

Sequential boundary eigenvalue destabilisation (SeBEDes): an expert method for parameter screening and estimation in complex ecosystem models.

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Abstract

We present a new method to find parameter sets that allow all populations to co-exist in multi-trophic level food web models in which the outcome of competition between populations at each trophic level is determined by R^* theory. The method involves sequentially destabilising an eigenvalue at the boundary equilibrium point of the winning population at each trophic level. We illustrate the procedure on a six population, three trophic level ecosystem model of a pelagic Antarctic ecosystem.

We used the method to find an initial parameter set for which all populations coexisted. Only three model evaluations were required to find a parameter set that allowed coexistence. In contrast, a random search of parameter space required an average of 250 model evaluations to find each coexistence parameter set. The method is useful for identifying regions of parameter space that have high densities of coexistence solutions.

Introduction

The estimation of parameters for ecological models remains a significant challenge (Lignell et al., 2013). In some disciplines model inter-comparison projects have been usual to “smooth out” differences in model predictions and to improve correlations of model predictions with observed data (for example, Bopp et al., 2013; Hashioka et al., 2013; Sailley et al., 2013; Vancoppenolle et al., 2013). However, the dimensionality of even moderate complexity ecological models, and uncertainty due to a paucity of information to guide choices of process formulations and parameter values, results in solution spaces that cannot be searched in any meaningful way by “naïve” algorithms (Cropp and Norbury, 2013). Here by “naïve” searches we mean random sampling of the functional form / parameter spaces for model solutions that look like the real world. It is well known among ecological modellers that parameter sets that allow coexistence of all model populations are rare in parameter space, but that given sufficient parameters, any model can produce any solution. Hence substantial amounts of computer time are expended to tune parameter sets to produce “real world” solutions that may be produced by parameter sets that bear no relation to “real world” parameter values.

The distribution of “real world” solutions in the parameter spaces of moderate to high complexity ecosystem models is a problem to which the computing demands of randomly

searching high-dimensional parameter spaces preclude an answer. Further, there is evidence that multiple regions of ecological verisimilitude exist in such spaces. For example, Franks (2009) observed that even in very simple NPZ models, that were “well-cited” and consequently we may assume to be well regarded by the plankton modelling community, fundamental, common parameters such as half-saturation constants varied by over two orders of magnitude. This suggests that within parameter spaces that are renowned for their overall paucity of “real world” solutions there may be multiple regions that provide model solutions that reflect the dynamics of real world systems, but that do not reflect the properties of real world systems.

There are many sophisticated algorithms and approaches available to search parameter spaces for real world solutions, ranging from Markov Chain Monte Carlo (MCMC) (for example, Lignell et al., 2013) through smoothed ensemble Kalman filters (SEnKF) (for example, Chen et al., 2008) to iterative, nonlinear regressions (for example, Necpalova et al., 2015). Generally, these methods do not fully exploit some of the fundamental properties of ecological models, in particular, the fact that the dynamics of living populations are described in most ecosystem models by ordinary differential equations that have Kolmogorov form (Kolmogorov, 1936). This property allows analytical expressions for the boundary eigenvalues (BEVs) of the populations to be obtained with little effort (Cropp and Norbury, 2012), where we define a BEV as the eigenvalue associated with a population at any boundary equilibrium point (BEP) where that population is zero. A BEP is any ecologically realistic boundary equilibrium point of a model (i.e. an equilibrium that lies on the boundary of the space that contains all valid solutions to the model (Cropp and Norbury, 2015)). BEPs have one or more populations equal to zero.

The BEVs are particularly important in determining the winner of competition within a trophic level, where competitive exclusion (Gause, 1932; Gause, 1934) often occurs and R^* theory (Tilman, 2007) can often decide the outcome. R^* theory simply says that the winner of any competition for a resource will be the population that leaves the least resource(s) for its competitor(s). Complex computer simulation models of ecosystems, such as those plankton systems commonly referred to as Dynamic Green Ocean Models (DGOMs, for example Le Quéré et al., 2005) currently being developed for climate prediction, usually explicitly represent the resources available to every population, facilitating the use of R^* theory to predict their behaviours. Further, these models typically represent their populations by differential

equations of Kolmogorov form, and hence their BEVs are analytically known. The analytic expressions for the BEVs are comprised of parameters that express key attributes of the population that is zero at the BEP, such as growth and mortality rates, and the steady state values of the other extant populations. The steady state values of the other populations are determined by their parameter values, and the parameter values of the populations that interact with them.

The attributes of BEVs make them ideal candidates for the application of Sequential Boundary Eigenvalue Destabilisation (SeBEDes). The sequential nature of the method, considering BEPs and BEVs sequentially from the lowest trophic level to the highest, is important in constraining the parameters that need to be considered at each step. The sequential approach also ensures that only lower trophic level populations are involved in each step, and their parameter values have been previously determined. The method may be used to identify regions of parameter space that contain ecologically sensible solutions. Once identified, the properties of the models in each region may be assessed and ecologically reasonable regions searched with the usual algorithms for solutions that correlate with the real world.

We demonstrate the utility of the SeBEDes approach by deriving a parameter set for a “sufficiently” complex model of a Southern Ocean ecosystem. This model is of a form first considered qualitatively by May et al. (1979) in the context of managing multispecies fisheries that is particularly useful for this demonstration as it has three trophic levels within each of which two populations compete for resources. The increasing exploitation of marine Antarctic living resources makes understanding these fragile systems an imperative. However, the constraints placed on developing complex models of Southern Ocean ecosystems are many, with a paucity of data on parameter values being one of a number of knowledge gaps identified (Murphy et al., 2012).

The Southern Ocean is one of the world’s major marine systems, supporting iconic species and ecosystems, influencing climate and in many ways isolating Antarctica from the rest of the world. Southern Ocean living resources have long been exploited, with sealing and whaling active since the late 18th century. The need for management of these resources has often focussed on the key role of krill, which is a key prey species for many Southern Ocean predators (Boyd, 2002; Ichii and Kato, 1991; Lockyer, 1981). Some of the early work on the

consequences of harvesting living resources expounds the need for ecosystem approaches to understand the impacts of Southern Ocean fisheries on krill populations (May et al., 1979). Since the early work of May et al, over 40 models of the impact of harvesting of krill populations on Southern Ocean ecosystems have been published (Hill et al., 2006). The paucity of measurements parameter values or data to validate/calibrate models of Southern Ocean ecosystems remains a significant impediment to the development of mechanistic models of these systems (Murphy et al., 2012). While it is important that our models are assessed in “reasonable” regions of parameter space, the SOE model is used as an example to demonstrate the efficacy of the SeBEDes method rather than as an example of an actual Southern Ocean ecosystem.

We present SeBEDes as an “expert” methodology rather than an algorithm, as in the examples we provide, it requires an “expert operator” to implement the method and make decisions at each step that guide the method towards a particular desired solution. We take this approach in order that we may demonstrate two different outcomes. However, it is possible, and perhaps even desirable, to define rules for these decisions so that the method may be implemented as an algorithm and consistently produce specific outcomes. We demonstrate the SeBEDes approach by finding a parameter set for a six-population, three trophic level model that has competition at each trophic level. The method is applicable to models of any complexity, but is perhaps of most use for those complex models that have solution spaces that cannot be computationally explored in human time scales. As ecosystem modellers are well aware, this includes most ecosystem models, even of quite low complexity. After demonstrating the method of implementation of the SeBEDes method, we show that it can identify regions of increased “desirable solution” density in the solution space that may then be searched for “real world” solutions. We also show that it is possible to derive parameter sets with different dynamical properties (for example high versus low resilience) by making subtly different choices of parameter values at each step.

The Southern Ocean Ecosystem (SOE) model structure

The food web that we examine has an interesting structure for theoretical studies in that it is comprised of three trophic levels with a competing pair of populations in each trophic level. At the base of the food web two autotrophs, ice algae (*A*) and phytoplankton (*P*) compete for the

inorganic nutrient (N). The phytoplankton can grow all year round, subject to the availability of light, but the ice algae are constrained to grow only in winter when sea ice is present, but irradiance is low.

In the second trophic level in the model, the herbivorous populations of salps (S) and krill (K) compete for phytoplankton resource, but the krill have the advantage of a secondary food source of ice algae. This is particularly important for juvenile krill that settle on the underside of the sea ice and graze the ice algae over winter. The third trophic level is composed of the carnivores, fish (F) and whales (W). The whales graze only on krill, but the fish consume both krill and salps. The whales may represent resident populations or, in the forced version of the model, populations that feed seasonally. The W population may be considered surrogates for all populations that seasonally feed in Antarctica in summer, such as baleen (Humpback, Blue and Minke) whales and migratory seabirds, and the F population as all resident populations such as fish, penguins and seals that feed on krill year-round.

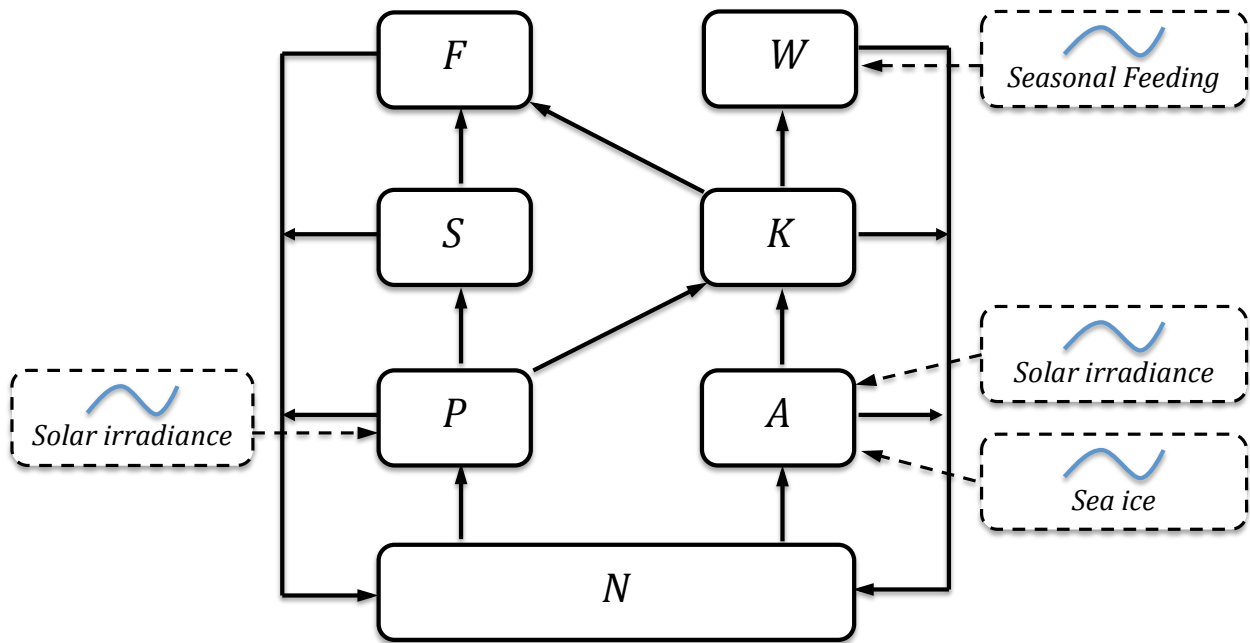


Figure 1. Food web structure for the SOE model. Each solid box represents the size of a living population (A , P , K , S , F or W) or nonliving nutrient (N), all measured in terms of the fraction of total limiting nutrient that they contain. The solid arrows show flows of mass of nutrient due to photosynthesis, grazing, mortality or microbial remineralisation. The latter is implicit in the model, but shown by solid arrows from the

other populations to the N compartment. The dashed boxes represent environmental forcings and the dashed arrows indicate which populations are affected by each forcing.

Figure 1 summarises the trophic structure of the SOE food web. We note that this model has a similar structure to the model proposed as a ‘canonical’ Southern Ocean ecosystem food web by May et al. (1979) and consistent with the recent developments in Southern Ocean ecosystem modelling articulated in Murphy et al. (2012). The key attributes of the model are that all populations, including nonliving (mostly inorganic) nutrient, are measured in a common currency of the key limiting nutrient (usually nitrogen in the ocean) and are expressed as the fraction of the total nutrient they contain. Recycling of nutrient is revealed by the arrows returning nutrient to the nutrient pool, N , with implicit microbial remineralisation.

The SOE model may be forced with environmental changes. Seasonal changes in solar irradiance and sea ice are used to modify the growth parameters of the ice algae and phytoplankton. Similarly the seasonal feeding behaviour is used to modify whale predation on krill. The latter forcing is unusual in models of trophic systems, as environmental forcings are usually applied to autotrophs; behaviourally forced ecosystem models have rarely been considered. Further effects, such as human harvesting of krill, fish and whales may be considered in addition to the environmental forcings on the lower-level populations. For simplicity and clarity of exposition of the method we do not consider the environmental forcings, seasonal feeding or human harvesting when demonstrating the application of the SeBEDes method to the model, but such forcings may be included in practical applications.

The SOE model without external forcings is composed of the following equations that describe the endogenous dynamics of the six populations:

$$\frac{dA}{dt} = A \left(\frac{\mu_A N}{N + \kappa_A} - \frac{\varphi_{AK} K}{A + P + \kappa_K} - \sigma_A \right), \quad (1)$$

$$\frac{dP}{dt} = P \left(\frac{\mu_P N}{N + \kappa_P} - \frac{\varphi_{PK} K}{A + P + \kappa_K} - \frac{\varphi_{PS} S}{P + \kappa_S} - \sigma_P \right), \quad (2)$$

$$\frac{dK}{dt} = K \left(\frac{\varphi_{AK} (1 - \psi_{AK}) A + \varphi_{PK} (1 - \psi_{PK}) P}{A + P + \kappa_K} - \frac{\varphi_{KF} F}{K + S + \kappa_F} - \frac{\varphi_{KW} W}{K + \kappa_W} - \sigma_K \right), \quad (3)$$

$$\frac{dS}{dt} = S \left(\frac{\varphi_{PS}(1-\psi_{PS})P}{P+\kappa_S} - \frac{\varphi_{SF}F}{K+S+\kappa_F} - \sigma_S \right), \quad (4)$$

$$\frac{dF}{dt} = F \left(\frac{\varphi_{KF}(1-\psi_{KF})K + \varphi_{SF}(1-\psi_{SF})S}{K+S+\kappa_F} - \sigma_F - \varepsilon_F F \right), \quad (5)$$

$$\frac{dW}{dt} = W \left(\frac{\varphi_{KW}(1-\psi_{KW})K}{K+\kappa_W} - \sigma_W - \varepsilon_W W \right). \quad (6)$$

Each equation represents the basic processes of growth via consumption of resources, whether inorganic nutrient or another population, mortality due to grazing or predation by other populations, mortality due to natural causes, and in the case of the highest trophic level, mortality due to predation by higher trophic level populations not explicitly represented in the model (Steele and Henderson, 1981). The first term in equations (1) and (2) represent the nutrient limited growth rates of the phytoplankton populations ice algae (A) and pelagic phytoplankton (P) and use standard Michaelis-Menten kinetics (Michaelis and Menten, 1913). The predation terms are all of the Holling Type II grazing form and where a predator has more than one prey we use the generalist multi-prey form that assumes that predators do not selectively graze, but consume whatever prey they encounter (Koen-Alonso, 2007). All populations are subject to density-independent mortality but the populations in the top trophic level also are subject to density-dependent mortality, which represents predation by higher trophic levels (Steele and Henderson, 1992).

The parameters in the SOE model are defined in Table 1, and note that ε_W and ε_F represent mortality due to higher predation by populations that are not explicitly represented in the model. Such terms can stabilise the model dynamics and may be used as perturbation parameters to investigate the influence of a quadratic closure term on the model dynamics.

Table 1. Parameter definitions for the SOE model.

Parameter	Role
μ_A	Maximum growth rate of Ice Algae
κ_A	Ice Algae half-saturation coefficient for nutrient uptake
σ_A	Ice Algae mortality rate
μ_P	Maximum growth rate of Phytoplankton
κ_P	Phytoplankton half-saturation coefficient for nutrient uptake
σ_P	Phytoplankton mortality rate

ϕ_{AK}	Rate of Krill grazing on Ice Algae
ψ_{AK}	Fraction of Ice Algae grazed by Krill that is lost due to sloppy feeding, respiration and excretion
ϕ_{PK}	Rate of Krill grazing on Phytoplankton
ψ_{PK}	Fraction of Phytoplankton grazed by Krill that is lost due to sloppy feeding, respiration and excretion
κ_K	Half-saturation coefficient for Krill grazing on Ice Algae and Phytoplankton
σ_K	Krill mortality rate
ϕ_{PS}	Rate of Salps grazing on Phytoplankton
ψ_{PS}	Fraction of Phytoplankton grazed by Salps that is lost due to sloppy feeding, respiration and excretion
κ_S	Half-saturation coefficient for Salps grazing on Phytoplankton
σ_S	Salps mortality rate
ϕ_{KF}	Rate of Fish grazing on Krill
ψ_{KF}	Fraction of Krill grazed by Fish that is lost due to sloppy feeding, respiration and excretion
ϕ_{SF}	Rate of Fish grazing on Salps
ψ_{SF}	Fraction of Salps grazed by Fish that is lost due to sloppy feeding, respiration and excretion
κ_F	Half-saturation coefficient for Fish grazing on Krill and Salps
σ_F	Fish mortality rate
ϕ_{KW}	Rate of Whales grazing on Krill
ψ_{KW}	Fraction of Krill grazed by Whales that is lost due to sloppy feeding, respiration and excretion
κ_W	Half-saturation coefficient for Whales grazing on Krill
σ_W	Whales mortality rate
ε_F	Fish closure coefficient
ε_W	Whale closure coefficient

Note also that the food web structure, together with local mass balance of net fluxes of the nutrient pool leads to the following equation for the quantity of nonliving nutrient N :

$$\frac{dN}{dt} = -\frac{dA}{dt} - \frac{dP}{dt} - \frac{dK}{dt} - \frac{dS}{dt} - \frac{dF}{dt} - \frac{dW}{dt} \Leftrightarrow N + A + P + K + S + F + W = 1. \quad (7)$$

This suggests that the food web is isolated with respect to its key, limiting nutrient. This reflects that in a system in which the limiting nutrient is very efficiently recycled (as is generally the case in pelagic marine ecosystems) it is reasonable to consider the system as closed to inputs and outputs and consider the total mass of the limiting nutrient N_T to be a finite constant. Note that we have scaled the populations in the system by the total mass of

cycling, limiting nutrient so that the size of each population is expressed in terms of the fraction of the total limiting nutrient that it contains.

Equilibrium points of the SOE model

The Kolmogorov form of the SOE model ($\dot{x}_i = x_i f_i(x_1, x_2, \dots, x_n)$) means that the model has $2^6 = 64$ sets of equations that define the equilibrium points of the system. For ease of discussion we shall refer to each of these sets of equations as describing ‘an equilibrium point’ but bear in mind that the solution to any set of equations may define more than one point in

the ecospace $E = \left\{ 0 \leq x_i < 1; \quad 0 \leq \sum_{i=1}^n x_i < 1 \right\}$.

Number of equilibrium points

We describe the possible equilibrium points as 0 or 1 according to whether the populations $[APKSF\bar{W}]$ are zero ($x_i = 0$) or not ($f_i = 0$) where $x_{1-6} = A, P, K, S, F, W$. The possible equilibrium points range from the origin (000000) where all populations are extinct to the internal point (111111) where all populations coexist. The 63 potential points where one or more populations are zero are referred to as boundary equilibrium points (BEPs). Of the 64 potential equilibrium points the food web structure (Figure 1) allows us to identify the following cases:

- Sixteen points of the form 00xxxx collapse to the origin point 000000;
- Four points of the form xx0011 are not possible (i.e. no K or $S \Rightarrow$ no F or W), of which one is already captured under 00xxxx above;
- Four points of the form xx0001 are not possible (i.e. no K or $S \Rightarrow$ no W), of which one is already captured under 00xxxx above;
- Four points of the form xx0010 are not possible (i.e. no K or $S \Rightarrow$ no F), of which one is already captured under 00xxxx above;
- Sixteen points of the form x0x1xx are not possible (i.e. no $P \Rightarrow$ no S), of which eight are captured under 00xxxx above;
- Sixteen points of the form xx0xx1 are not possible (i.e. no $K \Rightarrow$ no W), of which four are already captured under 00xxxx above, a further four are captured under xx0011 above, another four are captured under xx0001, and a further two are captured under x0x1xx. This leaves just an additional two points excluded under this rule.

Thirty-five potential equilibrium points can therefore be excluded from consideration. This leaves 29 potential equilibrium points that may need to be considered when applying the SeBEDes method (Table 2).

Table 2. Feasible equilibrium points for each trophic level of the SOE model. The order is $[APKSFW]$. Recall that a 1 indicates the population is nonzero at the equilibrium point, and a 0 indicates that the population is extinct at that point.

Trophic Level	Equilibrium Points			Total
Level zero:	000000			1
Level one:	010000	100000	110000	3
Level two:	101000	011000	010100	7
	011100	111000	110100	
	111100			
	101001	101010	011001	
Level three:	011001	011010	011011	18
	010110	011101	011110	
	101011	111001	111010	
	011111	110110	111011	
	111101	111110	111111	

The SeBEDes method may consider any of the BEPs in Table 1 as it progresses up the trophic levels. It initially destabilises the origin (000000), then one of the three Level One BEPs, then one of the seven Level Two BEPS, and then one of the 17 Level Three BEPs. Finally, it manipulates the closure terms to bring the system to the interior coexistence point (111111).

Parameter estimation using SeBEDes

Parameter estimation for complex ecological models presents a significant computational problem, especially for models to be applied in remote parts of the world such as the Southern Ocean where there is little data available to calibrate models against. This is a particular problem for models with competing populations due to the apparent paucity of parameter sets that allow coexistence of competitors in models. For example, Cropp and Norbury (2010) noted that randomly sampling one million parameter sets from a parameter space constrained

by measured parameter values did not find any parameter sets that allowed coexistence of competing populations in a simple model with two zooplankton populations that grazed on a single phytoplankton population.

A common approach to find parameter sets for complex models is to randomly choose a parameter set from a parameter space, use the parameter set to integrate the model for a predefined time, and then evaluate the final state of the system to determine if it has the desired attributes. This often involves comparing the model predictions to observed data, but may include determining if the solution has desired properties such as stable coexistence of all populations. The random sampling of parameter spaces presents a challenging computational problem and even relatively simple ecosystem models can have parameter spaces that cannot feasibly be explored (Cropp and Norbury, 2013), and many schemes have been proposed to improve the convergence of parameter searches to optimal, or even acceptable, solutions.

Bates et al. (2015) demonstrated a new method of parameter estimation for complex ecosystem models called Boundary Eigenvalue Nudging – Genetic Algorithm (BENGA). Bates et al. (2015) used the method to estimate the parameter values of an Antarctic ecosystem model with 21 populations ranging from plankton to whales with much less computational effort than is normally expended on parameterising such models. The BENGA method utilises the boundary eigenvalues of a model (that is, the eigenvalues associated with populations that are zero at an equilibrium point, i.e. on the boundaries of the model's ecospace (Cropp and Norbury, 2015)) to 'nudge' the parameter values towards a solution where all populations coexist. (Analytic expressions for the boundary eigenvalues are simply obtained for equations of Kolmogorov form (Kolmogorov, 1936) that are commonly used to describe population dynamics in ecosystems.) The BENGA method randomly chooses a parameter set and uses it to compute a model solution. It then examines that solution and chooses parameter values to change the signs of the boundary eigenvalues associated with the populations with zero abundance.

The Sequential Boundary Eigenvalue Destabilisation (SeBEDes) method also uses boundary eigenvalues to improve the efficiency of searches for model parameters. Rather than randomly sampling the parameter space as the BENGA method does, the SeBEDes method approaches the system from the 'bottom up' to find a parameter set that allows coexistence of all

competitors at plausible population levels. The method is straightforward and the algorithm may be implemented by hand (using a computer to numerically integrate the system) using the ‘expert knowledge’ of the operator to choose appropriate parameter values at each step. We demonstrate that approach here, but note that the expert decisions may be made *a priori* and included in the algorithm.

Theoretical basis

The SeBEDes method relies on two cornerstones of ecological theory: the Principle of Competitive Exclusion (Gause, 1934) and R^* theory (Tilman, 2007). These rubrics arose from *in vitro* experiments with simple ecosystems but have also been observed *in silico*. Gause’s principle states that when multiple populations at the same trophic level compete for a single resource all but one of the populations will go extinct. This principle has much experimental support *in vitro* and is commonly observed *in silico*, but its inability to predict outcomes in the real world led to the Paradox of the Plankton (Hutchinson, 1961). Tilman’s R^* theory says the winner of a competition for a resource will be the population that leaves the least resource for its competitors. The effect of competitive exclusion and R^* theory at any trophic level in an ecosystem model is evident in the existence of stable boundary equilibrium points (BEPs, defined by the equilibrium value of one or more populations being zero). A stable BEP for any trophic level represents the equilibrium population of the winner of the competition for the resource, and destabilises the BEPs of all other populations at that trophic level. The SeBEDes method works by sequentially destabilising the BEPs of the winning populations, starting from the lowest trophic level and moving up the food web, using the predators at the each higher trophic level to destabilise the trophic level below. The stable BEP at the highest trophic level is then destabilised by using quadratic mortality terms to tilt the zero isosurfaces, as these populations do not have higher predators. Note that top trophic level populations have parallel zero isosurfaces if they only have linear mortality terms.

Every population that is described by an equation of Kolmogorov form (Kolmogorov, 1936) $\dot{x}_i = x_i f_i(x_1, x_2, \dots, x_n)$ has a number of BEPs, depending on the number of populations in the model, where its population x_i^* is zero. The eigenvalues associated with each BEP of a population (its ‘boundary eigenvalues’, BEVs) are given by $\lambda_i = f_i \Big|_{x_i^*=0}$. Parameters that appear

in the BEVs of populations that feed on the non-zero population(s) of a stable BEP of a trophic level, (i.e. populations at the next trophic level) may be used to destabilise the BEP. For example, at the origin of the ecospace of any ecosystem model the eigenvalues of all non-autotroph populations are negative. If any population in the model is to exist, at least one BEV of at least one autotroph must be positive. Destabilisation of the origin (the ‘nutrient trophic level’) is therefore achieved by manipulating the eigenvalues of the next trophic level, the autotrophs.

The mechanism of R^* theory ensures that the winning population at any trophic level (i.e. the population with a stable BEP) destabilises the BEPs of all its competitors. This means that, in general, the SeBEDes method needs to consider only one BEP at each trophic level. Competitive Exclusion and R^* theories are predicated on the use of density-independent mortality for competing populations, which precludes coexistence of competing populations as the zero isosurfaces for such populations are functions of their resources only (i.e. their zero isosurfaces are parallel). Introducing predation by a higher trophic level, an *in silico* implementation of the “kill-the-winner” hypothesis (Thingstad and Lignell, 1997), allows the competitors to coexist. The SeBEDes method sequentially considers the BEPs for each trophic level after setting all the populations in higher trophic level to zero, which removes all predators from consideration. This imposes R^* theory outcomes on that level (assuming only linear mortalities are used for populations other than those of the highest trophic level). This principle allows us to start by destabilising the origin of the ecospace, and identifying the winning population at the next trophic level. We then choose parameter values for the populations that predate on the winning population so that its BEV destabilises the winner’s BEP, and so on up the trophic levels until we consider the competing populations at the highest trophic level.

The top trophic level populations have no explicit predators represented in the model, and hence no populations that can be used to destabilise their boundary equilibrium points. However, the quadratic mortality (closure) terms are commonly used to ‘close’ these systems (Steele and Henderson, 1992) and make these ‘invisible’ higher trophic level predators ‘visible’ in the model. It is this higher predation that allows the top trophic level populations to coexist (Freedman and Waltman, 1984). Manipulating the quadratic mortality terms of the top trophic level does not affect the stabilities of the BEPs that have previously been destabilised by the winner of competition in the top trophic level. The quadratic mortality terms cannot directly

modify the BEVs of top trophic level populations, as they are zero when the population is zero. Instead of moving the zero isosurface of a predator population to destabilise a BEP, as is done for lower trophic levels, in the highest trophic level we use the quadratic mortality parameters to tilt the winner's isosurface and move its stable BEP until it crosses the loser's zero isosurface, destabilising the winner's previously stable BEP.

The use of quadratic mortality coefficients to destabilise the top trophic level BEPs is therefore not as straight-forward as the procedure for the lower trophic levels. The relationship between the winner's BEP and the loser's zero isosurface determines when the quadratic mortality coefficient has been increased sufficiently. For very simple systems we can calculate the location of the BEP that we must destabilise and the relevant edge of the zero isosurface and choose quadratic mortality coefficients that result in the desired arrangement. For more complex systems, we may need to proceed by trial and error until the coefficients are sufficiently large. The interior equilibrium point we create using this approach is an attractor (i.e. it may be a stable point or an unstable point with a stable limit cycle or chaotic attractor around it).

Note that purely quadratic mortality for all top trophic level populations (i.e. all linear mortality coefficients are zero) will automatically ensure the existence of a stable internal equilibrium point, as it causes all the zero isosurfaces to intersect the origin, and hence intersect each other. Further, it is not necessary to impose quadratic mortality on all top level populations to ensure coexistence, however, it may be desirable to do so to reflect higher predation for all top level populations and have a 'more realistic' model.

Finally, we note that heuristics may be implemented in the SeBEDes method to find parameter sets that imbue the models with specific properties. For example, modelling scenarios that require the ecosystem model to respond strongly to changes in environmental forcings such as temperature need highly resilient models (DeAngelis, 1980). Measuring the resilience of complex ecosystems models is difficult and sometimes impossible, as many systems do not have stable interior equilibrium points. Therefore it is sometimes advisable to use a surrogate metric of resilience. We use the equilibrium remineralisation flux of nutrient, most easily measured as the rate of influx of nonliving material to the nutrient pool N , as a surrogate for the resilience of the internal equilibrium point. This indicates that we increase the loss

parameters of the system to increase its resilience, which must then be balanced by an increase in certain growth parameters to ensure the required BEVs are positive. This suggests that a key decision in implementing the SeBEDes method is, when defining the magnitude of any BEV, whether to choose parameters such that the value of the BEV is determined by the difference between two large numbers, resulting in a high resilience system, or the same difference between two small numbers, resulting in a low resilience system.

Application

The SeBEDes method proceeds as follows:

- i. Set the initial conditions for all populations to zero and set all parameters to zero;
- ii. Set the initial condition for the autotroph populations to a non-zero value. Choose values for the growth and mortality parameters of these populations so that their BEVs at the origin are positive and evaluate their BEPs (this may be done analytically for simpler models or by integrating the system for more complex models);
- iii. Use the BEP of the winner or the final state of the integration to calculate the BEVs of the next trophic level (i.e. all populations that feed on the currently extant populations) at the BEP. If integrating the system to find the BEP use either the end state if the system comes to a steady state, or the averages of the populations after transients have been eliminated if not a steady state. Note that the expressions for the BEVs of the extant populations at any BEP should be zero – evaluating these provides an indication of how close the estimate provided by the average of the populations is to the actual BEP;
- iv. Adjust the parameter values of the next trophic level populations so that their BEVs are positive at the winner's BEP;
- v. Set the initial condition for the newly parameterised population(s) to be non-zero and integrate the system again. Return to step (iii) and repeat until all populations are parameterised with the exception of the nonlinear mortality terms of the highest trophic level;
- vi. Integrate the system with all population initial conditions non-zero and determine the final state. Increase the quadratic mortality coefficient of the winning population until its competing populations become non-zero at steady state. If there are more than two populations at the highest trophic level, sequentially increase the quadratic mortalities

of all populations while simultaneously reducing their linear mortality coefficients until they all coexist. Increasing the quadratic mortality coefficient of the winning population in the highest trophic level is not necessary but may be desirable for ecological verisimilitude.

We demonstrate the procedure with its application to the SOE model (1) - (6). Note that the values are chosen using ‘expert knowledge’ of typical values for these parameters and are balanced to give relatively small positive eigenvalues that reduce in magnitude for populations at higher trophic levels. Note also that calculating the average of each population over a limit cycle only provides an estimate of the location of the BEP. In this case the BEVs of the non-zero populations indicates how accurate the estimate is as they are identically zero at the equilibrium point.

Applying SeBEDes to the SOE model

Here we demonstrate a different method of using the boundary eigenvalues to parameterise the SOE ecosystem model. In this case, we have three competing pairs of populations: ice algae and phytoplankton compete for inorganic nutrients; krill and salps compete for phytoplankton; and whales and fish compete for krill. Finding parameter sets that allow coexistence of these competitors is usually difficult. We will demonstrate two parameterisations of the SOE model for relatively weak and strong resilience.

The BEVs (λ_i^B) of the six populations of the SOE model are given by:

$$\lambda_A^B = \frac{\mu_A N^*}{N^* + \kappa_A} - \frac{\varphi_{AK} K^*}{A^* + P^* + \kappa_K} - \sigma_A, \quad (8)$$

$$\lambda_P^B = \frac{\mu_P N^*}{N^* + \kappa_P} - \frac{\varphi_{PK} K^*}{A^* + P^* + \kappa_K} - \frac{\varphi_{PS} S^*}{P^* + \kappa_S} - \sigma_P, \quad (9)$$

$$\lambda_K^B = \frac{\varphi_{AK}(1-\psi_{AK})A^* + \varphi_{PK}(1-\psi_{PK})P^*}{A^* + P^* + \kappa_K} - \frac{\varphi_{KF}F^*}{K^* + S^* + \kappa_F} - \frac{\varphi_{KW}W^*}{K^* + \kappa_W} - \sigma_K, \quad (10)$$

$$\lambda_S^B = \frac{\varphi_{PS}(1-\psi_{PS})P^*}{P^* + \kappa_S} - \frac{\varphi_{SF}F^*}{K^* + S^* + \kappa_F} - \sigma_S, \quad (11)$$

$$\lambda_F^B = \frac{\varphi_{KF}(1-\psi_{KF})K^* + \varphi_{SF}(1-\psi_{SF})S^*}{K^* + S^* + \kappa_F} - \sigma_F - \varepsilon_F F^*, \quad (12)$$

$$\lambda_W^B = \frac{\varphi_{KW}(1-\psi_{KW})K^*}{K^* + \kappa_W} - \sigma_W - \varepsilon_W W^*, \quad (13)$$

where the asterisk beside each population indicates that the value of the population at the appropriate BEP is used. The utilisation of these BEVs and closure parameters to destabilise each of the trophic levels in turn is described in Table 3. Stable BEPs at each trophic level are destabilised by the BEVs of higher trophic level populations. In the case of the highest trophic level explicitly represented in the model, the stable BEPs are destabilised by the parameters that represent implicit predation by higher trophic levels.

Table 3. The BEVs, or in the case of the highest trophic level the parameters, that are used to destabilise each trophic level of the SOE model.

Trophic Level	Destabilising BEVs	
0	λ_P^B	λ_A^B
1	λ_K^B	λ_S^B
2	λ_F^B	λ_W^B
Trophic Level	Destabilising parameters	
3	ε_F	ε_W

We use the equilibrium flux of the system, most easily measured as the rate of influx of nonliving material to the nutrient pool N , as a surrogate for the resilience of the internal equilibrium point and hence the tendency of the system to track an external forcing:

$$\begin{aligned} \frac{dN_{REMIN}}{dt} = & \sigma_A A + \sigma_P P + \sigma_K K + \sigma_S S + \sigma_F F + \sigma_W W + \varepsilon_F F^2 + \varepsilon_W W^2 + \frac{\varphi_{PS}\psi_{PS}PS}{P + \kappa_S} \\ & + \frac{\varphi_{AK}\psi_{AK}AK + \varphi_{PK}\psi_{PK}PK}{A + P + \kappa_K} + \frac{\varphi_{KF}\psi_{KF}KF + \varphi_{SF}\psi_{SF}SF}{K + S + \kappa_F} + \frac{\varphi_{KW}\psi_{KW}KW}{K + \kappa_W}. \end{aligned} \quad (14)$$

This provides the useful heuristic that to increase the resilience of the system, and hence its tendency to track environmental forcings, we need to increase the loss terms for each population.

The final stage of SeBEDes considers the two populations at the top trophic level of the model and must tilt the zero isosurfaces in a specific manner to ensure the creation of a stable internal equilibrium point. The populations at the top trophic level of the SOE model are F and W . We consider just these populations with their common resource K (equations (3) - (6)). We consider the equilibrium points of this subsystem and hence replace A , P and S with their equilibrium values A^* , P^* and S^* . The BEP involving K and W is given by:

$$K_W^* = \frac{\kappa_W (\sigma_W + \varepsilon_W W^*)}{\varphi_{KW} (1 - \psi_{KW}) - \sigma_W - \varepsilon_W W^*}, \quad (15)$$

$$W^* = \frac{(\Phi^* - \sigma_K)(K_W^* + \kappa_W)}{\varphi_{KW}}, \quad (16)$$

where

$$\Phi^* = \frac{\varphi_{AK} (1 - \psi_{AK}) A^* + \varphi_{PK} (1 - \psi_{PK}) P^*}{A^* + P^* + \kappa_K}. \quad (17)$$

Note that K^* is a constant for $\varepsilon_W = 0$. The BEP involving K and F is given by:

$$K_F^* = \frac{\kappa_F (\sigma_F + \varepsilon_F F^*) - [\varphi_{SF} (1 - \psi_{SF}) - \sigma_F - \varepsilon_F F^*] S^*}{\varphi_{SF} (1 - \psi_{SF}) - \sigma_F - \varepsilon_F F^*}, \quad (18)$$

$$F^* = \frac{(\Phi^* - \sigma_K)(K_F^* + S^* + \kappa_F)}{\varphi_{KF}}. \quad (19)$$

where Φ^* is again given by (17). Note that the availability of a second food resource S for F causes a reduction in the amount of resource that F leaves for its competitor (K_F^*) and consequently improves its chances of winning the R^* competition. Further, we see that K_F^* determines the value of F^* when $\varepsilon_F = 0$ but that increasing $\varepsilon_F > 0$ introduces a feedback.

Assume that integrating the system reveals that F is the winner of the competition between F and W (i.e. integrating the system comes to a stable BEV involving A , P , K , S and F). We then have estimates for K_F^* and F^* . We use the winner's quadratic mortality coefficient ε_F to tilt its zero isosurface so that the K - F BEP crosses to the other side of the W isosurface, that is, we require $K_W^* < K_F^*$. We can either solve the quadratic for K_F^* defined by (18) and (19) or proceed by trial and error by incrementing ε_F by small amounts and then integrating the

system to determine if the objective has been achieved. In either case we end up with $\lambda_F^B > 0$ at the $K-W$ BEP and $\lambda_W^B > 0$ at the $K-F$ BEP indicating that the interior equilibrium point we have just created must be an attractor (i.e. it may be a stable point, or an unstable point with a stable limit cycle or chaotic attractor around it).

Example steps of SeBEDes applied to SOE model

Step 1: All parameters are set to zero and we examine the BEVs of the autotroph populations A and P at the origin of the state space, as the BEVs of all other populations must be negative here. Equation (7) indicates that $N^* = 1$:

$$\lambda_A^B = \frac{\mu_A}{1 + \kappa_A} - \sigma_A, \quad (20)$$

$$\lambda_P^B = \frac{\mu_P}{1 + \kappa_P} - \sigma_P. \quad (21)$$

We choose values for the parameters in equations (20) and (21) so that both these eigenvalues are positive. In this case we set $\mu_A = 1 = \mu_P$ to reflect that many phytoplankton grow at an average rate of one per day; we choose $\kappa_A = 0.1 = \kappa_P$ to reflect that the autotrophs typically utilise nutrient very efficiently, and choose $\sigma_A = 0.0001$ and $\sigma_P = 0.00005$ to reflect the very low natural mortality rates of most phytoplankton. We choose σ_A to be double σ_P as P is grazed by both K and S but A is only grazed by K . These parameter values result in the boundary eigenvalues $\lambda_A^B = 0.90899$ for ice algae and $\lambda_P^B = 0.90904$ for phytoplankton as they destabilise the origin. The extinction of all populations is now not possible in this model.

Step 2: This step may be done analytically as the BEPs and associated BEVs for the two autotroph populations are easily obtained:

$$A^* = \frac{\mu_A - \sigma_A(1 + \kappa_A)}{\mu_A - \sigma_A} = 0.999999, \quad N^* = 1 - A^* = 0.000001, \quad (22)$$

$$P^* = \frac{\mu_P - \sigma_P(1 + \kappa_P)}{\mu_P - \sigma_P} = 0.999995, \quad N^* = 1 - P^* = 0.000005, \quad (23)$$

From (20) and (21) the autotroph BEVs at these points are $\lambda_A^B = -3.4 \times 10^{-5}$ for ice algae at the P^* point and $\lambda_P^B = 5 \times 10^{-5}$ for phytoplankton at the A^* point indicating that the P^* point is stable. Integrating the system confirms this. We choose salps and krill parameters to destabilise this point – for the salps we choose the parameters $\phi_{PS} = 0.33$, $\psi_{PS} = 0.20$, $\kappa_S = 0.20$, and $\sigma_S = 0.005$ to give the BEV for the salps population at this point:

$$\lambda_S^B = \frac{\phi_{PS}(1-\psi_{PS})P^*}{P^* + \kappa_S} - \sigma_S = 0.20 . \quad (24)$$

We choose $\phi_{PK} = 0.25$, $\psi_{PK} = 0.25$, $\kappa_K = 0.20$, and $\sigma_K = 0.10$ to give a value for the krill BEV of

$$\lambda_K^B = \frac{\phi_{PK}(1-\psi_{PK})P^*}{P^* + \kappa_K} - \sigma_K = 0.0563 . \quad (25)$$

We also choose $\phi_{AK} = 0.50$, and $\psi_{AK} = 0.25$ at this point, although it does not affect the krill's BEV.

Step 3: We integrate the model with these parameter values and the A , P , S and K populations non-zero and arrive at a periodic solution with the estimated BEP:

$$A^* = 0.1285, \quad P^* = 0.0093, \quad K^* = 0.3466, \quad S^* = 0.1940, \quad N^* = 0.3216 . \quad (26)$$

The “BEVs” of the A , P , K and S populations are zero at this BEP, so evaluating equations (8) - (11) provides an indication of how close to the location of the BEP the estimated position is. The values of equations (8) - (11) evaluated at (26) are:

$$\lambda_A^B = 0.2498, \quad \lambda_P^B = 0.2006, \quad \lambda_K^B = 0.0478, \quad \lambda_S^B = 0.0068, \quad (27)$$

indicating that the estimate is not very good. Consequently we may need to experiment with and/or set larger than expected BEVs to ensure destabilisation if the actual location is too distant from the estimate.

We choose fish and whale parameters to destabilise this BEP – for the whales we choose the parameters $\phi_{KW} = 0.05$, $\psi_{KW} = 0.50$, $\kappa_W = 1.00$, $\sigma_W = 0.0015$ and $\varepsilon_W = 0$ to give the BEV for the whale population at the estimated point:

$$\lambda_W^B = \frac{\phi_{KW}(1-\psi_{KW})K^*}{K^* + \kappa_W} - \sigma_W - \varepsilon_W W = 0.0049 , \quad (28)$$

We choose $\varphi_{KF} = 0.25$, $\varphi_{SF} = 0.25$, $\psi_{KF} = 0.50$, $\psi_{SF} = 0.50$, $\kappa_F = 0.90$, $\sigma_F = 0.01$ and $\varepsilon_F = 0$ to give a value for the fish BEV of:

$$\lambda_F^B = \frac{\varphi_{KF}(1-\psi_{KF})K^* + \varphi_{SF}(1-\psi_{SF})S^*}{K^* + S^* + \kappa_F} - \sigma_F - \varepsilon_F F = 0.0369, \quad (29)$$

This completes the parameter estimations with the exception of the quadratic mortality coefficients.

Step 4: We integrate the model with these parameter values and non-zero initial conditions for all populations and obtain a periodic solution with a slowly decaying W population and an estimated BEP:

$$\begin{aligned} A^* &= 0.2231, & P^* &= 0.2520, & K^* &= 0.0629, \\ S^* &= 0.0209, & F^* &= 0.3783, & W^* &= 0.0573, & N^* &= 0.0053 \end{aligned} \quad (30)$$

suggesting that F will eventually win the competition at the highest trophic level if we integrate the system long enough. The “BEVs” of the A , P , K , S and F populations are zero at the *APSOEF* BEP, so we evaluate equations (8) - (12) at (30) to obtain an indication of how close the estimated position is to the actual location of the BEP:

$$\lambda_A^B = 0.0060, \quad \lambda_P^B = 0.0146, \quad \lambda_K^B = 0.0052, \quad \lambda_S^B = 0.0471, \quad \lambda_F^B = 0.0005. \quad (31)$$

This suggests that the estimate is crude as might be expected from inspection of the time series of the integration, which shows the W population still declining (not shown). The final step of the SeBEDes method is to destabilise the *APSKF* BEP to allow the W population to exist.

Step 5: We now increase the quadratic mortality coefficient of the F population to tilt its zero isosurface so that it intercepts the zero isosurface of the W population by setting $\varepsilon_F = 0.02$.

Integrating this system leads to a stable limit cycle around an average population distribution:

$$\begin{aligned} A^* &= 0.1591, & P^* &= 0.0555, & K^* &= 0.0645, \\ S^* &= 0.0298, & F^* &= 0.1811, & W^* &= 0.5011, & N^* &= 0.0088 \end{aligned} \quad (32)$$

Evaluating equations (8) - (13) at this point again demonstrates that the estimate of the equilibrium point is not very accurate, but inspection of the solution indicates that it is not changing and the apparent limit cycle is stable. In the interests of ecological “completeness” we now add quadratic mortality to the W population to represent higher order predation on that population. We set $\varepsilon_W = 0.001$ and integrate the system to obtain a stable limit cycle with the average value:

$$\begin{aligned} A^* &= 0.1695, & P^* &= 0.0806, & K^* &= 0.0831, \\ S^* &= 0.0378, & F^* &= 0.2339, & W^* &= 0.3842, & N^* &= 0.0112 \end{aligned} \quad (33)$$

The final parameter set obtained by implementing the SeBEDes method is given in the centre column of Table 4. Integrating the SOE model with these parameters results in an interesting 'limit cycle' shown in Fig. 2.

Table 4. Parameters estimated for the SOE model using the SeBEDes method. The first application of the method is described as “Parameter Set 1” and the increased resilience application is described as “Parameter Set 2”.

Parameter	Parameter Set 1	Parameter Set 2
μ_A	1.00	1.00011
κ_A	0.10	0.10
σ_A	0.0001	0.0002
μ_P	1.00	1.000055
κ_P	0.10	0.10
σ_P	0.00005	0.0001
ϕ_{AK}	0.50	0.99
ψ_{AK}	0.25	0.50
ϕ_{PK}	0.25	0.61512
ψ_{PK}	0.25	0.50
κ_K	0.20	0.20
σ_K	0.10	0.20
ϕ_{PS}	0.33	0.38003
ψ_{PS}	0.20	0.40
κ_S	0.20	0.20
σ_S	0.005	0.01
ϕ_{KF}	0.25	0.6084
ψ_{KF}	0.50	0.75
ϕ_{SF}	0.25	0.6084
ψ_{SF}	0.50	0.75
κ_F	0.90	0.90
σ_F	0.01	0.02
ϕ_{KW}	0.05	0.1880
ψ_{KW}	0.50	0.75
κ_W	1.00	1.00
σ_W	0.0014	0.0030

ϵ_F	0.02	0.01
ϵ_W	0.001	0.01

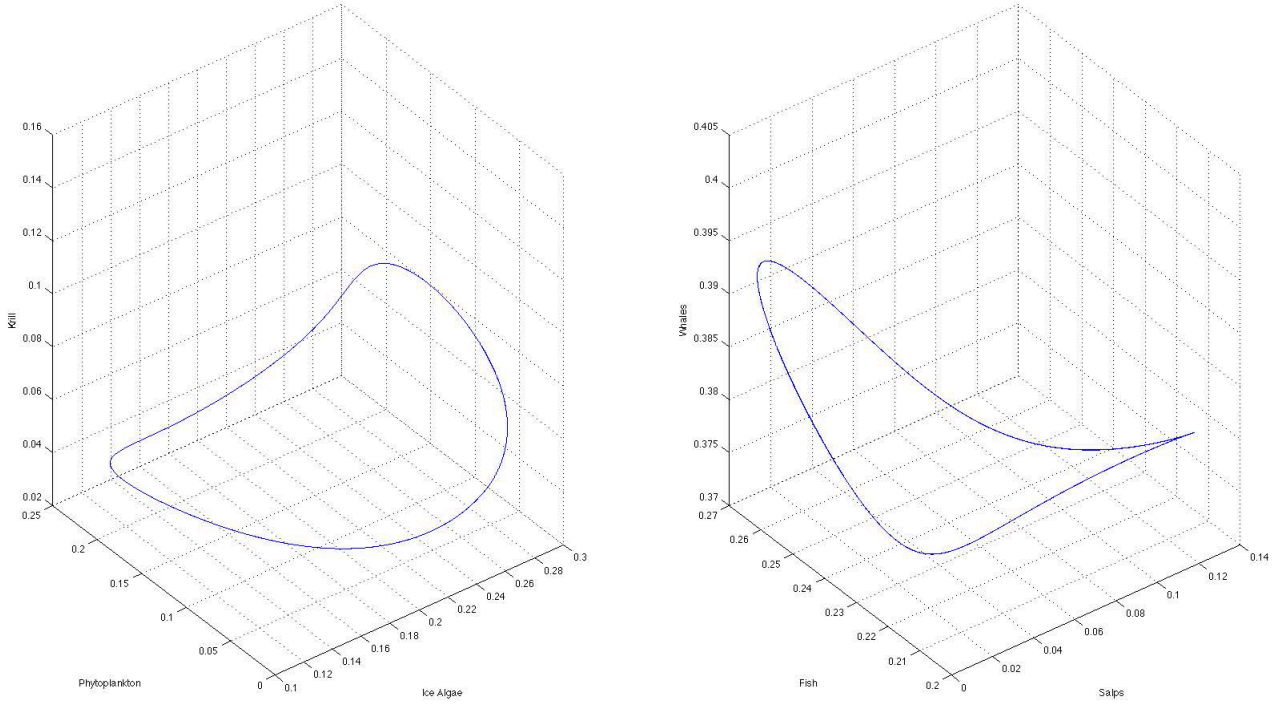


Figure 2. State space plots of populations for parameter set 1 from SeBEDes parameter estimation method showing all populations coexisting in a stable limit cycle. Parameter values are given in the second column of Table 4.

Alternative choices

SeBEDes is implemented by making choices of parameter values for predator populations so that their BEVs are positive at the BEP of the winning population at the trophic level below. Essentially there are two fundamental ways of doing this for any particular positive BEV: choose parameter values so that the BEV is the difference between two small numbers (i.e. growth minus loss) or choose parameter values so that the BEV is the same difference between two large numbers. The effect of this is demonstrated by the ‘remineralisation’ equation (14) - the former choice applied to all BEVs results in a small ‘remineralisation’ flux and a low-resilience system that does not closely follow environmental forcings. In contrast, the latter choice results in higher ‘remineralisation’ fluxes and a high-resilience system that more closely tracks environmental forcings. The nonlinear mortality terms do not affect the BEVs, as the

relevant populations are zero at their BEPs, so here we focus on the predation coefficients φ_X , the respiration/excretion coefficients ψ_X and the linear mortality coefficients σ_X .

We implemented the alternative approach on the SOE model using the heuristic of doubling (where possible) the loss parameters φ_X , ψ_X , and σ_X for $X = A, P, K, S, F, W$, and then adjusting the other parameters to obtain approximately the same BEVs as in the original application of the method. The alternate parameter values obtained by this implementation are provided in the third column of Table 4 and the BEPs and BEVs at intermediate steps are compared in Table 5.

Table 5. BEP and BEV values chosen for the second application of the SeBEDes method to the SOE model. Associated parameter values are listed in Table 4.

TL	Parameter Set 1		Parameter Set 2	
	BEP	BEV	BEP	BEV
0	$A^* = 0.999999$ $P^* = 0.999995$	$\lambda_A^B = 0.90889$ $\lambda_P^B = 0.90904$	$A^* = 0.999980$ $P^* = 0.999990$	$\lambda_A^B = 0.90889$ $\lambda_P^B = 0.90904$
1	$P^* = 0.999995$ $N^* = 0.000005$ $A^* = 0.999999$ $N^* = 0.000005$	$\lambda_S^B = 0.20$ $\lambda_K^B = 0.0563$ $\lambda_K^B = 0.2125$	$P^* = 0.999990$ $N^* = 0.000010$ $A^* = 0.999980$ $N^* = 0.000020$	$\lambda_S^B = 0.20$ $\lambda_K^B = 0.0563$ $\lambda_K^B = 0.2125$
2	$A^* = 0.1285$, $P^* = 0.0093$ $K^* = 0.3466$, $S^* = 0.1940$ $N^* = 0.3216$	$\lambda_W^B = 0.0049$ $\lambda_F^B = 0.0369$	$A^* = 0.2781$, $P^* = 0.0276$ $K^* = 0.2021$, $S^* = 0.1224$ $N^* = 0.3698$	$\lambda_W^B = 0.0049$ $\lambda_F^B = 0.0369$
3	$A^* = 0.2231$, $P^* = 0.2520$, $K^* = 0.0629$, $S^* = 0.0209$, $F^* = 0.3783$, $W^* = 0.0573$, $N^* = 0.0053$,		$A^* = 0.3089$, $P^* = 0.0092$, $K^* = 0.0682$, $S^* = 0.0272$, $F^* = 0$, $W^* = 0.5715$, $N^* = 0.0150$,	$\lambda_F^B = -0.0054$
3	$A^* = 0.1695$, $P^* = 0.0806$ $K^* = 0.0831$, $S^* = 0.0378$ $F^* = 0.2339$, $W^* = 0.3842$ $N^* = 0.0112$	$N_{REMIN} = 0.0194$	$A^* = 0.3258$, $P^* = 0.2475$ $K^* = 0.1001$, $S^* = 0.0469$ $F^* = 0.1551$, $W^* = 0.0978$ $N^* = 0.0267$	$N_{REMIN} = 0.0614$

Although the dynamics of this second parameter set (Fig. 3) are similar to that of the first (Fig. 2) we see that the second system ($N_{REMIN} = 0.0614$) is approximately three times as ‘resilient’ as the first ($N_{REMIN} = 0.0194$). This increased resilience is evident as a reduced period of

transient dynamics, with the increased resilience system coming to its equilibrium state faster than the original system (Fig. 4). This is most noticeable in the whale population (panels (f) and (l) in Figure 4).

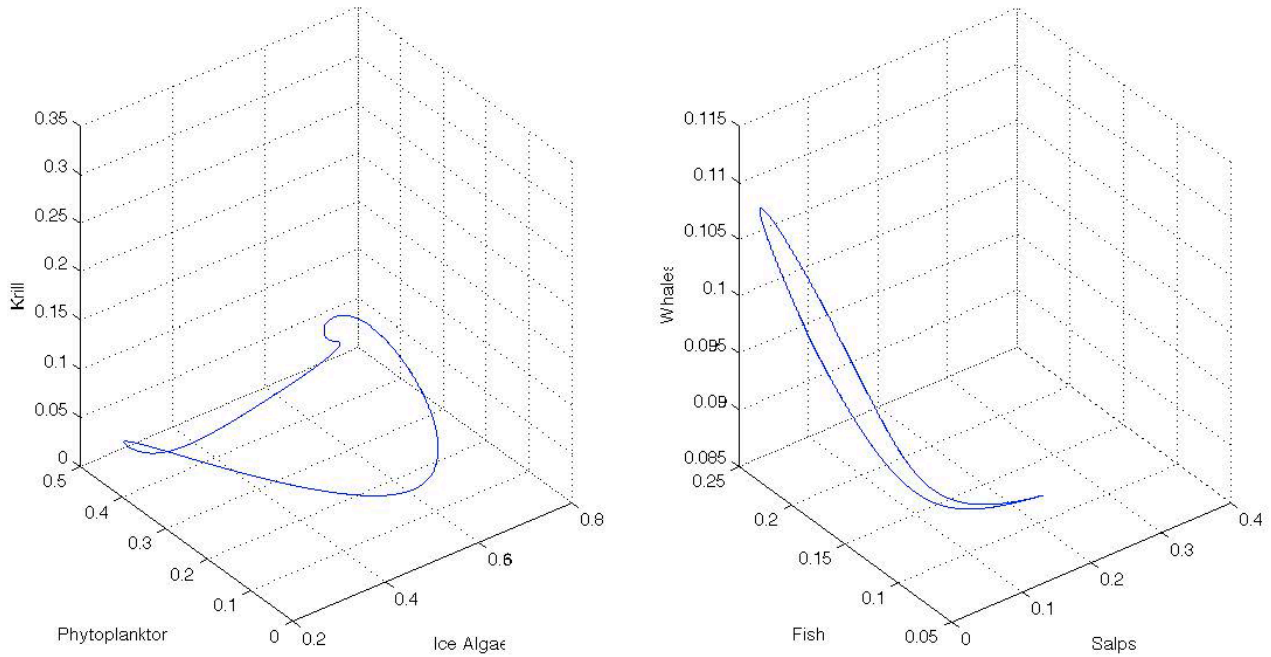


Figure 3. State space plots of populations for parameter set 2 from the SeBEDes parameter estimation method. This also shows all populations coexisting, but in a different stable limit cycle. Parameter values are given in the third column of Table 4.

Figure 3 suggests that the changed parameter sets has also affected the population sizes as well as the resilience of the system. The average sizes and standard deviations of the populations provide a measure of how the limit cycle of the model has changed with the more resilient parameter set and are shown in Table 6.

Table 6. Average sizes and standard deviations of the populations after integrating the SOE model for 10,000 time steps using the first and second parameter sets. Population sizes are expressed as the percentage of the total resource that they contain.

Parameter	Population average sizes and (standard deviations)						
Set	N	A	P	K	S	F	W
First	1.11	16.98	8.13	8.28	3.83	23.47	38.20
	(0.64)	(4.93)	(7.71)	(4.23)	(4.18)	(1.98)	(0.88)

Second	2.67 (3.74)	32.60 (7.60)	24.73 (18.68)	10.00 (9.42)	4.72 (6.16)	15.50 (4.80)	9.78 (0.77)
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Table 6 reveals that increasing the resilience of the system, although not dramatically changing the shape of the limit cycle, led to substantial redistribution of resources through the food web. While the changed parameter set maintained the general shape of the attractor it moved the location of the attractor in the state space. This is clearly evidenced by the percentage distribution of mass among the three trophic levels, which changes from 25 – 12 – 62 in the autotroph – herbivore – carnivore levels respectively with 1% in the nutrient pool, to 57 – 15 – 25 in the high resilience case with 3% in the nutrient pool. The shift of biomass from the top trophic level to the bottom with the increased resilience of the system is an interesting phenomena in the context of current theory on the structure and stability of food webs (Gunderson, 2000; McCann, 2012). The distribution of biomass observed in the “steady state” fact solutions for these parameter sets in the context of the very broad functional groupings we have used to represent populations suggests a fundamental “wasp-waisted” food web structure (Bakun, 2006) that is sometime associated with resilience (Condie et al., 2014; Madigan et al., 2012).

SOE model naïve parameter space search

The parameter space of the SOE model was explored by randomly selecting values for all 28 parameters from a uniform distribution then integrating the model for 10,000 time units using a 4-5th order Runge-Kutta adaptive step size integration routine with error tolerances set to machine epsilon ($\sim 2 \times 10^{-14}$). Population sizes were reported in steps of 0.1 time units. The last 10,000 time steps were used to determine the surviving populations and the state of the food web. Populations were deemed to be extinct if their average size over the last 10,000 time steps of the integration was less than 10^{-5} and the standard deviation was less than 10^{-2} . Note that such a measure over-estimates the number of extant populations as it may classify populations that may eventually go extinct as extant simply because the system has not been integrated for long enough. However, a compromise must be made between the probability of misclassification and integration times. Note that if both resources for a trophic level were classified as extinct then the populations were deemed to be extinct, which reduced the potential for misclassification.

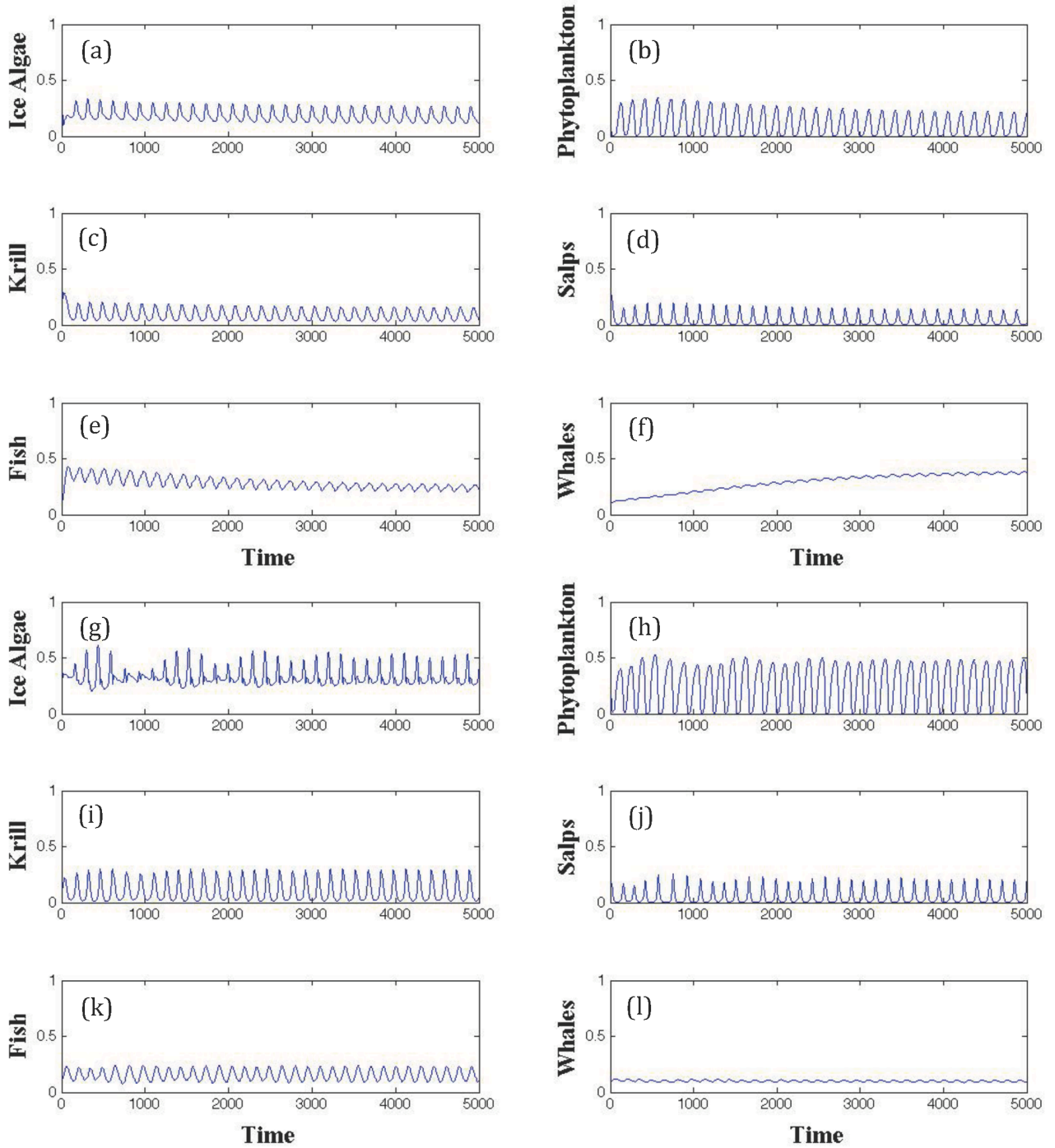


Figure 4. Time series plots of transient dynamics of populations for parameter set 1 (a - f) and parameter set 2 (g - l) from the same initial conditions. The plots show the increased resilience of the system with parameter set 2 values evidenced by a more rapid transition from the initial conditions to the long term stable limit cycle, particularly evident in the fish and whale populations (i.e. compare (e) with (k) and (f) with (l)).

The parameter range sampled for the “naïve” search was a uniform distribution between 0 – 1 for all parameters except the mortality coefficients, which were sampled from a uniform distribution that ranged between 0 – 0.1. Two thousand parameter sets were randomly generated and integrated. We repeated the random parameter space search undertaken above for an “informed” search in which, instead of arbitrarily defining a parameter space, we defined a space around the coexistence parameter set we had discovered using SeBEDes. The results of the parameter sampling are shown in Table 7 and Fig. 5.

Table 7. Frequency distribution of surviving populations after integrating the SOE model for 10,000 time steps using 2,000 randomly generated parameter sets from the naïve (upper rows) and informed (lower rows) parameter spaces.

Type of search		Number of surviving populations						
		0	1	2	3	4	5	6
Naive	Frequency	16	402	315	913	200	146	8
	(%)	0.8	20.1	15.8	45.6	10.0	7.3	0.4
Informed	Frequency	0	2	4	69	494	380	1050
	(%)	0	0.1	0.2	3.5	24.7	19.0	52.5

The most common food web found by the random parameter search shown in Fig. 5 was the single population food web 32 with only ice algae extant (*A*, 309 occurrences) – in contrast food web 16 containing only phytoplankton (*P*, 86 occurrences) was found much less frequently. The next most common food webs were the three-population / three-trophic level webs 41 (*AKW*, 240 occurrences) and 42 (*AKF*, 233 occurrences), followed by 26 (*PKF*, 145 occurrences) and 22 (*PSF*, 108 occurrences). The two-population / two-trophic level web 40 (*AK*, 161 occurrences) was the most common found in this category. The most commonly found five population food webs were 61 (*APKSW*, 49 occurrences) and 62 (*APKSF*, 53 occurrences), followed by the four population webs 60 (*APKS*, 56 occurrences) with two trophic levels and 43 (*AKFW*, 47 occurrences) with three trophic levels. The only other food web with more than two trophic levels found in significant numbers was 58 (*APKF*, 23 occurrences).

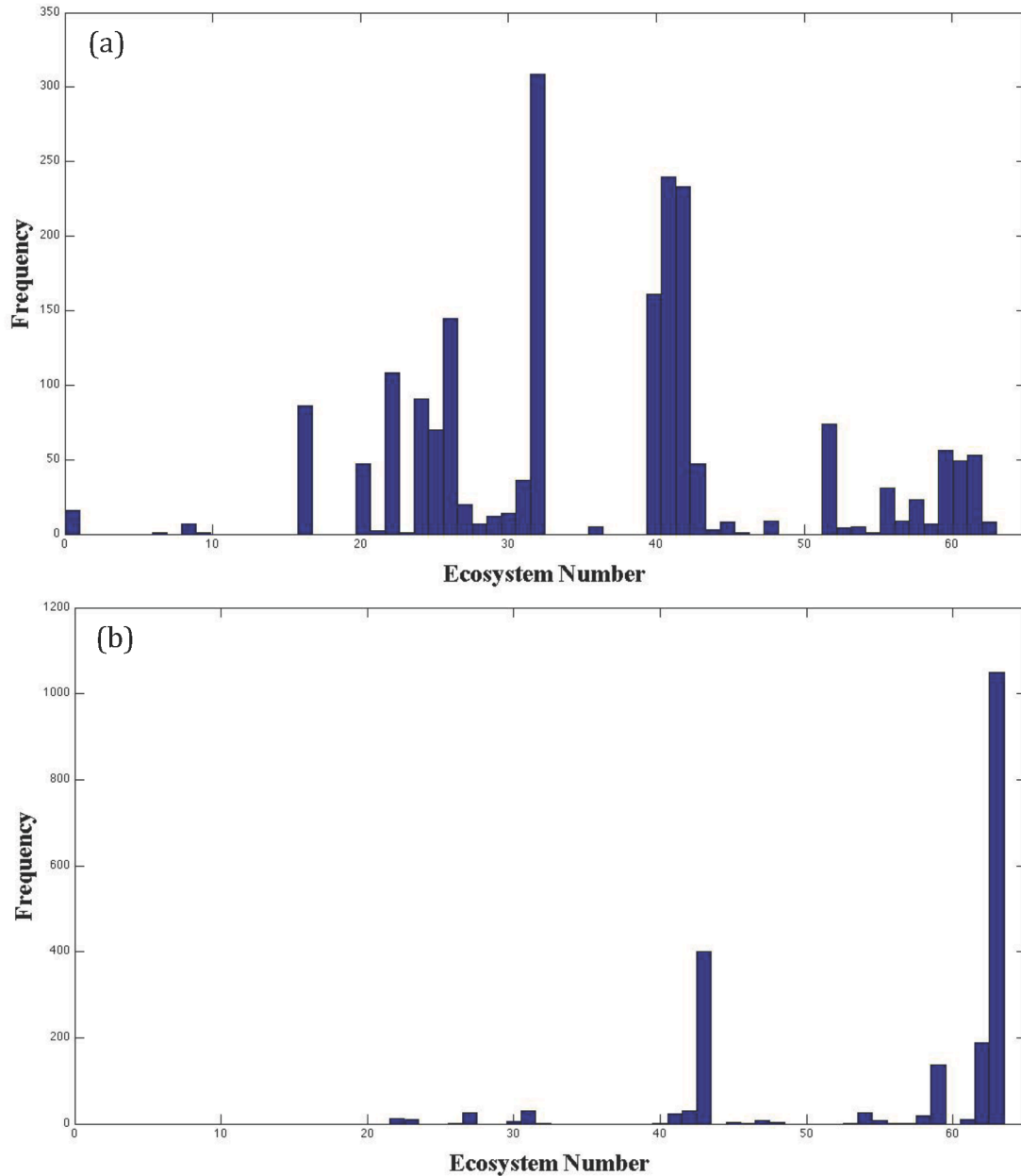


Figure 5. Distribution of stable food webs resulting from integrating 2,000 randomly chosen parameter sets from the naïve (a) and informed (b) parameter spaces. Food webs are identified by writing their presence (1) or absence (0) code in the order [APKSFW] as a binary number and then converting to decimal (i.e. $AKF = 101010 = 42$). Note the food webs 6 ($SF = 000110$), 8 ($K = 001000$) and 9 ($KW = 001001$) in (a) are not feasible. These ‘solutions’ are artifacts that arise from systems with populations that very slowly decay to extinction.

The results of the random search of the naïve parameter space reveal that the results of such undirected searches are dominated by food webs that have many extinct populations. Only

eight parameter sets (0.4% of samples) that allowed coexistence of all populations were found, with the random search mostly finding three-population food webs (46%) of which about 80% had three-trophic levels. Note each coexistence parameter set required approximately 250 model evaluations to find. In contrast, the informed search found a coexistence parameter set every second model evaluation.

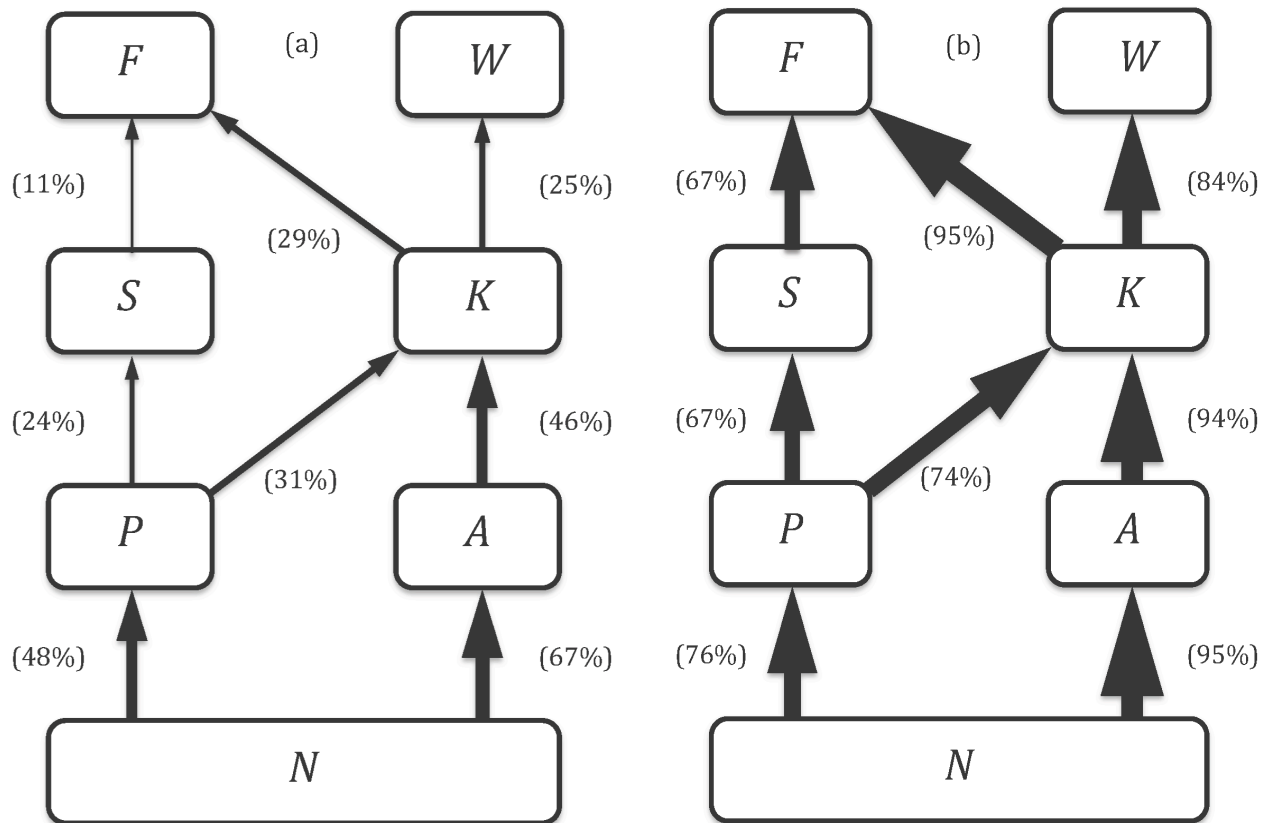


Figure 6. Frequency of links in food webs resulting from integrating 2,000 randomly chosen parameter sets from the naïve (a) and informed (b) parameter spaces (data as for Figure 5). The percentage of stable food webs in which each link is present is indicated by the thickness of the link, with the actual value shown in parentheses beside each arrow.

The random search of the informed parameter space resulted in over half of all parameter sets (1,050) having six coexisting populations. The next most common food web, with 400 instances, was 43 (*AKFW*), followed by 62 (*APKSF*, 188 instances) and 59 (*APKFW*, 137 instances). The remaining 225 cases (11%) were distributed across 19 different food webs. The key role of krill in moderating the properties of the ecosystem evident in Figure 6(b), being

involved in the transfer of almost all mass that moves from the primary producers to the highest trophic level, is consistent with krill's perceived role in producing "wasp-waisted" ecosystems (Atkinson et al., 2014). The lesser number of food webs that also include salps points to the dependence of the success of salps on environmental conditions, and allows for alternate pathways from the lowest to highest trophic levels as noted by Murphy et al. (2012).

These results demonstrate that the SeBEDes method can efficiently screen parameters to find regions of parameter space that contain coexistence parameter sets, can be directed to regions of parameter space that give the model particular properties, and that once appropriate regions of parameter space have been identified using SeBEDes, naïve parameter search methods may be used more effectively to find real world solutions due to the increased density of parameter sets that allow all populations to remain extant.

Discussion

The parameterisation of even moderately complex ecosystem models remains a problem that is mathematically challenging and computationally demanding (Lignell et al., 2013). Measured parameter values are few and generally not spatially or temporally cohesive and consequently not representative of any one system. Although it is the magnitude of parameter values in relation to other values in the system that is important, rather than the absolute magnitude, observations such as that of Franks (2009), that simple models that can reproduce real-world dynamics equally well can have values for the same parameter that span two orders of magnitude, confirms the well-known rubric attributed to the mathematician John von Neumann "with four parameters I can fit an elephant, and with five I can make him wiggle his trunk." (Dyson, 2004). Dyson goes on to note that in his case, the spurious fit of his model to observed data facilitated by "arbitrary parameters" occurred despite the fact that a fundamental aspect of the underlying theory was missing.

Many algorithms for estimating parameter values for ecosystem models have been proposed (for example, Chen et al., 2008; Lignell et al., 2013; Necpalova et al., 2015). In this work we propose a method based on some key ecological theories, the principle of competitive exclusion (Gause, 1932; Gause, 1934), R^* theory (Tilman, 2007) and the "kill-the-winner" hypothesis (Thingstad and Lignell, 1997). We show that the mathematical properties of

systems that have equations of Kolmogorov form (Kolmogorov, 1936), as most ecosystem models do, lend themselves to the application of these theories to provide a technique that allows parameter screening for complex models to be effectively undertaken by hand. SeBEDes proceeds as its name implies by sequentially destabilising the boundary eigenvalues of the boundary equilibrium points of the winners of competition at each trophic level.

Once the SeBEDes technique has identified a region of parameter space that contains parameter sets that provide the model with desirable properties, the usual parameter search techniques may be applied to find particular parameter sets that produce solutions to the particular model that match the real world. The ability of the investigator to direct the parameter screening process relatively easily to desirable regions of the parameter space, for instance, those regions with higher resilience in our example or regions where the parameter values are consistent with measured values, has the potential to constrain the space that needs to be naively searched and greatly reduce the computational demands of such searches. Here the computational search time reduction is shown to be several orders of magnitude, and allows the user to impose their own desired ecological constraints if desired.

An interesting outcome of the two example applications of the method to the SOE model, in which the second application seeks to increase the resilience of the system (which also forces the system to track any environmental forcing more closely when applied in realistic scenarios) is that increasing the resilience of the system is associated with a redistribution of the biomass from the highest trophic level to the lowest. Although the shape of the systems attractor is relatively similar for both parameter sets, the location of the attractor in the state space is very different. The 25 – 12 – 62 percentage distribution of biomass across the autotroph – herbivore – carnivore levels respectively of the low-resilience system becomes a 57 – 15 – 25 percentage distribution in the high resilience case, a re-allocation of some 30% of the total biomass in the system from the highest trophic level to the lowest. Such observations may provide useful rubrics for automated implementations of the method.

The SeBEDes method has been presented here as an expert system, that requires decisions to be made at various stages of its implementation. It is feasible that modellers may know *a priori* what dynamical attributes they wish their model to have, and may implement the method as an algorithm with the expert decisions prescribed. In such cases, the potential exists to couple the

SeBEDes with naïve search algorithms to develop an efficient, automatic method that first screens the parameter space for regions with parameter sets with particular attributes (coexistence, resilience, etc.) and then intensively searches a small, densely populated region of parameter space for real world solutions. An increased density of parameter sets that allows coexistence of all populations makes for an ecosystem model that can respond to environmental perturbations that change parameter values in a robust manner, and perhaps represents reality more robustly than an ecosystem model that is located in a region of parameter space that has few solutions that allow coexistence.

References

- Atkinson, A., Hill, S. L., Barange, M., Pakhomov, E. A., Raubenheimer, D., Schmidt, K., Simpson, S. J., Reiss, C., 2014. Sardine cycles, krill declines, and locust plagues: revisiting 'wasp-waist' food webs. *Trends Ecol Evol* 29, 309-316.
- Bakun, A., 2006. Wasp-waist populations and marine ecosystem dynamics: Navigating the "predator pit" topographies. *Progress in Oceanography* 68, 271-288.
- Bates, M., Bengtson Nash, S. M., Hawker, D. W., Norbury, J., Stark, J. S., Cropp, R. A., 2015. Construction of a trophically complex near-shore Antarctic food web model using the Conservative Normal framework with structural coexistence. *Journal of Marine Systems* 145, 1-14.
- Bopp, L., Resplandy, L., Orr, J., Doney, S., Dunne, J., Gehlen, M., Halloran, P., Heinze, C., Ilyina, T., Sfrian, R., Tjiputra, J., Vichi, M., 2013. Multiple stressors of ocean ecosystems in the 21st century: projections with CMIP5 models. *Biogeosciences* 10, 6225-6245.
- Boyd, I. L., 2002. Estimating food consumption of marine predators: Antarctic fur seals and macaroni penguins. *J Appl Ecol* 39, 103-119.
- Chen, M., Liu, S., Tieszen, L. L., Hollinger, D. Y., 2008. An improved state-parameter analysis of ecosystem models using data assimilation. *Ecol Model* 219, 317-326.
- Condie, S. A., Johnson, P., Fulton, E. A., Bulman, C. M., 2014. Relating food web structure to resilience, keystone status and uncertainty in ecological responses. *Ecosphere* 5, 1-16.
- Cropp, R. A., Norbury, J., 2010. Parameterizing competing zooplankton for survival in plankton functional type models. *Ecol Model*, 1852-1864.
- Cropp, R. A., Norbury, J., 2012. The mechanisms of coexistence and competitive exclusion in complex plankton ecosystem models. *Ecosystems* 15, 200-212, doi:10.1007/s10021-011-9503-1.
- Cropp, R. A., Norbury, J., 2013. Modelling plankton ecosystems and the Library of Lotka. *Journal of Marine Systems* 125, 3-13.
- Cropp, R. A., Norbury, J., 2015. Population interactions in ecology: a rule-based approach to modeling ecosystems in a mass-conserving framework. *SIAM Review* 57, 437-465.
- DeAngelis, D. L., 1980. Energy flow, nutrient cycling and ecosystem resilience. *Ecology* 61, 764-771.
- Dyson, F., 2004. A meeting with Enrico Fermi. *Nature* 427, 297.
- Franks, P. J. S., 2009. Planktonic ecosystem models: perplexing parameterisations and a failure to fail. *J Plankton Res* 31, 1299-1306.

- Freedman, H. I., Waltman, P., 1984. Persistence in models of three interacting predator-prey populations. *Math Biosci* 68, 213-231.
- Gause, G. F., 1932. Experimental studies on the struggle for existence. *J Exp Biol* 9, 389-402.
- Gause, G. F., 1934. *The Struggle for Existence*. Williams and Wilkins, Baltimore.
- Gunderson, L. H., 2000. Ecological resilience - in theory and application. *Annu Rev Ecol Syst* 31, 425-439.
- Hashioka, T., Vogt, M., Yamanaka, Y., Le Quere, C., Buitenhuis, E. T., Aita, M. N., Alvain, S., Bopp, L., Hirata, T., Lima, I., Sailley, S., Doney, S. C., 2013. Phytoplankton competition during the spring bloom in four plankton functional type models. *Biogeosciences* 10, 6833-6850.
- Hill, S. L., Murphy, E. J., Reid, K., Trathan, P. N., Constable, A., 2006. Modelling Southern Ocean ecosystems: krill, the food web, and the impacts of harvesting. *Biol Rev* 81, 581-608.
- Hutchinson, G. E., 1961. The paradox of the plankton. *Am Nat* 95, 137-145.
- Ichii, T., Kato, H., 1991. Food and daily food consumption of southern minke whales in the Antarctic. *Polar Biol* 11, 479-487.
- Koen-Alonso, M., 2007. A process-oriented approach to the multi-species functional response. In: Rooney, N., et al., Eds.), *From Energetics to Ecosystems: The Dynamics and Structure of Ecological Systems*, Vol. 1. Springer, Netherlands, pp. 1-36.
- Kolmogorov, A. N., 1936. Sulla Teoria di Volterra della Lotta per l'Esistenza. *Giornale dell' Istituto Italiano Degli Attuari* 7, 74-80.
- Le Quéré, C., Harrison, S. P., Prentice, I. C., Buitenhuis, E. T., Aumonts, O., Bopp, L., Claustre, H., Cotrim da Cunha, L., Geider, R. J., Giraud, X., Klaas, C., Kohfeld, K. E., Legrende, L., Manizza, M., Platt, T., Rivkin, R. B., Sathyendranath, S., Uitz, J., Watson, A., Wolf-Gladrow, D., 2005. Ecosystem dynamics based on plankton functional types for global ocean biogeochemistry models. *Global Change Biology* 11, 2016-2040.
- Lignell, R., Haario, H., Laine, M., Thingstad, F., 2013. Getting the "right" parameter values for models of the pelagic microbial food web. *Limnol Oceanogr* 58, 301-313.
- Lockyer, C., 1981. Growth and energy budgets of large baleen whales from the Southern Hemisphere., *Mammals in the Seas*, Vol. 3. FAO, Rome, pp. 379-487.
- Madigan, D. J., Carlisle, A. B., Dewar, H., Snodgrass, O. E., Litvin, S. Y., Micheli, F., Block, B. A., 2012. Stable isotope analysis challenges wasp-waisted food web assumptions in an upwelling pelagic ecosystem. *Scientific Reports* 2, 1-10.
- May, R. M., Beddington, J. R., Clark, C. W., Holt, S. J., Laws, R. M., 1979. Management of multispecies fisheries. *Science* 205, 267-277.
- McCann, K. S., 2012. The Structure and Stability of Food Webs. In: Levin, S., (Ed.), *The Princeton Guide to Ecology*. Princeton University Press, Princeton, pp. 305-311.
- Michaelis, L., Menten, M., 1913. Die kinetik der invertinwirkung. *Biochemische Zeitung* 49, 333-369.
- Murphy, E. J., Cavanagh, R. D., Hofmann, E. E., Hill, S. L., Constable, A. J., Costa, D. P., Pinkerton, M. H., Johnston, N. M., Trathan, P. N., Klinck, J. M., Wolf-Gladrow, D. A., Daly, K. L., Maury, O., Doney, S. C., 2012. Developing integrated models of Southern Ocean food webs: Including ecological complexity, accounting for uncertainty and the importance of scale. *Progress in Oceanography* 102, 74-92.
- Necpalova, M., Anex, R. P., Fienen, M. N., Del Grosso, S. J., Castellano, M. J., Sawyer, J. E., Iqbal, J., Pantoja, J. L., Barker, D. W., 2015. Understanding the DayCent model: Calibration, sensitivity, and identifiability through inverse modeling. *Environ Model Software* 66, 110-130.

- Sailley, S. F., Vogt, M., Doney, S., Aita, M. N., Bopp, L., Buitenhuis, E. T., Hashioka, T., Lima, I., Le Quéré, C., Yamanaka, Y., 2013. Comparing food web structures and dynamics across a suite of global marine ecosystem models. *Ecol Model* 261-262, 43-57.
- Steele, J. H., Henderson, E. W., 1981. A Simple Plankton Model. *The American Naturalist* 117, 676-691.
- Steele, J. H., Henderson, E. W., 1992. The role of predation in plankton models. *J Plankton Res* 14, 157-172.
- Thingstad, F., Lignell, R., 1997. Theoretical models for the control of bacterial growth rate, abundance, diversity and carbon demand. *Aquat Microb Ecol* 13, 19-27.
- Tilman, D., 2007. Interspecific competition and multispecies coexistence. In: May, R. M., McLean, A., Eds.), *Theoretical Ecology*. Oxford University Press, Oxford, pp. 257.
- Vancoppenolle, M., Bopp, L., Madec, G., Dunne, J., Ilyina, T., Halloran, P. R., Steiner, N., 2013. Ocean primary productivity from CMIP5 simulations: uncertain outcome, but consistent mechanisms. *Glob. Biogeochem. Cycles* 27, 605–619.