Automated parameter optimization for Ecopath ecosystem models

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Abstract
Ecopath is a mass-balance modeling approach that is widely used for incorporating ecosystem considerations into fisheries science. Up to now, users of Ecopath software who are constructing a model of a given area must carefully adjust input biomass, diets, and other parameters until the Ecopath parameterization is mass-balanced, a slow process leading to non-unique solutions. We present a new computer-automated iterative technique for mass-balancing Ecopath models which has the advantages of (1) reducing the lengthy process of and opportunity for encoding errors of the manual approach; (2) standardizing results for the same set of starting conditions; and (3) allowing exploration of alternative solutions, with consideration of the estimated confidence of each input parameter. Users can select random and/or gradient descent model perturbation of biomass and/or diet parameters, specify an objective (cost) function for optimization of the search, and modify decision logic, including simulated annealing. An objective function is defined to help target mass-balance solutions with minimum change to original input parameters. A Monte Carlo mode allows exploration of sensitivity to different starting conditions and random perturbations. The new procedure is implemented in the current version of the freely available Ecopath with Ecosim software (http://www.ecopath.org).

Keywords: Ecopath; Mass-balance; Ecosystem model; Simulated annealing; Search; Optimization

1. Introduction
Based on an approach originally proposed by Polovina (1984), and further developed by Christensen and Pauly (1992a), the Ecopath approach relies on straightforward mass-balance constraints to define trophic fluxes between functional groups. This, and the existence of detailed manuals documenting the use of successive versions (Polovina and Ow, 1983; Christensen and Pauly, 1992b; Christensen et al., 2000; Christensen and Walters, 2004) have enabled the approach and its supporting software to find a wide dissemination as evidenced by close to two hundred published applications (see http://www.ecopath.org).

The recent addition of routines for simulating biomass change over time (Walters et al., 1997; Walters et al., 2000) and space (Walters et al., 1999) has increased the demand for reliable parameterization of food webs constructed by Ecopath, an issue addressed through a quasi-Bayesian re-sampling technique (Christensen and Walters, 2004), and coded ‘pedigrees,’ quantifying the uncertainty associated with Ecopath input (Pauly et al., 2000).

Here, we address an issue concerning the parameterization of Ecopath models, by providing an algorithm as an alternative to the informative, but
subjective procedure so far involved in meeting the mass-balance requirements inherent in Ecopath. The new algorithm has been incorporated in the current version of the Ecopath with Ecosim software, freely available from http://www.ecopath.org.

In its simplest form, the master equation of Ecopath defines the mass-balance between consumption, production, and net system exports over a given time period for each functional group ($i$) in an ecosystem:

$$B_i \left( \frac{P_i}{B_i} \right) EE_i = Y_i + \sum_j B_j \left( \frac{Q_{ji}}{B_j} \right) DC_{ji}$$

(1)

where $B_i$ and $B_j$ are biomasses (the latter pertaining to $j$, the consumers of $i$); $P/B$ is the production/biomass ratio, equivalent to total mortality under most circumstances (Allen, 1971; Mertz and Myers, 1998); EE is ecotrophic efficiency which is the fraction of production ($P = B_i P_i/B_i$) that is consumed within, or caught from the system (by definition between 0 and 1); $Y_i$ is equal to the fisheries catch (i.e. $Y = FB$); $Q_{ij}$ is the food consumption per unit biomass of $j$; and $DC_{ji}$ is the contribution of $i$ to the diet of $j$, and the sum is over all predators ($j$). For simplicity, we have here excluded terms from the right hand side of Eq. (1) for biomass accumulation and migration in and out of the system.

Given appropriate input data, solving this system of linear equations is straightforward (Mackay, 1981). Once a solution is found, a quantified network of flows can be constructed from the biomass, production and consumption ($Q = B (Q/B)$) estimates, which can then be used to parameterize Ecosim and Ecospace models.

The problem, however, is that the estimates of biomass, $P/B$, $Q/B$, and DC diet composition data available for any given system usually do not lead to estimates of EE constrained between 0 and 1, as required for mass-balance. Rather, some EE values will be estimated as exceeding unity, implying that predation and/or fisheries catches from the groups in question exceed biological production.

Balancing a model then consists of identifying such groups, and changing input values to Eq. (1) until the resulting EE satisfies $0 \leq EE \leq 1$. In practice, this is usually achieved by modifying the diet composition of the ‘maximum predator’ of the most ‘unbalanced’ group (i.e. the predator having the greatest impact on the group with the highest EE), then solving Eq. (1) again, and identifying the next most unbalanced group, etc. until $EE \leq 1$ for all groups. The assumption here is that the fraction that a given group represents, on the average, in the diet of another one, is usually known with far less certainty than its biomass, which can be estimated directly for most groups, using various field methods. Best known, at least in principle, are the $P/B$ or $Q/B$ ratios, which are conservative, and largely predictable properties of animal species (Pauly, 1980; Palomares and Pauly, 1998).

This manual balancing procedure for Ecopath models, though so far, widely applied, has two several drawbacks:

- it is hard to teach and to learn, and some users never get the ‘hang’ of it; rather, they sometimes modify reliable inputs in their attempts to accommodate unreliable ones;
- it calls for knowledge and discipline to decide which changes to make and to keep track of the changes;
- the solutions reached are non-unique, and may not be reproducible.

A new automated parameter search procedure described below addresses these problems. We stress though that the ‘manual’ balancing provides very important feedback to modelers, and that it should not be abandoned because of the option provided with the new ‘automatic’ routine. Gross errors due notably to unit conversion errors (which are very common as part of model construction), will not necessarily be picked-up by the automatic routine. Also, the manual mass-balance procedure can provide a structured approach to examine the data and ecological relationships of a model, and make modelers reflect on the model definitions in a way that the automatic approach may well miss-out on. Why then have an automated approach at all? Notably, because it provides a well-structured way of getting from defined input data to a balanced model with clear-cut assumptions: given these data and assumptions, this is a physically possible mass-balance model with restricted changes to user input parameters, and how it is obtained is reproducible. The automatic mass-balance also facilitates database-driven model construction, a topic two of the authors are developing at present.
2. Methodology

Fig. 1 illustrates the software-controlled auto-balancing algorithm. An initial Ecopath model is iteratively adjusted, via perturbations to the diet, DC, and biomass, B, terms, until a model with EE $\leq 1$ for all species groups is obtained. At each iteration step, the ‘success’ of model adjustment is monitored by progress in reducing EE’s while keeping as low as possible the value of a cost function summarizing the amount of change from the original model. The cost function is linked to the manner in which uncertainty is accounted for in Ecopath models.

2.1. Input parameter uncertainty and cost function design

Ecopath is designed such as to allow explicit consideration of the uncertainty associated with input parameters. Specifically, users can either specify...
distributions (range, shape) around each input (\(B, P/B\), and \(Q/B\) ratios, DC, etc.), or accept default distributions associated with 'pedigrees' expressed in qualitative terms. The probability distribution assumed for the confidence interval can be selected (typically Uniform or Gaussian).

The auto-balancing routine presented below relies on these confidence intervals to constrain the extent of parameter perturbations away from the original values. Thus, parameter adjustments are larger for poorly known parameters (wide confidence interval), and conversely well-known parameters (narrow confidence interval) are allowed less adjustment.

An optimization search is generally guided by a cost function (or objective function), related to some measure of quality. We are looking for a model that achieves \(EE_i \leq 1\) for all groups \((i)\) but without excessive changes to the DC, and \(B\) input parameters, particularly those with narrow confidence interval (i.e. those that have been estimated more reliably). In this initial version of the auto-mass balance routine we allow only DC and \(B\) to be varied as these parameters are generally the most uncertain. However, we do intend to include other parameters in later versions of the routine.

At each iteration step, the model is perturbed by adjusting the biomass and diet components affecting groups with \(EE > 1\) (Fig. 1). Model perturbation, and identification of lower \(EE\) values may be performed in three different ways:

(1) Random lookup within confidence interval (no memory of current state).

(2) Random steps in the neighborhood of the current state.

(3) Gradient descent method.

Method (1) is similar to the Ecoranger routine of Ecopath (Christensen and Walters, 2004), except that we perturb only the parameters affecting groups with \(EE > 1\) at each step, while Ecoranger changes all parameters at once. At each iteration step, the new model has no relation to the previous model step, except that other groups which do not consume the groups with \(EE > 1\) are left untouched. This method is essentially an exhaustive random search of a pre-defined parameter space at each step. The search space may be too large to obtain low cost balanced models in an acceptable amount of computer time.

With method (2), parameters can be perturbed by a random amount in a small neighborhood surrounding the current parameter values. The decision logic can then choose to accept or reject the model at each step, depending on whether the objective function is moving in the desired direction. This method should have a faster convergence than method (1) but can get stuck at local minima or fail to converge, if the decision logic never accepts parameter perturbations causing worse values of the cost function.

Method (3) uses the 1st derivative of \(EE\) with respect to the parameter to be perturbed (DC or \(Q/B\)) to decide the direction and magnitude of perturbation so as to move the model toward lower EE. This method will generally offer the fastest convergence to a mass-balance solution, but again, the solution may get stuck at a local minimum which may not be the lowest cost solution.

The auto-balancing routine allows methods (2) and (3) to be combined, i.e. the fast convergence behavior of gradient descent is combined with random neighborhood perturbations, to allow solutions other than the gradient descent local optimum.

The convergence behavior can be explored, and local minima avoided, by:

- repeating iteration runs with randomly selected starting states (see below);
• varying perturbation step sizes;
• changing relative step size of random versus gradient descent perturbations;
• limiting perturbations to stay within the confidence intervals of the parameters (which may prevent convergence);
• changing the decision logic to accept some parameter steps which may make the objective function worse, at least temporarily (see Section 2.3).

2.2.1. Gradient descent algorithm for calculating parameter changes

The primary objective of $E_i \leq 1$ for all groups $(i)$ can, e.g. by be achieved through a directed gradient search procedure—the classic 'hill-climbing' technique (Gershenfeld, 1999). For our application, we choose a simple 'local' gradient search where parameters affecting each group with $E_i > 1$ are iteratively adjusted in small steps in a direction determined by the negative gradient (first derivative) of the $E_i$ equation with respect to each adjusted parameter, so as to reduce $E_i$.

For our purposes, the Ecopath master Eq. (1) can be rearranged so that $E_i$ is on the left side of the equation,

$$E_i = \sum \frac{B_j(Q/B)_jDCF_{ji} + y}{B_i(P/B)_i}$$  \tag{3}

Restricting parameter changes to biomass and diet terms, we solve below for the appropriate gradient steps $\delta B_j$ and $\delta DC_{ji}$ to subtract from the current values at each iteration step. Taking the partial derivative of $E_i$ with respect to biomass $B_j$ we obtain:

$$\delta E_i = \frac{\partial E_i}{\partial B_j} = \left( \frac{(Q/B)_jDCF_{ji} - E_i(P/B)_i}{B_j(P/B)_j} \right)$$  \tag{4}

for group $j = i$

$$\delta E_i = \frac{\partial E_i}{\partial DC_{ji}} = \left( \frac{E_i(P/B)_i - (Q/B)_jDCF_{ji}}{B_j(Q/B)_j} \right)$$  \tag{5}

for predator groups $j \neq i$

Solving for $\delta B_j$ and switching from $\delta$ indicating infinitesimally small differential steps to $\Delta$ indicating discrete steps $\Delta$,

$$\Delta B_j = \left( \frac{(Q/B)_jDCF_{ji} - E_i(P/B)_i}{(Q/B)_jDCF_{ji}} \right)$$  \tag{6}

for case $j = i$

$$\Delta B_j = \left( \frac{E_i(P/B)_i - (Q/B)_jDCF_{ji}}{(Q/B)_jDCF_{ji}} \right)$$  \tag{7}

for predators $j \neq i$

Typically the 'self-predation' term $DCF_{ii}$ (e.g. adult fish eating juveniles of their own species for cases which are not split in ontogenic groups) is small, so $\Delta B_i$ is negative and $E_i$ reduces with increasing biomass $B_i$. For the case of predators $j \neq i$, $E_i$ can be reduced by reducing the predator group $(j)$ biomass $B_j$ so that predator $(j)$ consumes less of group $(i)$.

Similarly, taking the partial derivative of $E_i$ with respect to diet $DC_{ji}$ we obtain:

$$\delta E_i = \frac{\partial E_i}{\partial DC_{ji}} = \left( \frac{B_j(Q/B)_j}{B_i(P/B)_i} \right)$$  \tag{8}

for all living groups $j$

Therefore, a decrease in $E_i$ by amount $\Delta E_i$ is accomplished by decreasing predator $(j)$ diet $DC_{ji}$ by:

$$\Delta DC_{ji} = \frac{\Delta E_i}{B_j(Q/B)_j}$$  \tag{9}

The above formulation is appropriate for living groups $(i)$ and $(j)$. Detritus groups have different flow equations (see Kavanagh, 2002, for the gradient step derivation for detritus groups used in the present approach). We have noticed that balancing detritus groups can conflict with efforts to balance living groups, which illustrates the connected nature of ecological networks helps constraint the possible parameter space.

2.2.2. Step size

The size of the adjustment steps should be small enough not to miss optimal solutions, yet large enough that the search is not unduly time-consuming. The gradient descent adjustment terms above are calculated based on the excess $E_i$. $\Delta E_i = E_i - 1$. The steps are

$$\Delta B_j = \left( \frac{(Q/B)_jDCF_{ji} - E_i(P/B)_i}{(Q/B)_jDCF_{ji}} \right)$$  \tag{10}

for predators $j \neq i$.
limited to a maximum step size specified by the user as some percentage of the original parameter value. As \( \Delta \text{EE} \) declines, the steps become finer, so as not to overstep the solution. The step size for random neighborhood perturbations is set by specifying a standard deviation of the additive zero mean Gaussian random noise (expressed as a percentage of the original parameter value).

2.2.3. Diet redistribution and renormalization

If the diet for predator \((j)\) of prey group \((i)\) is perturbed by \(\Delta \text{DC}_{ji}\), the other non-zero prey of predator \((j)\) are adjusted by an amount,

\[
-\frac{\Delta \text{DC}_{ji}}{\sum \text{DC}_{ji}} \sum \text{DC}_{ji} \tag{8}
\]

so that the diet sum is maintained. That is, the diet perturbation is redistributed in proportion to the original diet component size (which may cause the EE of other groups to increase).

2.2.4. Order of parameter adjustment

Because changes designed to reduce the EE of a group may increase that of others, convergence to a system with EE \(\leq 1\) for all groups will not necessarily be achieved by changing the parameters for one group at a time. Indeed, the routine may enter into an oscillatory loop from which it cannot escape. Countermasures implemented in the approach are,

- perturb \(\Delta \text{DC}_{ji}\) and \(B_j\) and for all predators \((j)\) of group \((i)\);
- perturb \(\Delta \text{DC}_{ji}\) and \(B_j\) only for the predator with the maximum impact on \((i)\);
- perturb \(\Delta \text{DC}_{ji}\) and \(B_j\) impacting all groups \((i)\) with EE’s exceeding unity;
- perturb \(\Delta \text{DC}_{ji}\) and \(B_j\) impacting only the highest EE group.

Typically, convergence is more rapid for the first and third of these strategies. Another strategy is to constrain predator biomass changes to groups with EE \(\leq 1\), so as to prevent further increases to EE for those groups.

2.3. Decision logic

At each iteration step, the auto-balancing algorithm chooses whether to accept or reject the change, depending on the progress in EE reduction and the parameter change cost function.

The simplest decision logic is to accept all steps of an iteration, regardless of the outcome, and to keep it going until the final objective (all EE \(\leq 1\)) is reached. This may be adequate for the local gradient descent directed method, but may not converge if the needs of each group conflict with each other. With random perturbations, this method can take a long time to converge depending on the size of the perturbations.

Another decision strategy is to accept only steps that lower the EE of the group for which the gradient steps are calculated. This method is not guaranteed to converge, as it focuses on locally optimal steps, ignoring a possible better solution obtained by locally higher cost but globally lower cost (better economy may be achieved in the long run by selecting higher cost steps).

To avoid local minima, we can instead accept only steps that lower a global objective equal to the sum of excess EE’s. Again, convergence is not guaranteed, as the adjustments for different groups may conflict. Adding random noise perturbations can sometimes help.

In the above, we are ignoring the parameter change cost in the search. The decision logic can be modified so that the conflicting goals of both minimizing the excess EE sum and the parameter change are considered in the decision. Alternatively, one can constrain the parameter adjustments to specified uncertainty limits and then proceed with reducing the EE excess only.

2.3.1. Step reversal

If a step is rejected, the parameter values backtrack to the value before the step. A variation to the decision logic is to reverse the parameter step sign to see if a better outcome is obtained.

2.3.2. Adaptation (gear-shifting)

Iterative optimization algorithms can be improved (or perhaps needlessly complicated) by using the objective function progress (or lack thereof) as a criterion for adapting the perturbation step size and the decision logic.

For the auto-balancing routine presented here, any such adaptation is ‘manual’: the user can run successive iteration runs starting with the end values of the previous iteration run. The parameters for each run can be adjusted to try to improve the final cost
2.3.3. Simulated annealing

Simulated Annealing is a technique where some higher cost steps are accepted with some probability, which can be varied throughout the iteration, either in a pre-defined or data adaptive method (Dowsland, 1993; Press et al., 1994; Gershenfeld, 1999). Given cost function $J_n$ at iteration $(n)$ then the decision logic is to accept the step if $\Delta J < 0$ (lower cost) where $\Delta J = J_n - J_{n-1}$. If $\Delta J > 0$ (higher cost) then the step is accepted with probability $P = e^{-\Delta J/T_n}$, where $T_n$ is a user-defined 'annealing temperature'. The higher the probability, the higher the chance of accepting a worse cost iteration step, but this may be what is needed to avoid local minima.

When beginning a search, the system is allowed high probabilities of accepting a larger portion of steps with higher cost. Later, as the final objective is approached, the system is made to accept only lower probabilities. We have implemented only a very simple linear annealing schedule where the 'temperature' $T_n$ is changed linearly between a start and finish temperature over the iteration period. The probability for accepting step $(n)$ is calculated as $P_n = e^{-\Delta J/T_n}$, so the higher temperature $T_n$ the greater the chance of accepting a higher cost step $\Delta J$. It is usually best to start with a high temperature ($P_n$ high) and end, hopefully near convergence, with a low temperature ($P_n$ low).

3. Application and discussion

Fig. 2 illustrates a typical iteration history for the auto-balancing of an Ecopath model for the Newfoundland-Labrador shelf (Bundy et al., 2000). The default gradient descent method was used, with
steps limited to 10% of the original B and DC parameter values and steps accepted which reduce the total sum of EE excess. The balanced model is quite different from the model defined by the raw inputs: biomass values changed up to 100% and diet fractions by up to 41% of their original values.

The order of parameter adjustment, noise perturbation, limits to confidence intervals, and decision logic were modified, to see if it was possible to balance the model with less change from the original parameter settings. In most cases, the gradient descent method achieved the fastest convergence compared to random perturbations, and the smallest differences between original and final values of the DC and B.

Simulated annealing often does not improve on the gradient descent solution. Moreover, constraining the gradient descent parameter adjustments to some percentage of the confidence intervals was better at finding lower cost solutions than were repeated random runs. The fully random parameter selection (not in the neighborhood of last step) was found to have least chance of converging to a solution with all $EE \leq 1$.

We find that balancing can be difficult to achieve for some models, probably because the needs of each group conflict with others. In these cases adding random noise and using simulated annealing can assist in the balancing and lead to improved results.

We intend to follow up on this research, notably by allowing parameters other than the diet compositions and the biomasses to be adjusted, by offering various additional constraints to acceptable solutions (e.g. $0.1 < P/Q < 0.3$, respiration $> 0$, or even Ecosim runs with pre-defined features), and by incorporating fuzzy logic instead of formal confidence intervals to describe the uncertainty inherent in certain data sets, notably the diet composition in FishBase (Froese and Pauly, 2000), a major data source of parameterization of Ecopath models. We also invite researchers working with EwE to participate in the further development of the approach presented here, as well as for EwE in general.

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