Modelling ecological communities as if they were DNA

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1 Abstract

Ecologists are interested in understanding and predicting how ecological communities change through time. While it might seem natural to measure this through changes in species' abundances, computational limitations mean transitions between community types are often modelled instead. We present an approach inspired by DNA substitution models that attempts to estimate historic interactions between species, and thus estimate turnover rates in ecological communities. Although our simulations show that the method has some limitations, our application to butterfly community data shows the method can detect signal in real data. Open source `C++` code implementing the method is available at `http://www.github.com/willpearse/lotto`.

2 Introduction

Many ecologists recognise broad habitat types and sub-types, grouping communities they define as being similar in structure. A good example is the British National Vegetation Classification system (Rodwell, 1991), which hierarchically classifies plant communities within the UK. Ecologists also recognise variability within these categories, and the recent interest in Neutral Theory (Hubbell, 2001) and stochastic variation at all spatial scales (reviewed in Vellend, 2010) suggests ecologists want to model this variation. However, models that allow for variation within habitat types are often over-parameterised, and summary statistics of structure do not necessarily facilitate the prediction of future species compositions.

One way to approach this problem has been to model a community as proceeding through a series of states, each state representing a particular community type with associated species compositions and abundances. The probability of moving among these states can be modelled using Markov chains, and thus predictions about future ecological composition can be made (reviewed in Logofet & Lesnaya, 2000). This is a natural way to model habitat types, but it cannot model variation within states, assumes that the history of a community is unimportant, and requires that a system reaches a final, stable state. Moreover, such methods require *a priori* definitions of states, and as such are not solely driven by the data themselves.

Our alternative is to model species turnover as a transition matrix, where the likelihood of an individual entering a community can be predicted as a function of the species of the individual it replaces. Such a model can be modified to allow the addition of individuals without replacement, and provides both species-level parameters of ecological interest and predictions about future species abundances. The problem of over-parameterisation can be solved by simplifying this matrix, analogously to procedures for simplifying DNA or protein substitution matrices. These simplifications are applied by allowing certain bases or amino acids (in our case species) to change with the same rate (*e.g.*, the Jukes-Cantor model where all characters evolve with the same rate; Jukes & Cantor, 1969). However, this method has the major drawback of requiring an accurate way of determining the history of species interactions in a community, which, unfortunately, is often unavailable and thus must be estimated from species composition data.

Species	Abundance	Species	Abundance
A	10	A	20
B	20	B	10
C	20	C	20
(a) First time-step		(b) Second time-step	

Table 1: The problem of estimating species turnover. What happened in the time between the first measurement of this community (a) and the second (b)? Did ten individuals of species B become replaced by ten of species A? Did ten individuals of species B die out without leaving descendants, and ten members of species A come from outside the community? Did ten individuals of species C become replaced by ten of species A, and another ten came in from outside the community? There are many possible transitions between the two communities, and no obvious way to determine what happened without already having a model for the likelihood of possible transitions.

	A	B	C	Death	Addition
A	reproduction	replacement	replacement	death	addition
B	replacement	reproduction	replacement	death	addition
C	replacement	replacement	reproduction	death	addition

Table 2: Example *transition matrix*. Each species is a represented by a letter ('A', 'B', and 'C'), and each element of the matrix represents a parameter of the model, as described in the text.

3 Methods

3.1 Overview and description of problem

We model the fate of each individual in a community over a number of discrete time-steps, assuming one of four events happens to each individual in each time-step:

- **Reproduction**. The individual dies and is replaced by another of the same species (implicitly its offspring). This is equivalent to, and indistinguishable from, the individual surviving until the next time-step.

- **Replacement**. The individual dies, and is replaced by another individual of a different species.

- **Death**. The individual dies, and is not replaced by another individual of any species. This allows communities to decrease in overall abundance.

- **Addition**. The individual enters the community, and does not replace any other individual. This allows communities to increase in overall abundance.

Although this model is conceptually straight-forward, it is difficult to estimate the parameters involved (the rate of reproduction, loss, death and addition); composition data do not reveal what happend during each time-step. Taking the community in table 1 as an example, it is difficult to disentangle what happened between the first and second measurements that led to species A increasing in number and species B becoming less abundant. Any attempt to infer what events were most likely to have happened requires an estimate of the relative likelihoods of those events taking place; this creates a circularity, since estimating the likelihoods requires some knowledge of the events.

3.2 Description of method

Open source `C++` code (named '*lotto*') that implements the method described below is available at `http://www.github.com/willpearse/lotto`. The program is also capable of simulating data with which to test the method.

The method assumes that community compositions are known perfectly, and all were repeatedly sampled at the same frequency. It starts by generating an initial *transition matrix* (table 2), which contains the relative rates of reproduction, replacement, death, and addition for each species. Within each row all bar the last column must sum to one, since each individual must do something in each time step. In the last column all the rows must sum to one, since every time an addition takes place the individual must be of a species.

Using the transition matrix, *lotto* must now estimate what happened between each time-step in each community. In random order, each individual is assigned its most likely source (a reproduction, replacement, or addition event) given the individuals in that community's previous time step not yet assigned to an event. Individuals undergo death events when a community has a lesser overall abundance than the previous time-step. This creates an *event matrix*, of the same dimensions as the transition matrix, with counts of the number of times each possible event in the transition matrix occurred in each community between each time-step.

	a	b	c	d	e	Death	Addition
a	**0.46**	0.11	0.11	0.11	0.11	0.11	0.20
b	0.07	**0.66**	0.07	0.07	0.07	0.07	0.20
c	0.02	0.02	**0.88**	0.02	0.02	0.02	0.20
d	0.03	0.03	0.03	**0.85**	0.03	0.03	0.20
e	0.09	0.09	0.09	0.09	**0.53**	0.09	0.20

(a) Real

	a	b	c	d	e	Death	Addition
a	**0.20**	0.16	0.16	0.16	0.16	0.16	0.20
b	0.16	**0.20**	0.16	0.16	0.16	0.16	0.20
c	0.16	0.16	**0.20**	0.16	0.16	0.16	0.20
d	0.16	0.16	0.16	**0.20**	0.16	0.16	0.20
e	0.16	0.16	0.16	0.16	**0.20**	0.16	0.20

(b) Initial

	a	b	c	d	e	Death	Addition
a	**0.65**	0.01	0.12	0.11	0.02	0.01	0.23
b	0.03	**0.84**	0.06	0.05	0.01	0.01	0.16
c	0.00	0.01	**0.96**	0.01	0.00	0.01	0.2771
d	0.01	0.01	0.01	**0.95**	0.01	0.01	0.01
e	0.01	0.06	0.04	0.052	**0.82**	0.01	0.32

(c) Estimated

Table 3: Values of the *transition matrix* used to generate the data (a), to start the search procedure (b), and given as the estimated result (c). Reproduction parameters have been highlighted. This example shows a general tendency of the program to under-estimate death, and to over-estimate the likelihood of an individual to reproduce.

We can now estimate the likelihood of the data (the event matrix) given the model (the transition matrix). *Lotto* repeats the process of calculating the event matrix given the transition matrix, conducting a maximum likelihood optimisation for each transition parameter in random order using Brent's method (Brent, 1973). Once each transition parameter has been optimised, the event matrix is rescaled so that the row and column totals conform to the restrictions above. This process of recalculating the entire transition matrix should be iterated until the parameter estimates converge, although at present *lotto* does not assess convergence.

4 Example with simulated data

We present an example of this method with ten random communities, each with ten years of data, starting with 100 individuals and having ten individuals added at each time-step. We used *lotto* to simulate these data, and then made one attempt (with five iterations) to estimate transition and event matrices. Tables 3 and 4 show the true and estimated transition and event matrices, along with the transition matrix used to initiate the search.

It is clear that the method has flaws. Although species with higher reproduction rates have higher estimated rates, these estimates are inflated, the method is poor at detecting death events, and underestimates rates of addition. This may stem from the special (but perhaps likely) case where transition and death rates for a species are identical, such that there may be equally likely ways of explaining the results. Repeated searches from different, randomised, starting transition matrices could help the program escape such local optima. There may also be identifiability issues relating to the death and addition rates; it is notable that the species with the lowest real death rate ('c') has the highest estimated rate of addition.

5 Example with ecological data

We used data from a well-recorded site (site 10, UK grid-reference NT590070) from the UK Butterfly Monitoring Scheme as a test-case of the method. We grouped the species' abundances into five groups of butterflies (the 'skippers', 'whites', 'hairstreaks, coppers and blues', 'fritillaries and nymphalids', and 'browns' as defined in Asher *et al.*, 2001) as input for the program to reduce the problem dimension. Grouping species according to their taxonomy is not unreasonable given the phylogenetic signal in species' traits and assemblage structure (WD Pearse unpublished obs.). The results, after only one search with five iterations, are shown in table 5.

Given the simulated results it is not appropriate to draw strong conclusions about these empirical results. However, a general point can be made: these transition matrices are more variable than those estimated from the simulated

	a	b	c	d	e	Death	Addition
a	**566**	121	148	150	131	136	169
b	125	**1234**	123	111	124	122	195
c	88	92	**2785**	79	80	63	173
d	108	93	92	**2447**	82	85	166
e	126	130	137	143	**786**	120	197

(a) Real

	a	b	c	d	e	Death	Addition
a	**896**	12	96	93	57	8	45
b	84	**1627**	78	24	26	0	63
c	11	34	**3104**	27	10	1	116
d	22	28	33	**2785**	38	1	106
e	34	101	31	61	**1215**	0	54

(b) Estimated

Table 4: Values of the *event matrix* used to generate the data (a), and estimated at the end of the run (b). Reproduction parameters have been emboldened. This example shows a general tendency of the program to under-estimate death, and to over-estimate the likelihood of an individual to reproduce.

	Whites	Blues	Skippers	Fritillaries	Browns	Death	Addition
Whites	**0.38**	0.01	0.02	0.01	0.01	0.57	0.04
Blues	0.30	**0.22**	0.04	0.01	0.07	0.35	0.03
Skippers	0.00	0.00	**0.99**	0.00	0.00	0.00	0.01
Fritillaries	0.15	0.01	0.08	**0.15**	0.15	0.45	0.68
Browns	0.01	0.00	0.01	0.00	**0.95**	0.01	0.24

(a) *Transition Matrix*

	Whites	Blues	Skippers	Fritillaries	Browns	Death	Addition
Whites	**16016**	590	76	64	1052	3556	2408
Blues	497	**2208**	237	153	481	119	443
Skippers	380	61	**863**	6	188	107	242
Fritillaries	168	30	71	**358**	73	40	78
Browns	2039	386	83	98	**6495**	930	1759

(b) *Event Matrix*

Table 5: Values of the *transition* and *event* matrices when the method was applied to real data. For ease of reading, the names of two of the groups are abbreviated to 'blues' and 'fritillaries' from 'hairstreaks, coppers and blues' and 'fritillaries and nymphalids', respectively. See text for further discussion, but note that these parameters do not resemble those of the simulated data, in particular having large 'death' parameter estimates.

data, suggesting the method may be picking up some signal (biological process) in the data. The low replacement parameters suggest that few of the clades seem to be interacting with other clades, with the exception of the blues replacing the whites.

6 Further work

The simulated example shows that the method is imperfect, and makes it clear that more work is needed. The butterfly data may still represent a good test case for the method once it has been refined, since few butterflies have overlapping generations and, in its current form, the method assumes there is no generational overlap.

Although the order in which individual events are assigned to the event matrix is randomised in each iteration of the program, the assignment of events according to whichever is the most likely is deterministic. This is another possible explanation for the inaccurate estimation of rates in the simulated data, and so more explicitly incorporating stochastic processes is an important next step. Preliminary experiments using MCMC (Markov Chain Monte Carlo; not shown) to both integrate over uncertainty and estimate confidence in model parameters suggest that this is a promising avenue of future work.

Currently, the method cannot be used with more than a handful of species or it takes too long to parameterise the event matrix, a step that needs further computation optimisation. However, allowing the user to specify a number of candidate restricted transition matrices that share parameters across species would not just allow more species to be analysed, but also allow explicit ecological hypotheses to be tested.

7 Acknowledgements

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