A stepwise Fitting Procedure for automated fitting of Ecopath with Ecosim models
Scott, Erin; Serpetti, Natalia; Steenbeek, Jeroen; Heymans, Johanna

Published in:
SoftwareX
Publication date:
2016
Publisher rights:
© 2016 The Authors. Published by Elsevier B.V.
The re-use license for this item is:
CC BY
The Document Version you have downloaded here is:
Publisher's PDF, also known as Version of record

The final published version is available direct from the publisher website at:
10.1016/j.softx.2016.02.002

Link to author version on UHI Research Database

Citation for published version (APA):

General rights
Copyright and moral rights for the publications made accessible in the UHI Research Database are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights:
1) Users may download and print one copy of any publication from the UHI Research Database for the purpose of private study or research.
2) You may not further distribute the material or use it for any profit-making activity or commercial gain
3) You may freely distribute the URL identifying the publication in the UHI Research Database

Take down policy
If you believe that this document breaches copyright please contact us at RO@uhi.ac.uk providing details; we will remove access to the work immediately and investigate your claim.

Download date: 25. Jan. 2020
A Stepwise Fitting Procedure for automated fitting of Ecopath with Ecosim models

Erin Scott\textsuperscript{a,∗}, Natalia Serpetti\textsuperscript{a}, Jeroen Steenbeek\textsuperscript{b}, Johanna Jacomina Heymans\textsuperscript{a}

\textsuperscript{a}Scottish Association for Marine Science, Oban, Argyll, PA37 1QA, UK
\textsuperscript{b}Ecopath International Initiative Research Association, Barcelona, Spain

Received 17 September 2015; received in revised form 10 December 2015; accepted 10 February 2016

Abstract

The Stepwise Fitting Procedure automates testing of alternative hypotheses used for fitting Ecopath with Ecosim (EwE) models to observation reference data (Mackinson et al. 2009). The calibration of EwE model predictions to observed data is important to evaluate any model that will be used for ecosystem based management. Thus far, the model fitting procedure in EwE has been carried out manually: a repetitive task involving setting >1000 specific individual searches to find the statistically ‘best fit’ model. The novel fitting procedure automates the manual procedure therefore producing accurate results and lets the modeller concentrate on investigating the ‘best fit’ model for ecological accuracy.

Copyright © 2016 Published by Elsevier B.V.

Keywords: Stepwise model fitting procedure; Ecopath with Ecosim; Ecological modelling; Model fitting

1. Motivation and significance

Ecopath with Ecosim (EwE) is an ecological modelling software suite that is freely accessible with over 6000 registered users from 164 countries [1,2]. It is used to build models of marine and freshwater as well as terrestrial ecosystems. Ecopath describes energy flows through a trophic web of functional groups. Ecosim provides a time-dynamic simulation of the ecosystem, with key initial parameters inherited from the base Ecopath model [1].

The calibration of Ecopath models by fitting model predictions to time series reference data (observations) is important, as it evaluates the assumptions made when parameterising the Ecopath model [3]. The model fitting procedure tests a
Table 1
The eight alternative hypotheses and changing factors parameterised and compared by the Stepwise Fitting Procedure. ☑ and ✗ indicate if a factor is included and not included respectively.

<table>
<thead>
<tr>
<th>Hypothesis</th>
<th>Fishing data</th>
<th>Trophic effects (Vulnerabilities)</th>
<th>PP anomaly</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baseline</td>
<td>✗</td>
<td>☑</td>
<td>✗</td>
</tr>
<tr>
<td>Baseline and trophic effects</td>
<td>✗</td>
<td>☑</td>
<td>✗</td>
</tr>
<tr>
<td>Baseline and PP anomaly</td>
<td>☑</td>
<td>✗</td>
<td>☑</td>
</tr>
<tr>
<td>Baseline, trophic effects and PP anomaly</td>
<td>✗</td>
<td>☑</td>
<td>☑</td>
</tr>
<tr>
<td>Fishing</td>
<td>☑</td>
<td>✗</td>
<td>☑</td>
</tr>
<tr>
<td>Fishing and trophic effects</td>
<td>☑</td>
<td>✗</td>
<td>☑</td>
</tr>
<tr>
<td>Fishing and PP anomaly</td>
<td>☑</td>
<td>✗</td>
<td>☑</td>
</tr>
<tr>
<td>Fishing, trophic effects and PP anomaly</td>
<td>☑</td>
<td>✗</td>
<td>☑</td>
</tr>
</tbody>
</table>

2. Software description

The novel Stepwise Fitting Procedure presented here automates the Ecosim model fitting procedure described in [3] and used by [4,5]. As [3] states it is convention and good practice to explore different search strategies for parameterisations that best explain the observation data to find the best-fit model. The automated procedure focuses on the impact of fishing, changes in the predator–prey dynamics (predation vulnerability settings), changes in primary production (PP), and all of the above [3]. A high level view of the stepwise fitting procedure is shown in Fig. 1. Eight alternative hypotheses are parameterised and compared. A more detailed description of the eight types of hypotheses can be found in [5] and are outlined for convenience in Table 1 which presents the factors which are included in each hypothesis.

The fitting procedure determines all the alternative hypotheses that may describe the observation data in equal measure and finds the ‘best-fit’ model. The alternative hypotheses are calculated by the fitting procedure from the maximum number of parameters that can be estimated \((m - 1)\) [6]. The maximum number of estimated parameters \(m\) is calculated by the procedure from the total number of loaded time series of type: relative biomass, total mortality, catch and average weight [6]. Here we assume that all the time series data are independent but that each data point in the time series are not independent from the other data points in that series. The hypotheses are listed as fitting iterations in the user interface of the stand-alone version (Fig. 2).

The fitting procedure calculates the total number of iterations for each hypothesis by calculating all combinations of number of parameters estimated \((K)\) based on \(m\) and/or the maximum number of spline points. For example, if \(m = 3\) then for the hypothesis “Baseline and trophic effects” the procedure would calculate 3 iterations where the value of \(K\) will be 1, 2 and 3 in each of the iterations. All forcing data including absolute biomass, forced biomass, time forcing data, effort data by gear type, fishing mortality, forced total mortality and forced catch time series are disabled in baseline iterations [6]. There is the option to include and enable absolute biomass time series to the calculation of \(m\) and to include these time series in baseline iterations. If a forcing function is applied to the PP in the model, anomaly and vulnerability plus anomaly iteration searches will be calculated and shown in the iteration list of the fitting procedure user interface. The spline point step size can...
The fitting procedure was created to automate and assist in finding a ‘best-fit’ model. The ‘best-fit’ model is found and determined by the minimum difference between model predictions to time series observations using the weighted sum of squared differences (SS) and the Akaike Information Criterion (AIC) [7], which penalises for fitting too many parameters based on the number of time series available for estimating...
the SS. The formula used for the AIC is defined as:

\[
AIC = n \cdot \log (\text{minSS}/n) + 2K
\]

where \( n \) is calculated by the fitting procedure as the total number of observations, or time series values, from the loaded times series of type: relative biomass, total mortality, catch and average weight. minSS is the minimum sum of squares calculated by the algorithm, and \( K \) is the number of parameters estimated. In addition the procedure also calculates the AICc [8], to address small sample size. The AICc is defined as:

\[
AICc = AIC + 2K \cdot (K - 1) / (n - K - 1)
\]

The fitting procedure calculates these values for each iteration and identifies the best-fit by the iteration which has the lowest AICc value.

The number of possible vulnerabilities that can be estimated are often significantly more than that of the data available to constrain the model, thus it is imperative to test the vulnerabilities that affect the most detectable change [3]. Before each iteration search is started a sensitivity search of sum of squares (SS) to the vulnerability parameters is carried out to find which of the vulnerability parameters creates the largest change on the SS, and therefore the most sensitive vulnerability parameters are used in the iteration search. The fitting procedure interface gives the choice to search by predator or predator/prey for all iterations, as is also the case in the search interface within EwE [1].

A variety of output results for further analysis can be chosen from the fitting procedure user interface: these are: no results, Ecosim results (similar to all the output results obtained from a usual Ecosim run), aggregated results (a smaller sub group of Ecosim results which include biomass, yield, mortality, vulnerabilities and anomaly shape) and both Ecosim and aggregated. Once all iteration searches are completed a csv file of the runs and fitting results is produced. Ecosim results are stored in separately named iteration folders. Aggregated results are stored in one folder and the file names identify the providence of the results. Anomaly shape results for all iteration searches are also stored in one csv file when Ecosim or aggregated result output is selected.

The fitting procedure can be used in three ways: command line, stand-alone and as an integrated plug-in within the EwE software suite. Iteration searches in the stand-alone version are faster than that of the integrated version. The stand-alone version has a user interface (Fig. 2) and has all the functionality of the integrated plug-in. The integrated plug-in will be available in the next release of the EwE software suite due for release in February 2016.

3. Example of the automated model fitting procedure

3.1. Iteration numbers and run times

The West Coast of Scotland model [5] is used as an example to demonstrate the fitting procedure. As stated previously there are 48 time series of catch or biomass, and therefore the fitting procedure calculates that a maximum of 47 parameters can be estimated. These parameters can be either vulnerabilities or PP spline points (up to the number of years in the time series). Thus 2–23 spline points (as there are 23 years in the time series, and one cannot have less than 2 spline points) or 47 vulnerabilities and a combination of these are possible. The fitting procedure calculates the number of observations \( n \) in the AIC formula in the time series as 1063 and that there is in total 1658 iteration searches. There is 829 iteration runs for both Baseline and Fishing. The time taken for the fitting procedure to complete all iteration runs was approximately 3.5 days. The number of different search iterations and the time taken for the fitting procedure to complete each are shown in Table 2.

3.2. Results

The fitting procedure user interface highlights the best fit model (the iteration with the lowest AICc value) which in this case includes fishing and 39 vulnerabilities and 7 PP anomaly spline points as shown in Fig. 2. Fig. 3 presents the AICc result output for all iteration searches. This shows a comparison between the baseline and fishing iterations. Baseline (without fishing) iterations have higher AICc values than fishing iterations which indicates that fishing is the main driver in this ecosystem. Although the fitting procedure can produce various output results, in the case of the West Coast of Scotland model, aggregated result output was selected. The fitting procedure can assist in the analysis of results by providing output that can be easily converted into different visualisations.

4. Impact

This fitting procedure will aid in the analysis of a variety of EwE models implemented by the high number of worldwide EwE registered users and encourage new users to the EwE software. The fitting procedure automates the Ecosim model fitting procedure described by calculating all alternative hypotheses and suggests the ‘best-fit’ model. This procedure is useful for exploratory analysis. It allows for broad exploration of the parameter space and can be useful if the drivers of the system are not clearly elucidated. This procedure will help identify key drivers in the system. The quality of the results obtained by this procedure is dependent on the quality and quantity of data used in the fitting and best practice in the parameterisation of the initial Ecopath with Ecosim modelling [3,8].

The choice in ‘best-fit’ model is still subjective as it only reflects the statistical fit, therefore the user should take care in selecting the best model on the basis of its fit to data, supporting ecological knowledge and reasoned justification [3]. There are other parameters within an Ecosim model that could also be estimated to find the ‘best-fit’ model such as the diet matrix [9] which the fitting procedure does not deal with and the user should also consider. In addition, this procedure does not address the issue of confirmatory analysis. Here the user assumes that the data is perfect and observation error is not resolved. For truly confirmatory analyses, suitable for management advice to policy makers, a limited number a priori candidate hypotheses should be tested (i.e. only a limited number of parameters estimated) and compared to see which hypothesis explains the data.
Table 2
The number of iterations and time taken to complete for each of the 8 alternative hypotheses of the West Coast of Scotland model. The stand-alone version of the fitting procedure was run on a PC running Windows 7 with an i7 core and 8 GB RAM.

<table>
<thead>
<tr>
<th>Hypothesis</th>
<th>No. of iterations</th>
<th>Time (min)</th>
<th>No. of parameters estimated</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baseline</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>Baseline and trophic effects (vulnerabilities)</td>
<td>47</td>
<td>82</td>
<td>1–47</td>
</tr>
<tr>
<td>Baseline and PP anomaly</td>
<td>22</td>
<td>9</td>
<td>2–23</td>
</tr>
<tr>
<td>Baseline and trophic effects (vulnerabilities) and PP anomaly</td>
<td>759</td>
<td>2333</td>
<td>4</td>
</tr>
<tr>
<td>Fishing</td>
<td>1</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>Fishing and trophic effects (vulnerabilities)</td>
<td>47</td>
<td>139</td>
<td>1–47</td>
</tr>
<tr>
<td>Fishing and PP anomaly</td>
<td>22</td>
<td>31</td>
<td>2–23</td>
</tr>
<tr>
<td>Fishing, trophic effects (vulnerabilities) and PP anomaly</td>
<td>759</td>
<td>2672</td>
<td>4</td>
</tr>
</tbody>
</table>

A combination of vulnerabilities and spline points up to the maximum number of estimated parameters (47).

5. Future work

This procedure uses a specific formulation of the AIC which is based on the work done by [3] and it balances model fit against overparameterisation. However, it is probably more suited to univariate analysis as it penalises the incorporation of too many time series or too long a time series, while in manual fitting more and longer time series data help constrain the model. Thus in future it would be useful to incorporate the likelihood formulation of the AIC as used by [10] or other multivariate model formulations. In addition the specific estimation of K in this program is based on the number of time series included, not the number of data points, as we assume that a time series is autocorrelated. This might be an assumption too far, and in future the value of K could be decided by the user, and not calculated by the procedure.

In addition, in EwE it is possible to weight the time series used for fitting based on its quality [11] and these weightings could be included in future programs, or these could be varied to undertake an ensemble approach to fitting EwE models.

6. Conclusion

The Stepwise Fitting Procedure automates testing of alternative hypotheses used for fitting EwE models to observation data [3]. The fitting procedure allows users to easily explore a range of possible ecological mechanisms that may contribute to ecosystem changes. It will assist in the integration of empirical investigations and help confront data issues [3]. The main benefit the fitting procedure provides is reducing the occurrences of human error and aids in finding the ‘best-fit’ model. This allows the user to concentrate on the ecological reasoning behind the model parameters and the justification of the ‘best fit’ model rather than on the model fitting procedure itself.

Uncited references

[12].

Acknowledgements

Erin Scott was funded by the Scottish Informatics and Computer Science Alliance (SICSA) Postgraduate Industry Internship Programme. Johanna J Heymans and Natalia Serpetti were supported by the Natural Environment Research Council and Department for Environment, Food and Rural Affairs under the project MERP: grant number NE/L003279/1, Marine Ecosystems Research Programme.

References


