13	7.38
lat.p05	T	1.57	2.48	2.77	1.73	1.75	1.75	2.23	2.01	2.74	1.49	1.54	1.73
lat.p05	PV	2.58	2.84	2.91	2.42	2.59	2.63	2.75	2.88	2.98	2.54	2.73	2.61
lat.p95	T	1.86	1.26	1.01	2.47	1.98	1.44	1.81	1.59	2.4	3.29	2.6	2.08
lat.p95	PV	6.06	5.65	5.21	5.73	3.65	2.64	8.42	6.2	5.95	6.73	5.51	2.1

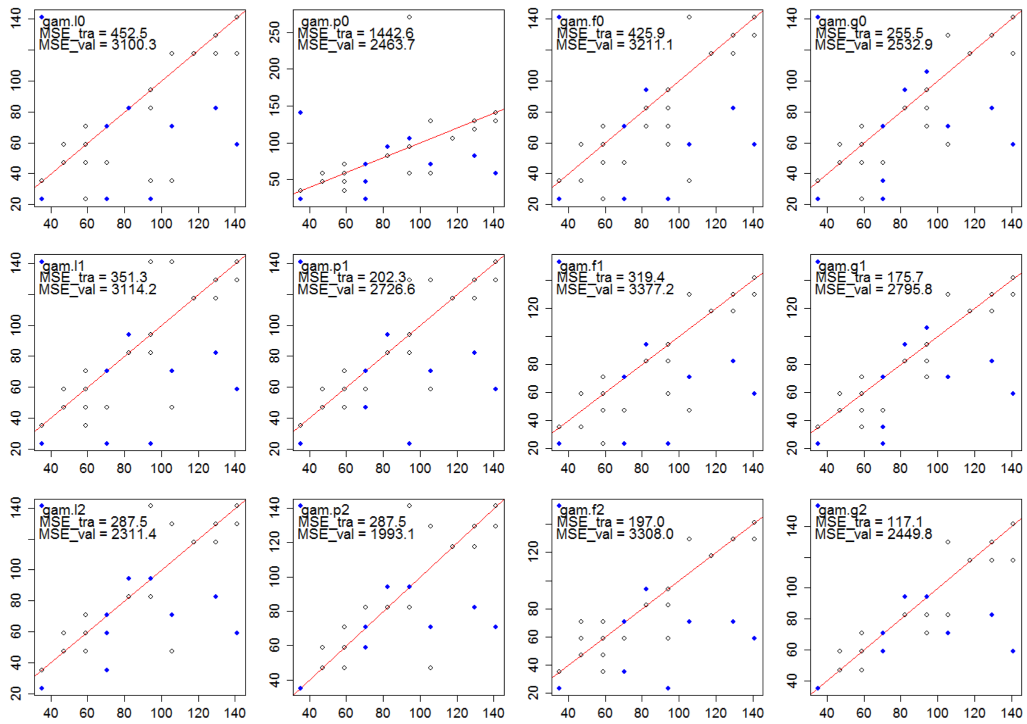

Figure 1. Modes of the distance to the coast distribution profile. The observed modes (x axis) against the predicted ones (y axis) are shown. The black dots correspond to the training period and the blue ones to the validation period. The red line is the y=x rect. The mean squared error (MSE) for the training period and the validation period for each model are shown.

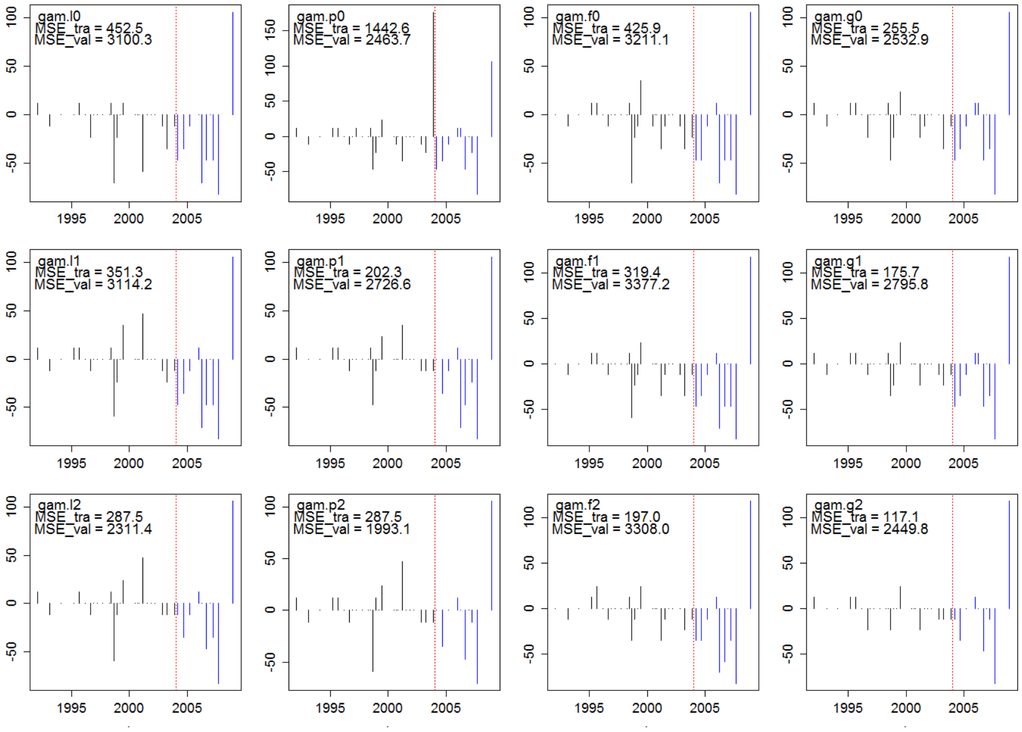

Figure 2. Time series of the residuals of predictions of the mode of the distance to the coast distribution profiles for jack mackerel.

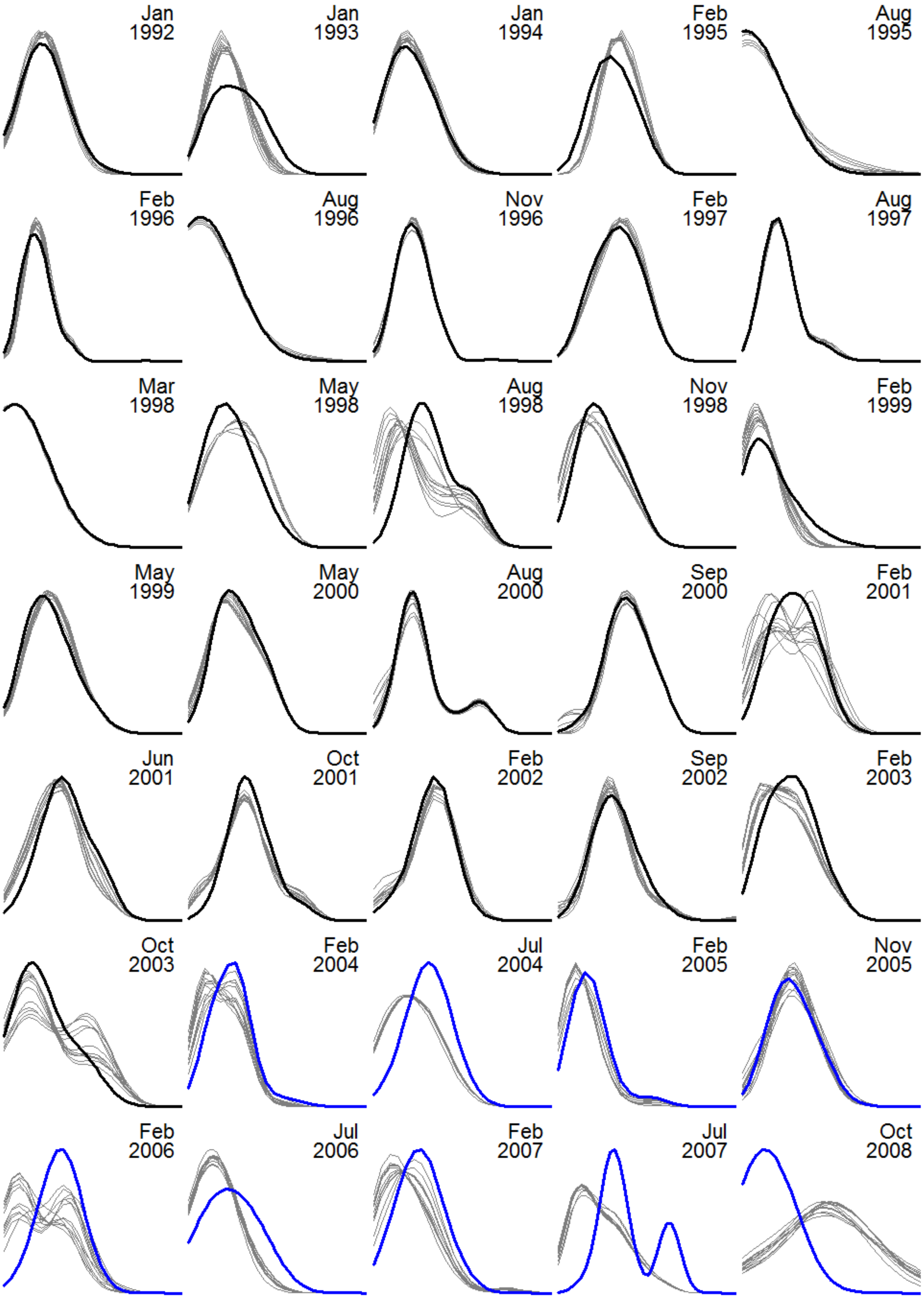

Figure 3. Profiles of the distance to the coast. The observed distribution from the coast (thick line) of jack mackerel for several research surveys and the predictions made by the considered GAM models (gray lines) are shown. The surveys before 2004 were used to train the model (black) and the rest were used to validate the model (blue).

4. Conclusions and perspectives

A good model in terms of classification (AUC, Cohen's Kappa) can poorly predict some particular spatial patterns, so that a complementary validation based on the predictions of spatial patterns is necessary, especially when these summarize important functional features for the ecosystem. Different spatial indicators can lead to the selection of a different model, so the objectives and subsequent uses of the SDMs must be known when analyzing the quality of the models and their validation with independent data is essential to detect and avoid problems with forecasting of distributions in time.

References

Aguirre-Gutierrez J, Carvalheiro LG, Polce C, van Loon EE, Raes N, et al. (2013) Fit-for-Purpose: Species Distribution Model Performance Depends on Evaluation Criteria – Dutch Hoverflies as a Case Study. PLoS ONE 8(5): e63708. doi:10.1371/journal.pone.0063708

Araújo, M.B., Pearson, R.G., Thuiller, W. & Erhard, M. (2005) Validation of species-climate impact models under climate change. Global Change Biology, 11, 1504–1513.

Aumont O. & L. Bopp. 2006. Globalizing results from ocean in situ iron fertilization studies. Gl. Biogeochem. Cyc.20(GB2017).doi:10.1029/2005GB002591.

Barría P. et al. 2001. Diagnóstico de la Pesquería Chilena de Jurel (Trachurus symmetricus murphyi).Instituto de Fomento Pesquero, Valparaíso. Pp. 123-141.

Behrenfeld M. & P. Falkowski. 1997. Photosynthetic rates derived from satellite-based chlorophyll concentration. Limnology and Oceanography 42(1): 1-20.

Bertrand A., Chaigneau A., Peraltilla S., Ledesma J., Graco M. &Monetti F. 2011. Oxygen, a fundamental property regulating pelagic ecosystem structure in the coastal Southeastern tropical Pacific.PLoS ONE, 6(12): e29558.

Chavez F. P., A. Bertrand, R. Guevara-Carrasco, P. Soler & J. Csirke. 2008. The northern Humboldt Current System: Brief history, present status and a view towards the future. Progress in Oceanography 79:95-105.

Chaigneau A., A. Gizolme& C. Grados. 2008. Mesoscale eddies off Peru in altimeter records: Identification algorithms and eddy spatio-temporal patterns. Prog.Oceanogr. 79: 106–119.

Chirichigno N., W. Fischer & C.E. Nauen, C.E. 1982.INFOPESCA. *Catálogo de especies marinas de interés económico actual o potencial para América Latina. Parte 2-Pacífico Centro y Suroriental.* Roma, FAO/PNUD, 588 p.

Czeschel R., L. Stramma, F. Schwarzkopf, B.S Giese, A. Funk & J. Karstensen. 2011. Middepth circulation of the eastern tropical South Pacific and its link to the oxygen minimum zone. Journal of Geophysical Research - Oceans, 116: C01015.

Demarcq H. & D. Dagorne. 2011. Case study 15. Biological Response Associated With a Coastal Upwelling Event In: Morales, J., Stuart, V., Olatt, T. and Sathyendranath,S. (Eds.). PRESPO/IOCCG. Handbook of Satellite Remote Sensing Image Interpretation: Applications for Marine Living Resources Conservation and Management, pp. 217-228, EU PRESPO and IOCCG, Dartmouth, Canada.

Drexler M, Ainsworth CH (2013) Generalized Additive Models to Predict Species Abundance in the Gulf of Mexico: An Ecosystem modeling tool. PLoS ONE 8(5):e64458.

Espinoza-Morriberon D., V. Echevin V., C.Y. Romero, J. Ledesma, R. Oliveros-Ramos & J. Tam. (Submitted) Validación del modelo acoplado ROMS-PISCES en el Pacifico Sudoriental.Parte II: Condiciones biogeoquimicas.

Garcia H.E., R.A. Locarnini, T.P. Boyer et al. 2010. World Ocean Atlas 2009, Volume 3: Dissolved Oxygen, Apparent Oxygen Utilization, and Oxygen Saturation. (NOAA Atlas NESDIS 70, U.S. Government Printing Office, Washington, DC).

Guisan A., Edwards T.C., Hastie T. (2002) Generalized linear and generalized additive models in studies of species distribution: setting the scene. Ecological Modelling 157:89-100.

Gutiérrez M. et al., 2000. Estimados de biomasa hidroacústica de los cuatro principales recursos pelágicos en el mar peruano durante 1983 -2000. Bol. Inst. Mar Perú. Vol. 19, n°1-2, pp. 136-156.

IMARPE, 2010. Informe sobre la quinta reunión de expertos en dinámica de población de la anchoveta peruana. Bol. Inst. Mar. Perú – Callao. Bol. Inst. Mar Perú 23(1-2).

Instituto de Fomento Pesquero (IFOP). 1994. Evaluación Directa del Stock de Jurel en la Zona Centro - Sur. Informes Técnicos FIP. FIP-IT/93-02.

Instituto de Fomento Pesquero (IFOP). 1996. Seguimiento de las Principales Pesquerías Chilenas 1995. Centro de Servicios Pesqueros. Pp. 274.

Instituto de Fomento Pesquero (IFOP). 1997. Estudio Biológico - Pesquero del Recurso Jurel en la Zona Norte (Regiones I y II). Fase II. Informes Técnicos FIP. FIP-IT/94-17.

Instituto de Fomento Pesquero (IFOP). 1998. Evaluación Hidroacústica del Recurso Jurel en la Zona Centro - Sur (Fase Crucero Metodológico). Informes Técnicos FIP. FIP-IT/95-07.

Instituto de Fomento Pesquero (IFOP). 1999. Monitoreo de las Capturas de Jurel en la Zona Centro - Sur. Informe Final Corregido. FIP N° 98-01.

Instituto de Fomento Pesquero (IFOP). 2001. Monitoreo de las Capturas de Jurel, 1999. InformesTécnicos FIP. FIP-IT/99-02.

Instituto de Fomento Pesquero (IFOP). 2007a. Evaluación Hidroacústica de Jurel en la Región Oceánica, de la I y II Regiones. Informe Final. Proyecto FIP N° 2006-08.

Instituto de Fomento Pesquero (IFOP). 2007b. Evaluación Hidroacústica del Recurso Jurel entre la V y X Regiones, verano, año 2006. Informe Final. Proyecto FIP N° 2006-02.

Instituto de Fomento Pesquero (IFOP). 2008a. Evaluación Hidroacústica de Jurel en la I y II Regiones, año 2007. Informe Final. Proyecto FIP N° 2007-09.

Instituto de Fomento Pesquero (IFOP). 2008b. Monitoreo de las condiciones bio-oceanográficas entre la I y IV Regiones, año 2007. Informe Final. Proyecto FIP N° 2007-11 (Segunda licitación).

Instituto de Fomento Pesquero (IFOP). 2009. Evaluación Hidroacústica de jurel en la I-II Regiones, año 2008. Informe Final. Proyecto FIP N°2008-07.

Instituto de Investigación Pesquera Octava Región (IIPOR). 2003. Condición Biológica del Jurel en Alta Mar, 2001. Informe Final. Proyecto FIP N°2001-12.

Instituto de Investigación Pesquera Octava Región (IIPOR). 2001. Condiciones Biológicas del Jurel en Altamar. InformesTécnicos FIP. FIP-IT/99-14.

Instituto de Investigación Pesquera Octava Región (IIPOR). 1995. Estudio Biológico - Pesquero del Recurso Jurel en la Zona Centro - Sur (V a IX Regiones). InformesTécnicos FIP. FIP-IT/93-18.

Kondrashov D. & M. Ghil. 2006. Spatio-temporal filling of missing points in geophysical data sets. Nonlin. ProcessesGeophys. 13: 151-159.

Martínez C. & M. Gabriela Böhm S. 2005. Análisis Biológico-Pesquero de los Recursos Pelágicos de la I y II Región de Chile. 11° Taller IFOP/IMARPE. Lima.

Martínez C. et al., 2009. La Pesquería Pelágica del Norte de Chile. Evaluación conjunta de los stocks de anchoveta y sardina. 13° Taller IFOP/IMARPE. Lima.

Metzger M. J., Bunce R. G. H., Jongman R. H. G., Mücher C. A. and Watkins J. W. (2005). A climatic stratification of the environment of Europe. Global Ecology and Biogeography 14(6): 549–563.

Morón O. 2000. Características del ambiente marino frente a la costa peruana. Boletín Instituto del Mar del Perú 19, 179–204.

Muck P. &Sanchez G. 1987. The importance of mackerel and jack mackerel predation for the Peruvian anchoveta stock (a population and feeding model). p. 276-293 *In* D. Pauly and I. Tsukayama (eds.) *The Peruvian anchoveta and its upwelling ecosystem: three decades of change.*ICLARM Studies and Reviews. 15.

NOAA's Pacific Marine Environmental Laboratory. 2013. http://ferret.pmel.noaa.gov/Ferret/

Ñiquen M, Bouchon M., 2004. Impact of El Niño event on pelagic fisheries in Peruvian waters. Deep-Sea Research II 51:563-574.

Oliveros-Ramos R., D. Espinoza-Morriberón, C. Wosnitza-Mendo, A Alegre, C. Quispe-Ccalluari& T. Dioses. Jack mackerel (*Trachurusmurphyi*) and chub mackerel (*Scomberjaponicus*) off the Peruvian coast and their predation on anchoveta (*Engraulisringens*). Submitted to Scientia Marina.

Penven P., V. Echevin, J. Pasapera, F. Colas, & J. Tam. 2005. Average circulation, seasonal cycle, and mesoscale dynamics of the Peru Current System: A modeling approach. J. Geophys. Res. 110: C10021.

Penven P., P. Marchesiello, L. Debreu& J. Lefevre. 2008. Software tools for pre- and post-processing of oceanic regional simulations. EnvironmentalModelling and Software 23(5): 660-662.

Quispe et al. 2010. Comparative analysis between satellite and in situ chlorophyll-a in the Peruvian Upwelling Ecosystem, between 1998 – 2007. Ecología Aplicada, 9(2): 151-159.

Romero C.Y., D. Espinoza-Morriberon, R. Oliveros-Ramos & J. Tam (Submitted). Validación del modelo acoplado ROMS-PISCES en el Pacifico Sudoriental. Parte I: Condicionesfísicas.

Serra R. 1991. Important life history aspects of the Chilean jack mackerel, *Trachurussymmetricusmurphyi*. *Invest Pesq (Chile)*, 36: 67-83.

Shin Y.-J., Cury P., 2001. Exploring fish community dynamics through size-dependent trophic interactions using a spatialized individual-based model. Aquatic Living Resources, 14(2): 65-80.

Shin Y.-J., Cury P., 2004. Using an individual-based model of fish assemblages to study the response of size spectra to changes in fishing. Canadian Journal of Fisheries and Aquatic Sciences, 61: 414-431.

Swartzman G, A. Bertrand, M. Gutiérrez, S. Bertrand, L. Vasquez. 2008. The relationship of anchovy and sardine to water masses in the Peruvian Humboldt Current System from 1983 to 2005. Progress In Oceanography 79(2-4):228-237.

Thuiller W, Lafourcade B, Araujo M (2010). Presentation Manual for BIOMOD.http://r-forge.r-project.org/scm/viewvc.php/*checkout*/pkg/inst/doc/Biomod_Presentation_Manual.pdf

Zuta S., O. Guillén. 1970. Oceanografía de las aguas costeras del Perú. Boletín del Instituto del Mar del Perú 5:157-324.

1.3.2 Prediction of the spatial distribution of modeled fish in the NHCE

Similar models and methods as described in the previous subsection for Jack mackerel were applied to the other species explicitly modeled in OSMOSE (macrozooplankton, anchovy, sardine, chub mackerel, mesopelagic fish, red lobster or munida, jumbo squid and the Peruvian hake). The seasonal patterns of the distribution as a summary of these results are shown in the next figures.

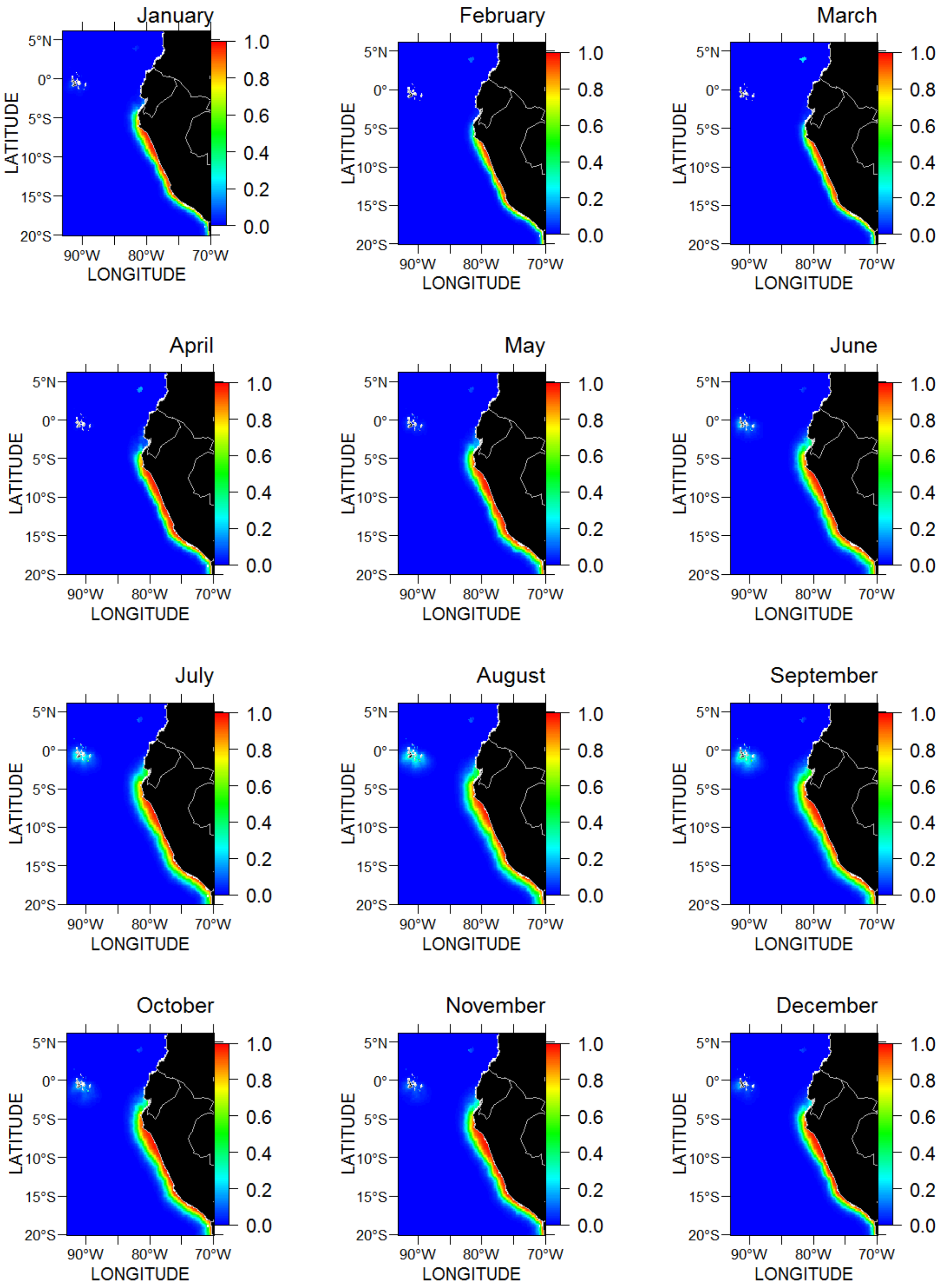

Figure 1.2: Seasonal patterns of the distribution of Peruvian anchovy as predicted by the species distribution models used to build the interannual maps for the NHCE OSMOSE model.

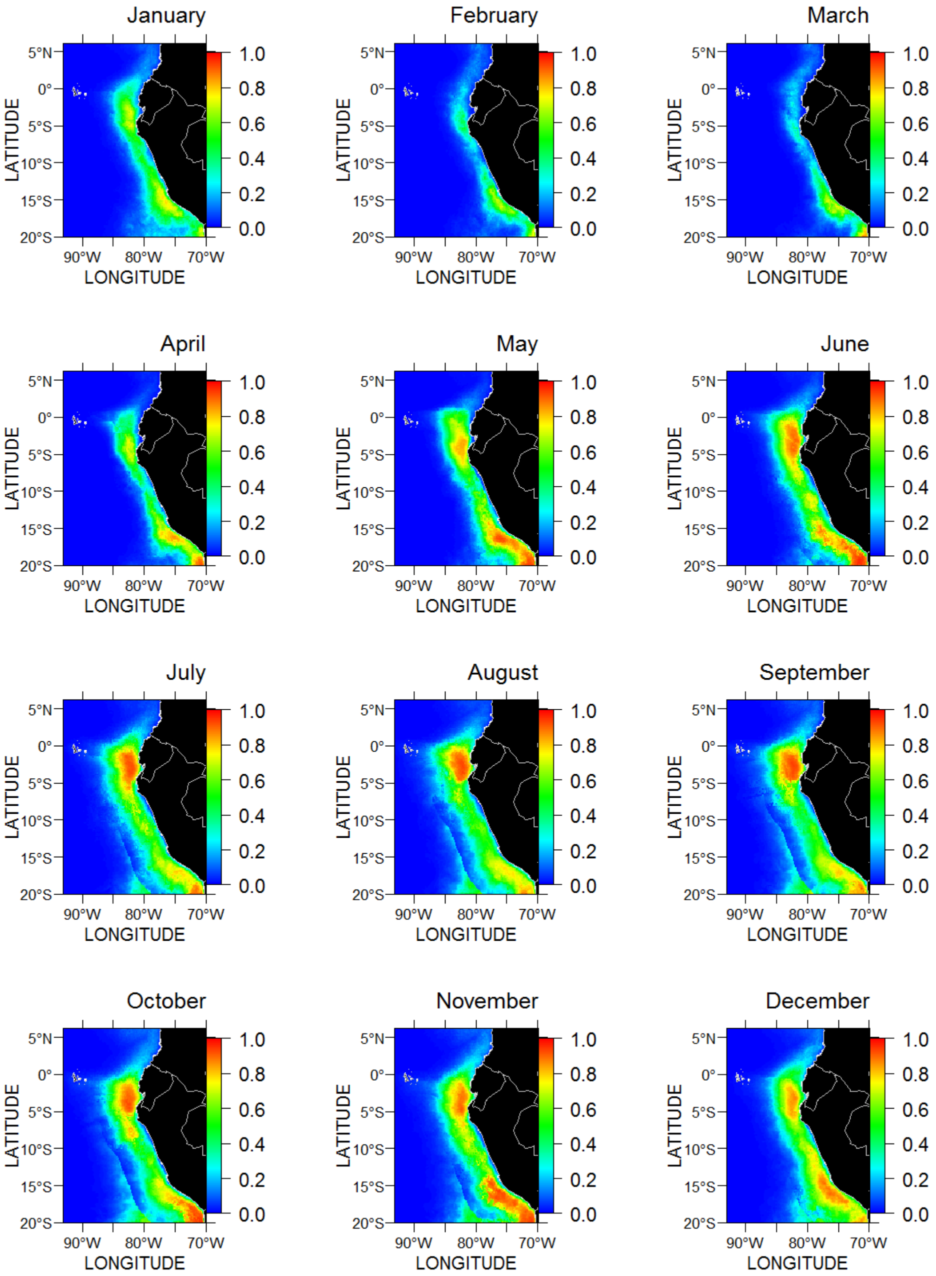

Figure 1.3: Seasonal patterns of the distribution of Jack mackerel as predicted by the species distribution models used to build the interannual maps for the NHCE OSMOSE model.

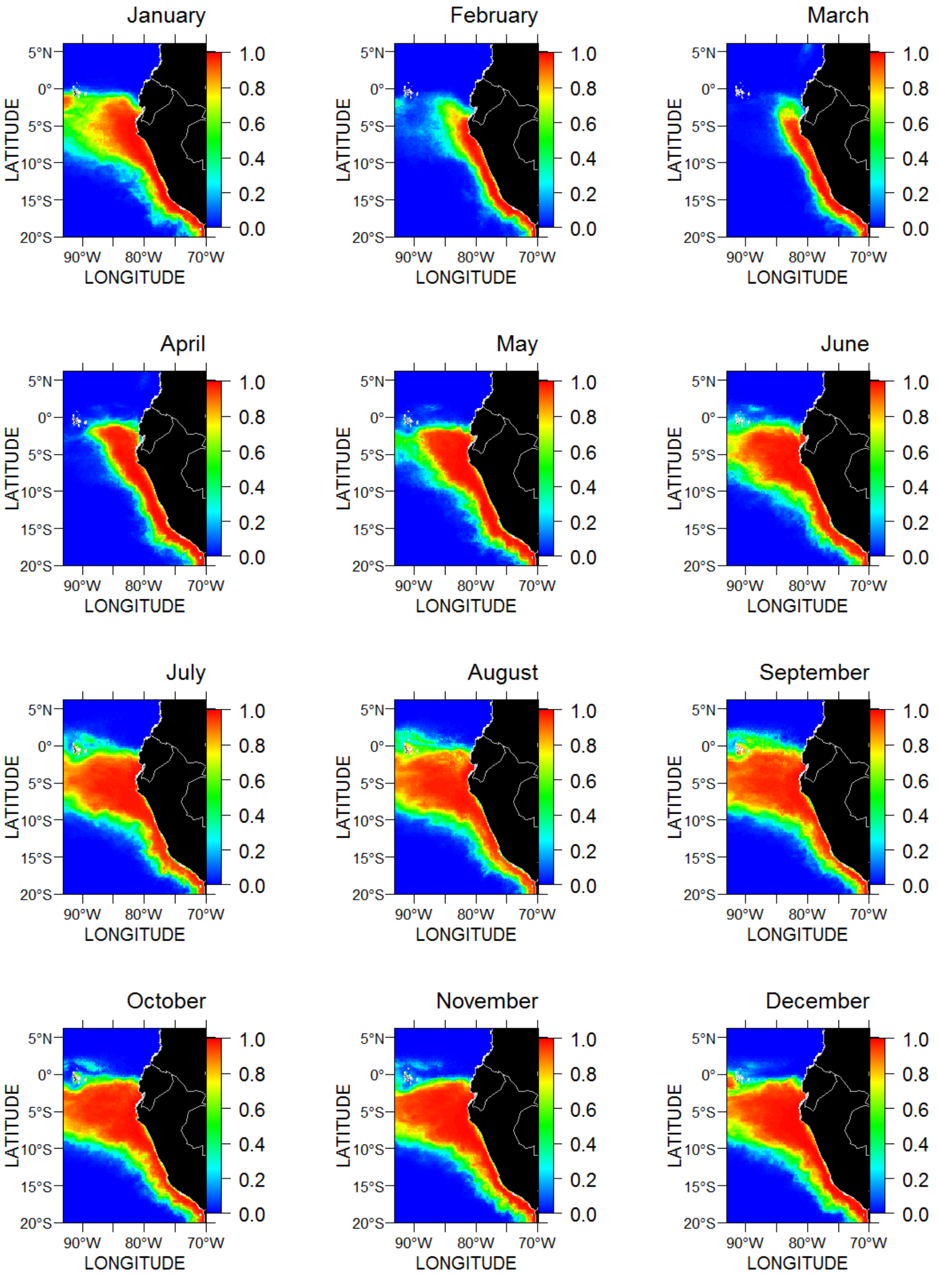

Figure 1.4: Seasonal patterns of the distribution of macrozooplankton as predicted by the species distribution models used to build the interannual maps for the NHCE OSMOSE model.

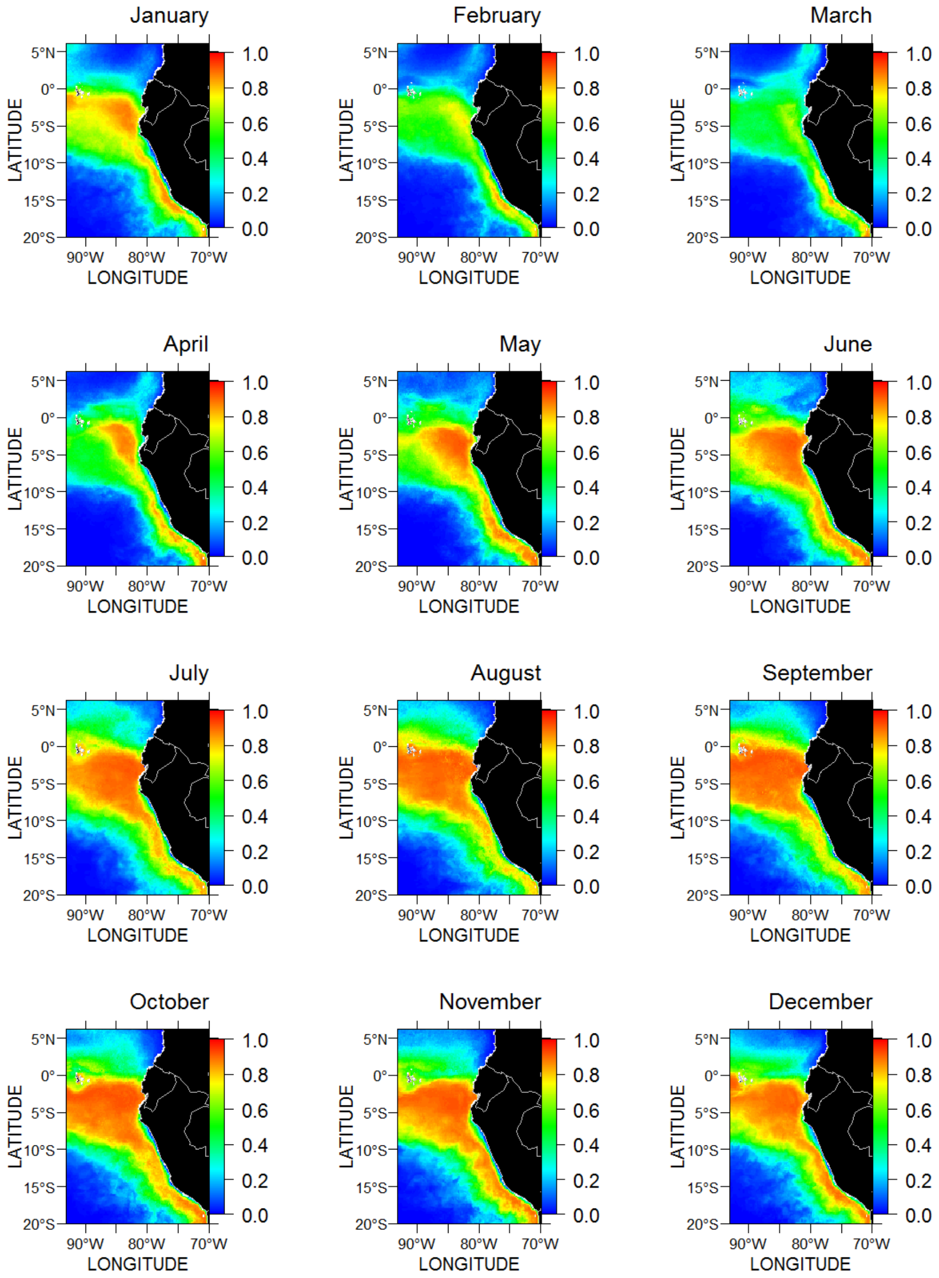

Figure 1.5: Seasonal patterns of the distribution of Humboldt squid as predicted by the species distribution models used to build the interannual maps for the NHCE OSMOSE model.

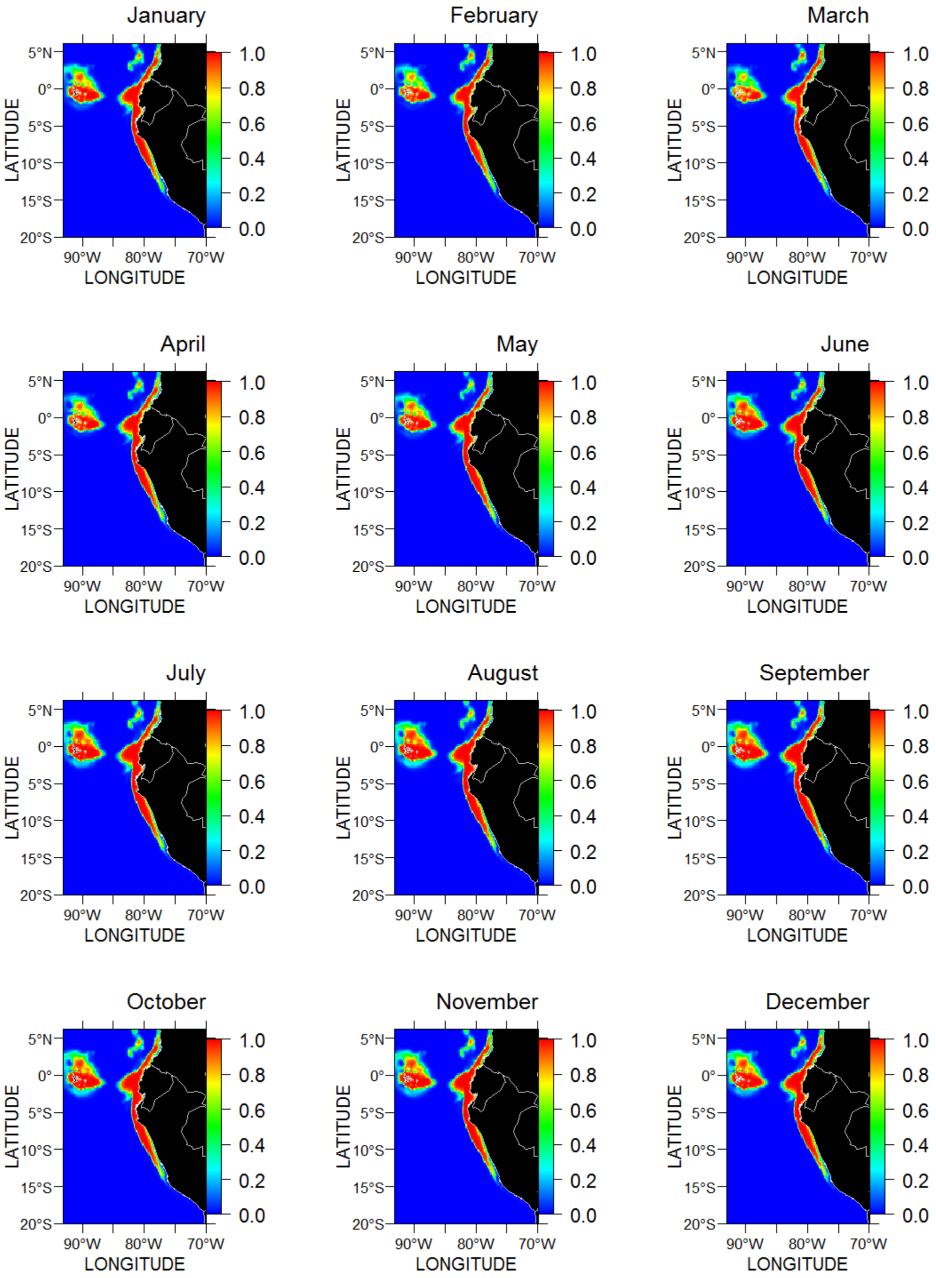

Figure 1.6: Seasonal patterns of the distribution of Peruvian hake as predicted by the species distribution models used to build the interannual maps for the NHCE OSMOSE model.

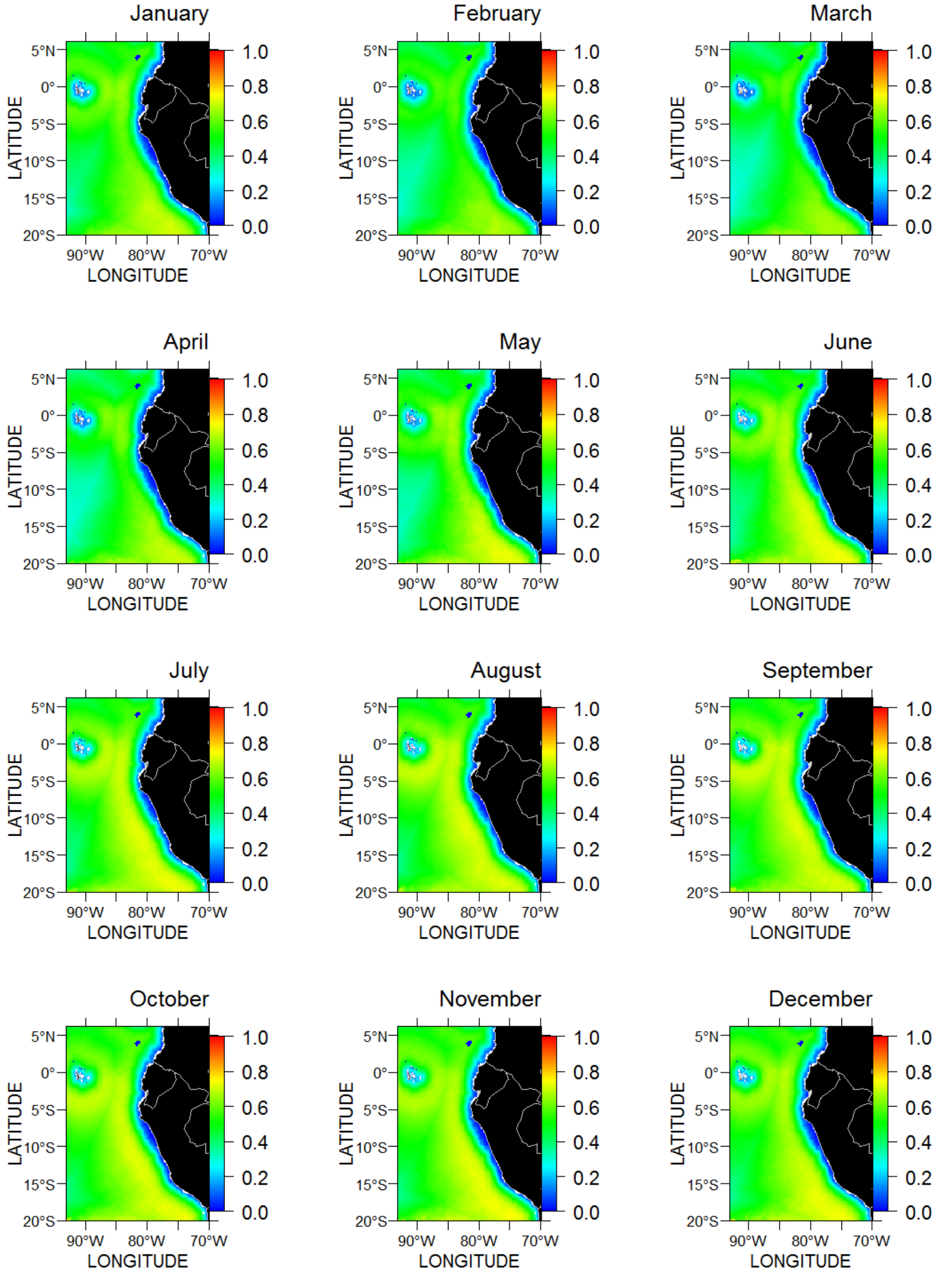

Figure 1.7: Seasonal patterns of the distribution of mesopelagic fish as predicted by the species distribution models used to build the interannual maps for the NHCE OSMOSE model.

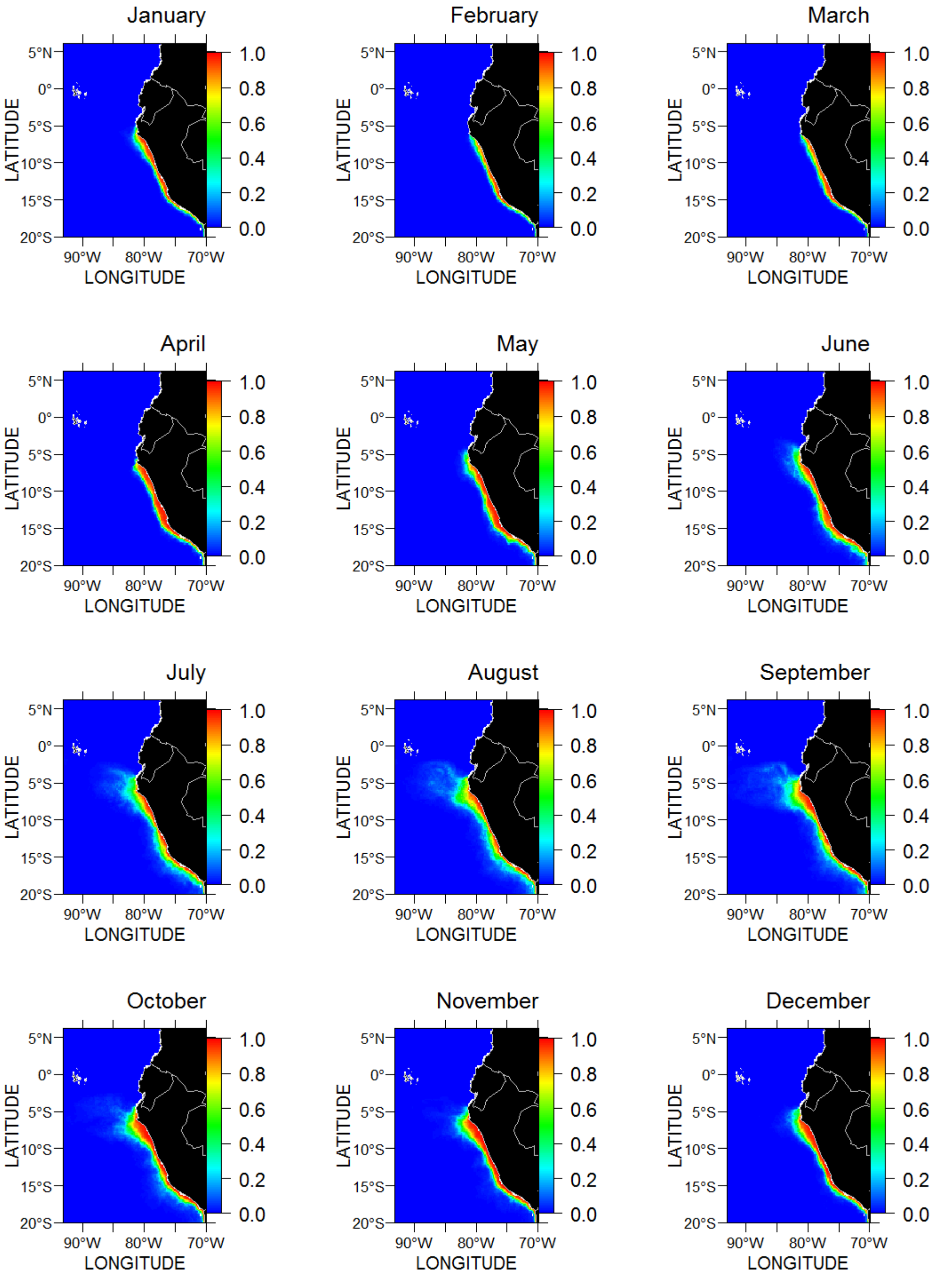

Figure 1.8: Seasonal patterns of the distribution of Munida as predicted by the species distribution models used to build the interannual maps for the NHCE OSMOSE model.

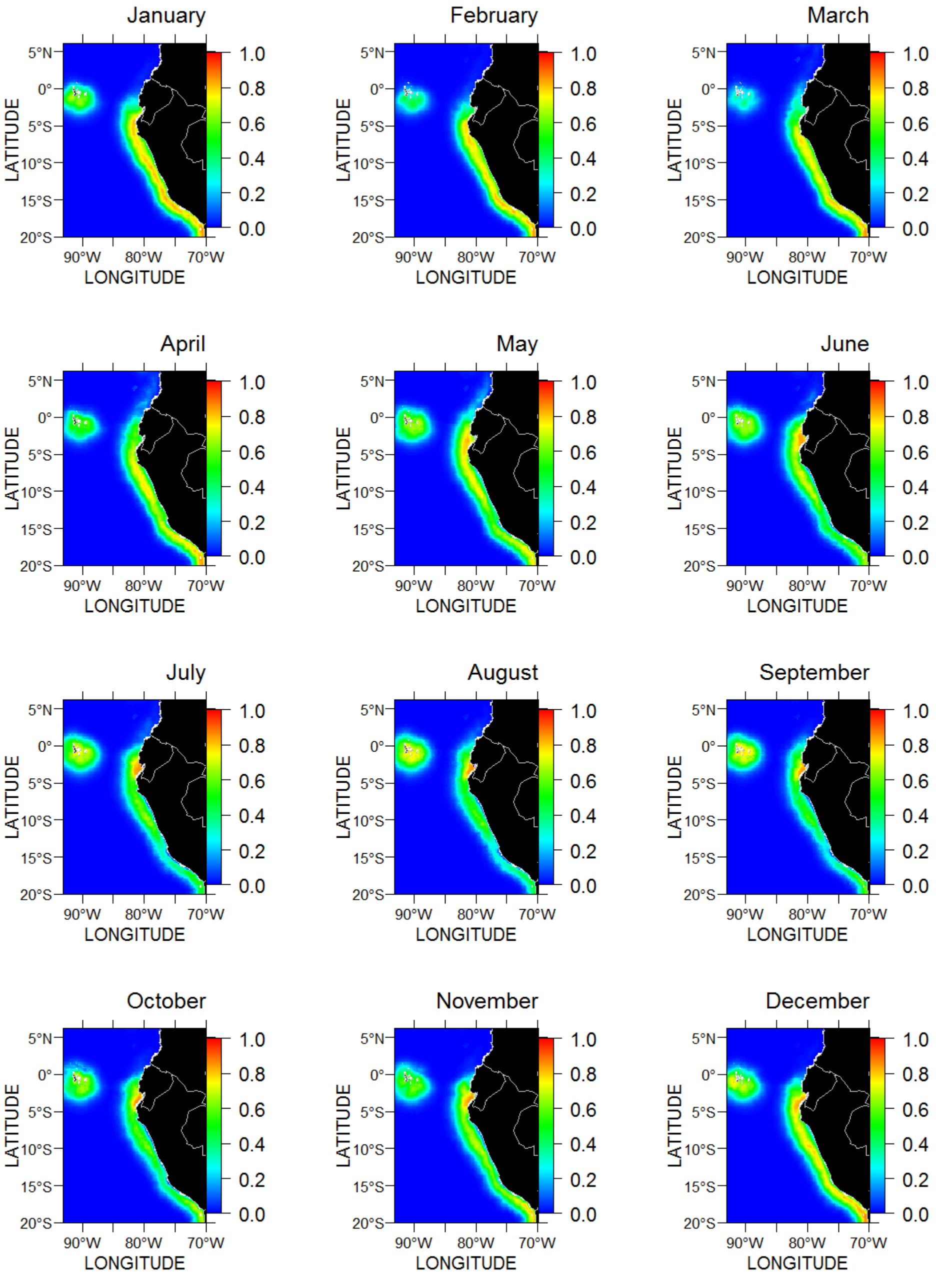

Figure 1.9: Seasonal patterns of the distribution of mackerel as predicted by the species distribution models used to build the interannual maps for the NHCE OSMOSE model.

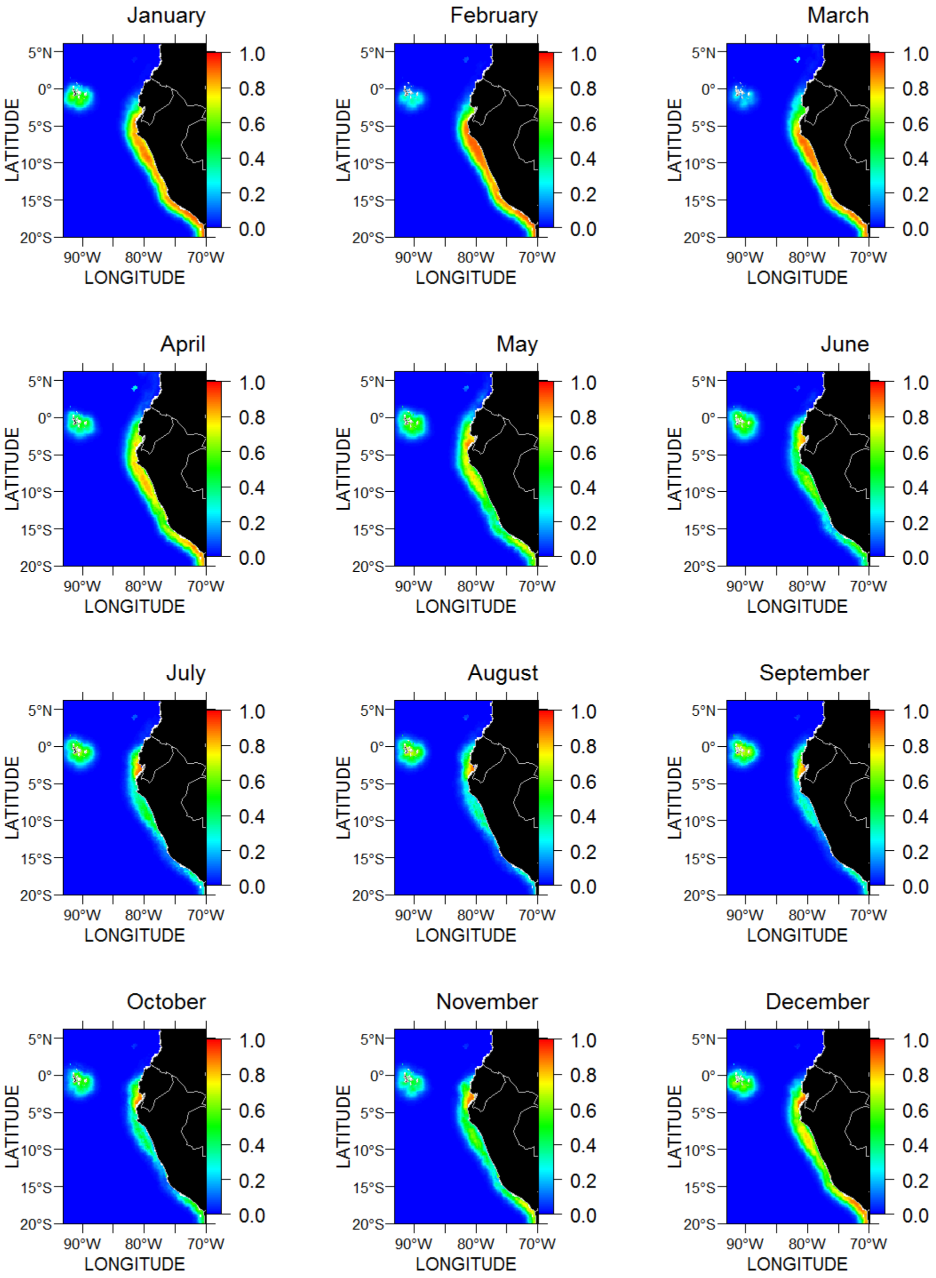

Figure 1.10: Seasonal patterns of the distribution of sardine as predicted by the species distribution models used to build the interannual maps for the NHCE OSMOSE model.

References

Aumont O. and Bopp L. 2006. Globalizing results from ocean in situ iron fertilization studies. Gl.Biogeochem.Cyc. 20:GB2017.

Budgell, W.P., 2005: Numerical simulation of ice-ocean variability in the Barents Sea region, Ocean Dynamics, DOI 10.1007/s10236-005-0008-3.

Cambon G.,Goubanova K., Marchesiello P., et al. 2013. Assessing the impact of downscaled atmospheric winds on a regional ocean model simulation of the Humboldt system. Ocean Modelling 65:11-24.

Colas, F., X. Capet, J. C. McWilliams, et al. 2008. 1997–1998 El Nino off Peru: A numerical study. Prog. Oceanogr.79:138–155.

Da Silva A.M., Young C.C. Levitus S. 1994. Atlas of surface marina data 1994. Technical report, Natl. Oceanogr. And Atmos. Admin. Silver Spring Md.

Di Lorenzo, E., 2003: Seasonal dynamics of the surface circulation in the southern California Current System, Deep-Sea Res., Part II, 50, 2371-2388.

Dinniman, M. S., J. M. Klinck, and W. O. Smith Jr. (2003), Cross shelf exchange in a model of the Ross Sea circulation and biogeochemistry, Deep-Sea Res., Part II, 50, 3103-3120.

Echevin V., Goubanova K., Dewitte B., A., et al. 2012. Sensitivity of the Humboldt Current system to global warming: a downscaling experiment of the IPSL-CM4 model. Clim. Dyn. 38(3-4):761-774.

Espinoza-Morriberón D. 2012. Impacto de la circulaciónecuatorialen la zonamínima de oxígenopresenteen el nortedelEcosistema de la Corriente de Humboldt.Thesis to obtain the degree of Master in Marine Sciences. Unidad de PostgradoVíctorAlzamora. Facultad de Ciencia y Filosofía. Universidad PeruanaCayetano Heredia, Lima. 115 pp.

Espinoza-Morriberón D., Echevin V., Romero Y., Ledesma J., Oliveros-Ramos R., Tam J., (submitted) Validation of ROMS-PISCES Coupled Model in the Southeast Pacific. Part II: Biogeochemical conditions.

Gruber N., Frenzel H., Doney S.C., et al. 2006. Eddy-resolving simulation of plankton ecosystem dynamics in the California Current System. Deep Sea Res. 1(53): 1483-516.

Haidvogel, D. B., H. G. Arango, K. Hedstrom, A. Beckmann, P. Malanotte-Rizzoli, and A. F. Shchepetkin (2000), Model evaluation experiments in the North Atlantic Basin: Simulations in nonlinear terrain-following coordinates, Dyn. Atmos. Oceans, 32, 239-281.

Montes I., Colas F., Capet X., et al. 2010. On the pathways of the equatorial subsurface currents in the eastern equatorial Pacific and their contributions to the Peru Chile Undercurrent. J. Geophys. Res. 115: C09003.

Penven P., Echevin V, Pasapera J, et al. 2005. Average circulation, seasonal cycle, and mesoscale dynamics of the Peru Current System: A modeling approach. J. Geophys. Res. 110: C10021. DOI:10.1029/2005JC002945.

Redfield A.C., Ketchum B.H. and Richards F.A. 1963. The influence of organisms on the composition of the sea-water. En: Hill M.N. (Eds.). Interscience 2: 26-77.

Risien C.M. and Chelton D.B. 2008. A Global Climatology of Surface Wind and Wind Stress Fields from Eight Years of QuikScatscatterometer Data. J. Phys. Oceanogr. 38: 2379-2413.

Romero Y., Espinoza-Morriberón D., Oliveros-Ramos R., Tam J., Echevin V. (submitted) Validation of ROMS-PISCES Coupled Model in the Southeast Pacific. Part I: Physical conditions.

Peliz, A., J. Dubert, D. B. Haidvogel, and B. Le Cann (2003), Generation and unstable evolution of a density-driven Eastern Poleward Current: The Iberian Poleward Current, J. Geophys. Res., 108(C8), 3268, doi:10.1029/2002JC001443.

Shchepetkin, A.F., McWilliams, J.C., 2005. Regional Ocean Model System: a split-explicit ocean model with a free-surface and topography-following vertical coordinate. Ocean Modelling 9, 347-404.

Warner, J.C, C.R. Sherwood, H.G. Arango, and R.P. Signell (2005) Performance of four Turbulence Closure Methods Implemented using a Generic Length Scale Method. Ocean Modelling, 8, 81-113.

Wilkin, J.L., H.G. Arango, D.B. Haidvogel, C.S. Lichtenwalner, S.M. Durski, and K.S. Hedstrom, 2005: A regional Ocean Modeling System for the Long-term Ecosystem Observatory. J. Geophys. Res., 110, C06S91, doi:10.1029/2003JC002218.

Chapter 2

On the calibration of ecosystem models using time series data

An original Evolutionary Algorithm has been developed during the thesis for the purpose of calibrating complex stochastic models. The concepts and details are provided in section 2.1.

This optimization algorithm and the tools related to the calibration of ecological models have been implemented in an R package, `calibrar`, which is also described in this chapter (manuscript 2).

2.1 An evolutionary algorithm for the calibration of ecological models using maximum likelihood estimation

Evolutionary algorithms (EA) are computer programs designed for the automatic solving of complex problems such as minimization of functions, and are inspired by the process of Darwinian evolution (Jones 1998). The three main types of EA are Genetic Algorithms (GA), Evolutionary Programming (EP) and Evolutionary Strategies (ES). Historically, Evolutionary Programming and especially Genetic Algorithms were designed with a broader range of applications (Bäck and Schewefel, 1993) while Evolutionary Strategies (ESs) were specifically designed for parameter optimization problems (Jones, 1998). For optimization problems, EAs work over a population of "individuals" searching over the space of solutions. Each individual encodes a solution (e.g. a vector of parameter values for a model) to the problem which performance can be assessed. EAs rely on three main processes: selection, recombination and mutation. The selection process is intended to select the individuals which will produce offspring (i.e the population for the next generation). The recombination process allows inbreeding the selected individuals (parents) in an attempt to enhance their performance. Finally, the mutation process produces random variability in the population, normally by modifying the solution encoded by the parents.

The next sections describe the material presented in the Supplementary material 1 of the manuscript presented in section **??**

2.1.1 Evolutionary strategies

In ESs, selection and recombination are deterministic parametric processes. Additionally, EAs include some ?meta-parameters? controlling the behavior of the algorithm itself (e.g. the mutation rates). ESs also include “self-adaptation” procedures allowing to make the meta-parameters of the algorithm vary to improve their performance over the evolutionary process. ESs focus on mutation as the main search operator, and it has been pointed out that it is necessary to use recombination in connection to self-adaptation to improve the performance of the algorithm (Thomas and Schewefel, 1993). A comprehensive synthesis of Evolutionary Strategies can be found in Beyer and Schwefel (2002).

We consider a population $\{x_i\}$, with $x_i \in \mathbb{R}^n$, for $i = 1, \ldots, \lambda$ and n the dimension of the problem (i.e the number of parameters to estimate). We also need to define an objective function f (so called fitness function) to be minimized. So, for each x_i we can calculate $f(x_i)$ and we can sort the individuals of the population by their fitness values:

$$f(x_{1:\lambda}) \leq f(x_{2:\lambda}) \leq \cdots \leq f(x_{\lambda:\lambda}) \tag{2.1}$$

Where $x_{i:\lambda}$ encodes the i-th lower value for the function f among the population. This allows us to carry on the selection of the best $\mu < \lambda$ individuals of the population, which will constitute the parents for the next generation.

The recombination of the parents can follow different rules. It can be as simple as taking the mean (or weighted mean) of the μ selected parents. Finally, the mutation process is used to produce a new generation, for example by sampling the new x_i from a multivariate normal distribution:

$$x_i \sim N(m, C)$$

where m is an n-dimensional vector resulting from the recombination of the parents and C is a covariance matrix. During the course of the evolutionary process, m will converge to an optimal solution.

In the algorithm developed in this work, we introduce a new method for an adaptative hierarchical recombination (AHR), optimized for parameter estimation of models using several sources of information (i.e calibration using several sources of data). Additionally, in order to improve the convergence and search capabilities, we implement self-adaptation procedures to improve the adaptation of the covariance matrix C during the optimization.

In order to introduce a self-adaptation process in our algorithm, we assume C is a diagonal matrix, while extending the results to a generic covariance matrix is a work under progress. In the next section, the algorithm developed is described in detail.

2.1.2 The AHR-ES Algorithm

Objective function

We are considering a general class of objective functions f:

$$f(x) = f_0(x) + \sum_{k=1}^{K} f_k(x), \tag{2.2}$$

where $x \in \mathbb{R}^n$ is a parameter vector and f_k, $k = 0, \ldots, K$ are the *partial fitnesses*. The objective of the calibration is to optimize $f(x)$, the search being directed by the recombination between individuals with "local" success (optimizing f_k, $k = 1, \ldots, K$).

It is important to notice that we are not sorting the parents according to the partial fitness for the f_0 component, but this component contributes to the total fitness and the initial selection. In particular, f_k could be the likelihood function associated to each calibration variable. By using likelihood functions, it is straightforward to build fitness functions to calibrate variables with data time series. Also, this choice makes a handful of statistical procedures available to test the goodness of fit, to estimate confidence intervals, etc. On the other hand, likelihood fitness functions could be very complex and highly multimodal, especially when handling a model with non-linear relationships and stochasticity. Optimizing likelihood functions for complex models could be prone to premature stagnation and requires more generations to find optimal solutions, reason why it is important to reduce population sizes (to reduce computing time) and to use properly defined self-adapted mutation rates (to increase rate of convergence).

2.1.3 Selection

We select the $\mu < \lambda$ parents $\tilde{x}_i$ $(i = 1, \ldots, \mu)$ which have the lowest value of the objective function f. Then, for each partial fitness f_i $(i = 1, \ldots, K)$ we will sort the parents as in Equation (2.1):

$$f_k(\tilde{x}_{1:\mu,k}) \leq f_k(\tilde{x}_{2:\mu,k}) \leq \cdots \leq f_k(\tilde{x}_{\mu:\mu,k}) \tag{2.3}$$

for each $m = 1, \ldots, K$ partial fitness.

2.1.4 Recombination

As a first step, we will recombine the parents according to their success at optimizing each partial fitness f_k, given a set of weights w_i $(i = 1, \ldots, \mu)$:

$$\begin{aligned} x_k &= \textstyle\sum_i w_i \tilde{x}_{i:\mu,m} & (2.4) \\ \sigma_k^2 &= \textstyle\sum_i w_i \tilde{x}_{i:\mu,m}^2 - x_k^2 & (2.5) \end{aligned}$$

such that $w_i \geq w_j$ for $i < j$ and $\sum_i w_i = 1$. Note that x_k^2 is taken entry–wise, i.e. squaring each component of x_k independently (Hadamard product). This initial recombination allows to better use the information in all selected individuals, and particulary to reduce the impact of selecting an individual with a good fitness value just by chance, especially when dealing with stochastic models. As part of the recombination we also calculate σ_k which provides information about the variability of each parameter value among the parents.

Then, we exploit all the historical information on x_k and σ_k by exponentially weighting the past of the recombined parents:

$$\begin{aligned} \mathbf{x}_k(g) &= (1-\alpha)\,\mathbf{x}_k(g-1) + \alpha x_k & (2.6) \\ \mathbf{s}_k^2(g) &= (1-\alpha)\left(\mathbf{x}_k^2(g-1) + \mathbf{s}_k^2(g-1)\right) + \alpha\left(\sigma_k^2 + x_k^2\right) - \mathbf{x}_k^2(g) & (2.7) \end{aligned}$$

for each $m = 1, \ldots, K$ partial fitness, and generation g. Here, $\mathbf{x}_k(g)$ and $\mathbf{s}_k(g)$ are calculated as moving average and variance for generation g, to take into account past information with exponentially decreasing weights given by $\alpha \in [0, 1]$, a meta-parameter of the algorithm, which controls the rate at which the algorithm learns from the current parents. Particularly, $\mathbf{s}_k$ provides information on how important a particular parameter is for the minimization of the objective function, since the more important the parameter the smaller the variability that we would expect across the generations. Now, let's define $\mathbf{s}_k^{(\min)} = \min_n \mathbf{s}_k$ and $\mathbf{s}_k^{(\max)} = \max_n \mathbf{s}_k$, the minimum and maximum over the n entries of $\mathbf{s}_k$, respectively to calculate:

$$\hat{w}_k = \left[\frac{\mathbf{s}_k^{(\max)} - \mathbf{s}_k}{\mathbf{s}_k^{(\max)} - \mathbf{s}_k^{(\min)}} \right]^{\beta} \tag{2.8}$$

$$w_k = \frac{\hat{w}_k}{\|\hat{w}_k\|_1} \tag{2.9}$$

for $\beta \geq 1$, and $\|\hat{w}_k\|_1$ is the L_1 norm of $\hat{w}_k$, taken to make the sum of w_k equal to 1. Again, the quotient and the power are taken entry–wise . w_k ponderates the relative importance of each parameter to the partial fitness m. When parameters are bounded, the vector $\mathbf{s}_k$ can be divided by the ranges of each parameter before the recombination stage for rescaling purposes.

Finally, we recombine all parents to produce the *parental genotype* $\mathbf{x}$ by using the weights given by w_k and the first recombined parents given by $\mathbf{x}_k$:

$$\mathbf{x}[i] = \frac{\sum_{m=1}^{M} w_k[i]\mathbf{x}_k[i]}{\sum_{m=1}^{M} w_k[i]}, \tag{2.10}$$

where $i = 1, \ldots, n$ represents the position of a particular parameter in the vectors.

This final recombination uses dynamically changing weights which take into account the variability of each parameter independently and its importance to minimize every partial component of the objective function.

2.1.5 Mutation

The new individuals of the population in generation $g + 1$ will be produced by mutating the parental genotype $\mathbf{x}$ using a multivariate normal distribution:

$$x_i^{(g+1)} \sim N(\mathbf{x}^{(g)}, \sigma_{size}^{(g)} C^{(g)}) \tag{2.11}$$

for $i = 1, \ldots, \lambda$. The matrix $C^{(g)}$ is constructed following the self-adaptation algorithm techniques (Covariance Matrix Adaptation CMA-ES; Hansen and Ostermeier 2001) and σ_{size} is the step size control calculated as in Hansen and Ostermeier (2001). The reader can read the source code for details on this particular implementation.

Additionally, when the parameters are bounded, a truncated multivariate normal distribution is used for the mutation process instead of a multivariate normal distribution.

2.2 calibrar: an R package for the calibration of ecological models

In this section we include a manuscript submitted to the journal “Methods in Ecology an Evolution” (manuscript MEE-14-10-625).

calibrar: an R package for the calibration of ecological models

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Word count: 4379

Summary

1. The calibration of complex ecological models is a challenging optimization task, with a notable lack of tools for the calibration of stochastic models.

2. calibrar is a new R package for the calibration of stochastic ecological models, including Individual Based Models. It is a generic tool that can be used for any type of model, especially those with non-differentiable objective functions.

3. calibrar supports multiple phase calibrations and constrained optimization. It implements maximum likelihood estimation methods and automated construction of the objective function from simulated model outputs.

4. User-level expertise in R is necessary to handle calibration experiments with calibrar, but there is no need to modify the model's code, which can be programmed in any language. For more experienced users, calibrar allows the implementation of user-defined objective functions.

5. The package source code is fully accessible and can be installed directly from github (htpps://roliveros-ramos.github.com/calibrar).

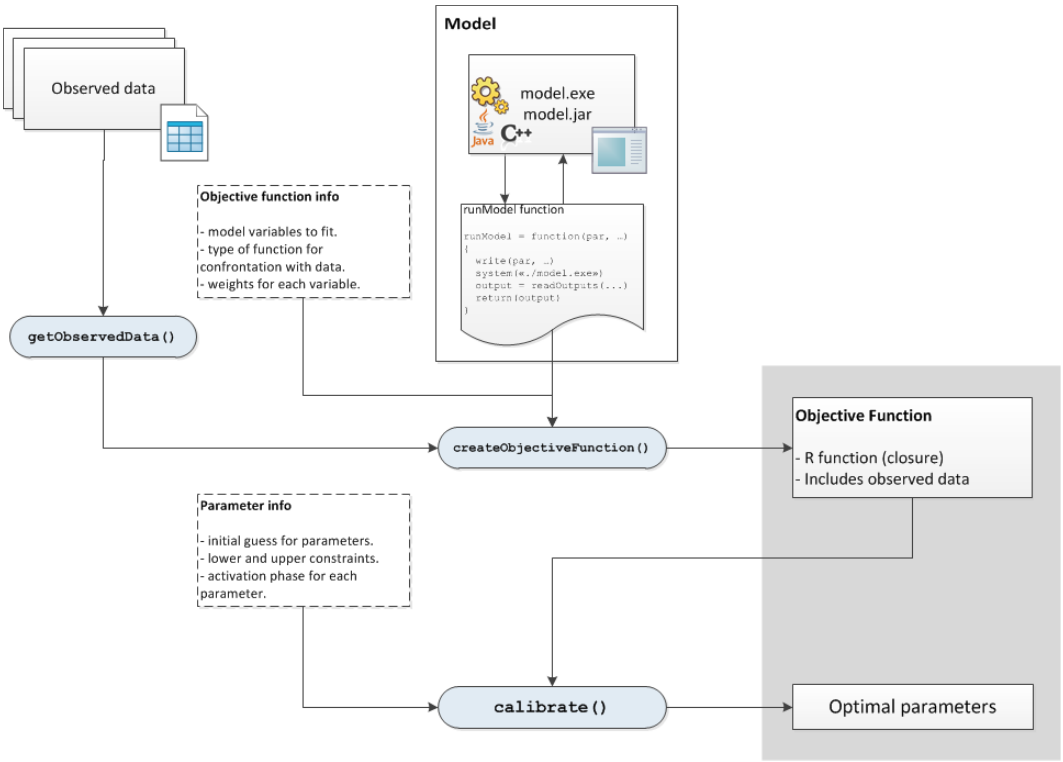
Keywords: black-box optimization, inverse problem, parameter estimation, evolutionary algorithms, stochastic model, individual based model, OSMOSE model.

Introduction

The ability to achieve accurate inverse parameter estimation is one important criterion to assess the usefulness of ecological models (Bartell 2003). Given a model, the selection of the best possible parameter set is based on the optimization of a scalar *objective function* (e.g. log-likelihood, residual sum of squares) with respect to the model parameters (Walter and Pronzato 1997, Bolker et al. 2013). Once the objective function is properly defined, parameter estimation is essentially an optimization problem which can be a difficult task because of model characteristics such as non-linearity, high dimensionality as well as low quantity and quality of observed data (Tashkova et al. 2012). These diverse factors have hampered the development of calibration algorithms and methodologies that are sufficiently flexible and generic, and only sparse documentation has been produced on fitting complex models (Bolker et al. 2013). Additionally, complex ecosystem models can be numerically intensive and require long simulation runs, adding an extra layer of difficulty to their calibration.

There are some dedicated tools for non-linear parameter estimation, AD Model Builder (ADMB, Fournier et al. 2012) being one of the most robust and fast (Bolker et al. 2013). Among other advantages, ADMB provides support for calibration in multiple phases (Nash and Walker-Smith 1987), which can be of great interest for the calibration of complex ecosystem models (Oliveros-Ramos et al. submitted). It also provides support for constraining optimization, which can be helpful for regularizing hard optimization problems (Bolker et al. 2013). However, the model and the objective function itself need to be coded in C++ (using the ADMB scripting), which can be an obstacle for calibrating complex models already implemented in other languages (e.g. Java, Fortran). In addition, as ADMB is based on automatic differentiation, which allows to provide accurate estimates of derivatives (Griewank and Corliss 1992), the tool is not suited for stochastic models for which derivatives cannot be computed.

Parameter estimation methods have been developed for stochastic non-linear models, such as continuous time, finite state Markov models and individual-based models (IBMs), for which the probability of state transitions or the master equation can be written (Ionides et al. 2006, Newman et al. 2009, Ross et al. 2009, Walker et al. 2006). However, many IBMs can only be simulated numerically and are too complex for mathematical analysis and explicit parameter estimation (Black and McKane 2012), resulting in more attention being given to the exploration of model behaviour than to a rigorous confrontation with data. As alternative methods, meta-heuristic algorithms have been developed (Cropper and Anderson 2004, Poovathingal and Gunawan 2010, Duboz et at. 2010, Tashkova et al. 2012, Travers-Trolet et al. 2013), and have in some cases shown better performance than derivative-based optimization methods (Tashkova et al. 2012).



```
runModel = function(par, …)
{
  write(par, …)
  system(«./model.exe»)
  output = readOutputs(...)
  return(output)
}
```

Figure 1. Diagram representing the functioning of the calibrar package. The grey area groups the outputs produced for the package (the objective function and the optimal parameters of the model). Rectangles with broken border lines show user inputs which are needed to configure the calibration. Rounded rectangles show main package functions.

However, the scientific community lacks generic and flexible enough tools for the calibration of different types of ecological models with different degrees of complexity.

Here we present a new R package, calibrar, designed for, but not exclusive to, the calibration of complex stochastic models. The optimization routine is based on an original Evolutionary Algorithm (EA) optimized for maximum likelihood estimation. The package provides support for multiple phase calibration and parameter constraint optimization. In particular, by using a "black-box" approach, the package allows the calibration of models implemented in any programming language. It provides a generic interface with models and allows the construction of the objective function in R, without requiring changes in the models' code. Parallel support for computationally intensive models is also provided, and can be used with high performance computing systems.

General description of the package

The calibrar package is written in R (R Development Core Team 2014), and can be installed from github ("roliveros-ramos/calibrar"). The package is designed for the optimization of "black-box" functions (Jones et al. 1998), where analytical information about the function to be optimized and the model source code are assumed to be unavailable or impractical to modify (Rios and Sahinidis

2013). Our approach is hence “non-intrusive”, making the model interact with the optimizer, i.e. the calibrar package, in two ways: i) receiving a set of parameters to run, and ii) providing the model outputs to be confronted with the observed data. calibrar also helps in the construction of the objective function to be optimized in order to estimate a model's parameters (Figure 1).

Table 1. Functions of the calibrar package.

Function	**Returned objects**	**Description**
calibrate	An object of class “calibration” summarizing the calibration results.	Performs a sequential calibration of a model using multiple phases.
getObservedData	A list with the observed values (the data)	Create a list with the observed data with the information provided by its main argument.
createObjectiveFunction	A function, integrating the simulation of the model and the comparison with observed data.	Create a new function, to be used as the objective function in the calibration, given a function to run the model within R, observed data and information about the comparison with data.
getCalibrationInfo	A data.frame with the information necessary to create the objective function using createObjectiveFunction	Basically a wrapper for read.csv checking column names and data types for the table with the calibration information.
optimES	A list with the results of the optimization	For completeness, the optimizer is provided as a function. It takes the par, fn, upper and lower arguments. See ?optimES for details.
plot, summary, predict, coef, print		R S3 methods for visualizing the results of the calibration

The package has been designed such that minimal expertise in R is necessary to handle the calibration. The user intervention is mainly required in the construction of the function to run the model (runModel function, Figure 1) and in retrieving the simulation output. However, given R’s flexibility and features for data manipulation, it is rather straightforward to develop such a function. Some models have dedicated packages oriented to the analysis of their outputs that could be used to link with calibrar, e.g., RNetLogo (Thiel et al. 2012) for IBMs implemented in netLogo or osmose2R (www.osmose-model.org) for the OSMOSE model. Additionally, two functions, getObservedData and createObjectiveFunction are provided to simplify the organization of the observed data and construct the objective function for the calibration, respectively.

In order to create the objective function, the user needs to specify some information about the model outputs used for the calibration and how to combine them (Figure 1). More experienced users can create the objective function by directly integrating the simulation of the model (the main purpose of the runModel function; details in the next section).

Additionally, the user needs to specify information on the parameters to estimate. We recommend that lower and upper thresholds are provided for each parameter, but unconstrained optimization is also supported. If initial approximate estimates for the parameters are provided, this would simplify the calibration process, but this step can be omitted if no information is available. In case of a multiple phase calibration, the user must indicate the phase of the calibration where the estimation of a parameter must be included (details provided in the next section).

The optimization is solved using a novel algorithm based on Evolutionary Strategies (ES), a type of EA especially designed for parameter optimization problems (Jones 1998). The reader can refer to Bäck and Schewefel (1993) for an overview of EAs for parameter estimation, as well as to Beyer and Schwefel (2002) for a general introduction to ESs. ESs concentrate on “mutation” as the main search operator, and to improve its performance it is necessary to complement it with “recombination” and “self-adaptation” processes (Bäck and Schewefel 1993). The main novelty of the algorithm developed in calibrar is the implementation of a recombination process that takes into account: i) the variability in the parameters, which provides a better fit for each data type, and ii) the probabilistic nature of the likelihood approach to weight the potential candidates to parameter solutions (full technical details in Appendix S1). Also, a similar approach for self-adaptation as in Hansen and Ostermeier (2001) has been implemented to avoid a premature convergence. These modifications have shown a great increase in performance compared to other ESs used for the calibration of complex stochastic models, like in Duboz et al. (2010).

Implementation of a simple example

The main function of the package is calibrate, which performs minimization of an objective function. It has a similar syntax as optim (Table 2), a common optimization function in R, and as most optimization functions in other R packages. We illustrate the use of this function by minimizing the SphereN function (Sphere function with random noise), defined as:

$F(x) = \sum_{i=1}^{n} x_i^2 + e$, where $x = (x_1, x_2, \ldots, x_n)$ and $e \sim N(0, \sigma)$.

This function has a minimum expected value of 0 at the origin. The two obligatory arguments of the calibrate function, with no default values, are par and fn, i.e. the starting parameter values for the search and the function to minimize, respectively (Table 2). For n=5, the minimization can be run as follows:

```
calibrate(par=rep(NA, 5), fn=Sphere)
```

When `NA` (not available) values are provided as initial search points, the function will try to choose an appropriate start value (see the help page of the function for details). However, providing good start values based on prior knowledge of the parameters would improve the performance of the calibration of complex models (Bolker et al. 2013), even when using a global optimization algorithm as in `calibrar`. It is also possible to provide lower and upper bounds for the parameters. In this example, only one value is provided (instead of a vector) for all parameters:

```
calibrate(par=rep(0.5, 5), fn=SphereN, lower=-5, upper=5)
```

As the objective function is stochastic, the search surface depends on the particular realization of the random variables involved. Here we can specify the number of replicate simulations to run, and the expected value of the objective function is the average over the replicates.

```
calibrate(par=rep(0.5, 5), fn=SphereN, lower=-5, upper=5, replicates=3)
```

Finally, the calibration can be run in multiple phases, by specifying at which phase the parameters are included in the optimization (Table 2):

```
calibrate(par=rep(0.5, 5), fn=SphereN, lower=-5, upper=5,replicates=c(1,1,4), phases=c(1,1,1,2,3))
```

This call will perform three sequential optimizations. In the first one, only the first three parameters are estimated, the last ones remaining constant at the start value (0.5). In the second phase, the fourth parameter becomes activated with the first three, and a second optimization is carried out, keeping the last parameter constant. The main difference from the first phase is that the starting points for the first three parameters are the optimal values obtained from the first phase. Then the final optimization is carried out with all parameters. Negative integers or `NA` in `phases` mean that the corresponding parameter is never activated and remains constant throughout the calibration. This can be particularly useful to test simpler models with some constant parameters, without needing to change the objective function. Lastly, the above calibrate example indicates a different number of replicates for each phase. Since the objective of the initial phases is to get an improved vector of start values for the final calibration phase, it can be useful to reduce the computer time by using fewer replicates in the initial phases. The default value for the replicates is 1, but using more replicates in the last phase can reduce the stochasticity of the search surface, which can help to estimate the optimal parameters for very “noisy” problems.

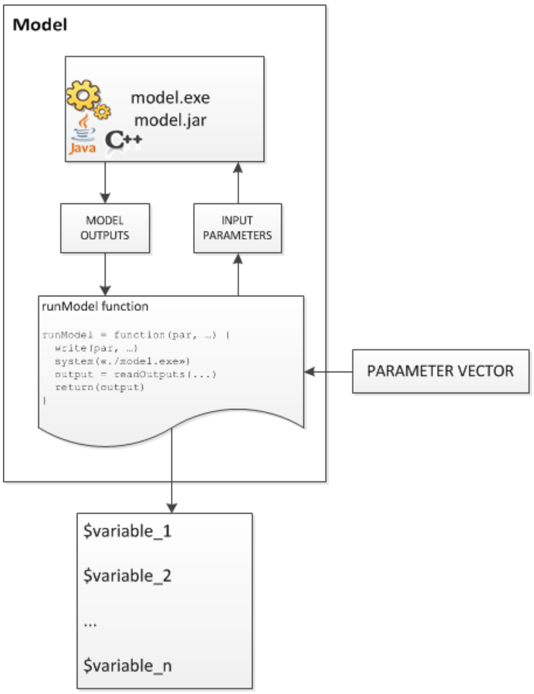
Table 2. Main arguments of the calibrate function.

Argument	Description
par	A numeric vector. The length of the par argument defines the number of parameters to be estimated (i.e. the dimension of the problem).
fn	The function to be minimized
upper	Upper threshold value(s) for parameters. One value or a vector of the same length as par. If one value is provided, it is used for all parameters. NA means Inf. By default Inf is used (unconstrained).
lower	Lower threshold value(s) for parameters. One value or a vector of the same length as par. If one value is provided, it is used for all parameters. NA means -Inf. By default -Inf is used (unconstrained).
phases	An optional vector of the same length as par, indicating the phase at which each parameter becomes active. If omitted, default value is 1 for all parameters.
replicates	The number of replicates of model simulation to evaluate the objective function. One value or a vector of length max(phases), to specify a different number of replicates for each phase. The default value is 1.
aggFn	Default is weighted.sum (and default weights all equal to 1).
control	Fine control of the optimization, see function help for details and Table 3.

Linking to models and data

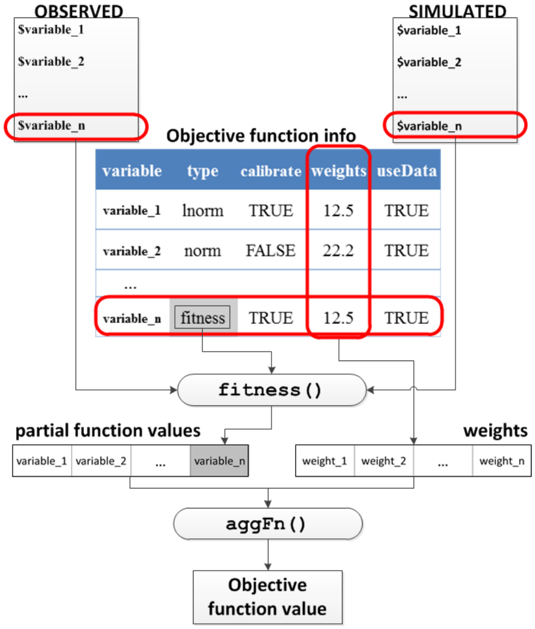
The calibration of complex models is the main purpose of the package, for which we first need to define the objective function. Having adopted a non-intrusive black-box optimization approach, the code of the model to calibrate does not need to be modified, but can be directly evaluated for a given set of parameters. Hence, the role of the runModel function is to i) write a set of parameters in the format the model is able to read, ii) run the model with this set of parameters and iii) read the model outputs back into R (Figure 2). The output of runModel is a list, each element being one of the variables to calibrate. R facilities to process and analyse data in different formats allows to handle model outputs independently of the language used for coding the model.

After the construction of the runModel function, the second step consists of providing information for the construction of the objective function. Output variables listed in runModel need to be documented (name of "variable", "type", "calibrate", "weight" and "useData"; Figure 3) as a data.frame which will be used as an argument for the functions getObservedData and createObjectiveFunction. The getObservedData function reads data from the disk to produce a list with the same structure as the outputs of the runModel function. The function createObjectiveFunction combines observed data and the runModel function to create the objective function for the calibration problem (Figure 3), which in turn will be the fn argument for the calibrate function.



```
runModel = function(par, …) {
  write(par, …)
  system(«./model.exe»)
  output = readOutputs(...)
  return(output)
}
```

Figure 2. Scheme of the link between the model and the calibration. The R function runModel receives a vector of parameters to test, writes the parameters in a form readable for the model (e.g. via txt or csv files), runs the model (possibly via system) then captures and processes the model outputs. The result of the function is a “list” object with all the variables to be confronted to observed data.



variable	type	calibrate	weights	useData
variable_1	lnorm	TRUE	12.5	TRUE
variable_2	norm	FALSE	22.2	TRUE
...				
variable_n	fitness	TRUE	12.5	TRUE

Figure 3. Scheme of the calculation of the value of the objective function for a given set of parameters. For each variable, a partial value of the objective function is calculated by applying the function fitness (specified in the column ‘type’) to the observed and simulated values. The final value of the objective function is calculated by applying the aggFn to the partial function values and the weights specified in the "objective function info" table.

To build the objective function, the ‘type’ of each variable is the function that combines observed and simulated data to produce a scalar value, measuring the fit between the model and the observations. Some negative log-likelihood functions are already implemented in calibrar (e.g. normal, lognormal, multinomial; type `?fitness` for available functions). User defined functions can also be provided, having two vector arguments (`obs` and `sim`) and returning a scalar value:

```
userFunction = function(obs, sim, ...) {
          value = sum((obs-sim)^2, na.rm=TRUE)
          return(value)
          }
```

The ‘calibrate’ column in the objective function information flags the variables to be used for the calibration. The ‘useData’ column indicates whether data are read from the disk. If `useData=TRUE`, a file called `variable_n.csv` is searched for "variable_n". If `useData=FALSE`, the observed value is set to `NULL`, and the 'type' function is expected to use simulated data only. The latter option can be particularly useful to set penalties in the model outputs or parameters, where no observed data are needed. Finally, the ‘weight’ column provides the relative weights to combine the partial objective values obtained for each variable (Appendix S2).

The `calibrate` function takes a list as a control argument, where fine control options for the calibration and the optimization are provided, particularly to activate the calibration in parallel which is based on the `foreach` package (Revolution Analytics and Weston 2014). Before using the parallel implementation, a parallel ‘cluster’ should be created, using the `parallel` or `snow` R packages (see appendix S2 for an example). The user can fully control the configuration of the parallel runs in different computer systems, from computers with multicore processors to high-performance supercomputers. Once the cluster is created, only the `parallel=TRUE` and `ncores` control options should be provided (Table 3). Additionally, since each model run could require files to be written to the disk (which will be read by the `runModel` function after the simulation), different folders need to be assigned for each parameter combination that is tested by the optimization algorithm; the `run` control option specifies a directory where all simulations are run (subfolders named `i0`, `i1`, …, `in` will be automatically created as needed). By default, no folders are created, so a path should be specified if the model needs to write files to the disk. All the parameter input files (Figure 2) are written in temporary folders (e.g. `run/i0`). The control option `master` specifies a folder for which all contents are copied to the temporary folders. Only files that need to be changed between individual runs are recommended to be put in the master folder; the use of absolute or relative paths is recommended for common heavy files needed to run the model. Since the calibration of numerically intensive models can run for a long time, a ‘restart’ option is also available, allowing an interrupted calibration to be continued (see appendix S2 for an example).

Table 3. Some options for the control argument of the function calibrate.

Option	Description
maxit	Maximum number of executions of the objective function
maxgen	Maximum number of generations for the evolutionary strategy. Ignored if maxit is provided, and recalculated accordingly.
parallel	Boolean, TRUE or FALSE to activate the parallel execution of the optimization.
ncores	The number of cores available in the parallel cluster for the active session. If parallel=TRUE, the default is to get the number of cores of the system.
run	An optional folder path to create all the temporary folders needed to run the simulations for each parameter combination tested by the optimization algorithm. The folders are recycled every generation.
master	An optional folder path. All the contents of the designated folder will be copied to each temporary folder.
save	Number of generations after saving a new restart object, which contains all the information necessary to restart the calibration at that point. The default is NULL, and no restart files are created.
restart.file	Filename for the restart file to be created.

Comparison with other software

General purpose optimizers can be found in R (see Optimization and Mathematical Programming Task View at CRAN: http://cran.r-project.org/web/views/Optimization.html). Two very useful features for model calibration are the performance of constrained optimization (limiting the search to a box by defining lower and upper boundaries to parameter values) and the calibration in multiple phases (to improve the search of the global minimum by performing a sequential approximation). The former option is implemented in several R packages, including the optim function (providing the "L-BFGS-B" method, Byrd et al. 1995) and several others wrapped in the optimx package (Nash and Varadhan 2011). The latter option is available in some R packages (e.g. Rcgmin, Rvmmin and bnmle) for a single phase optimization, but a sequential calibration, as described here, would have to be performed manually. For the calibration of stochastic models, several meta-heuristic and non-derivative based algorithms are now available in R, from EAs (e.g. genalg, DEoptim and cmaes packages) to other nature-inspired algorithms (e.g. Simulated Annealing 'SANN' method in optim and the Particle Swarm Optimization (PSO) algorithm in the hydroPSO package, Zambrano-Bigiarini and Rojas 2013). However, while all these packages and algorithms allows constrained optimization, none of them provides support for keeping fixed parameters during the course of a single optimization, and multiple phase calibration would have to be performed manually by modifying the objective function for each trial. Furthermore, a very important feature for the calibration of complex models is the parallel implementation of the optimization routine. The PSO algorithm in the hydroPSO has its parallel implementation tied to the core of the function and does not allow its use in high-performance clusters, especially under a queue system (e.g. TORQUE), and only the DEoptim package provides a more flexible externally configured parallelization.

Additionally, in the construction of the objective function, our approach allows an easy transferability of the calibration problem by using other general purpose optimizers, which can be useful under certain circumstances (e.g. see Bolker et al. 2013). There is "no free lunch" in optimization, and no optimization algorithm will perform best for every type of optimization problems (Wolpert and Macready 1997). Other calibration oriented packages like hydroPSO provide functions to write parameters and read outputs, but this approach breaks the "objective function" approach for the optimization, and while the hydromad package (Andrews et al. 2011) offers support for the automated construction of an objective function in a standard way, it is restricted to some specific cases in hydrological modelling. In these regards, our calibration package calibrar is meant to be generic enough to be used in a variety of optimization problems, including the calibration of complex (e.g. non-linearity, high-dimensionality) and stochastic models. calibrar has, for example, been successfully applied to the interannual calibration of the OSMOSE model (Shin and Cury 2001, 2004), a multispecies spatially-explicit IBM implemented in the Java language (Oliveros et al. under revision). Three features of calibrar render it particularly useful for the calibration of computationally intensive stochastic models: the parallelization of the simulations, the ability to handle replicate simulations in the evaluation of the objective function and the 'restart' option, which allows the calibration to be handled under restricted access to high performance resources (e.g. clusters with queue systems and fixed walltime).

Conclusions and perspectives

A successful model calibration implies several computational, theoretical and practical challenges. The calibrar package intends to provide a framework to simplify the calibration of complex models, in particular stochastic ones, for which fewer tools exist compared to those for deterministic and differentiable models. We adopted a "black-box" and "non-intrusive" approach, since most complex models are computationally intensive and most likely implemented in fast low-level languages; their recoding for calibration purposes is not the best option. The next step envisaged is the inclusion of other optimization algorithms in calibrar so the users are provided with a suite of tools to solve a variety of calibration problems in a transparent way. In future, more tests with other models will help to improve the package, its flexibility and the robustness of the optimization algorithm.

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References

Andrews, F.T., Croke, B.F.W. &Jakeman, A.J. (2011) An open software environment for hydrological model assessment and development. Environmental Modelling & Software 26:1171-1185.

Bäck, T. & Schewefel, H.-P. (1993) An Overview of Evolutionary Algorithms for parameter optimization. Evolutionary Computation 1:1-23.

Bartell, S.M. (2003) Effective use of ecological modeling in management: The toolkit concept. Ecological modeling for resource management (ed V. Dale), pp. 211-220. Springer Verlag, Berlín.

Black, A.J. & McKane, A.J. (2012) Stochastic formulation of ecological models and their applications. Trend in Ecology and Evolution 27(6):337-345. DOI: http://dx.doi.org/10.1016/j.tree.2012.01.014

Beyer, H.-G. & Schwefel, H.-P. (2002) Evolution strategies: a comprehensive introduction, Natural Computing 1:3-52.

Bolker, B.M., Gardner, B., Maunder, M., Berg, C.W. , Brooks, M., Comita, L., Crone, E., Cubaynes, S., Davies, T., de Valpine, P., Ford, J., Gimenez, O., Kéry, M., Kim, E.J., Lennert-Cody, C., Magnusson, A., Martell, S., Nash, J., Nielsen, A., Regetz, J., Skaug, H. & Zipkin, E. (2013) Strategies for fitting nonlinear ecological models in R, AD Model Builder, and BUGS. Methods in Ecology and Evolution 4: 501–512.

Byrd, R. H., Lu, P., Nocedal, J. & Zhu, C. (1995) A limited memory algorithm for bound constrained optimization. SIAM J. Scientific Computing, 16, 1190–1208.

Cropper, W.P. Jr. & Anderson, P.J. (2004) Population dynamics of a tropical palm: use of a genetic algorithm for inverse parameter estimation. Ecological Modelling 177: 119–127.

Duboz, R., Versmisse, D., Travers, M., Ramat, E. & Shin, Y.-J. (2010) Application of an evolutionary algorithm to the inverse parameter estimation of an individual-based model. Ecological Modelling 221(5):840-849.

Fournier, D.A., Skaug, H.J., Ancheta, J., Ianelli, J., Magnusson, A., Maunder, M.N., Nielsen, A. &Sibert, J. (2012) AD Model Builder: using automatic differentiation for statistical inference of highly parameterized complex nonlinear models. Optimization Methods and Software, 27:2, 233-249, DOI: 10.1080/10556788.2011.597854.

Griewank, A. & Corliss, G.F. (1992) Automatic Differentiation of Algorithms: Theory, Implementation, and Application. SIAM, Philadelphia, PA, USA.

Hansen, N., & Ostermeier, A. (2001) Completely de-randomized self-adaptation in evolution strategies. Evolutionary Computation 9(2):159–195.

Ionides, E. L., Breto, C. & King, A.A. (2006) Inference for nonlinear dynamical systems. PNAS 103(49): 18438–18443.

Jones, D.R., Schonlau, M. & Welch, W.J. (1998) Efficient Global Optimization of Expensive Black-Box Functions. Journal of Global Optimization 13: 455–492.

Jones, G. (1998) Genetic and evolutionary algorithms. In Encyclopedia of Computational Chemistry (Schleyer, P .v.R. et al., eds), pp. 1127–1136, John Wiley & Sons.

Nash, J.C & Varadhan, R. (2011) Unifying Optimization Algorithms to Aid Software System Users: optimx for R. Journal of Statistical Software, 43(9), 1-14. http://www.jstatsoft.org/v43/i09/.

Nash, J.C. & Walker-Smith, M. (1987) Nonlinear Parameter Estimation: an Integrated System in BASIC. Marcel Dekker, New York. 493pp.

Newman, K.B., Fernández, C., Thomas, L. & Buckland, S.T. (2009) Monte Carlo Inference for State–Space Models of Wild Animal Populations. Biometrics 65, 572–583.

Oliveros-Ramos, R., Verley, P. & Shin, Y.-J., unpublished. A sequential approach to calibrate ecosystem models with multiple time series data. Submitted to Progress in Oceanography.

Poovathingal, S.K & Gunawan, R. (2010) Global parameter estimation methods for stochastic biochemical systems, BMC Bioinformatics 11:414.

R Core Team (2014) R: A language and environment for statistical computing. R Foundation for Statistical Computing, Vienna, Austria. URL http://www.R-project.org/. [accessed 09 June 2014]

Revolution Analytics & Weston, S. (2014) foreach: Foreach looping construct for R. R package version 1.4.2. http://CRAN.R-project.org/package=foreach. [accessed 09 June 2014]

Rios, L.M. & Sahinidis, N.V. (2013) Derivative-free optimization: a review of algorithms and comparison of software implementations. Journal of Global Optimization 56:1247–1293.

Ross, J.V., Pagendam, D.E. & Pollet P.K. (2009) On parameter estimation in population models II: Multi-dimensional processes and transient dynamics. Theoretical Population Biology 75: 123132.

Shin, Y.-J. & Cury, P. (2001) Exploring fish community dynamics through size-dependent trophic interactions using a spatialized individual-based model. Aquatic Living Resources, 14(2): 65-80.

Shin, Y.-J. & Cury, P. (2004) Using an individual-based model of fish assemblages to study the response of size spectra to changes in fishing. Canadian Journal of Fisheries and Aquatic Sciences, 61: 414-431.

Tashkova, K., Silc, J., Atanasova, N. & Dzeroski, S. (2012) Parameter estimation in a nonlinear dynamic model of an aquatic ecosystem with meta-heuristic optimization. Ecological Modelling 226: 36– 61.

Thiele, J.C, Kurth, W. & Grimm, V. (2012) RNetLogo: an R package for running and exploring individual-based models implemented in NetLogo. Methods in Ecology and Evolution 3:480-483.

Travers-Trolet, M., Shin, Y.-J. & Field, J.G. (2013) An end-to-end coupled model ROMS-N2P2Z2D2-OSMOSE of the southern Benguela foodweb: parameterisation, calibration and pattern-oriented validation, African Journal of Marine Science, 36:1, 11-29, DOI:10.2989/1814232X.2014.883326

Walker, D.M., Pérez-Barbería, F.J. & Marion, G. (2006) Stochastic modelling of ecological processes using hybrid Gibbs samplers. Ecological Modelling 198:40-52.

Walter, E. and Pronzato, L. (1997) Identification of parametric models from Experimental data. Springer Masson. 413pp.

Wolpert, D.H. & Macready, W.G. (1997) No Free Lunch Theorems for Optimization. IEEE Transactions on Evolutionary Computation, 1(1):67-82.

Zambrano-Bigiarini, M. & Rojas, R. (2013) A model-independent Particle Swarm Optimisation software for model calibration. Environmental Modelling & Software 43:5-25.

Appendix S1. Full description of the algorithm.

Appendix S2. Scripts with examples.

Supplementary material 2:

Scripts with examples

calibrar: an R package for the calibration of ecological models

Ricardo Oliveros–Ramos, Yunne–Jai Shin

1 Examples from the paper

```
calibrate(par=rep(NA, 5), fn=SphereN)
calibrate(par=rep(NA, 5), fn=SphereN, replicates=3)
calibrate(par=rep(0.5, 5), fn=SphereN, replicates=3, lower=-5, upper=5)
calibrate(par=rep(0.5, 5), fn=SphereN, replicates=3, lower=-5, upper=5,
   phases=c(1,1,1,2,3))
calibrate(par=rep(0.5, 5), fn=SphereN, replicates=c(1,1,4), lower=-5,
   upper=5, phases=c(1,1,1,2,3))
# this calibration save results on the disk for restart purposes
calibrate(par=rep(0.5, 5), fn=SphereN, replicates=3, lower=-5, upper=5,
   phases=c(1,1,1,2,3), control=list(restart.file="sphere"))
# this calibration take no time, starts from (already finished) previous one
calibrate(par=rep(0.5, 5), fn=SphereN, replicates=3, lower=-5, upper=5,
   phases=c(1,1,1,2,3), control=list(restart.file="sphere"))
```

2 Parallel execution and restart functionality

```
# Restarting a calibration -------------------------------------------------

# this calibration save results on the disk for restart purposes
calibrate(par=rep(0.5, 5), fn=SphereN, replicates=3, lower=-5, upper=5,
   phases=c(1,1,1,2,3), control=list(restart.file="sphere"))
# this calibration take no time, because starts from (already finished)
   previous one
calibrate(par=rep(0.5, 5), fn=SphereN, replicates=3, lower=-5, upper=5,
   phases=c(1,1,1,2,3), control=list(restart.file="sphere"))

# Parallel execution -------------------------------------------------------

nCores = 6 # number of cores to be used
myCluster = makeCluster(nCores)
registerDoSNOW(myCluster) # register the parallel backend
# this is slower than sequential for very fast models
```

```
calib = calibrate(par=rep(0.5, 5), fn=SphereN,
                  replicates=3, lower=-5, upper=5,
                  phases=c(1,1,1,2,3),
                  control=list(parallel=TRUE, nCores=nCores))
stopCluster(myCluster) # close the parallel connections
```

3 A simple linear model fitting as benchmarking

```
require(calibrar)
require(optimx)
require(hydroPSO)
require(cmaes)

N = 9 # number of variables in the linear model
T = 100 # number of observations
noise = FALSE # add gaussian noise to the model
shift = FALSE # add a random shift to the slopes
sd = runif(1) # standard deviation of the gaussian noise

# observed data
x = t(matrix(rnorm(N*T, sd=sd), nrow=N, ncol=T))

# slopes for the linear model (real parameters)
slope = seq_len(N) + shift*sample(c(-100, 100), N, replace=TRUE)
# intercept for the linear model (real parameters)
intercept = pi
# real parameters
real = c(intercept, slope)

# function to simulate the linear model
linear = function(x, slope, intercept) {
  stopifnot(length(x)==length(slope))
  out = sum(x*slope) + intercept
  return(out)
}

# simulated data
y = apply(x, 1, linear, slope=slope, intercept=intercept) +
   noise*rnorm(nrow(x), sd=mean(sd))

# objective function (residual squares sum)
obj = function(par, x, y) {
  intercept = par[1]
  par = par[-1]
  slope = par[seq_len(ncol(x))]
  out = apply(x, 1, linear, slope=slope, intercept=intercept)
  out = sum((out - y)^2)
  return(out)
}

# initial guess for optimization
```

```
start = rep(0, N+1)

cat("Running optimization algorithms\n")
cat("\t", date(), "\n")

cat("Running calibrar AHR-ES (unconstrained)\n")
print(system.time(es  <- optimES(par=start, fn=obj, x=x, y=y)))

cat("Running calibrar AHR-ES (constrained)\n")
print(system.time(es2 <- optimES(par=start, fn=obj, x=x, y=y,
                           lower=rep(-100, length(start)),
                           upper=rep(100, length(start)))))

cat("Running linear model\n")
print(system.time(mod <- lm(y ~ x)))

cat("Running optim CG\n")
print(system.time(opt  <- optim(par=start, fn=obj, x=x, y=y, method="CG")))

cat("Running optim SANN\n")
print(system.time(sann <- optim(par=start, fn=obj, x=x, y=y, method="SANN")))

cat("Running optimx Nelder-Mead + BFGS\n")
print(system.time(optx <- optimx(par=start, fn=obj, x=x, y=y)))

cat("Running hydroPSO\n")
print(system.time(pso  <- hydroPSO(par=start, fn=obj, x=x, y=y,
               lower=rep(-100, length(start)),
               upper=rep(100, length(start)))))

cat("Running cmaes CMA-ES\n")
print(system.time(cma <- cma_es(par=start, fn=obj, x=x, y=y,
             lower=rep(-100, length(start)),
             upper=rep(100, length(start)))))


comps = rbind(real=real,
             'AHR-ES'=es$par,
             'AHR-ES (constrained)'=es2$par,
             lm=coef(mod),
             SANN=sann$par,
             PSO=pso$par,
             'CMA-ES'=cma$par,
             optx[,seq_along(start)],
             CG=opt$par
             )

print(comps)
```

4 Fitting an Autoregressive Poisson mixed model

```r
require(calibrar)
require(optimx)
require(cmaes)

path = NULL # NULL to use the current directory

# create the demonstration files
demo = calibrarDemo(path=path, model="PoissonMixedModel", L=4, T=20)

# set.seed(12345) # updated to T=20 and L=40 for comparative purposes.
# Parameter information
parInfo = read.csv(file.path(demo$path, "parInfo.csv"), row.names=1)

# get calibration information
calibrationInfo = getCalibrationInfo(path=demo$path)

# get observed data
observed = getObservedData(info=calibrationInfo, path=demo$path)

# read forcings for the model
forcing = read.csv(file.path(demo$path, "master", "environment.csv"),
                   row.names=1)

# Defining ’runModel’ function
  runModel = function(par, forcing) {

    # forcing is a matrix with the values of environmental variables
    T = nrow(forcing) # get number of time steps
    L = ncol(forcing) # get number of sites

    # create parameter list in a format readable by model
    parList = list()
    parList$alpha = par[1]
    parList$beta  = par[2]
    parList$gamma = par[2 + seq_len(T-1)]
    parList$sd = par[T+2]
    parList$mu_ini = par[T + 2 + seq_len(L)]

    # get the model
    model = calibrar:::.PoissonMixedModel
    # run the model
    output = model(par=parList, forcing=forcing)
    output = as.list(as.data.frame(output)) # return a list with the results
    # names of the outputs matching observed data names
    names(output) = paste0("site_", sprintf(paste0("%0", ceiling(log10(L+1)),
       "d"), seq_len(L)))

    output = c(output, list(gammas=parList$gamma))
    return(output)

  }
```

```
x = runModel(parInfo$guess, forcing)
print(x)
names(x)

obj  = createObjectiveFunction(runModel=runModel, info=calibrationInfo,
   observed=observed, forcing=forcing)
obj2 = createObjectiveFunction(runModel=runModel, info=calibrationInfo,
   observed=observed, forcing=forcing, aggregate=TRUE)
cat("Starting calibration...\n")

calib = calibrate(par=parInfo$guess, fn=obj, lower=parInfo$lower,
                  upper=parInfo$upper, phases=parInfo$phase,
                  control=list(weights=calibrationInfo$weights,
                               REPORT=10, trace=5))

cat("Running optimization algorithms\n")
cat("\t", date(), "\n")

cat("Running optim CG\n")
opt = optim(par=parInfo$guess, fn=obj2)

cat("Running optimx BFGS\n")
optx = optimx(par=parInfo$guess, fn=obj2, lower=parInfo$lower,
              upper=parInfo$upper, method="L-BFGS-B")

cat("Running cmaes CMA-ES\n")
cma = cma_es(par=parInfo$guess, fn=obj2, lower=parInfo$lower,
   upper=parInfo$upper)

cat("Running optim SANN\n")
sann = optim(par=parInfo$guess, fn=obj2, method="SANN")

comps = rbind(real=unlist(demo$par),
              'AHR-ES'=calib$par,
              SANN=sann$par,
              'CMA-ES'=cma$par,
              optx[,seq_along(parInfo$guess)],
              CG=opt$par
)

print(comps)
```

Chapter 3

Parameterization and calibration of the end-to-end ROMS-PISCES-OSMOSE model of the Northern Humboldt Current Ecosystem

In this chapter we address the key calibration phase of the end-to-end (E2E) ecosystem model ROMS-PISCES-OSMOSE for the Northern Humboldt Current Ecosystem. For this purpose, we highlight some issues related to the confrontation of complex ecosystem models to data and propose a methodology for a sequential multi-phases calibration of ecosystem models (section 3.1). We first propose two criteria to classify the parameters of a model: the model dependency and the time variability of the parameters. Then, these criteria and the availability of approximate initial estimates are used as decision rules to determine which parameters need to be estimated, and their precedence order in the sequential calibration process.

The E2E model is calibrated using an the evolutionary algorithm described in chapter 2 and a likelihood approach to fit monthly time series data of landings, abundance indices and catch at length distributions from 1992 to 2008.

3.1 A sequential approach for the calibration of ecosystem models

In this section we include a manuscript submitted to the journal “Progress in Oceanography” (manuscript PROOCE-S-14-00115).

A sequential approach to calibrate ecosystem models with multiple time series data

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Abstract

Ecosystem approach to fisheries requires a thorough understanding of fishing impacts on ecosystem status and processes as well as predictive tools such as ecosystem models allowing to provide useful information for management. The credibility of such models is essential when used as decision making tools, and data comparison is one major criterion to assess such credibility. However, more attention has been given to the exploration of model behavior than to a rigorous confrontation to observations, as the calibration of ecosystem models is challenging in many ways: first, ecosystem models can only be simulated numerically and are generally too complex for mathematical analysis and explicit parameter estimation; secondly, the complex dynamics represented in ecosystem models allow species-specific parameters to impact other species parameters through ecological interactions; thirdly, critical data about non-commercial species are often poor; lastly, technical aspects can be impediments to the calibration with regard to the high computational cost potentially involved and the scarce documentation published on fitting complex ecosystem models to data. This work highlights some issues related to the confrontation of complex ecosystem models to data and proposes a methodology for a sequential multi-phases calibration of ecosystem models. We first propose two criteria to classify the parameters of a model: the model dependency and the time variability of the parameters. Then, these criteria and the availability of approximate initial estimates are used as decision rules to determine which parameters need to be estimated, and their precedence order in the sequential calibration process. The end-to-end (E2E) ecosystem model ROMS-PISCES-OSMOSE applied to the Northern Humboldt Current Ecosystem is used as an illustrative case study. The model is calibrated using an original evolutionary algorithm and a likelihood approach to fit monthly time series data of landings, abundance indices and catch at length distributions from 1992 to 2008.

Keywords: Stochastic models, ecosystem model, model calibration, inverse problems, time series, ecological data, Humboldt Current Ecosystem, Peru.

1. Introduction

The implementation of an ecosystem approach to fisheries not only requires a thorough understanding of the impact of fishing on ecosystem functioning and of the ecological processes involved, but also quantitative tools such as ecosystem models to provide useful information and predictions in support of management decision. Yet, the use of ecosystems models as decision making tools would only be possible if they are rigorously confronted to data by means of accurate and robust parameter estimation methods and algorithms (Bartell 2003). In many respects, the calibration of ecosystem models is a complex task. In particular, the dynamics represented in ecosystem models allow species-specific parameters to have an impact on one another through ecological interactions, which results in highly correlated parameters, while additionally, critical information and observations on non-commercial species can be missing or poor. Furthermore, the high number of parameters and the long duration of the simulations can be an obstacle to calibrate a model. These diverse reasons hampered the development of flexible and generic enough calibration algorithms and methodology for ecosystem models, and only sparse documentation has been produced on fitting complex models (Bolker et al. 2013).

Given that the calibration of complex ecosystem models requires a lot of data and potentially involves a high number of parameters to estimate, common practice in the field has been to i) reduce the number of parameters to estimate by using estimates provided by other models (Marzloff et al. 2009, Lehuta et al. 2010) or available for similar species or ecosystems (Bundy 2005, Ruiz and Wolff 2011), ii) use other models outputs as data to calibrate the model (Mackinson and Daskalov 2007), or both (Shannon et al. 2003, Guénette et al. 2008, Friska et al. 2011, Travers-Trolet et al. 2013). These different strategies allow to calibrate complex models while attempting to synthesize the maximum of available information. However, as the parameters or outputs used rely on different model assumptions, they may lead to the fitting of artificial parameter values or to inconsistent behavior of the model by trying to reproduce other models' dynamics.

When calibrating complex non-linear models, it can be useful to fix some parameters in preliminary calibration trials when guess estimates of these parameters can be obtained from independent data, other models or expertise (Nash and Walker-Smith 1987). In particular, assigning initial guess values for completely unknown parameters before proceeding to a full calibration of all parameters can ease the estimation of model parameters (Nash and Walker-Smith 1987, Fournier et al. 2012). This multiple phases calibration approach is supported by some optimization softwares, like specialized R packages or the AD Model Builder software (Bolker et al. 2013). However, it is difficult to find in the literature a clear roadmap or strategy to guide the users and help them to determine what parameters should be estimated in the successive phases. It appears that the final organization of the calibration phases is most often an empirical process and is the result of trials and errors in the calibration procedure (Fournier 2013).

The objective of this paper is to highlight some issues related to the confrontation of complex ecosystem models to data and propose a methodology to a sequential calibration of ecosystem models, illustrating it with the calibration of the ecosystem model OSMOSE (Shin and Cury 2004, Travers et al. 2009) applied to the northern Humboldt Current Ecosystem. The first important step in a calibration is to be able to categorize the parameters of a model. To do so, we propose two criteria: the model dependency and the time variability of the parameters. Then, we use these criteria and the availability of approximate initial estimates of the parameters to determine which parameters need to be estimated, and their precedence in the sequential calibration process. We finally compare our sequential approach with the results of a single step calibration of all parameters.

2. Material and methods

2.1. Parameterization and calibration

2.1.1 Types of parameters

Several classifications of model parameters can be found in the literature (e.g. Jorgensen and Bendoricchio 2001). In this work, we classified the parameters according to two criteria: 1) the independence of the parameter value from the model structural assumptions, and 2) the time variability of the parameter in relation to its use in the model. The categorization of the parameters is defined as follows:

Model dependency: Parameters are considered to be model dependent when their values can vary between models due to different model structures or assumptions. For example, fishing mortality can be categorized as being model-dependent (which depends on the value of natural mortality, structural equations of the fishing process and assumptions on the selectivity or seasonal distribution of fishing effort). On the contrary, model-independent parameters can be estimated directly from data and observations by simple models or consistent theoretical relationships. For example, length-weight parameters, or von Bertalanffy growth parameters can be considered to be independent of the overarching ecosystem model structures and assumptions.

Time variability: Some parameters of the model are expected to have temporal variability at the time scale of the model and the data. For example, fish larval mortality rates which determine the fish annual recruitment success and which are related to environmental conditions are expected to vary annually. Other parameters of an ecosystem model are not expected to have significant temporal variability at the time scale of the model and the data time series, for example the parameters of predators’ functional response.

The classification of the parameters in terms of model dependency is necessary in order to avoid the misleading use of parameters' values which have been estimated in other models and not directly from observations. If some parameters are fixed to values which are inconsistent with the model structure currently used to fit the data, the other parameter estimates obtained from the calibration can be highly uncertain and only artifacts to fit the data. This can also impede the convergence of the objective function and lead to a calibration failure (Gaume et al. 1998, Whitley et al. 2013).

The classification in terms of temporal variability can be more arbitrary since many parameters (especially the ones characterizing the populations) are expected to vary with time. The cutoff we propose for a parameter to be considered as time varying results from the following considerations: i) the identification of a process leading to such time variability, ii) the existence of theoretical assumptions about the importance of such process in the dynamics of the modeled ecosystem, iii) the non-explicit representation of the process in the model, and iv) the significance of the time variability compared to the time scale of the model and the length of the data time series. Some parameters can be assumed to be constant at shorter time scales (e.g. a few years) but can exhibit variability at longer time scales (e.g. several decades). For example, the length at maturity for a given species can decrease in response to heavy fishing (Shin et al. 2005), but can be considered as constant in the model for periods short enough, or if the variability is not considered to cause significant changes in the functioning of the multispecies assemblage.

Despite the apparent dichotomous classification presented, the degree of temporal variability or model-dependency in the parameters can vary, and a qualitative classification of the parameters should be attempted. In the OSMOSE ecosystem model, such classification could be proposed for the parameters characterizing modelled multispecies fish assemblages (Figure 1; see Appendix A for details about the parameterization of OSMOSE).

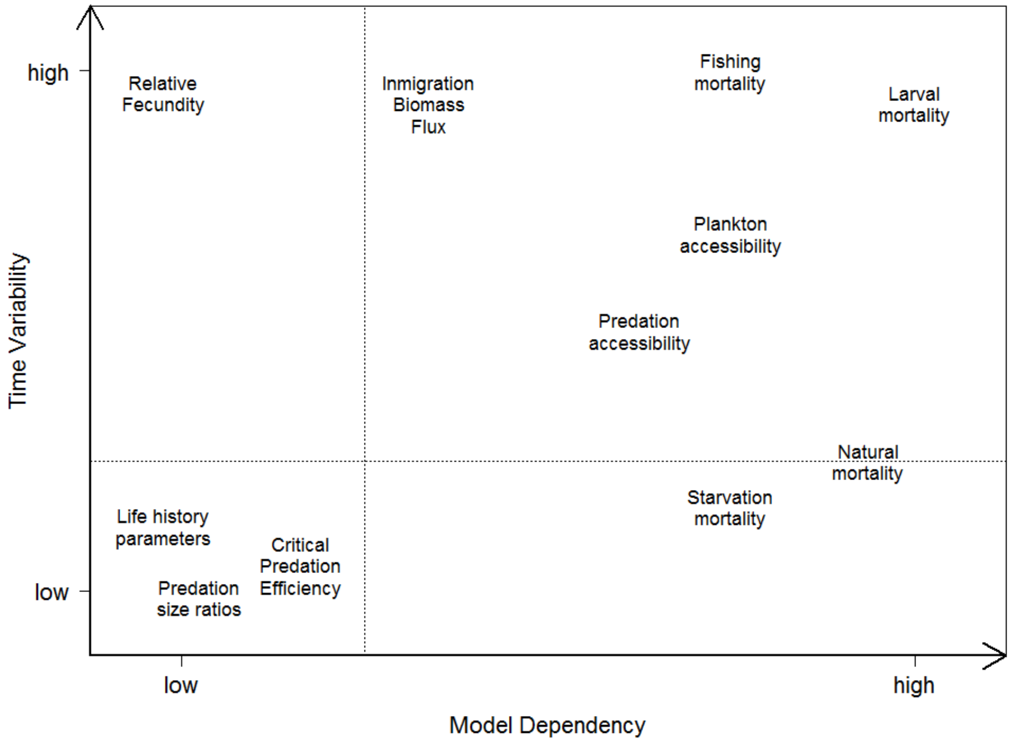

Figure 1. Proposed classification of OSMOSE model parameters depending on the time variability and the model dependency criteria.

2.2 Approach for the sequential calibration

2.2.1 Progressive time resolution of the parameters

The number of parameters to estimate in a model can be high, particularly when time-varying parameters are included, so that fitting the model to data can be challenging (e.g. see Schnute 1994). Additionally, the way a model is parameterized will define the objective function to be optimized to estimate the parameters; just by rescaling or transforming the parameters this objective function can be changed and improve the parameter estimation process (Bolker et al. 2013).

There are several ways to model the time variability in the parameters, taking into account the assumed shape of the variability and the degree of time resolution one wants to introduce (see Megrey 1989, Methot and Wetzel 2013 for examples in fishery models). However, in practical terms, there is a limit in the number of parameters which can be used, which depends on the quality of the available data to estimate such parameters. The data must provide information on the time variability of the parameters at the right resolution, otherwise the risk is high to end fitting the noise in data or simply failing in the parameter estimation. This means the decision to keep a parameter constant or to model its time variability has to take into account both the complexity of the parameter estimation and the quality of the data used for the calibration of the model (Jorgensen and Bendoricchio 2001).

We considered different models to represent the temporal variability in the parameters (Appendix B, Table B.1, Figure B.1), where the variability can be split into three components: the mean value of the parameter, the high frequency variability (seasonal or non-periodical) and the low frequency variability (interannual). This type of parameterization allowed us to define several nested models, i.e. models which can gradually be complexified from the simplest models' parameterization (setting to zero the random effects in the yearly component for the time varying parameters) to full consideration of low and high frequency variability. For example, the mean value of time-varying parameters over the time series should be estimated in priority, with the interannual deviations fixed to zero.

If the different components of time variability in a given parameter can be introduced progressively, the final parameter estimation can be improved by providing good initial values for the more important variability components after preliminary calibration of simpler versions of the model. We therefore propose a general calibration strategy which consists in modelling the time-varying parameters such that the several components of variability are independent and can be nullified by fixing some parameters to constant values (nested models).

2.2.2. Calibration in multiple phases

According to the parsimony principle, given two models with similar accuracy, the simplest model is the best compromise with regard to the available data. In particular, for nested models, the complexity of a model is directly related to the number of parameters to estimate, so the parsimony principle implies to estimate the lowest number of parameters as possible. On the other hand, it is possible to increase the goodness of fit of the model just by increasing the number of parameters, but this can lead to overfitting (Walter and Pronzato 1997, Bolker 2008). However, there is no way to know a priori if all parameters will be identifiable, i.e. if we can estimate them properly from the available data.

Based on the criteria of time variability and model dependency of the parameters, we propose a set of rules for a hierarchical approach to select the parameters to estimate in a model and the order at which the parameters should be estimated in the different phases of the calibration. Also, we propose some criteria to design nested models for taking into account time variability by using simple time series models which allow to assess the usefulness of the additional temporal parameters introduced in the model calibration.

The first rule relates to the model dependency of the parameters. Independently of the time variability, parameters with low model dependency should be assigned values directly from observations, simple models or from dedicated designed experiments. On the contrary, parameters with high model dependency should always be estimated through model calibration, because even though the theoretical meaning of the parameters is not necessarily model-dependent, different model structures will introduce differences in the actual meaning and value of the parameters within the model.

The second rule relates to the time variability of the parameters. Along with the decision on what components of the variability need to be included (e.g. seasonal or interannual), it is also necessary to assume which time component is more important to explain the total variability of the parameter. These choices allow to progressively increase the variability of the time-varying parameters during different phases of the calibration. The order of the calibration phases is different depending on whether the seasonal component (Figure 2 A and C) or the interannual component (Figure 2B and D) dominates the temporal dynamics.

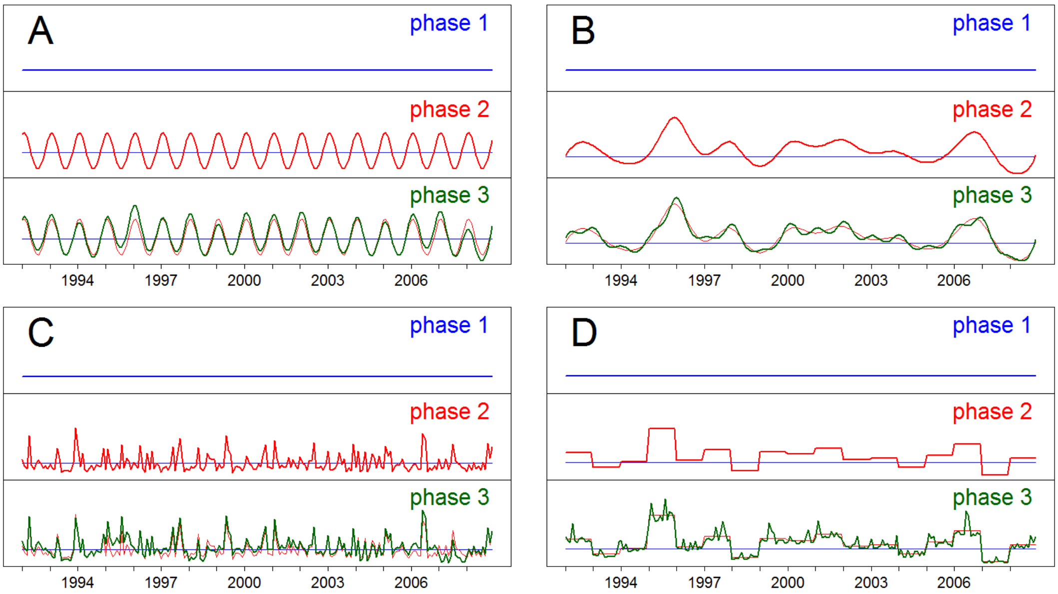

Figure 2. Progressive increase in the time variability of parameters in the case of a 3-phases model calibration. The A and C plots show predominance in the seasonal variability, while interannual variability is the dominant signal in plots B and D plots. The upper plots correspond to type-A models and the lower plots to type-B models described in the appendix B.

A third rule relates to the availability of initial estimates for the parameters to calibrate. Even in case of model-dependency, estimates from other models can be used as initial values to start the calibration. For time-varying parameters, the deviations estimated from other models (e.g. single species models) or approximate relationships can be used as proxies of the interannual variability if they are estimated from the same dataset used for the current calibration. Another alternative is to use parameters estimated from models with a similar structure, such as previous versions (likely simpler) of the same model (e.g. a steady-state one). It is important to note that the proxies or initial estimates will only be used to start the calibration in a given parameter space but the parameters will be fully estimated during the calibration, which means the final estimates can be far from the initial values (Sonnenborg et al. 2003).

Considering all these rules together, we propose a hierarchy in the order of parameters' estimation using a sequential calibration approach (Figure 3).

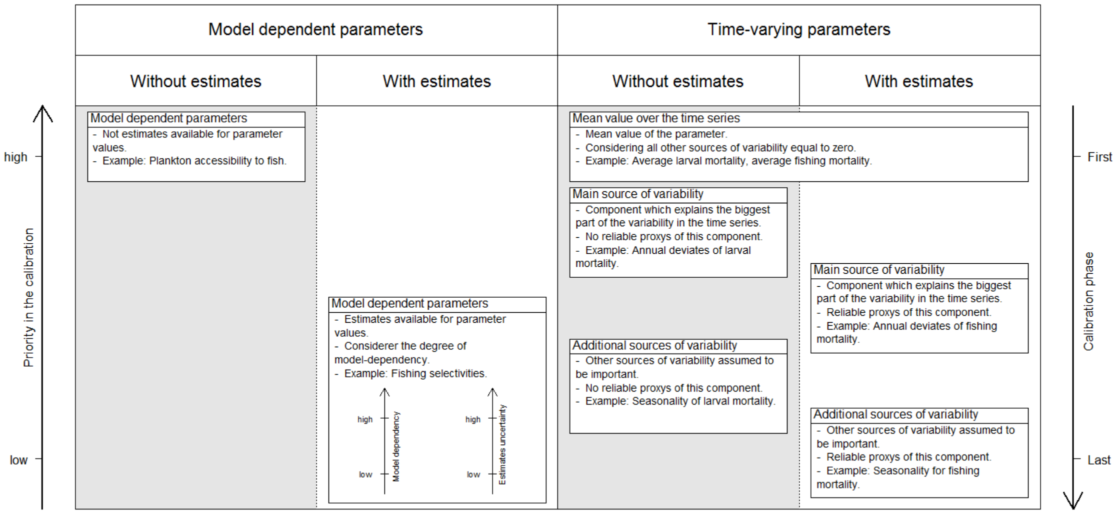

Figure3. Proposed hierarchy in the order of parameters' estimation using a sequential calibration approach.

If we consider the initial phase of the calibration with some parameters fixed as a way to improve the final calibration, it is possible to make changes in the objective function across the different phases of the calibration (Fournier 2013). However, by keeping constant the objective function and running a full optimization at each phase, it is possible to analyze the improvement in the fitting process as a result of the increased complexity of the calibration. It therefore allows to test the usefulness of the additional parameters and to perform model selection by detecting which parameters do not improve the data fitting.

2.3. Case model: OSMOSE for Northern Humboldt Current Ecosystem

To illustrate our calibration methodology, we applied the OSMOSE model to the Northern Humboldt Current Ecosystem (NHCE) inhabited by the main stock of "anchoveta" or Peruvian anchovy (*Engraulis ringens*). As the paper focuses on the calibration methodology, we do not present the OSMOSE model in detail; this is done by Shin and Cury (2001, 2004) and Travers et al. (2009, 2013), and the application to the Humboldt ecosystem is detailed by Oliveros et al. (in prep.) as well as in Appendix A. OSMOSE is a multispecies individual-based model (IBM) which focuses on high trophic level (HTL) species. This model assumes size-based opportunistic predation based on the spatial co-occurrence of a predator and its prey. It represents fish individuals grouped into schools, and models the major processes of fish life cycle (growth, predation, natural and starvation mortalities, reproduction and migration) and the impact of fisheries. The modeled area ranges from 20°S to 6°N and 93°W to 70°W covering the extension of the Northern Humboldt Current Ecosystem and the Peruvian Upwelling Ecosystem (Figure 4), with 1/6° of spatial resolution. The model explicits the life history and spatio-temporal dynamics of 9 species (1 macro-zooplankton group, 1 crustacean, 1 cephalopod and 6 fish species), between 1992 and 2008.

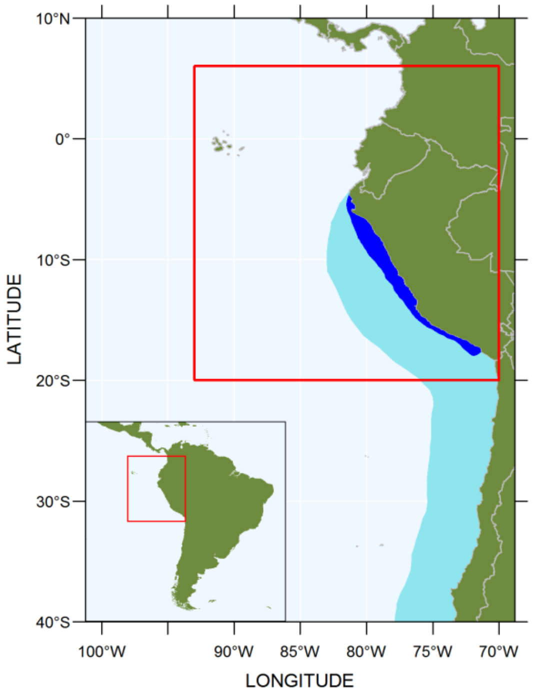

Figure 4. Map of the modeled area. The model spatial domain is limited by the red square. The light blue area shows the extension of the Humboldt Current Large Marine Ecosystem, and the dark blue area the extension of the Peruvian Upwelling Ecosystem.

The NHCE exhibits a high climatic and oceanographic variability at several scales (e.g. seasonal, interannual and decadal), the major source of interannual variability being the interruption of the upwelling seasonality by the El Nino Southern Oscillation ENSO (Alheit and Ñiquen 2004), having direct effects on larval survival and fish recruitment success (Ñiquen and Bouchon 2004). Additionally, the fishing activity can also be highly variable, depending on the variability in the abundance and accessibility of the main fishery resources. Due to these different sources of temporal variability, it was important to model the variability in some processes which are implicit in OSMOSE: the larval and the fishing mortality. This variability was modeled using time varying parameters, which were estimated considering interannual and seasonal variability. For both processes, we estimated the mean value and annual deviations. The natural mortality (due to other sources of mortality not included in the model) and plankton accessibility to fish coefficients were also estimated.

The data used to calibrate our model were: i) biomass indices from hydro-acoustic scientific surveys (Gutierrez et. al 2000; IMARPE 2010) and ii) total reported landings for the main commercial species (IMARPE 2009, IMARPE 2010). Additionally, catch-at-length data were available for anchovy and jack mackerel and catch-at-age for hake. A summary of the data available, the time resolution of the information and the period of availability is shown in Table 1. The model was confronted to data using a likelihood approach described in Appendix A. The optimization of the likelihood function was carried out using an evolutionary algorithm developed by Oliveros-Ramos and Shin (submitted), since for stochastic models it is not possible to apply derivative-based methods (see Appendix A for more details).

Table 1.Summary of data available for the calibration of the model. Years for data availability are indicated, M (monthly) and Y (yearly) indicates the time resolution of the data.

	Catch-at-age	**Catch-at-length**	**Landings**	**Acousticindex**
Euphausiids			No fishing	2003 - 2008 (Y)
Anchovy (*Engraulis ringens*)		1992 - 2008 (M)	1992 - 2008 (M)	1992 - 2008 (Y)
Sardine (*Sardine sagax*)			1992 - 2008 (M)	1992 - 2008 (Y)
Jack Mackerel (*Trachurus murphyi*)		1992 - 2008 (Y)	1992 - 2008 (M)	1992 - 2008 (Y)
ChubMackerel (*Scomber japonicus*)			1992 - 2008 (M)	1992 - 2008 (Y)
Mesopelagic fish			No fishing	1999 - 2008 (Y)
Red lobster (*Pleuroncodes monodon*)			No fishing	1999 - 2008 (Y)
Jumbo squid (*Dosidicus gigas*)			1992 - 2008 (M)	1999 - 2008 (Y)
Peruvian hake (*Merluccius gayi*)	1992-2008 (Y)		1992 - 2008 (M)	1992 - 2008 (Y, trawl)

2.4. Calibration experiments

For the OSMOSE model of the Northern Humboldt Current Ecosystem (NHCE), 5 types of parameters needed to be estimated (Table 3): i) larval mortality rates, ii) fishing mortality rates, iii) coefficients of plankton accessibility to fish, iv) natural mortality rates (due to other sources of mortality not explicit in OSMOSE) and, v) fishing selectivities. Additionally, we needed to estimate the immigration flux of the biomass of munida in the system. The calibration strategy proposed was applied to our model calibration and resulted in a pre-defined order of phases for the estimation of the parameters of the model (Table 2).

Table 2. Order of estimation of parameters in the calibration of the NHCE OSMOSE model.

Phase	Parameters	Remarks
1	**Time varying parameters:** - **Larval mortality:** mean for all species. - **Fishing mortality:** mean for all species. **Non time-varying (without estimates):** - **Natural mortality:** all species. - **Inmigration:** total immigrated biomass, peak of migration flux (munida).	**Number of parameters estimated: 51.** - Larval and fishing mortalities are assumed to vary with time. - Natural mortality is assumed to not vary with time.
2	**Previous parameters** **+ Time varying parameters:** - **Larval mortality:** annual deviates (all species). - **Fishing mortality:** annual deviates without proxys (6 first years for squid).	**Number of parameters estimated: 208** (including previous 51). - Main source of variability for the larval and fishing mortality is assumed to be interannual.
3	**Previous parameters** **+ Time varying parameters:** - **Fishing mortality:** annual deviates (all remaining parameters and species).	**Number of parameters estimated: 299** (including previous 208). Main source of variability for fishing mortality is assumed to be interannual.
4	**Previous parameters** **+ Time varying parameters:** - **Larval mortality:** seasonal variability (anchovy). **+ Non time-varying (with estimates):** - **Selectivity parameters:** anchovy, hake, jack mackerel.	**Number of parameters estimated: 307** (including previous 299). - Seasonal variability was only included for anchovy due to data limitations. - Selectivity is assumed to not vary with time.

We considered larval and fishing mortality as time-varying parameters, and modeled them using the functions described in appendix B (Table B.1). The immigration flux of munida biomass was also treated as a time-varying parameter, but is parameterized with two non time-varying parameters (total biomass immigrated in the system and the time at the peak of the migration) using a "gaussian pulse" as described in appendix B. The other parameters (natural mortality, plankton accessibility and fishing selectivities) were considered constant during the simulation and are ranked according to our evaluation of their model dependency (Figure 1).

Table 3. Models used for the time variability of larval and fishing mortalities, according to the functional forms described in Appendix B.

Species	*Time-varying parameters*		*Abundance index quality*	*Time resolution of the information*	
	Larval mortalities	*Fishing mortalities*		*Catch*	*Catch at age/length*
1. Abundance index, stage structured fishing information.					
Anchovy	A.3	B.2	High	Monthly	Monthly
Hake	A.2	B.2	High	Monthly	Yearly
Jack mackerel	A.2	B.2	Low	Monthly	Yearly
2. Abundance index, aggregated fishing information.					
Sardine	A.2	B.2	High	Monthly	Not available
Chub mackerel	A.2	B.2	Medium	Monthly	Not available
Humboldt Squid	A.2	B.2	Low	Monthly	Not available
3. Abundance index.					
Munida	A.2	Not required	High	-	-
Euphausiids	A.2		Low		
Mesopelagics	A.2		Low		

A steady state calibration of the NHCE-OSMOSE model was performed first, corresponding to the initial conditions prevailing in 1992, which is the first year of the data time series. Munida was not included because it immigrates in the NHCE after 1992, during the 1997/98 El Niño event. This first calibration allowed to provide estimates of the average value of the larval and natural mortality rates for the modelled species. For the fishing selectivity parameters, values used in stock assessment were used, while we chose to estimate only the ones for the species including age or length composition data (anchovy, hake and jack mackerel). We used the ratio between catch and biomass, estimated directly from data, as a proxy of the variability of the fishing mortality rate. This ratio was split into seasonal and interannual deviations from the average value.

In order to evaluate the performance of the sequential calibration approach in the parameter estimation, we compared it to other calibration experiments:

- We first run a one-phase calibration where all parameters were estimated at once, while trying to keep constant the total number of function evaluations (i.e. the number of times we run the simulation model) to make both calibrations comparable.
- Additionally, we also run a sequential multi-phases calibration where some parameters were fixed. Concretely, we fixed the natural

and fishing mortality variability to values reported in the literature. As in previous OSMOSE applications (Marzloff et al. 2009, Duboz et al. 2010), natural and fishing mortalities from the Ecopath with Ecosim model for the same system (Tam et al. 2008) were used. In this case, only larval mortalities, coefficients of fish accessibility to plankton, the immigration flux of munida and average fishing mortality were estimated.

- Finally, we run a calibration without including the annual deviates, estimating only the long term mean of the larval mortality and the average fishing mortality, to analyze the effect of considering time-varying parameters in the calibration results.

In all calibration experiments, we considered commercial landings data as the most reliable source of information, compared to estimates of species biomass derived from scientific surveys. In consequence, more weight was given to catch data (i.e. less uncertainty; CV=0.05) than to the biomass indices (CV=0.15, 0.10 for anchovy), so the fit to catch data contributed the most to the total value of the likelihood function we tried to optimize during the calibration process.

3. Results and discussion

3.1 Calibration in multiple phases

As we considered commercial landings as the most reliable source of information in the likelihood function, catch output from the NHCE-OSMOSE model should have the better fit from all the information used for the calibration. The simulated landings we obtained are in good agreement with data, at monthly and yearly scale (Figures 5 and 6), with high correlations between observed and simulated values. The landings for the Humboldt squid are the ones with the poorest fitting, which can be partially explained by the lack of information of abundance indices and proxys for the variability in the fishing mortality for the initial years. Landings for anchovy are the ones with the highest variability, since fishing mortality has a strong seasonality (Oliveros-Ramos et al. 2010), with no fishing over several months and the setting of two quotas per year. A refined modeling of the variability of the fishing mortality for anchovy (two parameters per year, instead of one for example) could help to better reproduce the variability in the observed landings. However, with the current calibration, the fit of the NHCE-OSMOSE model to anchovy landings can be considered as satisfactory, capturing most of the interannual variability observed for this fishery. The landings of hake are overestimated for most of the simulated period, but the trends in variability are properly reproduced, having the highest correlation between observed and simulated landings among all the species. Jack mackerel and sardine are the ones presenting the best fit, while there is a significant overestimation of the landings for the chub mackerel during 1999 and 2000. The simulated landings were produced from the estimated fishing mortalities and our initial choice of the selectivity functions. The fishing mortality rates for a given length or age class are highly variable over time for all target species (Figure 7).

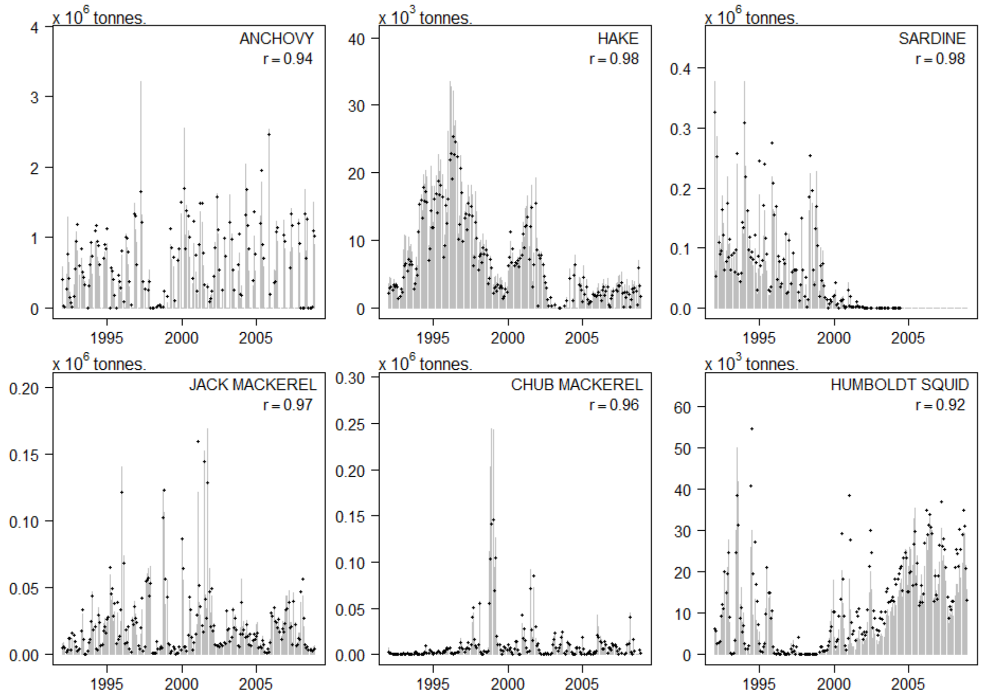

Figure 5. Fit of the NHCE-OSMOSE model to the monthly landings data for the multiple phases reference calibration. The grey bars represent the monthly landings predicted by the model and the dots the observed landings, for each modelled species targeted by Peruvian fisheries.

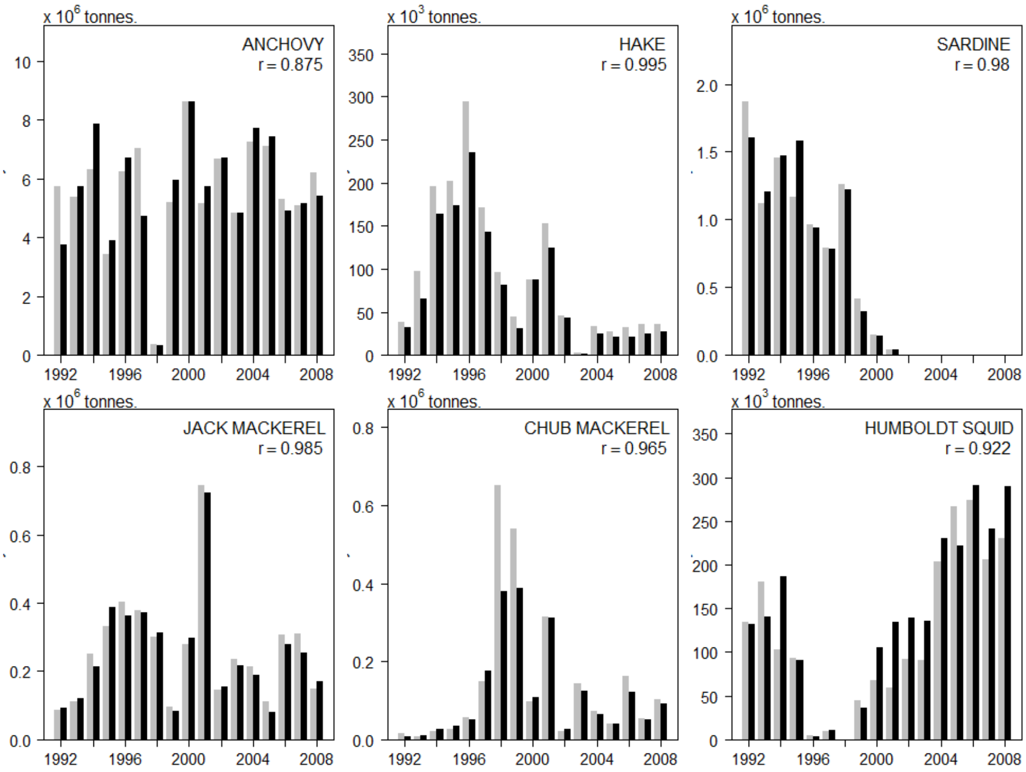

Figure 6. Fit of the NHCE-OSMOSE model to the annual landings data for the multiple phases reference calibration. The grey and black bars represent the annual landings predicted by the model and the observed landings, respectively, for each species with active fisheries.

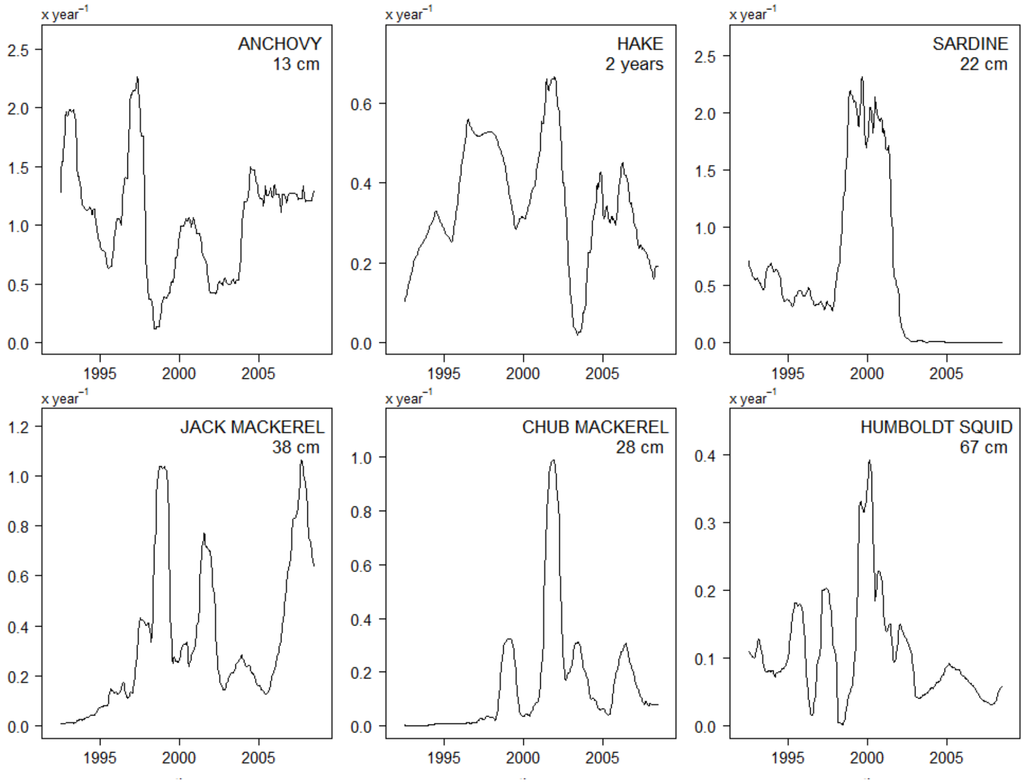

Figure 7. Estimated average fishing mortality rates (year^{-1}) for the most representative length or age class observed in the fishery.

For the age and length distributions of fish abundance (Figure 8), we obtained a good fit considering we assumed only one selectivity pattern over the whole studied period, while time varying selectivity is more standard in fishery modeling. For anchovy, the model predicts more young adults (12-14cm) and less juveniles (< 12cm) in average, but in the temporal patterns of the residuals, there are both over and underestimation of fish density for the same length classes. The model does not include spatial variability in the fishing effort, which usually concentrates in the central part of Peru (IMARPE 2010). In addition, anchovy biomass spatial distribution by size can be also very variable, depending on the environmental conditions (Bertrand et al. 2004, Gutierrez et al. 2007, Swartzman et al. 2008). Including these sources of variability properly could help to explain better the variability patterns in the catch at size without introducing time variability in the selectivity. For jack mackerel, main differences are localized in a few years. The discrepancy could be due to the fact that Jack mackerel is a straddling stock which can show high variability in spatial distribution (Dioses 2013, Segura and Aliaga 2013, Ayón y Correa 2013), and we did not model the spatial distribution of fishing effort which is concentrated inside the Peruvian EEZ (Ñiquen et al. 2013, Zuzunaga 2013). In addition, the bimodal shape of the distribution of observed catch at length is related to a higher than usual proportion of juveniles in the landings in 2004 (Diaz 2013). The model is predicting more juveniles in the range of 15 to 25 cm in order to properly fit the small mode around 15cm. OSMOSE being a spatial model, these issues can possibly be handled in future by improving the spatial definition of the habitat for different classes of jack mackerel, without adding ad hoc assumptions on selectivity changes. Finally, for hake, the landings of the main age classes exploited by the trawl fishery (1 to 3 years) are well represented while landings of older classes are in general overestimated. However, these older age classes are normally not accessible to the industrial trawl fishery. This could represent a misspecification of the model we could not handle with a simple lognormal selectivity model as used here (appendix A).

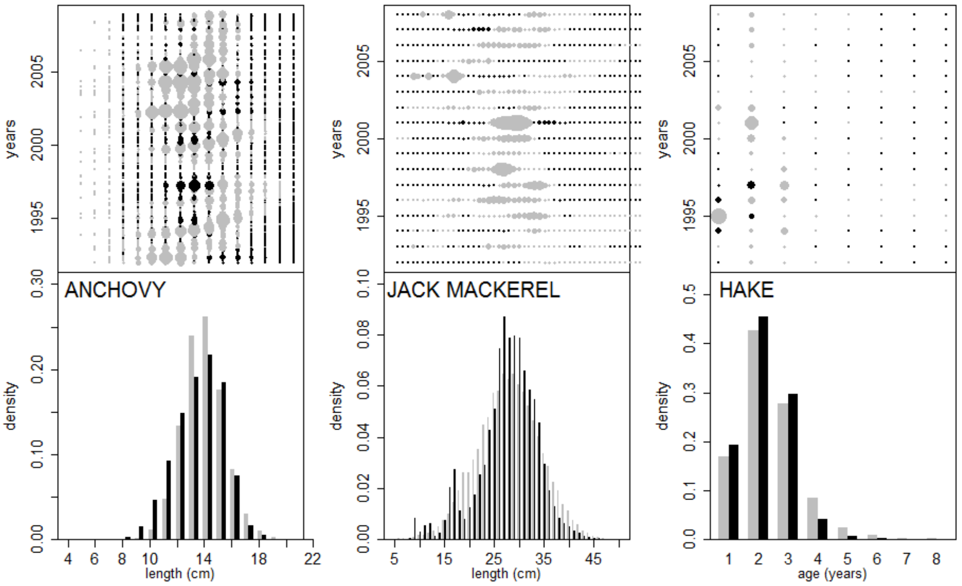

Figure 8. Fit of the NHCE-OSMOSE model to catch at length/age data for the multiple phases reference calibration. The upper panels show the raw residuals; the size of the circle is proportional to the magnitude of the error, grey means that the simulated density is lower than observed, and black means the simulated density is higher than observed. The bottom panels show the average size or age distributions of fish abundance, grey bars represent simulated outputs and black bars observed values.

The second important source of information for the calibration was provided by the time series of surveyed biomass indices. The model captured properly the more important trends in the time series of the abundance indexes (Figure 9), but mesopelagic fish and euphausiids. Two main problems with these two species groups could explain the poor fit: a lack of abundance data during the first years of the simulation and because both species are not harvested, there are no landings data that could be used for the calibration of the dynamics of these species. For mesopelagic fish, the simulated biomass is within the range of observed biomass but the simulations do not reproduce the observed interannual variability pattern. For euphausiids, there is a systematic overestimation of the biomass, which combined with a low larval mortality (Figure 10) suggests a incompatibility of the model configuration with the observed biomass, and indicates that the system would require more macrozooplankton biomass to be consistent with observed levels of biomass of the other species. With regard to these results, it is worth mentioning that Ballon et al. (2011) suggested that there might be an underestimation of euphausiid biomass directly derived from scientific surveys using traditional methods.

The estimated larval mortalities for all species are shown in Figure 10. A more detailed analysis and validation of the estimated larval mortalities is necessary to assess the temporal signals in these parameters, since there is a potential risk that some of its variability is an artifact to fit properly the observed biomass. In particular, for species where length structured information was used, it is possible to better estimate the larval mortalities since this will help to disentangle possible confounding effects with other parameters like the base natural mortality (representing all other sources of mortality not included in the model) which affects all length classes uniformly.

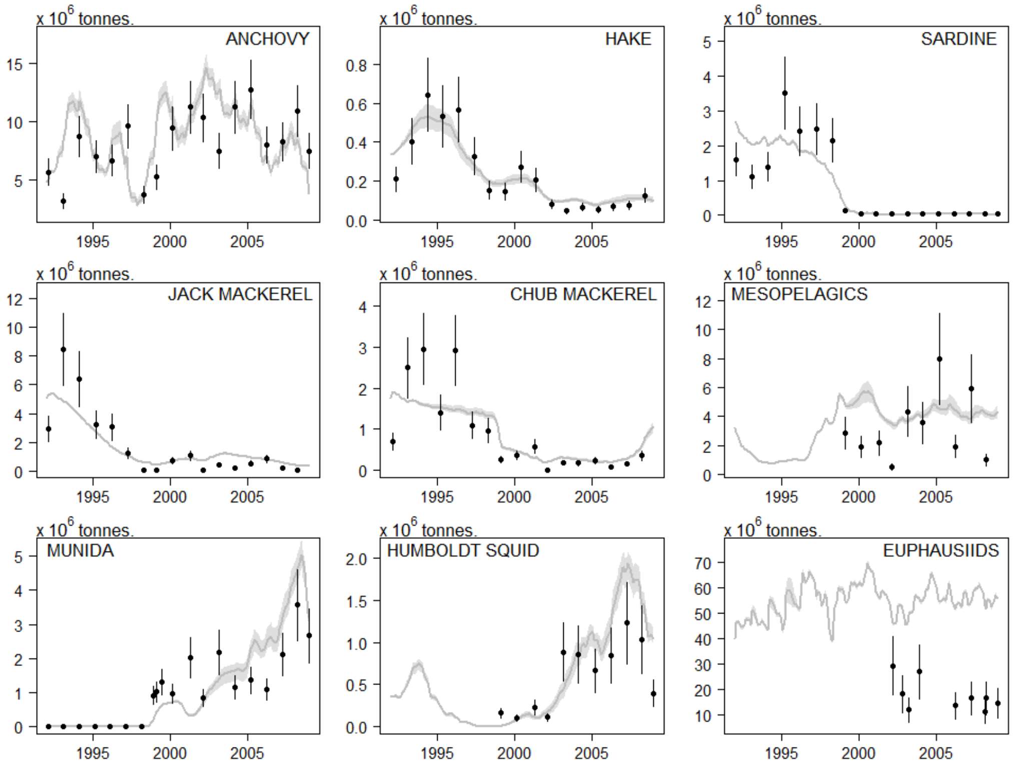

Figure 9. Fit of the NHCE-OSMOSE model to the monthly survey biomass for the reference multiple phases calibration. The shaded area represent the 95% confidence interval for the simulated biomass, considering the model stochasticity only. The black dots and bars represent the observed value and 95% confidence intervals for the observations, given the CV assumed for the data errors in the calibration.

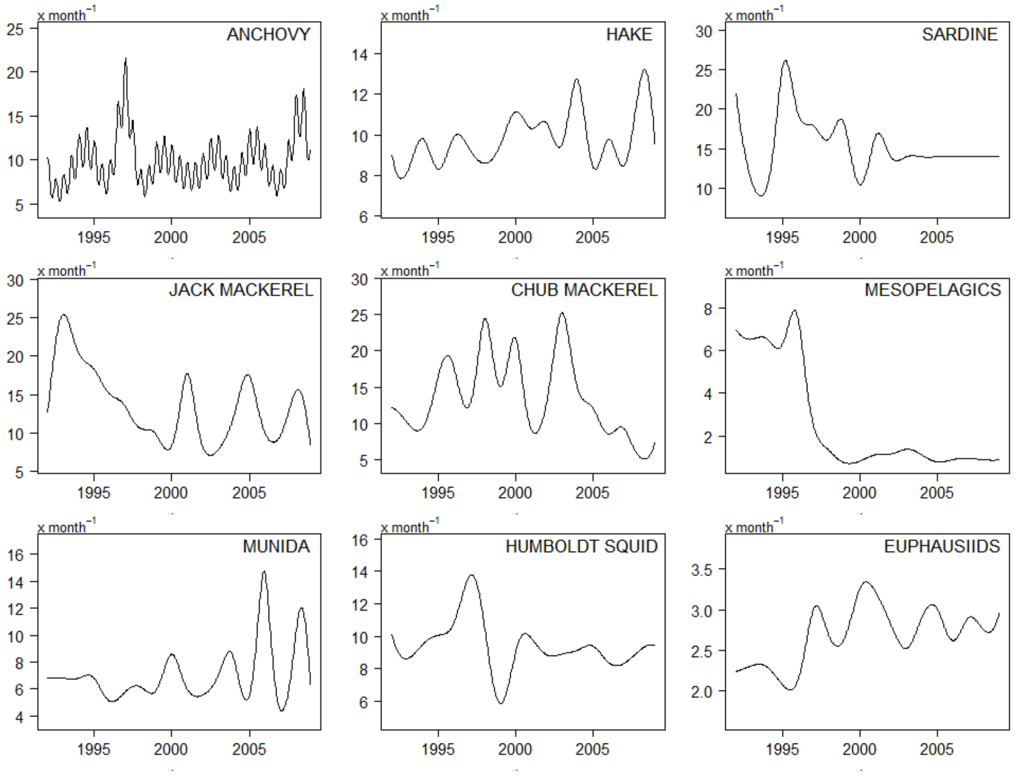

Figure 10. Larval mortality rates estimated by the reference multiple phases calibration for all modelled species.

3.2 Comparison with other calibration experiments

Since the same data has been used for all the calibration experiments, the likelihood contribution of each source of information is comparable between models. In particular, the first two experiments (multiple and single phases calibrations) are directly comparable since the only difference is the strategy used for the calibration of the same model configuration and for the same number of parameters. The results show clearly that the multiple phases calibration allowed to improve the optimisation (lower AIC and negative log-likelihood; Table 4). The calibration run with some parameters fixed from the literature, was not able to fit the landings as well as do the other calibrations, probably because the variability in the fishing mortality rates was fixed and these parameters are model dependent. Also, there is a poorest fit to the abundance indices, which can be more related to the mis-specification of the natural mortalities. The calibration without interannual parameters is not able to fit properly the landings nor the biomass indices, and the interannual variability observed in the simulations come from the forcing effect of fish habitat distribution and from the plankton dynamics (ROMS-PISCES output forcing OSMOSE – Appendix A). Larval mortality can be strongly affected by the environment and this parameter can have an important impact, particularly for the dynamics of short lived species which depend more on the level of recruitment, like Peruvian anchovy (Oliveros-Ramos and Peña-Tercero 2011). Since OSMOSE does not include an explicit sub-model for such variability in eggs and larval survival, the estimation of the interannual variability in the larval mortality was necessary. Similar reasoning can be applied to the case of fishing mortality since the variability in this parameter can be related not only to the availability of the resource biomass but also to social and economical constraints.

Table4.Summary of the likelihood for the different calibration experiments of the NHCE-OSMOSE model.

Calibrationexperiment	Number parameters	AIC	Negative log-likelihood			
			Total	Landings	BiomassIndex	Catch-at-age/length
Multiple phases	307	74807.8	37096.9	26958.7	1778.4	8333.2
Single phase	307	101030.1	50208.1	39356.8	2267.8	8543.3
Fixed parameters	207	142731.0	71158.5	57943.8	2855.9	10287.9
Without interannual parameters	56	280353.0	140120.5	128809.7	3319.5	7985.0

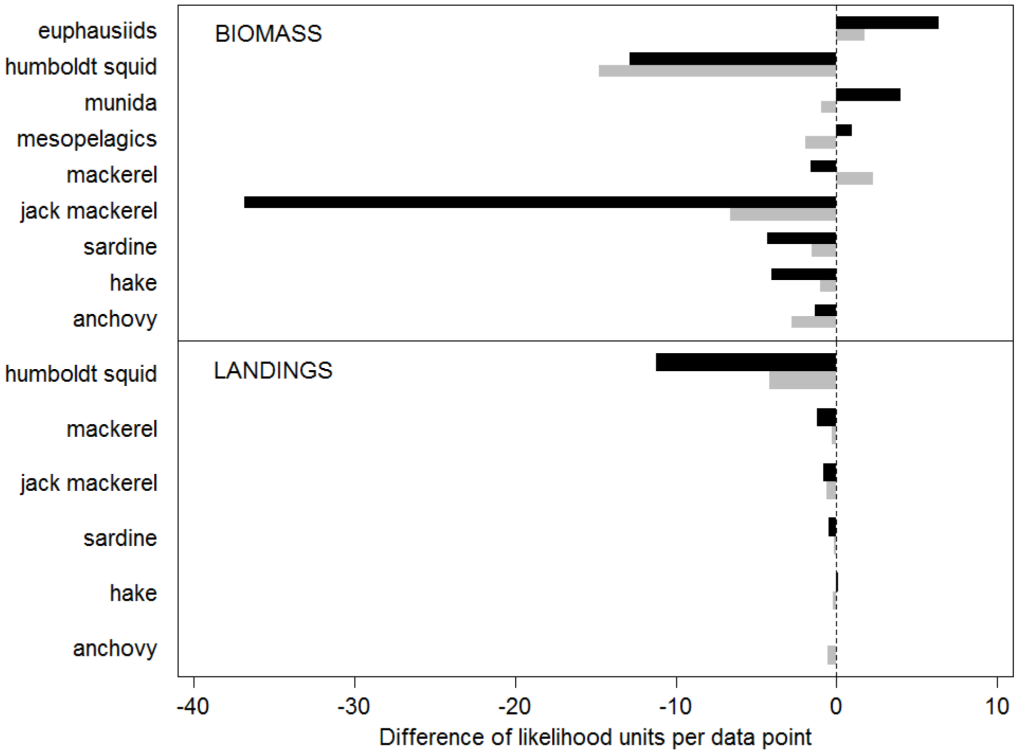

Figure 11. Comparison of the likelihood components for the different calibration experiments. The difference between the calibration experiment and the reference calibration (multiple phases) is shown. A negative difference means that the reference calibration fitted the data better for that particular component. The one phase calibration is shown in grey and the calibration with fixed parameters in black.

Globally, the comparative calibration experiments show that the reference calibration (multiple phases) fits better the landing data than do the other calibrations (one phase and fixed parameters), except for hake where the difference is negligible (Figure 11). The reference calibration fits better the biomass data as well for most species. However, the reference calibration clearly performs better in comparison to the other two calibrations. Considering the temporal variability of the log-normal errors for the simulated landings (Figure 12), the two calibrations with the full parameterization (one or multiple phases) fit the data better than the calibration with fixed parameters. Hake is the exception for which the reference calibration produces a systematic overestimation of the landings. The temporal patterns of the lognormal residuals of the landings are similar for all three calibrations, which can be due to the proxys of monthly fishing mortality variability which are common for all calibration experiments. Nonetheless, the reference calibration produces consistently smaller residuals. In addition, for all harvested species but hake, the total likelihood of the landings is lower in the reference multi-phases calibration experiment.

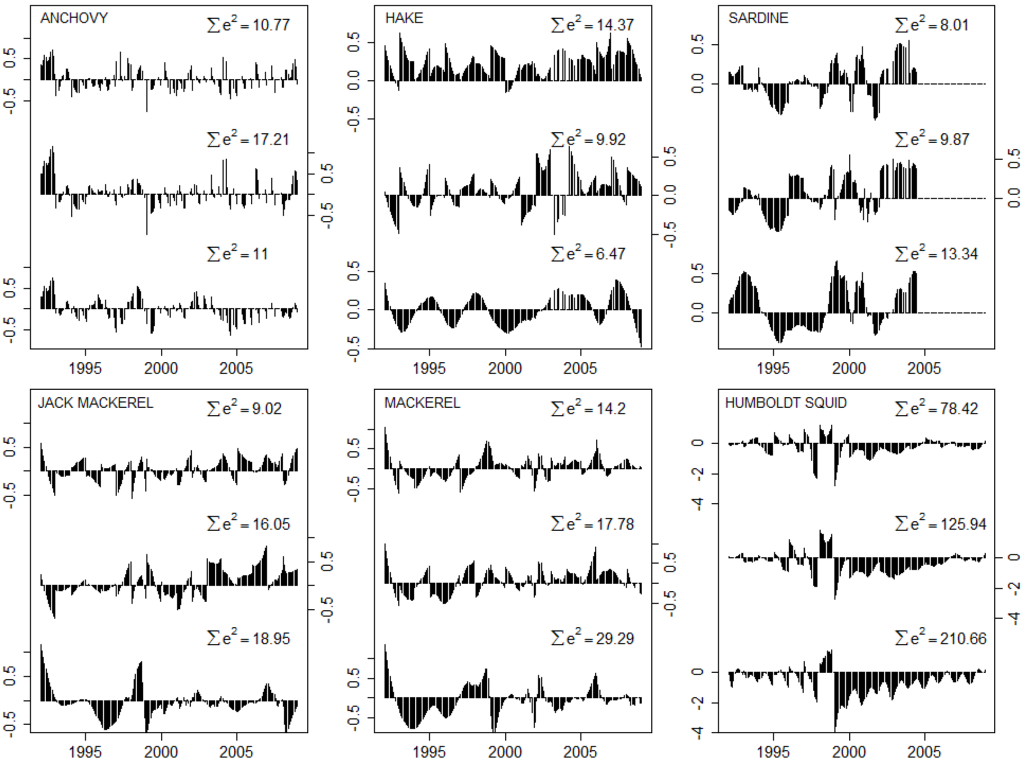

Figure 12. Comparison of the lognormal residuals of the monthly landings for the different calibration experiments. For each species, the multiple phases (top), the single phase (center) and the fixed parameters (bottom) calibration results are shown.

The calibration experiments were also compared with regard to the predicted species biomass (Figure 13). The simulated trends are very similar across the calibrations for some species (i.e. hake, sardine and chub mackerel) while more discrepancies can be reported for other species. In particular, the reference calibration captured better the interannual variability for anchovy and Humboldt squid. All the calibrated models failed to reproduce the dynamics of the biomass of mesopelagic fish and euphausiids. However, the behavior of the simulations for these species shared a common pattern: steady biomass for both species, overestimation of the euphausiids biomass and average biomass of mesopelagic fish in the range of observed biomass.

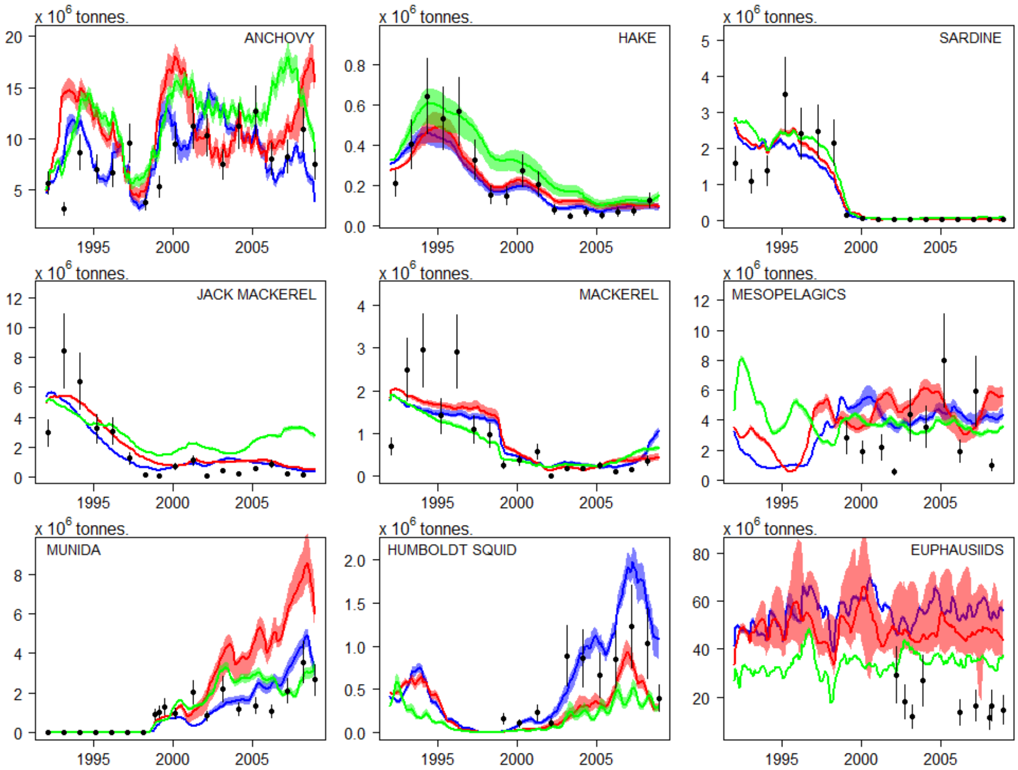

Figure 13. Comparison of the fit of the NHCE-OSMOSE model to surveyed biomass in the different calibration experiments. The shaded area represent the 95% confidence interval for the simulated biomass and considering the model stochasticity only. The black dots and bars represent the observed value and 95% confidence intervals for the observations, given the CV assumed for the data in the calibration. The calibration fixing parameters from other models estimates (green) is compared to the one phase calibration (red). The reference calibration in multiple phases (blue) is also shown.

For all our experiments, we have used the standard information used in fishery models (landings, abundance indices, catch at age or length). Since ecosystem models can provide more outputs to be confronted to data (e.g. diets, size spectrum, and other community indicators), the availability and use of these additional information could help selecting the more appropriate parameterization among different alternatives. On the other hand, if this type of data is not available, this could direct new objectives in data collection (Rose 2012) which can lead to important and necessary improvements of ecosystem models in general.

4. Conclusions and perspectives

Using a dedicated global search optimization method (Oliveros-Ramos and Shin, in prep.), we proposed a sequential multi-phases calibration approach which allowed to improve significantly the estimation of the model parameters and to lead to a better agreement between the model and the data. Our main objective was to provide guidelines to improve the calibration of ecosystem models. We focused on model dependency and time variability to categorize the parameters since these are two criteria which are usually considered to reduce the parameters' space. This preliminary parameters' classification can lead to fixing parameter values from other models or species/ecosystems or to ignoring time variability in the parameters (Lehuta et al 2013). However, in the present study, we have not considered other useful criteria such as results from sensitivity analyses which can provide a rationale to reduce the number of parameters to estimate (Megrey et al. 2007, Dueri et al. 2012, Lehuta et al 2013). Additionally, a successful calibration does not mean that a model is reliable (Gaume et al. 1998), and a proper validation is always required, eventually providing information to improve the model and to revise the calibration (Walter and Pronzato 1997, Jorgensen and Bendoricchio 2001).

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References

Alheit J., Ñiquen M., 2004. Regime shifts in the Humboldt Current ecosystem. Progress in Oceanography 60:201–222.

Ayón P. and Correa J., 2013. Spatial and temporal variability of Jack mackerel *Trachurus murphyi* larvae in Peru between 1966 –2010. Rev. peru. biol. 20(1):083- 086.

Bäck T., Schewefel H.-P., 1993. An Overview of Evolutionary Algorithms for parameter optimization. Evolutionary Computation 1:1-23.

Ballon M., Bertrand A., Lebourges D. A., Gutierrez M., Ayon P., Grados D., Gerlotto F., 2011. Is there enough zooplankton to feed forage fish populations off Peru? An acoustic (positive) answer. Progress in Oceanography 91 (4):360-381.

Bartell S.M., 2003. Effective use of ecological modeling in management: The toolkit concept. In Dale V (editor).Ecological modeling for resource management, Springer Verlag.

Bakun A. and Parrish R., 1982. Turbulence, transport, and fish in California and Peru currents. Calcofi Rep. Vol. xxiii. 99-112.

Bertrand A., Segura M., Gutiérrez M., Vásquez L., 2004. From small-scale habitat loopholes to decadal cycles: a habitat-based hypothesis explaining fluctuation in pelagic fish populations off Peru. Fish and Fisheries 5:296–316.

Bolker B.M., 2008. Ecological models and Data in R. Princeton University Press. 408pp.

Bolker B.M., Gardner B., Maunder M., Berg C.W. , Brooks M., Comita L., Crone E., Cubaynes S., Davies T., de Valpine P., Ford J., Gimenez O., Kéry M., Kim E.J., Lennert-Cody C., Magnusson A., Martell S., Nash J., Nielsen A., Regetz J., Skaug H., Zipkin E., 2013. Strategies for fitting nonlinear ecological models in R, AD Model Builder, and BUGS. Methods in Ecology and Evolution 4: 501–512.

Bundy A., 2005. Structure and functioning of the eastern Scotian Shelf ecosystem before and after the collapse of ground fish stocks in the early 1990s. Canadian Journal Of Fisheries And Aquatic Sciences 62:1453-1473.

Diaz E., 2013. Estimation of growth parameters of Jack mackerel Trachurus murphyi caught in Peru from length frequency analysis. Rev. peru. biol. 20(1):061- 066.

Dioses T., 2013. Abundance and distribution patterns of Jack mackerel Trachurus murphyi in Peru. Rev. peru. biol. 20(1):067- 074.

Duboz R., Versmisse D., Travers M., Ramat E., Shin Y.-J., 2010. Application of an evolutionary algorithm to the inverse parameter estimation of an individual-based model. Ecological Modelling 221(5):840-849.

Dueri S., Faugeras B., Maury O., 2012. Modelling the skipjack tuna dynamics in the Indian Ocean with APECOSM-E – Part 2: Parameter estimation and sensitivity analysis. Ecological Modelling 245:55-64.

Echevin V., Goubanova K., Dewitte B., Belmadani A., 2012. Sensitivity of the Humboldt Current system to global warming: a downscaling experiment of the IPSL-CM4 model, Climate Dynamics. doi:10.1007/s00382-011-1085-2.

Fournier D.A., Skaug H.J., Ancheta J., Ianelli J., Magnusson A., Maunder M.N., Nielsen A., Sibert J., 2012. AD Model Builder: using automatic differentiation for statistical inference of highly parameterized complex nonlinear models. Optimization Methods and Software, 27:2, 233-249, DOI: 10.1080/10556788.2011.597854.

Fournier D.A., 2013. An introduction to AD Model Builder for use in Nonlinear Modeling and Statistics. ADMB Foundation, Honolulu. 212pp.

Friska M.G., Miller T.J., Latour R.J., Martell S.J.D., 2011. Assessing biomass gains from marsh restoration in Delaware Bay using Ecopath with Ecosim. Ecological Modelling 222:190–200.

Gaume E., Villeneuve J.-P., Desbordes M., 1998. Uncertainty assessment and analysis of the calibrated parameter values of an urban storm water quality model. Journal of Hydrology 210: 38–50.

Guénette S., Christensen V., Pauly D., 2008. Trophic modelling of the Peruvian upwelling ecosystem: Towards reconciliation of multiple datasets. Progress in Oceanography 79: 326–335.

Gutiérrez M. et al., 2000. Estimados de biomasa hidroacústica de los cuatro principales recursos pelágicos en el mar peruano durante 1983 -2000. Bol. Inst. Mar Perú. Vol. 19, n°1-2, pp. 136-156.

Gutiérrez M., Swartzman G., Bertrand A., Bertrand S., 2007. Anchovy (*Engraulis ringens*) and sardine (*Sardinops sagax*) spatial dynamics and aggregation patterns in the Humboldt Current ecosystem, Peru, from 1983–2003. Fish. Oceanogr. 16:2, 155–168.

IMARPE, 2009. Informe sobre la tercera reunión de expertos en dinámica de evaluación de la merluza peruana. Bol. Inst. Mar. Perú – Callao. Bol. Inst. Mar Perú 24(1-2).

IMARPE, 2010. Informe sobre la quinta reunión de expertos en dinámica de población de la anchoveta peruana. Bol. Inst. Mar. Perú – Callao. Bol. Inst. Mar Perú 23(1-2).

Jones G., 1998. Genetic and evolutionary algorithms. Encyclopedia of Computational Chemistry. John Wiley and Sons.

Jorgensen S.E. and Bendoricchio G., 2001. Fundamentals of Ecological Modelling. Third Edition. Elsevier. 530pp.

Lehuta S., Mahévas S., Petitgas, P., Pelletier D., 2010. Combining sensitivity and uncertainty analysis to evaluate the impact of management measures with ISIS–Fish: marine protected areas for the Bay of Biscay anchovy (Engraulis encrasicolus) fishery. ICES J. Mar. Sci. 67, 1063–1075.

Lehuta S., Petitgas P., Mahévas S., Huret M., Vermard Y., Uriarte A., Record N.R., 2013. Selection and validation of a complex fishery model using an uncertainty hierarchy. Fisheries Research 143:57– 66.

Mackinson S., and Daskalov G., 2007. An ecosystem model of the North Sea for use in research supporting the ecosystem approach to fisheries management: description and parameterisation [online]. (CEFAS, Lowestoft.) Available from www.cefas.co.uk/publications/techrep/tech142.pdf.

Marzloff M., Shin Y.-J., Tam J., Travers M., Bertrand A., 2009. Trophic structure of the Peruvian marine ecosystem in 2000–2006: Insights on the effects of management scenarios for the hake fishery using the IBM trophic model Osmose. Journal of Marine Systems 75: 290-304.

Maunder M.N. and Deriso R.B., 2003. Estimation of recruitment in catch-at-age models. Can. J. Fish. Aquat. Sci.60: 1204–1216.

Megrey B.A., 1989. A Review and Comparison of Age-Structured Stock Assessment Models from Theoretical and Applied Points of View. NWAFC Processed Report 88-21. 124pp.

Megrey B.A., Rose K.A, Klumb R.A, Hay D.E, Werner F.E, Eslinger D.L, Smith S.L., 2007. A bioenergetics-based population dynamics model of Pacific herring (Clupea harengus pallasi) coupled to a lower trophic level nutrient–phytoplankton–zooplankton model: Description, calibration, and sensitivity analysis. Ecological Modelling 202:144–164.

Methot R.D. Jr. and Wetzel C.R., 2013. Stock synthesis: A biological and statistical framework for fish stock assessment and fishery management. Fisheries Research 142: 86–99.

Nash J.C. and Walker-Smith M., 1987. Nonlinear Parameter Estimation: an Integrated System in BASIC. Marcel Dekker, New York. 493pp.

Ñiquen M., Bouchon M., Ulloa D., Medina A., 2013. Analysis of the Jack mackerel Trachurus murphyi fishery in Peru. Rev. peru. biol. 20(1):097-106.

Ñiquen M, Bouchon M., 2004. Impact of El Niño event on pelagic fisheries in Peruvian waters. Deep-Sea Research II 51:563-574.

Oliveros-Ramos R., Guevara-Carrasco R., Simmonds J., Cirske J., Gerlotto F., Peña-Tercero C., Castillo R., Tam J., 2010. Modelo de evaluación integrada del stock norte-centro de la anchoveta peruana Engraulis ringens. BolInst mar Perú 25(1-2):49-55.

Oliveros-Ramos R., Peña-Tercero C., 2011. Modeling and analysis of the recruitment of Peruvian anchovy (Engraulis ringens) between 1961 and 2009. Ciencias Marinas 37(4B):659-674.

Oliveros-Ramos R. and Shin Y.-J. Unpublished results. calibraR: an R package for the calibration of individual based models. (Submitted to Methods in Ecology and Evolution).

Oliveros-Ramos et al. Unpublished results. An end-to-end model ROMS-PISCES-OSMOSE of the northern Humboldt Current Ecosystem. In preparation.

Oliveros-Ramos et al. Unpublished results. Pattern oriented validation of habitat distribution models: application to the potential habitat of main small pelagics in the Humboldt Current Ecosystem. In preparation.

Rose K., 2012. End-to-end models for marine ecosystems: Are we on the precipice of a significant advance or just putting lipstick on a pig? Scientia Marina 76:195-201.

Ruiz D.J, Wolff M., 2011. The Bolivar Channel Ecosystem of the Galapagos Marine Reserve: Energy flow structure and role of keystone groups. Journal of Sea Research 66 (2011) 123–134.

Schnute J.T., 1994. A general framework for developing sequential fisheries models. Can. J. Fish. Aquat. Sci. 51:1676-1688.

Segura M. and Aliaga A., 2013. Acoustic biomass and distribution of Jack mackerel Trachurus murphyi in Peru. Rev. peru. biol. 20(1):087- 096.

Shannon L.J., Moloney C.L., Jarre A., Field J.G., 2003. Trophic flows in the southern Benguela during the 1980s and 1990s. Journal of Marine Systems 39:83 – 116.

Shin Y.-J., Cury P., 2001. Exploring fish community dynamics through size-dependent trophic interactions using a spatialized individual-based model. Aquatic Living Resources, 14(2): 65-80.

Shin Y.-J., Cury P., 2004. Using an individual-based model of fish assemblages to study the response of size spectra to changes in fishing. Canadian Journal of Fisheries and Aquatic Sciences, 61: 414-431.

Shin Y.-J., Rochet M.-J., Jennings S., Field J., Gislason H., 2005. Using size-based indicators to evaluate the ecosystem effects of fishing. ICES Journal of marine Science 62(3): 394-396.

Sonnenborg T.O., Christensen B.S.B., Nyegaard P., Henriksen H.J., Refsgaard C., 2003. Transient modeling of regional groundwater flow using parameter estimates from steady-state automatic calibration. J. Hydrol. (Amsterdam) 273:188–204.

Swartzman G., Bertrand A., Gutiérrez M., Bertrand S., Vasquez L., 2008. The relationship of anchovy and sardine to water masses in the Peruvian Humboldt Current System from 1983 to 2005. Progress in Oceanography 79 (2008) 228–237.

Tam J., Taylor M.H., Blaskovic V., Espinoza P., Ballón M., Díaz E., Wosnitza-Mendo C., Argüelles J., Purca S., Ayón P. et al., 2008. Trophic modeling of the Northern Humboldt Current Ecosystem. Part I: Comparing trophic linkages under La Niña and El Niño conditions. Progress In Oceanography 79(2-4):352-365.

Travers M., Shin, Y.-J., Jennings, S., Machu, E., Huggett, J.A., Field, J.G., Cury, P.M., 2009. Two-way coupling versus one-way forncing of plankton and fish models to predict ecosystem changes in the Benguela. Ecological modelling 220: 3089-3099.

Travers-Trolet M., Y.-J. Shin & J.G. Field., 2013. An end-to-end coupled model ROMS-N2P2Z2D2-OSMOSE of the southern Benguela foodweb: parameterisation, calibration and pattern-oriented validation, African Journal of Marine Science, 36:1, 11-29, DOI:10.2989/1814232X.2014.883326

Walter E. and Pronzato L., 1997. Identification of parametric models from Experimental data. Springer Masson. 413pp.

Whitley R., Taylor D., Macinnis-Ng C., Zeppel M., Yunusa I., O’Grady A., Froend R., Medlyn B. and Eamus D., 2013. Developing an empirical model of canopy waterflux describing the common response of transpiration to solar radiation and VPD across five contrasting woodlands and forests. Hydrol. Process. 27: 1133–1146.

Zuzunaga J., 2013. Conservation and fishery management regulations of Jack mackerel Trachurus murphyi in Peru. Rev. peru. biol. 20(1):107 - 113.

Appendix A. Description of the OSMOSE model for the Northern Humboldt Current Ecosystem.

For the NHCE OSMOSE model, we considered 13 species (Table A.1), 9 being explicitly modeled in OSMOSE (1 macrozooplankton, 1 crustacean, 1 cephalopod and 6 fish species) and 4 plankton groups being represented in the ROMS-PISCES model. Total plankton biomass and average distribution from ROMS-PISCES model during the study period is shown in Figure A.1. Using Generalized Additive Models, we built maps for the spatial distribution of the species explicitly modeled in OSMOSE (Oliveros-Ramos et al. in prep. b). Providing the probability of occurrence of a species given some environmental predictors (temperature, salinity, chlorophyll-a, oxygen and bathymetry), annual maps were produced with seasonal time resolution for all species (4 maps per year) except euphausiids, for which monthly resolution (12 maps per year) was used. The average spatial distributions over the modeled period for each species are shown in Figure A.2.

Table A.1. Species or functional groups considered in the NHCE OSMOSE model. The main representative species of the functional groups are marked with an asterisk.

Group	**Species or functional groups**	**Spanish name**	**Scientific name**	**Model**
Phytoplankton	Nanophytoplankton			ROMS-PISCES
	Diatoms			ROMS-PISCES
Zooplankton	Microzooplankton			ROMS-PISCES
	Mesozooplankton			ROMS-PISCES
	Euphausiids		*Euphausia mucronata**	OSMOSE
Small pelagics	Anchovy	Anchoveta	*Engraulis ringens*	OSMOSE
	Sardine	Sardina	*Sardinops sagax*	OSMOSE
Medium pelagics	Jack Mackerel	Jurel	*Trachurus murphyi*	OSMOSE
	Chub Mackerel	Caballa	*Scomber japonicus*	OSMOSE
Other pelagics	Mesopelagics		*Vinciguerria sp.**	OSMOSE
	Red lobster	Munida	*Pleuroncodes monodon*	OSMOSE
	Jumbo squid	Pota	*Dosidicus gigas*	OSMOSE
Demersal	Peruvian hake	Merluza	*Merluccius gayi peruanus*	OSMOSE

To compare the model biomass with the estimated by scientific surveys, we estimate a catchability coefficient *q* from the average ratio between the distribution area and the area covered by the scientific surveys. This value was close to 1 for five species with a more coastal distribution and a good coverage of the surveys (anchovy, sardine, chub mackerel, munida and hake), while lower than 1 for four species (jack mackerel, mesopelagics, euphausiids and Humboldt squid).

We considered a constant selectivity over the whole model period, but used different models (logistic, normal and lognormal) for each species. A logistic selectivity was used for sardine, chub mackerel and Humboldt squid; a normal selectivity for anchovy and jack mackerel; and a log-normal selectivity for hake. All selectivities were length-based but for hake we used an age-based selectivity.

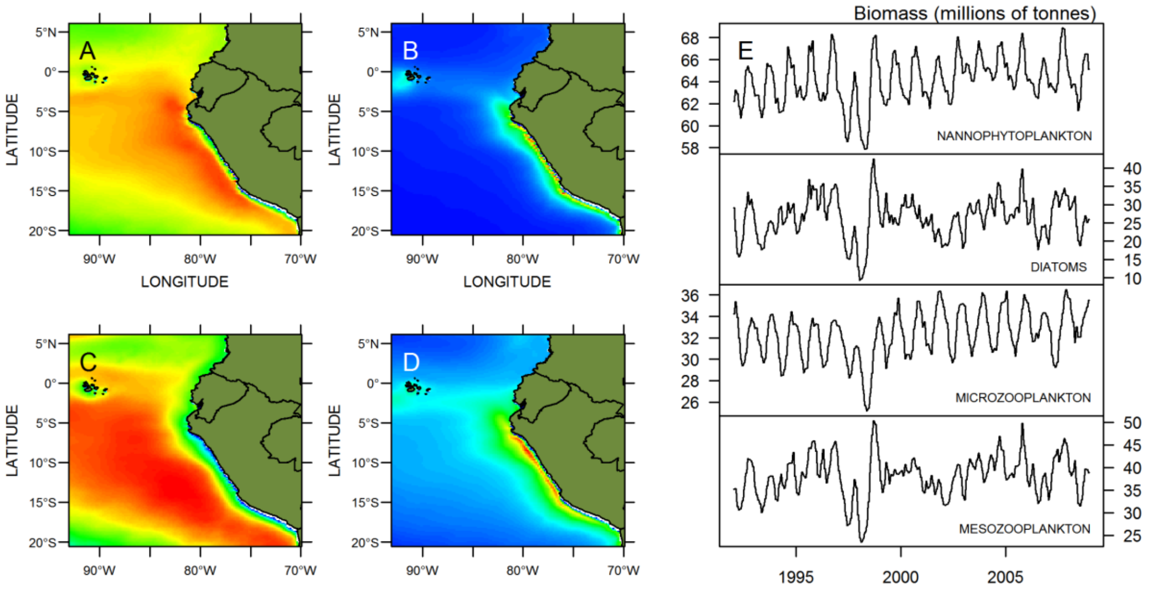

Figure A.1. Summary of the LTL biomass simulated by ROMS-PISCES model and forcing OSMOSE. Average spatial distribution for nanophytoplankton (A), diatoms (B), microzooplankton (C) and mesozooplankton (D) (red is high, blue is low, following the light visible spectrum). Simulated temporal dynamics of the total biomass (millions of tonnes) of the four plankton groups (E) is also shown.

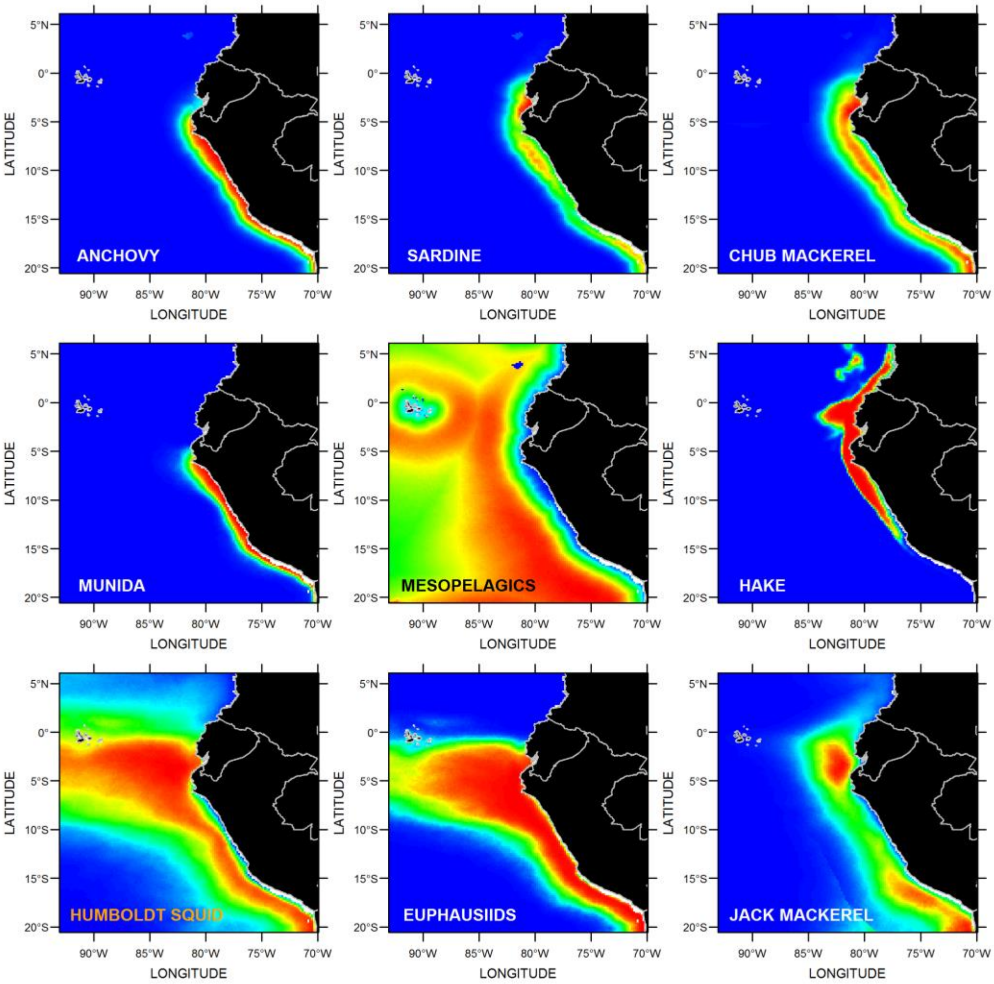

Figure A.2. Average probability distribution maps for OSMOSE species as predicted by generalized additive models (Oliveros-Ramos et al. in prep.). Probability distributions are constructed from the GAM outputs (red is high, blue is low, following the light visible spectrum).

The objective function for the calibration was a penalized negative log-likelihood function. For the likelihoods, we considered three main components: i) the errors in the biomass indices (e.g. acoustic, trawl), ii) the errors in the landings and iii) the errors in the proportions of catch-at-length or catch-at-age. A log-normal distribution was assumed for the biomass indices and landings errors, while for the age and length composition data the likelihood proposed by Maunder and Deriso (2003) was used. We also added penalties to constrain the variability in the time-varying parameters, in order to avoid overfitting. A full description of the components of the objective function is provided in Table A.2.

Table A.2. Components of the objective function.

Likelihood/Penalty component	Equations of the likelihoods	Remarks
Likelihoods		
Biomass Index	$L_1 = \sum_s \lambda_{s,1} \sum_t \log\left(\frac{q_s B_s(t) + 0.01}{\hat{I}_s(t) + 0.01}\right)^2$	$\lambda_{s,1} = 22.2$ for all species s but anchovy $\lambda_{anchovy,1} = 50$
Monthly Landings	$L_2 = \sum_s \lambda_{s,2} \sum_t \log\left(\frac{Y_s(t) + 0.01}{\hat{Y}_s(t) + 0.01}\right)^2$	$\lambda_{s,2} = 200$ for all exploited species s
Catch-at-length	$L_3 = \sum_s T_{s,l} \sum_{y=1}^{T} \sum_l -\ln\left[\exp\left(\frac{-(P_s^l(y) - \hat{P}_s^l(y))^2}{2\sigma_s^2}\right) + 10^{-3}\right]$	$T_{anchovy,l} = 5$ $T_{jack\_mackerel,l} = 10$
Catch-at-age	$L_4 = \sum_s T_{s,a} \sum_{y=1}^{T} \sum_a -\ln\left[\exp\left(\frac{-(P_s^a(y) - \hat{P}_s^a(y))^2}{2\sigma_s^2}\right) + 10^{-3}\right]$	$T_{hake,a} = 10$
Penalties		
Larval mortality annual deviates	$P_1 = \sum_s p_{s,3} \sum_{y=1}^{T} \Lambda_y$	$p_{s,3} = 2$ for all species but $p_{anchovy,3} = 1$, $p_{squid,3} = 8$, $p_{euphausiid,3} = 4$.
Natural mortality monthly deviations from proxy	$P_2 = \sum_s p_{s,4} \sum_{y=1}^{T} m(t)$	$p_{s,4} = 0.5$ for all species
Objective function		
	$L = \sum_{i=1}^{5} L_i + \sum_{i=1}^{2} P_i$	

The optimization problem related to minimizing the negative log-likelihood ***L*** was solved using an evolutionary algorithm developed by Oliveros-Ramos and Shin (submitted), since for stochastic models it is not possible to apply derivative-based methods (e.g. gradient descent or quasi-Newton methods). Evolutionary algorithms (EAs), which are meta-heuristic optimization methods inspired by Darwin's theory of evolution (Jones 1998), have shown their capability to yield good approximate solutions in cases of complicated multimodal, discontinuous, non-differentiable, or even noisy or moving response surfaces of optimization problems (Bäck and Schewefel 1993). They prove to be useful alternatives for the calibration of stochastic and complex non-linear models. In this EA, different parameter combinations are tested as possible solutions to minimize the ***L*** function. At each generation (i.e iteration of the optimization process), the algorithm calculates an "optimal parent" which results from the recombination of the parameter sets which provide the best solution for each objective (e.g. likelihood for biomass, yield, age/length structure). The optimal parent is then used to produce a new set of parameter combinations. To calculate this optimal parent, potential solutions are weighted according to the variability of each parameter across generations, using the coefficient of variation to take into account differences in the order of magnitude between different parameters.

Appendix B. Models used for time varying parameters.

We considered three type of models to represent the variability of time varying parameters (A, B and C-type models).

The A-type models assume continuous changes in the parameter value, with a smooth interannual variability and a periodic seasonality linked to environmental drivers. The B-type models assume discrete changes for the interannual variability (e.g. driven by annual changes in management measures), and with a seasonal pattern potentially very variable between years (Table B.1). These models allow us to define nested models, for example, for A and B type models, by setting to zero the monthly and yearly effects, we reduce the parameterization to A.0 or B.0, respectively.

Finally, the C-type models assume the parameters taken non-zero values only for a shorter period of time, in this case following a Gaussian.

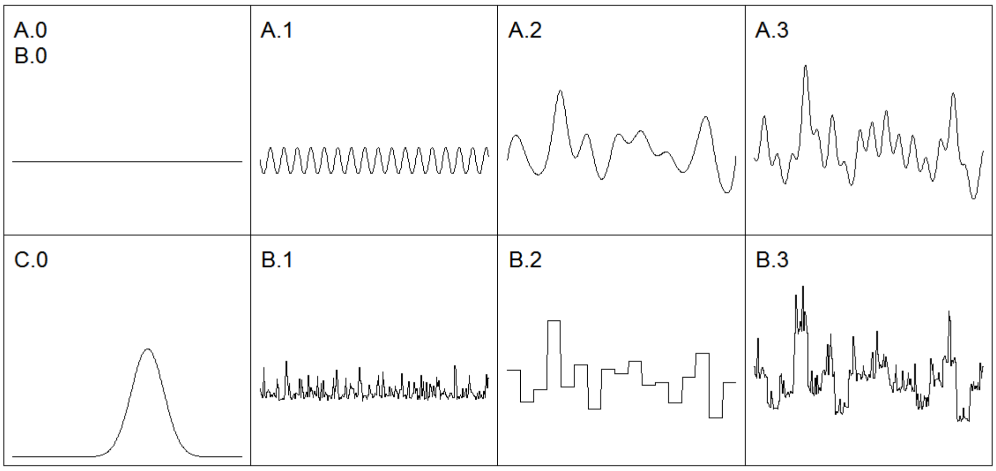

Figure B.1. Examples of the different models used for time-varying parameters.

Table B.1 Different models used for temporal variability in parameters. For each model, X(t) is the value of the parameter at time *t*, $\bar{x}$ is the mean value of the parameter, m(t) and y(t) the month and year, respectively, at time t. The equations and the number of parameters (depending on the number of years of the simulation, T) are shown.

Model	Seasonal	Interannual	Model equation	Parameters	Number of parameters
A. Continuous and smooth interannual changes and periodic seasonality					
A.0	None	None	$\log X(t) = \log \bar{x}$	$\bar{x}$	1
A.1	Periodic	None	$\log X(t) = \log \bar{x} + A \sin 2\pi d(t - a)$	$\bar{x}, A, d, a$	1 + 3
A.2	None	Spline	$\log X(t) = \log \bar{x} + \mathrm{spline}(t \mid x_1, \dots, x_{T+1})$	$\bar{x}, x_1, \dots, x_{T+1}$	1 + (T+1)
A.3	Periodic	Spline	$\log X(t) = \log \bar{x} + \mathrm{spline}(t \mid x_1, \dots, x_{T+1}) + A \sin(2\pi d(t - a))$	$\bar{x}, A, d, a, x_1, \dots, x_{T+1}$	1 + (T+1) + 3
B. Discontinuous interannual changes with aperiodic seasonality					
B.0	None	None	$\log X(t) = \log \bar{x}$	$\bar{x}$	1
B.1	Pattern	None	$\log X(t) = \log \bar{x} + x_{m(t)}$	$\bar{x}, x_{m_1}, \dots, x_{m_{12T}}$	1 + 12T
B.2	None	Deviates	$\log X(t) = \log \bar{x} + x_{y(t)}$	$\bar{x}, x_{y_1}, \dots, x_{y_T}$	1 + T
B.3	Pattern	Deviates	$\log X(t) = \log \bar{x} + x_{y(t)} + x_{m(t)}$	$\bar{x}, x_{y_1}, \dots, x_{y_T}, x_{m_1}, \dots, x_{m_{12T}}$	1 + T + 12T
C. Interannual variability as a short pulse					
C.0	None	Gaussian pulse	$\log X(t) = \log \bar{x} - \frac{(x - t_0)^2}{2\sigma^2} - \log 2\sigma$	$\bar{x}, \sigma, t_0$	3

Concluding remarks and perspectives

Confronting ecosystem models to data

Confronting ecosystem models to data is essential to increase their credibility and to start using them in support to management decision. A successful model calibration implies several computational, theoretical and practical challenges. The `calibrar` R package intends to provide a framework to simplify the calibration of complex models, in particular stochastic ones, for which fewer developments have been done compared to those for deterministic and differentiable models. There is "no free lunch" in optimization, and no optimization algorithm will perform bestfor every type of optimization problems (Wolpert and Macready 1997). In this direction, the next step we envisage is the inclusion of other optimization algorithms in our `calibrar` package so the users are provided with a suite of tools to solve a variety of calibration problems in a transparent way without additional technical complications. In parallel, more tests with other models and real-world calibration problems are required to improve the generality of the package, its flexibility and the robustness of the optimization algorithm.

However, calibration is only one step in the process of rigorous model development and application. One important step we did not prioritize here due to time constraints, is a full sensitivity analysis for the OSMOSE model, which could have greatly helped in the calibration process by providing a rationale to reduce the number of parameters to estimate (Megrey et al. 2007, Dueri et al. 2012, Lehuta et al 2013). Complementary to this first approach and expected to be developed in close future is an uncertainty analysis on the parameters of the E2E model, relying on the calibration phase but also on the analysis of the uncertainties due to the different component models (ROMS-NPZD, OSMOSE, climate niches) and how they can combine together into an assessment of different management scenarios in the HCE. Additionally, a successful calibration does not mean that a model is reliable (Gaume et al. 1998), and a proper validation is always required, eventually providing information to improve the model and to revise the calibration (Walter and Pronzato 1997, Jorgensen and Bendoricchio 2001). In particular, a more detailed validation of our model results including alternative sources of information (e.g. trophic ecology) could help to increase the credibility of the model.

Bridging ecosystem models with single species models

Management strategy evaluation (MSE) is a set of simulation-based procedures to compare alternative management procedures (Butterworth 2007, De Lara and Martinet, 2008). More precisely, MSE consists in defining a set of operational objectives and to evaluate, by means of simulations, the performance of alternative management procedures in relation to the set of objectives defined, and taking into account the uncertainties related to the modeling process (Sainsbury et al. 2000, Butterworth 2007). One of the weakest points in some MSE applications is the use of the same model as the operative model (used to generate artificial data) and the assessment model (used to evaluate the status of the population given the artificial data generated by the assessment model). Even if the operative model is a more complex version of the assessment model, it is likely that the results would be artificially better than if an independent model with a different structure was used to generate the data. Additionally, by doing so, it is implicit that the assumptions of the model are correct, i.e. the reality is driven by the processes included in the operative model, which can lead to important model misspecifications and bias in the MSE because model uncertainty would not have been taken into account. In particular, when using single-species models as operative models, the impact of species interactions and their variability is not taken into account (or at least not directly) which could bias long term projections. In this respect, future MSE in the HCE could rely on a fully calibrated ecosystem model as the operative model while still using the current single-species assessment models for management purposes.

A weakness of some single-species models is to take as constants some parameters which are expected to have a strong variability, like natural mortality, which greatly depends on the changes in the environmental conditions and trophic structure of the ecosystem, as well as the life stage of the individuals. Ecosystem models can provide information about such variability, which can be incorporated as a forcing or additional source of uncertainty in single-species models. By doing so, it would be possible to understand the impact of other sources of variability (e.g. the environment) in single-species models, which normally rely on the (phenomenological) estimation of time series of deviates to incorporate the impact of such sources of variability. On the other hand, keeping multi- and single-species models independent (not using outputs from one as input to the other) allows us to provide insights into the impact of different assumptions and resolution of the model processes and structure, e.g. single-species models being more fishery oriented (e.g selectivity modeling) and ecosystem models being more trophic oriented (e.g. predation modeling).

Applications to EBFM

Despite some attempts to move towards EBFM around the world, most commercial species remain managed using single-species management procedures (MP). Therefore, one interesting application would be to evaluate the impact of neglecting the interspecific interactions in the ecosystem as well as the interactions between single species MPs leading to concrete multispecies management strategies. This can be done by replicating the single-species management procedures using ecosystem models to eventually help to develop more robust MPs in an ecosystem context. Additionally, current single-species reference points (RP) cannot take into account important ecosystem processes, particularly here in the HCE the environmentally-induced changes in the ecosystem structure. Ecosystem models will allow to estimate ecosystem RPs taking into account the complex dynamics of the ecosystems while simultaneously allowing to work in a single-species context. However, by counting with ecosystem-based RPs (like multi-species MSY) and operational ecosystem models, a further step would be to carry out an integrated ecosystem MSE. Since several criteria are used to estimate "optimal" strategies for fisheries management, but most of them rely on single-species models, the solutions under the same criteria can be totally different by considering an ecosystem approach. Furthermore, ecosystem models can be better at forecasting the impacts of the environmental variability in the dynamics of exploited populations. Currently, physical models can provide synthetic scenarios of natural and human-induced environmental variability which can be used for MSE purposes. On the other hand, single-species models normally need to rely on simpler time-series of environmental variability to force the models, while spatial ecosystem models, like OSMOSE, can better exploit the variability given by ocean and biogeochemical models.

OSMOSE modelling platform

The version of OSMOSE implemented in this thesis (OSMOSE 3 release 1, `www.osmose-model.org`) includes several improvements with respect to the versions used in previous published applications (OSMOSE 2), particularly related to the incorporation of interannual variability in the model. The OSMOSE model for the NHCE is also the first interannual application using OSMOSE. However, in all OSMOSE versions, the impact of fishing is simplified as it does not explicitly handle multiple fisheries but just species catches or fishing mortalities. OSMOSE 3 includes more flexible selectivity specifications (in addition to the original knife-edge selectivity), but a more general approach is needed to explore options for real management applications in a multiple fisheries context, e.g. one species being targeted by more than one fisheries (possibly in different areas) and one fishery targeting more than one species (possibly, with different selectivities and catchabilities). This approach will lead fisheries to be modeled similarly to other predator species which can have access to all the other species inside the limits specified by the size-specific predation hypothesis of OSMOSE.

Another improvement to bringing OSMOSE to better represent the NHCE ecosystem dynamics is a finer specification of land-based predators, like mammals and birds. This can be handled in OSMOSE 3 by using a time-varying size-specific natural mortality instead of a constant one as is the case in the current implementation. This approach will need to specify i) a proxy of the natural mortality induced by the land-based predators (e.g. time series of abundance or consumption), ii) the shape of the selectivity of the predator (equivalent to the ratios for the size-dependent predation for other predators), iii) the target preys (equivalent to the accessibility matrix for other predators) and iv) the estimation of the average natural mortality induced by the land-based predators during the calibration process. For example, data is available in the NHCE to apply such approach for seabirds preying upon anchovy. Other possibility for the inclusion of land-based predators is to assimilate their parameterization to that of a ”fishery” in a multi-fisheries implementation as discussed before.

Finally, the interannual implementation of OSMOSE required to model the spatial distribution of fish, which is one of the current forcings in OSMOSE, and to construct interannual maps of fish distributions. However, fish spatial distribution is currently disrupted as discrete maps drive fish spatial dynamics. To reduce the potential disruptive effect, we refined the forcing by using seasonal maps for most of the species (four maps per year), but further details and mechanisms should be included in the movement sub-model in OSMOSE, particularly to smooth the transitions between maps and to not lose the spatial structure created in the model.

HCE modelling

A model cannot be better than the information used to build it. Ecosystem models in particular rely on a great quantity and quality of information in order to be able to properly reproduce the observed dynamics of the ecosystem and identify the parameters of the model. In this sense, gathering the information needed to build an interannual OSMOSE model for the Northern Humboldt Current Ecosystem was by itself a complex task, requiring a lot of pre-processing work in terms of data standardization. To review and standardize the information needed for this application has motivated the launch of an on-going IMARPE project ("Estimation of fishery-biological parameters for the sustainable management of marine resources", funded by RM-350-2013-PRODUCE) that has the objective to improve the IMARPE's database (IMARSIS) and to digitalize and concentrate all the sources of information pertinent for modeling purposes. Also, improvements in the standardization of abundance indices are needed, as the main source of information on the variability of the exploited populations. Currently, two master theses are under way at IMARPE to address i) a review of the fishery-independent abundance indices for Jack mackerel and ii) the development of empirical echo-abundance indices when length data from surveys is not appropriate to estimate biomass from acoustic data, mainly for less common non-commercial species.

In terms of the spatial distribution modelling, the current implementation of OSMOSE-NHCE uses the same distribution for all the schools of the same species, independently of the age or size. As data exist for different stages of anchovy (larvae, juveniles, recruits and adults), another master thesis is in progress to refine the spatial distribution models. Also, munida (squad lobster) requires more detailed modeling of its spatial distribution since the larger individuals start to develop demersal habits in comparison to the smaller ones which are pelagics off Peru. Finally, a more detailed pattern oriented validation is needed for all modelled species to ensure that the maps produced fulfill the requirements for our modeling objectives.

References

De Lara M. and Doyen L. 2008. Sustainable Management of Natural Resources. Mathematical Models and Methods. Springer-Verlag, Berlin, 2008.

Dueri S., Faugeras B., Maury O.,2012. Modelling the skipjack tuna dynamics in the Indian Ocean with APECOSM-E – Part 2: Parameter estimation and sensitivity analysis. Ecological Modelling 245:55-64.

Gaume E., Villeneuve J.-P., Desbordes M., 1998. Uncertainty assessment and analysis of the calibrated parameter values of an urban storm water quality model. Journal of Hydrology 210: 38–50.

Lehuta S., Petitgas P., Mahévas S., Huret M., Vermard Y., Uriarte A., Record N.R.,2013. Selection and validation of a complex fishery model using an uncertainty hierarchy. Fisheries Research 143:57– 66.

Jorgensen S.E. and Bendoricchio G., 2001. Fundamentals of Ecological Modelling. Third Edition. Elsevier. 530pp.

Megrey B.A., Rose K.A, Klumb R.A, Hay D.E, Werner F.E, Eslinger D.L, Smith S.L., 2007. A bioenergetics-based population dynamics model of Pacific herring (Clupeaharenguspallasi) coupled to a lower trophic level nutrient-–phytoplankton—zooplankton model: Description, calibration, and sensitivity analysis. Ecological Modelling 202:144–164.

Sainsbury K. J., Punt A. E. and Smith A. D. M. 2000. Design of operational management strategies for achieving fishery ecosystem ob¬jectives. ICES Journal of Marine Science, 57: 731-741.

Walter E. and Pronzato L., 1997. Identification of parametric models from Experimental data. Springer Masson. 413pp.

Wolpert, D.H. and Macready, W.G. (1997) No Free Lunch Theorems for Optimization. IEEE Transactions on Evolutionary Computation, 1(1):67-82.