The statistical mechanics of community assembly and species distribution

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Supplementary material

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Maximum entropy, priors and alien species

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Abstract. Theoretically, communities at or near their equilibrium species number resist entry of new species. Such ‘biotic resistance’ recently has been questioned because of successful entry of alien species into diverse natural communities. Data on 10,409 naturalizations of 5350 plant species over 16 sites dispersed globally show exponential distributions for both species over sites and sites over number of species shared. These exponentials signal a statistical mechanics of species distribution, assuming two conditions. First, species and sites are equivalent, either identical (‘neutral’), or so complex that the chance a species is in the right place at the right time is vanishingly small (‘idiosyncratic’); the range of species and sites in our data disallows a neutral explanation. Secondly, the total number of naturalisations is fixed in any era by a ‘regulator.’ Previous correlation of species naturalization rates with net primary productivity over time suggests that regulator is related to productivity. We conclude that biotic resistance is a moving ceiling, with resistance controlled by productivity. The general observation that the majority of species occur naturally at only a few sites but only a few at many now has a quantitative [exponential] character, offering the study of species’ distributions a previously unavailable rigor.
Introduction

The effects, accidental or otherwise, that humans may have on natural systems are a classic source of insight into the fundamental processes governing those systems (Darwin 1859; Elton 1958). Here we use distributions of plant species’ naturalization* to characterize the factors determining entry of new species into a standing species complement, the fundamental building block of natural communities. Ecological theory of community assembly predicts that mature communities – those at or near their equilibrium species number – will resist the entry of new species. Such ‘biotic resistance’ is proposed to occur either through in situ coevolution filling all available niche space, or by ecological sorting to find the combination of species best able to exploit available resources. The resulting complex matrix of interactions is supposed to leave little niche space in the existing community into which a newcomer may easily insert itself, thus regulating community diversity (Elton 1958; Hutchinson 1959; MacArthur 1965; May 1973; Pimm 1991; Tilman 2004).

Biotic resistance has been interpreted on a practical level to mean that highly diverse communities are protected from invasion by species not currently a part of the community, and small-scale manipulations under natural conditions largely support this expectation (Levine 2000; Kennedy et al. 2002). However, two patterns of species’ naturalisation at greater geographic scales and incorporating longer time-spans seem to contradict these observations: regional inventories of species occurrences show highly diverse communities readily invaded by naturalized species (Lonsdale 1999; Stohlgren et al. 1999; Sax 2002); successful naturalizations are not being offset by the concomitant extinctions of native species that would be expected if

* Here we use ‘naturalized’ to denote merely having an established population; ‘invasive’ (pest) species are a subset of naturalized species, but not all naturalized species become pests.
niche filling regulates community assembly (Sax and Gaines 2003). These observations challenge the idea that complex interactions regulate the successful entry of new species into natural communities, and pose the question as to what, then, determines entry of a species into a community.

In this study we exploit the global-scale ‘natural experiment’ created by the escalation of species naturalizations over the last century. We employ these data to examine the large-scale patterns of species naturalizations and community assembly through the high-power lens of statistical mechanics. Statistical mechanics uses probability theory to provide a framework relating the properties of large numbers of individual units to the bulk properties of the whole, revealing emergent properties that give insight into the regulators of individual behavior not available from considering one or a few individuals independently. Statistical mechanics underlies much of the realm of the physical sciences, but also has been useful in problems such as the distribution of wealth (Drăgulescu and Yakovenko 2001) and the ubiquitous lognormal distribution of individuals among species in ecological communities (Pueyo et al. 2007; Dewar and Porté 2008; Harte et al. 2008; Bowler and Kelly 2010).

Our approach has produced new insights into several fundamental ecological processes. First, we have derived an analytical explanation of community assembly able to incorporate naturally all the above observations. From this, we are able to conclude that biotic resistance exists, but as a moving ceiling regulated by some external factor; combining these findings with earlier work (Woodward and Kelly 2008), we infer that external factor to be net primary productivity (NPP) or some process innately linked to NPP. Secondly, we have identified a quantitative (exponential) character to the general observation that the majority of species are of restricted distribution and only a few are widespread. This pattern is an emergent property deriving from the fundamental nature of niches themselves and does not require the operation of any particular trait of any particular niche. Lastly, the simple exponential distributions make
possible analytical tools carrying with them a degree of rigor not previously available to the
cumparative study of species’ distributions (see Gotelli et al. 2009).

**Materials and Methods**

We collated data on 10,409 naturalizations of 5350 unique plant species over 16 sites
dispersed globally, determining the number of sites at which each unique species occurred. We
also recorded the number of species in common between sites, grouping sites first into all
possible pairwise combinations, next into all possible triplet combinations, and finally into all
possible quadruplet combinations.

Because species naturalization is largely tabulated at the country scale, our study is at this
scale. Site selection was dictated by the availability of naturalized species lists including all
known established alien pteridophyte, gymnosperm and angiosperm species, and not restricted to
invasive pests. The 16 sites meeting these criteria and included in the study are: Chile (Castro et
al. 2005), Czech Republic (Pysek et al. 2002), Estonia (Anonymous 2007e), Galapagos (Tye
2001), Hawai’i (Wester 1992), Israel (Dafni and Heller 1990), Japan (Anonymous 2007d), Latvia
(Anonymous 2007c), New Zealand (Healy and Edgar 1980; Webb et al. 1988; Edgar and Connor
1999), Poland (Anonymous 2007b), Singapore (Corlett 1988), Swaziland (Braun), Switzerland
(Wittenberg 2005), Taiwan (Wu et al. 2004), United Kingdom (Preston et al. 2006), and
Wyoming (Anonymous 2007a). Subspecies were subsumed under the name of their parent
species in determining the number of unique species.

In order to investigate the possible effect of dispersal on the observed distributions, we
performed a Mantel test of correlation between geographical distance and number of species
shared between pairs of sites (table A1) using the R-package MANTEL module (with 9999
permutations) (Casgrain and Legendre 2001).
Observations

Three important properties were revealed by our treatment of the data. First, species naturalizations show an exponential distribution of the number of naturalized species $S(n)$ found at $n$ sites (fig. 1). To correspond to the analyses illustrated in figs. 2 and 3, the exponential is fit to $n \geq 2$ using maximum likelihood; the relationship is

$$S(n+1) = 0.59S(n) \quad \text{or} \quad S(n) = S_0 e^{-0.52n}$$

where $S_0$ is 2343 and the coefficient in the exponent (-0.52) is uniquely related to the number of naturalized species summed over sites, which we term the alien footprint, $M_1 = \sum nS(n)$ (see Appendix B).

Figure 1. Number of species as a function of number of sites. The number of naturalized species $S(n)$ falls exponentially with the number of sites $n$ at which each is found. To correspond to the analyses illustrated in figs. 2 and 3, the exponential is fit to $n \geq 2$ using maximum likelihood, with goodness of fit assessed using the appropriate one-sample $\delta$-corrected Kolmogorov-Smirnov analysis [$p > 0.20$; (Khamis 2000)].

Secondly, there is no correlation between the number of naturalized species common to a pair of sites and the separation of those sites (fig. 2). The comparison of matrices of distance between two sites and the number of species shared pairwise showed no relationship between the
two factors (p > 0.22). Some correlation might be present for distances ≤ 5000 km, but if so, it is not sufficient to affect the overall conclusion that at the global scale, the proportion of sites sharing a large number of species does not depend on distance. The number of shared species for each site-pairing are given in table A1.

Finally, the number of pairs of sites sharing a given number of naturalized species falls exponentially with the number of shared species (fig. 3a). The observed distribution is an exponential $y = 60e^{-0.01x}$, fitted to the individual values in fig. 2 using maximum likelihood, with goodness of fit assessed using the appropriate one-sample δ-corrected Kolmogorov-Smirnov analysis [p > 0.20; (Khamis 2000)]. As we show below, it is also predicted from $S(n)$, assuming only that the distribution is exponential. In particular, the coefficient in the exponent is given by the number of pairs (120) divided by what we refer to as the overlap measure $M_2 = \sum n(n-1)S(n)/2$. The exponentials illustrated in figs. 3b and 3c are similarly predicted.
Figure 3. Distribution of groups of sites over shared species. In fig. 3a the y-axis represents the number of pairs of sites sharing the number of species counted along the x-axis. The data are binned and the exponential is calculated from $S(n)$. Figs. 3b and 3c are similarly for triplets and quadruplets of sites. The ubiquity of exponentials at every level of site grouping corroborates the robustness of our findings over alternative explanations of species shared between sites (details in Appendix A: Dispersal; fig. A1).

The Model

No reasonable model of exponential attenuation of propagules spreading stepwise (through dispersal and transport) can produce the exponential distribution of fig. 1; even extremely contrived models are at odds with the lack of distance correlations shown in fig. 2 (see Appendix A: Dispersal; fig. A1). There is, however, an explanation that includes naturally the complexity of the biological world and this lack of correlation: the statistical behaviour of complex systems involving large numbers of components yields exponential distributions of the kind observed in figs. 1 and 3. Such systems function subject to certain constraints, in this case of biological or environmental origin. The techniques of statistical mechanics are mostly employed in the physical sciences but have also found some applications in ecology (Shipley et al. 2006; Pueyo et al. 2007; Dewar and Porté 2008; Harte et al. 2008). Ecologists have long been familiar with the attempt by (MacArthur 1957; MacArthur 1960) to account for species abundance distributions in terms of a statistical model known as the ‘broken stick.’ MacArthur postulated that a finite resource (the stick) is partitioned at random into a given number of pieces, taken to represent species with the abundances given by the lengths. This postulate leads to an exponential distribution of species abundance as the most probable configuration subject to those constraints and can be obtained using just the techniques we discuss below. The model is not correct for
most species abundance distributions but does serve as model for the distribution of alien species
over the sites at which they are naturalized, a very different ecological problem we enlarge on
below.

The logical structure of our investigation is that we started with the hypothesis that a simple
argument in statistical mechanics accounts for the observed exponential distribution of species
over sites. We identified the necessary general conditions and constraints and found them to
account also for the exponential distribution of pairs of sites over numbers of species held in
common (fig. 3a). We were then able to predict successfully the exponential distributions shown
in figs. 3b and c, further supporting our hypothesis of the nature of our original observation.
Below, we start with the mathematical framework of our model.

Suppose we have $S$ objects [of so far unspecified nature] assigned to classes such that the
class labelled $n$ contains $s_n$ objects. The number of ways of arranging $S$ objects over the
different classes so as to achieve a configuration $\{s_n\}$, characterised by numbers in each class
$s_1, s_2, \ldots, s_n, \ldots$ is simply

$$ W = \frac{S!}{\prod s_n!} \quad (1) $$

where $\prod$ represents the continued product.

The quantity $W$ is proportional to the probability of finding this configuration $\{s_n\}$, provided that
each arrangement has equal weight; without further conditions, every object has the same
probability of being found in every class. If this is not true, an additional weight factor can be
introduced (a prior) and the form of that prior is determined by the nature of the problem to be
addressed (Bowler and Kelly 2010; Haegeman and Etienne 2010). In statistical mechanics the
origin of such a factor is to be found in the dynamics of the system; this is further discussed (with examples) in Appendix D.

**MacArthur’s broken stick**

To match the mathematics of Eq. (1) to reality it is necessary to specify the nature of the $S$ objects and the classes labelled by $n$. In MacArthur’s broken stick, the objects are species and the class labelled by $n$ is the class of all species with population $n$ individuals (see also Pueyo et al 2007). The environmental constraints to be applied are first that there are a given number of species $S$ (the number of pieces into which the stick is to be broken) and secondly that $\sum ns_n$ is fixed – this is the length of the stick; the sum of all the pieces is equal to the original length. The most probable of the configurations $\{s_n\}$ is found by maximising (1) subject to the constraints – an operation which is mathematically well defined – where the constraints are on the number of species and available resources to be subdivided. The solution is

$$s_n = s_0 \exp(-\beta n)$$  \hspace{1cm} (2)

(the parameters of this exponential are determined by the values of the constraints; see Appendix B). If the stick is broken randomly then the distribution of species with population $n$ as a function of $n$ is exponential, provided Eq. (1) contains the essential underlying biology and the constraints are the only ones that matter in this problem. For most guilds, (2) is not an acceptable species abundance distribution (Rosenzweig 1995). The above conditions are not sufficient for this problem and indeed the papers by Pueyo et al (2007), Dewar and Porte (2008) and Harte et al (2008) are attempts to identify additional assumptions or constraints required to produce a log series distribution, and the biological nature of such additions (see Appendix D). That particular problem has been solved by Bowler and Kelly (2010).

**The distribution of species over sites**
In our problem of the distribution of naturalized species over a number of sites, the objects in Eq. (1) are naturalized species and the classes are defined by the number of sites at which a species is to be found. Thus here we identify $s_n$, general in Eq. (1), with the number of species found at $n$ sites, $S(n)$. The most probable configuration $\{s_n\}$ is obtained by maximising Eq. (1) with respect to all $s_n$, subject to conditions dictated by the nature of this problem. The first is that a given number of species $S$ is involved and the second is that the sum $\sum nS(n) = M_1$ is fixed – this is the analog of the length of MacArthur’s stick (and so must correspond to some fixed resource, over 16 sites, to be partitioned) and it is the total number of alien establishments over the 16 sites available to us. It is of such importance that we have given it a name; the alien footprint introduced earlier. When (1) is maximised with respect to all $S(n)$ subject to these constraints, the most probable distribution of species over the number of sites $n$ at which they are found is given by

$$S(n) = S_0 \exp(-\beta n)$$

(3)

The mathematical constraint on the number of naturalized establishments found in the 16 sites considered $M_1 = \sum nS(n)$, which is also the sum of site diversities, implies a biological constraint. The rate at which the exponential decreases is controlled by the mean alien footprint for these 16 sites, $\bar{n} = \sum s_n n / S = M_1 / S$, the number of sites reached averaged over all species and in (3) the value of $\beta$ is determined by the value of $1/\bar{n}$ [$\beta = -\ln(1-1/\bar{n}-1)$]; see fig. 1. [The constants $S_0$ and $\beta$ are obtained from (3) by evaluating the sums over $S(n)$ and over $nS(n)$. This is discussed in greater detail in Appendix B.]

Thus the observed exponential in fig. 1 is reproduced by two ecological assumptions. First, that the alien footprint has a fixed value (it is a conserved quantity) and the value is determined by ecological constraints. Secondly, the nature of the world is such that Eq. (1) is indeed proportional to the probability of finding some specified configuration; there is a sense in which species are equivalent. Any other ecological forces then do not affect this distribution. The origin
of the ecological forces that do fix the alien footprint has not been completely established, but
MacArthur’s idea of partitioning a limited resource is extremely suggestive. Resource availability
is limited – ultimately by the degree of insolation, water availability and CO₂ – and is reflected in
productivity. Species diversity has been shown to be highly correlated with net primary
productivity, and naturalization rates with increases in productivity over time (Woodward and
Kelly 2008). This is considered further in the discussion at the end of the paper.

There is of course nothing special about 16 sites – they were merely those for which
appropriate data were found. It should be clear that the conserved alien footprint defined above is
for that sample of 16 sites and that as time goes on the alien footprint for those particular sites
stays pretty much constant. If more sites were available the alien footprint for the larger sample
would be bigger, but would not change much with time. Thus the slope of the exponential in \( n \) is
a function of the number of sites in the sample. It would be expected that if the fractional variable
\( n/N \) is defined for the case of \( N \) sites then the mean alien footprint per site would be independent
of \( N \) and the slope of the exponential expressed as a function of \( n/N \) would not depend on \( N \). This
is not easy to test with any precision, but on selecting a random sub-sample of 8 sites from the 16
it is indeed the case that the mean alien footprint is halved and the mean alien footprint per site
remains the same. Computer simulations for the random distribution of species over sites in such
a way that (3) is satisfied yields the equivalent result for sub-samples of various numbers of sites.
Thus the mean alien footprint per site is fixed regardless of the number of sites.

**The distribution of sites over species**

Figure 3a shows the distribution of the number of pairs of sites over the number of
naturalized species common to both and is again an exponential. This distribution follows from
the subsidiary ecological assumptions that Eq. (1) is proportional to the probability of finding
some specified configuration of pairs \([ s_n \text{ in (1)}]\) over \( n \) species in common; that there is a sense in
which sites are equivalent. A constraint equivalent to the length of MacArthur’s stick is wholly
determined by the exponential distribution \( S(n) \) for \( S(n) \) species over \( n \) sites; it is that the sum of

the number of pairs with \( m \) alien species in common multiplied by that number \( m \) of common

species is constrained. This sum is easily evaluated. Pairs can be chosen from a set of \( n \) sites in

\( n(n-1)/2 \) different ways and so a species found at \( n \) sites will also be found at \( n(n-1)/2 \) pairs of

sites. Summing over all \( n \) yields a total overlap measure \( M_2 \) given by \( M_2 = \sum n(n-1)S(n)/2 \)

which counts up all pairs of sites and sums the number of common species over all pairs and is

thus the required sum. Because \( S(n) \) is already determined, \( M_2 \) is fixed, essentially by the same

biological constraints that limit \( M_1 \). The coefficient in the exponential in fig. 3a is given by the

number of pairs (120) divided by the overlap measure \( M_2 \).

Our hypotheses now allow us to predict that the distribution of triplets of sites over the

number of species common to all three will also be exponential and with parameters given by the

numbers \( S(n) \) for the distribution of species over the number of sites. The quantity

\[ M_3 = \sum n(n-1)(n-2)S(n)/6 \]

is the analogue of \( M_2 \) and is again fixed; we obtain an exponential
distribution with coefficient equal to the number of triplets (560) divided by \( M_3 \). This is shown

in fig. 3b, together with the exponential for quadruplets, with a coefficient given by the number

of quadruplets (1820) divided by the analogous moment \( M_4 \), in fig. 3c. The calculated

exponentials are again in agreement with the data and support our hypotheses.

Finally, consider the distribution of single sites over the number of naturalized species. The

mean number of species per site is given by \( M_1 / N \) \( \left( \sum nS(n)/N \right) \), the alien footprint divided by

the number of sites, and this singlet distribution is also exponential under the statistical

assumptions. With only 16 sites the distribution is not very well defined by the data, but

maximum likelihood and a Kolmogorov-Smirnov test (Khamis 2000) show them to be consistent

with being drawn from the exponential.
The distributions of sites over species and of various multiplets of sites holding species in common all contain information. The exponentials observed show that in every case the distribution corresponds to the maximum amount of missing information (the distributions most likely to be encountered) after fixing the alien footprint.

The ecological implications of the success of our assumptions in reproducing the observed distributions are first that the overlap measures $\mathcal{M}_n$ are fixed (already ensured by the form of the distribution of species over sites) and secondly that sites are (without constraints) indifferent to the classes of the number of species, pairs of sites similarly indifferent to the classes of the number of species held in common and so on; Eq. (1) is applicable to all these classes. Thus these distributions imply that sites are in some sense equivalent, just as the distribution of species over sites implies an equivalence of species.

Discussion

While it is widely observed that, in nature, species are generally restricted in distribution and relatively few species are widely distributed (Pielou 1979; Brown 1995; Gaston 2003), no definitive quantitative pattern of species distribution has previously been revealed (Gotelli et al. 2009). The number of species $S(n)$ at $n$ sites might fall with $n$ in many different ways, and the exponential observed here is new information revealing underlying processes.

The distribution of species naturalizations contains an analog of the mean energy term $kT$ in the theory of gases in the mean alien footprint per site, the number of alien establishments averaged over all species and all sites. With fixed numbers of naturalized species and of sites, increasing the mean number of sites per species ($\bar{n}$) dictates an increase in the average number of species per site; for a given number of species distributed among a given number of sites, the sum of sites over naturalized species is equal to the sum of species over sites. For naturalized species we suggest that the determinant of this fixed number of alien establishments per site, an
ecological analogue of thermodynamic temperature $T$, may be associated with productivity, in the 
light of the relationship between plant species naturalization rate and increasing net primary 
productivity (NPP) over time (Woodward and Kelly 2008). An increase in productivity would 
then increase this ‘ecological temperature,’ to produce a new most probable exponential in which 
species are found at more sites, and more species are found per site. This would be so regardless 
of whether total number of naturalized species increases or not [where species do not increase, 
the analog is heating a box of gas from outside; where species increase, an injection of hotter gas 
into the box].

The fixed nature of the number of naturalizations per site does not imply that no further 
naturalizations are possible; such an extreme interpretation is not necessary. The model is not 
likely to be perfect and the world is not likely to be in equilibrium. There are also stochastic 
effects with a small sample, such as only 16 sites. Finally, we envisage the lid on the total 
number of naturalizations being raised as global climate changes.

The relevant point is that the dynamic ‘relaxes’ rapidly into the (quasi) equilibrium 
configuration, achieving a new maximum number of species within the time scale over which 
changes in productivity occur. Evidence for this may be found in the observed exponential itself 
and, independently, in the close tracking of net primary productivity (NPP) by local (site) 
naturalization rates shown in (Woodward and Kelly 2008) using a large proportion of the data 
included here (Online Appendix C: The nature of equilibrium). In this picture biotic resistance is 
best portrayed as a moving ceiling responding to generally increasing productivity levels; the 
apparent 'failure' of biotic resistance is rather a reflection of its innate character. In such a picture 
the current escalation of species naturalizations, carrying with it potentially destructive invasive 
weeds (Rejmánek and Randall 2004; Ricciardi and Kipp 2008), will continue as long as NPP 
continues to increase, a phenomenon generally attributed to ongoing global climate change and
potentially tied into increasing levels of atmospheric carbon dioxide (Woodward and Kelly 2008).

Our central premise in obtaining the most probable distributions by maximising Eq. (1) is that, without the specified conditions, every object (species or sites or groups of sites) has the same probability of being in any class. From the observed exponential distribution of naturalized species over sites, we infer that every species in our data set has the same a priori probability of being in any class and all arrangements corresponding to a given configuration are equally probable, similarly for sites over species. One ecological model of this would be that every species is identical and further that every site is identical; the wide range of environments and species comprising our data set and the reported variety of mechanisms for individual cases of naturalisation (Mack et al. 2000; Mitchell et al. 2006) disallows this assumption.

A reasonable basis for the observed distributions and the consequent inference of independence in the action of the component species and sites is provided by the concept of idiosyncrasy (Pueyo et al. 2007). Idiosyncratic species each operate within the aegis of a unique, highly complex niche which dictates that any species plucked at random has the same probability of ending in the class characterised by that species being found at \( n \) sites. Like Hutchinson’s classic ‘\( n \)-dimensional hypervolume’ (Hutchinson 1957), idiosyncratic niches contain the full range of factors permitting a species to persist at a site, environmental conditions, competitors, consumers, infectious diseases and mutualists as well as resources. With this definition, the distribution of naturalized species over the number of alien sites reached \( (n) \) is given by an exponential once we maximise the number of equivalent configurations with Eq. (1). Similarly, the distribution of (idiosyncratic) pairs of sites over classes defined by the number of species in common is given by an exponential once the number of configurations is maximised. That potential species (and potential niches) are so varied is the underlying assumption of the
idiosyncratic model of species abundance, so that ‘the bits of information which are different in
different [ecological] models cancel out’ (Pueyo et al. 2007).

Previous applications of statistical mechanics to community assembly have focused on the
lognormal distribution of individuals over species within a guild (ecologically similar taxa) of a
single community, and so have not had information necessary to discriminate between neutral
and idiosyncratic explanations [although recent analyses have demonstrated that even highly
similar co-occurring species cannot be assumed to meet the fundamental neutrality criterion of
species interchangeability (Kelly et al. 2008; Leibold 2008; Kelly et al. 2010). The relation
between our treatment of naturalized species, (Pueyo et al. 2007), and other recent works
employing statistical mechanics in ecology (Dewar and Porté 2008; Harte et al. 2008; Bowler and
Kelly 2010) is discussed in Online Appendix D: Statistical mechanics in ecology.

Independent evidence ties our findings directly into the fundamental nature of community
assembly: free-living heteroflagellate communities show a similar exponential distribution of
species across sites (Patterson 2003), as do tree species from the tropical deciduous forest of
México (Trejo and Dirzo 2002). This is not particularly surprising: the relationship between
productivity and diversity in naturalized species reported in Woodward and Kelly (2008)
suggests general correlation of species diversity with productivity and the determinants of
productivity (Mittelbach et al. 2001; Hawkins et al. 2003; Gillman and Wright 2006; Kreft and
Jetz 2007). The natural inference is of a similarly general directionality between productivity and
diversity, an inference in accord with recent theoretical treatments relating diversity to both
complexity and productivity (Tokita 2004; Tokita 2006; Dewar and Porté 2008; Harte et al.
2008). At smaller scales, the reverse has been observed, with productivity apparently causally
affected by diversity (Flombaum and Sala 2008). Scale-dependence in the directionality of the
relationship is an intuitively satisfying integration of these differences, with productivity
determining the population process of species entry as proposed in Tilman (2004), along the
major axis of the relationship, and filtering of species (sampling) through subsequent species interactions affecting the variation at any particular point along that axis as in Flombaum and Sala (2008).

In conclusion, the primary result of our treatment of species naturalization is a new window on the fundamental processes governing community assembly and diversity – identifying the significance of the alien footprint, the implications of a causative role for productivity and the rapidity with which equilibrium species number can be reached – but it also generates subsidiary insights. Regardless of the extent to which an assumption of idiosyncrasy holds, the data of figs. 1-3 make it most unlikely that any single pronounced signature will reveal species that can easily naturalize; while there may be geographically or taxonomically local generalities, no one solution will be universal, consistent with recent reviews of empirical species’ naturalization studies (Mack et al. 2000; Mitchell et al. 2006). The implication of species idiosyncrasy also provides an explanation in the same vein for the general observation that the majority of species have a restricted distribution and few species are widespread over many sites; this pattern is an emergent property deriving from the fundamental nature of niches themselves, and does not require the operation of any particular trait of any specific niche (cf. Brown 1984; Brown 1995). We have shown here a quantitative [exponential] character to that general observation, making possible an analytical tool carrying with it a degree of rigor not previously available to the comparative study of species’ distributions.

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### Supplementary Table 1. Number of species shared between sites.

Authors can be found in Literature Cited section of the main text.

|                | Chile | Czech Republic | Estonia | Galapagos | Hawai‘i | Israel | Japan | Latvia | New Zealand | Poland | Singapore | Swaziland | Switzerland | Taiwan | UK |
|----------------|-------|-----------------|---------|-----------|---------|--------|-------|--------|-------------|--------|------------|-----------|-------------|--------|----|
| Chile          | 0     | 225             | 0       | 0         | 0       | 0      | 0     | 0      | 0           | 0      | 0          | 0         | 0           | 0      |    |
| Czech Republic | 0     | 225             | 0       | 0         | 0       | 0      | 0     | 0      | 0           | 0      | 0          | 0         | 0           | 0      |    |
| Estonia        | 0     | 0               | 100     | 372       | 0       | 0      | 0     | 0      | 0           | 0      | 0          | 0         | 0           | 0      |    |
| Galapagos      | 0     | 0               | 22      | 47        | 21      | 0      | 0     | 0      | 0           | 0      | 0          | 0         | 0           | 0      |    |
| Hawai‘i        | 0     | 0               | 128     | 147       | 62      | 99     | 0     | 0      | 0           | 0      | 0          | 0         | 0           | 0      |    |
| Israel         | 0     | 0               | 28      | 44        | 24      | 19     | 41    | 0      | 0           | 0      | 0          | 0         | 0           | 0      |    |
| Japan          | 0     | 0               | 248     | 413       | 211     | 68     | 25    | 52     | 0           | 0      | 0          | 0         | 0           | 0      |    |
| Latvia         | 0     | 0               | 75      | 299       | 340     | 15     | 47    | 21     | 162         | 0      | 0          | 0         | 0           | 0      |    |
| New Zealand    | 0     | 0               | 294     | 442       | 256     | 55     | 264   | 42     | 479         | 199    | 0          | 0         | 0           | 0      |    |
| Poland         | 0     | 0               | 33      | 188       | 142     | 9      | 28    | 12     | 78          | 127    | 94         | 0         | 0           | 0      |    |
| Singapore      | 0     | 0               | 7       | 10        | 3       | 27     | 57    | 10     | 61          | 3      | 18         | 3         | 0           | 0      |    |
| Swaziland      | 0     | 0               | 43      | 54        | 30      | 48     | 94    | 28     | 89          | 23     | 14         | 17        | 0           | 0      |    |
| Switzerland    | 0     | 0               | 48      | 189       | 118     | 13     | 43    | 16     | 114         | 98     | 146        | 78        | 0           | 21     | 0   |
| Taiwan         | 0     | 0               | 59      | 81        | 40      | 57     | 158   | 31     | 197         | 24     | 103        | 17        | 54          | 62     | 23  |
| UK             | 0     | 0               | 134     | 487       | 295     | 34     | 109   | 35     | 281         | 207    | 437        | 129       | 4           | 56     | 168 |
| Wyoming        | 0     | 0               | 103     | 147       | 106     | 8      | 68    | 7      | 160         | 94     | 164        | 27        | 1           | 15     | 34  |
|                |       |                 |         |           |         |       |       |        |             |        |            |           |             |        |    |
Appendix A. Dispersal

Failure of models involving attenuation with distance.

It is natural to think of dispersal by diffusion as limiting the distance travelled by propagules and hence the number of sites reached. For a given diffusion parameter, the probability of a propagule ending up a certain distance $R$ from the source is a normal distribution. In two dimensions were all sites (or a fixed proportion thereof) within a circle of radius $R$ to be captured by a species ending up at $R$, then an exponential as in Figure 1 would in fact be generated, but the number of pairs of sites sharing a species would decrease rapidly with the separation of the members of the pair. In fact the idea that all sites within a circle of radius $R$ be captured is a red herring. In a random walk the number of sites visited on average grows almost linearly with the number of steps allowed (which corresponds to the diffusion parameter) and many of these sites are outside the circle possessing the final radius, the average value of which grows only with the square root of the number of steps. Fluctuations about the mean number of sites visited for a fixed number of steps cannot generate the desired exponential. Dispersal by diffusion is incapable of reproducing the data of fig. 1 (unless the number of steps allowed is exponentially distributed; see below), and cannot generate anything resembling fig. 2.

As an alternative, consider a process in which propagule drift is all one way and accidents attenuate the flux of propagules exponentially with distance. Each site a propagule passes is adopted but once a propagule suffers an accident it goes no further. This model is not realistic but was contrived to generate an exponential dependence (as in fig. 1) on $n$ of the probability of $n$ sites being taken. This it will do, provided the probability of getting from site $n$ to site $n+1$ is some universal constant $x$ (in an explicitly spatial picture this would correspond to successive sites having a fixed separation). Thus the probability of reaching site $n+1$ is conditional on the probability of site $n$ having already been reached and an equation of the form given in the caption to fig.1 results [where the value of $x$ is 0.59]. Because very few propagules make – say – 15 steps the probabilities of distances between species being above 10 units are very small in comparison with the probabilities of gaps of a few units only; quite unlike fig. 2. The number of species found at two sites separated by distance $d$ inevitably falls with $d$. It is easily shown that the number of pairs of sites separated by $d$ (integer) units falls as the factor $x^d$ an exponential.

It is not necessary in the above scenario for propagules to travel in straight lines, merely that each link is of constant length. An illustration of the problem is provided by fig. A1a, b. To make these figures we used a combination of random walk in two dimensions and attenuation, but attenuation is the driving feature. Species were launched on a two dimensional grid and executed a random walk of $D$ steps, where $D$ was chosen at random for each species from the same exponential probability distribution. For each species any site visited once or more was counted as taken; the origin could be crossed but not taken (because there the species would not be alien). Fig. A1a displays a good exponential – which it should because the model was designed to do just that. The distribution of pairs of sites as a function of their separation was calculated and the analogue of fig. 2 is shown in fig. A1b, quite unlike fig. 2. In both there are pairs of sites with several hundred species in common, but these are only closely separated in fig. A1b. The clusters of points at separations given by the lengths of the hypotenuse of right angled triangles with two integer sides is a reflection of the geography of our unrealistic two dimensional world, just as the vertical stripes in fig 2 reflect the geography of our planet. The observations summarised in figs.
1 and 2 can hardly have been generated by any kind of dispersal mechanism involving decreasing probability with distance.

![Graph of species distribution](image1.png)

**Figure A1.** Patterns expected from a diffusion process.  

- **a.** Distribution of number of species as a function of number of sites. The width of the exponential is set by a single species found at 19 sites.  
- **b.** Number of species shared pairwise between sites relative to distance between sites. Compare with the actual data shown in fig. 2 in the text.

To generate an exponential distribution of species with the number of sites reached the spread must proceed stepwise, with a single probability of each step or link in the propagation chain failing. It is not necessary that each step is over the same distance and if this is not the case the lack of correlation in fig. 2 may be less of an objection. However, abandoning that assumption does not increase the plausibility of this already highly contrived model. If species can easily reach sites at antipodes (as they can; fig. 2, table A1) and steps can be very long, propagation by a number of sequential steps is even more artificial. (Wyoming and New Zealand were both colonised from Western Europe; NZ was not colonised by settlers from Wyoming.) It is more
realistic to consider spread of a species from its homeland to sites at which it is an alien in a
number of independent steps, perhaps along trade routes ancient and modern.

\textbf{A single step approach.}

In a picture with independent single steps, species are launched a number of times and have a
certain fixed probability of hitting a target (an alien site at which a species becomes established).
The simplest version, that probability would be independent of species and of site, will not
produce the simple pattern observed. This is again a mechanistic model, but distances do not
enter explicitly. After a possibly large number of attempts, let the chance of a single species
having achieved one or more hits on any given target be \( p \), with \( N \) target sites. Then the
probabilities of a species occupying 1, 2, 3, … \( n \) sites are given by successive terms in the
binomial expansion

\[ P(n) = p^n (1 - p)^{N-n} \frac{N!}{(N-n)!n!} \]  

and the features of this distribution are entirely different from the exponential in \( n \) which is
observed. The model described in this section is ludicrously simple because the same probability
\( p \) has been taken for each species and every target. If instead different values are possible for
each species on every site the possibilities are enormously increased and this of itself suggests a
statistical approach, necessarily involving the complexity of the biological world. Simple
mechanistic explanations do not lead to any acceptable explanations of our observations.

\textbf{Appendix B. Maximization subject to constraints and determination of parameters}

The problem we have is to maximise the weight given by eq (1) of the text, subject to constraints.
This outline of the general case may help the reader to perceive the analogy between our
ecological problem and the statistical mechanics of gases. The function to be maximised is

\[ W = \frac{S!}{\prod s_n!} \]

with respect to all \( s_n \), subject to constraints. The first constraint simply imposes the condition that
we are working with a fixed number of objects, be they atoms or species. This condition is

\[ G(s_n) = \sum s_n - S = 0 \]

This is a zero order moment; the next condition is a first order moment. If the objects labelled by
\( n \) have some attribute which we denote generally by \( A_n \), then a second constraint which might
apply is

\[ H(s_n) = \sum s_n A_n - A = 0 \]

These two constraints would determine the average value of the attribute \( A \). In the statistical
mechanics of gases \( A \) is the total energy of the \( S \) atoms. (Higher order moments can be introduced
as constraints in the same way; we do not need to go further.)
It is convenient to maximise the function

\[ F(s_n) = \ln(W) \]

rather than \( W \) itself and the necessary condition to be satisfied for all \( s_n \) is

\[ \frac{\partial F}{\partial s_n} + \lambda \frac{\partial G}{\partial s_n} + \mu \frac{\partial H}{\partial s_n} = 0 \]

The quantities \( \lambda \) and \( \mu \) are at this stage undetermined but for non zero values impose the constraints. An elegant explanation of the principles behind the use of these Lagrangian multipliers may be found in appendix C.13 of Blundell and Blundell (2006).

Expanding the logarithms of the factorial functions using Stirling’s theorem, the condition for an extremum under constraints becomes

\[ \frac{\partial F}{\partial s_n} + \lambda + \mu A_n = 0 \quad \text{whence} \quad \ln s_n = \lambda + \mu A_n \]

and the exponential dependence of \( s_n \) on the attribute \( A_n \) follows.

In the statistical mechanics of gases, the number of atoms in a level of energy \( E_n \) decreases exponentially with that energy (the Boltzmann distribution). In the problem of the distribution of species over sites the \( s_n \) are the number of species \( S(n) \) in a class defined by a species being at \( n \) sites; the attribute is \( n \). Thus there are 873 at 2 sites, 184 at 5 sites and so on down to 1 species at 13 sites.

If the first moment of \( S(n) \), \( \sum nS(n) \) is constrained and the number of complexions maximised subject to this constraint, then an exponential distribution of \( S(n) \) over \( n \) results

\[ S(n) = S_0 \exp(-\beta n) \quad (A2) \]

where \( \beta \) is an undetermined multiplier. However, both the normalising constant \( S_0 \) and the constant \( \beta \) are determined by the total number of species and the value of the first moment.

Suppose we carry out summations from \( n = 1 \) to infinity – we have no information on what \( S(0) \) might be or even how meaningful it is. Then we define

\[ S_i = \sum S(n) \quad F_i = \sum nS(n) \quad (A3) \]

For a given number of species and given values of the number of species at each number of sites, these numbers can be calculated from the data without any assumption about the shape of the distribution. For the data collected for alien species the numbers are respectively 5350 and 10409.
The mean number of sites per species is given by \( n_1 = F_1 / S_1 \) and is, from the above numbers, 1.946 sites per species.

Now substitute the expression (A2) into eqs (A3). The sums can be calculated very simply (these are essentially sums over geometric series) and the following results are mathematically exact.

\[
S_1 = S_0 \exp(-\beta) / (1 - \exp(-\beta)) \\
F_1 = S_0 \exp(-\beta) / (1 - \exp(-\beta))^2
\]

and hence \( n_1 = 1 / (1 - \exp(-\beta)) \). The data are best represented here by an exponential for \( n \) greater than or equal to 2 and fig. 2 is restricted to \( n \geq 2 \).

Therefore define

\[
S_2 = \sum S(n) \\
F_2 = \sum nS(n)
\]

The numbers from the data are 2049 and 7108 respectively. The ratio \( n_2 = F_2 / S_2 \) is 3.47.

We can of course substitute (A2) into equations (A4) and calculate \( \beta \) in terms of the new average \( n_2 \). The calculations are again simple sums of series and the result is that \( \beta = -\ln(1 - 1/(n_2 - 1)) \).

The normalising constants are also easily calculated in terms of the sums. The exponential best fitted to the data points at \( n=2 \) and greater has \( \beta = 0.52 \) and the constant \( S_0 = 2343 \).

Appendix C. The nature of equilibrium

The distribution of species over the number of sites is exponential, as is the distribution of pairs of sites over the number of species in common. These exponentials are the most probable configurations subject to the relevant constraints. Most probable configurations correspond to the notion of equilibrium; once a system is in the vicinity of this configuration it is very unlikely to depart substantially from it.

The existence of such an equilibrium merely dictates an exponential distribution of alien species over the number of sites. It does not specify which species are found at 8 sites or anything of that kind – it does not even require that the same species are found at 8 sites at all times (atoms hop in and out of energy levels). Still less does this equilibrium require that the populations of alien species are unchanging; only the presence of a certain number of species at a certain number of sites.

It is particularly interesting that alien species have reached configurations close to equilibrium and quite quickly at that. Probably a global equilibrium with a single global ecotemperature is an oversimplification, but the data are close. Insofar as the role of human activity is concerned, this would reduce the relaxation time rather than determine the distribution. An analogous process is bringing boxes of gas at differing temperatures into better thermal contact.

Appendix D. Statistical mechanics in ecology.

Statistical mechanics, maximum entropy and ecological guilds
There have been several recent papers applying methods, similar to ours, from statistical mechanics to the structure of ecological guilds. The work of (Pueyo et al. 2007) derives the whole family of species abundance distributions from very few assumptions. The first is their idiosyncratic assumption: that every species is different (the antithesis of the assumptions of neutral models). The second is concerned with the statistical properties of large ensembles of complex ecological models; that the species abundance distribution can be obtained by applying the principle of maximum entropy so as to obtain a probability distribution for species abundance which contains minimal information (maximum entropy). In statistical mechanics this is a very likely configuration because it can be obtained in a vast number of ways – if the system explores these possibilities. [The problem is initially set up in terms of combinatorics, as in eq (1) in the main body of this paper. This formulation sheds particular light on the role of a priori probabilities (see below).] An important element is that rather than the entropy of information theory, a quantity called the relative entropy is maximised, which requires the introduction of a ‘prior’ (Jaynes 1968; Jaynes 2003) – this is equivalent to discarding the assumption that every species has the same a priori probability of having any abundance. The maximisation is subject to two constraints: first that the probability is normalised to unity and secondly that a mean of the number of individuals \( n \) is constrained [as in MacArthur’s broken stick model for species abundance (MacArthur 1960; Etienne and Olff 2005)]. The solution is then

\[
P(s_n) = P_\pi(n) e^{-\beta n} \quad (A5)
\]

where \( P_\pi(n) \) is the ‘prior’ relative to which the entropy is maximised; an a priori probability that must be applied before maximising the purely combinatorial weight, or maximising entropy. (Pueyo et al. 2007) imposed not the commonly employed uniform prior [corresponding to both MacArthur’s model (MacArthur 1960) and the statistical mechanics of gases (Bowler 1982)], but rather

\[
P_\pi(n) = \frac{A}{n} \quad (A6)
\]

where \( A \) is a constant. The prior is chosen before the total number of individuals is specified and Pueyo et al argued that this choice of prior is correct for species abundance distributions because it is in a certain sense scale invariant and in consequence contains no information on the geographic scale or sample size (Pueyo et al. 2007).

The result of the particular choice (A6) is the famous log series expression

\[
P(s_n) = \frac{A e^{-\beta n}}{n} \quad (A7)
\]

This choice of prior corresponds to equal intervals of log \( n \) being equally probable a priori. If the relative entropy is maximised subject to an additional condition on the mean value of log \( n \) then the result is

\[
P(s_n) = \frac{A e^{-\beta n}}{n^b} \quad (A8)
\]
and if a constraint is also applied on the average value of \((\log n)^2\) then a skewed log normal distribution results. We note here that (A7) is a particular member of the family of solutions (A8), as indeed is the broken stick solution of (MacArthur 1960).

The paper of (Dewar and Porté 2008) is similar in a number of respects. Again the relative entropy is maximised, but in this case the prior is taken as

\[
P_x(n) = \frac{A}{n + 1}
\]  

\text{(A9)}

Their motivation for this choice of prior is again that it in some sense contains the least information, but their criterion is drawn from coding theory rather than scale invariance.

Naturally a species abundance distribution close to the log series results.

Finally, the recent paper of (Harte et al. 2008) applies more constraints. In addition to the number of species and the total number of individuals in the guild being fixed, a measure of total metabolic rate is also taken as constrained. Their treatment employs a joint probability function \(R(n, \varepsilon)\); the probability of a species having \(n\) individuals and of an individual having energy requirement \(\varepsilon\). A uniform prior is assumed and the entropy maximised to yield this function. Integration over the continuous variable \(\varepsilon\) then results in a log series species abundance distribution.

**Maximum entropy, priors and alien species**

The principle of maximum entropy is used in more than one way, mathematically equivalent but different in interpretation. If all that is known of a function is the values of certain moments, then maximising the entropy subject to these constraints minimises the information contained in the resulting function, thus yielding the least biased estimate of the probability distribution consistent with limited information. In the statistical mechanics of gases the problem is different. The number of atoms in a box is known to be constrained by physics (impermeable walls) and the mean energy is known to be constrained (adiabatic walls and conservation of energy).

Application of maximum entropy yields the most probable distribution consistent with these constraints (the Boltzmann distribution). Here the constraints are real as opposed to being the result of inadequate information.

The role of a prior distribution is clear enough when it is used to incorporate already existing information and need not be mysterious. In the kinetic theory of gases each state with energy \(E_n\) has occupation given by eq (2) of the text, but if there are \(g_n\) different quantum states with this same energy, then the number of atoms with energy \(E_n\) is eq (2) multiplied by the degeneracy factor \(g_n\). The degeneracy factor plays the role of a prior [see for example (Bowler 1982)] and in this context pre-dates information theory. (Pueyo et al. 2007) and (Dewar and Porté 2008) appealed to principles of minimum knowledge for their priors (Pueyo et al. 2007), but in statistical mechanics one expects to see machinery driving the choice of prior. We note that the model of Harte et al (2008) contains a concrete realisation equivalent to the prior of Pueyo et al (2007). The complexity model of (Tokita 2004; Tokita 2006) is rather successful at producing species abundance distributions and the last equation on page 122 of (Hubbell 2001) contains factors which are identical to the prior of Pueyo et al. (2007), yet reached from a very different
argument. The origin of the prior of Pueyo et al (2007) has in fact been traced to a specific piece of biological machinery. This is the fundamental biological processes of the birth and death of individuals, so that a species with $n$ individuals exits that class at a rate proportional to $n$ (Bowler and Kelly 2010). Thus the prior of Pueyo et al (2007) is correct for species abundance distributions but need not apply to the distribution of alien species, a very different ecological problem.

In our application of statistical mechanics to naturalised species, we know not only the mean value $\bar{n}$ but also that the distribution is exponential. We do not need to estimate a distribution by using maximum entropy. All we need is the knowledge that with a uniform prior [the weight in eq (1) correctly representing probability] an exponential results if that mean value is determined by the properties of the world in which these species find themselves. This is in accord with the absence of any identifiable mechanism that could bias the probabilities of the $s_n$, a priori.

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