Punctuated equilibrium as an emergent process and its modified thermodynamic characterization

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ABSTRACT

We address evolutionary dynamics and consider under which conditions the ecosystem interaction network allows punctuated equilibrium (i.e., alternation between hectic and quasi-stable phases). We focus on the links connecting various species and on the strength and sign of those links. For this study we consider the Tangled Nature model, which allows considerable flexibility and plasticity in the analysis of interspecies interactions. We find that it is necessary to have a proper balance of connectivity and interaction intensities so as to establish the kind of mutual cooperation and competition found in nature. It suggests evolutionary punctuated equilibrium as an *emergent* process, thus displaying features of complex systems. To explicitly demonstrate this fact we consider an extended form of thermodynamics, defining (for the present context) relevant out-of-equilibrium "collective" functions. We then show how to characterize the punctuated equilibrium through entropy-like and free energy-like quantities. Finally, from a close analogy to thermodynamic systems, we propose a protocol similar to simulated annealing. It is based on controlling the species' rate of mutation during the hectic periods, in this way enhancing the exploration of the genome space (similar to the known behavior of bacteria in stressful environments). This allows the system to more rapidly converge to long-duration quasi-stable phases.

1. Introduction

The dynamics of living systems generally takes place at different hierarchical scales (Anteneodo and da Luz, 2010). As a result, evolutionary processes are usually studied on distinct levels: microevolution, associated with changes observed at the scale of individuals; and emergent macroevolution, patterns observed at large, say, meta-population, scales. On the one hand, the interactions between species, the resources available from the environment, and occasional genetic mutations control microevolution dynamics (Hendry and Kinnison, 2001) at short and intermediate times (on the order of generations). On the other hand, for an ecosystem as a whole, macroevolution determines (on longer time scales) the distribution of species, regarding their formation, extinction, and diversification (Maruvka et al., 2013). Empirically, data sources for macroevolution are mainly supplied by fossil records (Raup and Sepkoski, 1986), providing the fundamental link from modern taxa to ancient evolutionary mechanisms. For instance, fossil records are useful to investigate the origin of optimal foraging strategies (Sims et al., 2014) and to identify certain cycles in extinction processes (Lieberman and Melott, 2007).

Nonetheless, the connection between macroevolution and micro-

evolution is far from being completely understood. Fossil records do not support gradual transitions of species in time, something that might have been expected from natural selection rules at the scale of individuals (Gingerich, 2001; Reznick and Ricklefs, 2009; Simons, 2002). In fact, the creation and annihilation of species is not a steady (or even stable) process (Martín et al., 2015). Data seem to indicate that long term evolution is characterized by bursts of high evolutionary changes followed by metastable configurations (Solé et al., 1997, 1999). Such intermittency is known as *punctuated equilibrium* (Gould and Eldredge, 1977), with the punctuation corresponding to high activity (hectic) phases followed by periods of stasis.

The (minimal) necessary (Newman et al., 1985) mechanisms behind punctuated equilibria is a topic of intense debate. Proposals range from the occurrence of rare events, like meteor impacts (Raup and Sepkoski, 1984), to intrinsic nonlinear dynamics promoting self-organized criticality (Bak et al., 1988; Solé et al., 1997). Interestingly for the latter possibility, one does not need an intricate set of rules – i.e., involving inter-relations among the elements of the system – to produce punctuated equilibria (Bak and Boettcher, 1997; Paczuski et al., 1996). But despite much work, it is still not clear whether nature *does require* special events (like drastic climate change, Fischer, 1986)

or whether the phenomenon could arise from emergent dynamics alone. In fact, in certain instances it may be necessary to include both catastrophic and emergent factors (Brussate et al., 2015). Thus given the many open issues related to the microevolution/macroevolution interplay (Arnold et al., 2001; Futuyma and Agrawal, 2009; Reznick and Ricklefs, 2009), general conceptual frameworks and proper mathematical descriptions (Alicea and Gordon, 2014; Pennell et al., 2015) are essential in trying to characterize macroevolution and the underlying punctuated equilibria. As put in Alicea and Gordon (2014), although constituting simplifications of the actual problem, models must "attempt to retain major essential features of evolution, bridging the gap between empirical reality and formal theoretical understanding".

There is no doubt that the interaction network plays a fundamental role, accounting for the positive and negative interactions driving the coevolution of species (Bascompte et al., 2006) (e.g., on smaller time scales being related to the stability of communities, Thébault and Fontaine, 2010). But the actual portrayal of these networks is difficult because of the large number of elements and influences (and which can change in time) and the difficulty of quantifying their interaction strengths (Ings et al., 2009). Also, observation of extensive food web data has revealed small world properties, like high clustering and power-law scaling (Montoya and Solé, 2002). These features make the general characterization of connections along the network extremely laborious. Hence, in this context legitimate evolutionary models – specifying the essential interactions between the individuals and the environment through a set of laws establishing time evolution – become relevant. The interaction distribution (which can be regarded as related to food chains and other biological pressures, describing mutually beneficial, antagonistic and neutral relationships) as a function of time should unveil the system properties, like survival, stability, and the possibility of alternation between evolutionary states.

Here we analyze two of the most important interaction network features, the distribution of links and the strengths along those links. To do this, we consider the plastic Tangled Nature model (TNM) (Christensen et al., 2002; Hall et al., 2002; di Collobiano et al., 2003) used in evolutionary ecology. In the present context the TNM is useful because of two of its essential technical aspects: the general way the TNM handles the interaction network and its flexibility in allowing changes in the network links during time evolution.

We systematically study the conditions for punctuated equilibrium. As one would expect, the configurations yielding such behavior are akin to those already discussed in Christensen et al. (2002), Hall et al. (2002), and di Collobiano et al. (2003). But we further examine why punctuated equilibrium is partially or totally lost when one has too many or too few connections as well as too strong or too weak interactions. We find that punctuated equilibria stem from a balance in the number and magnitude of the interspecies interactions. Hence, the "punctuation" takes place only when the interaction network displays proper structure.

Specifically, since it is known that a key component for maintaining quasi-stable periods is mutual cooperation, we calculate the number of possible combinations of mutually cooperative pairs in the TNM interaction matrix and show that the system performs an exhaustive search for 'harmonious' pairs during a hectic period. The search may not succeed if the interaction network is weak and no quasi-stable phases of large diversity can emerge. In the opposite extreme, overly correlated networks can lead to punctuated equilibrium, but then diversity is affected in a drastic way: few species occur, and they account for almost all individuals in the population. As for the network connections, a high average number of links strongly abbreviates the quasi-stable phases. Conversely, interaction networks with a low number of links cannot display punctuated equilibrium. Moreover, there is a critical value for the mean number of links below which the system goes quickly to extinction. These facts, which seem decisive for long term stable ecosystems, agree with works pointing to the necessity

of diversity in the distribution of interactions for community stability (Paine, 1980; Mougi and Kondoh, 2012) as well as with an analysis demonstrating the essential role played by the network architecture (Thébault and Fontaine, 2010).

The above results indicate that punctuated equilibrium can be characterized as an emerging behavior.[1] This leads to our second principal finding: we characterize punctuated equilibrium as a collective process by drawing parallels between micro/macroevolution and statistical mechanics/thermodynamics. But to do so we must recall that evolution is not an equilibrium phenomenon (Goldenfeld and Woese, 2011), being closely related to the concept of complex systems (see Anteneodo and da Luz, 2010; Viswanathan et al., 2014 and references therein). Hence, we shall borrow ideas and methods from thermodynamics, but not using its standard formulation. Thus, we consider modified definitions of mesoscopic energy-like, entropy-like and temperature-like quantities, which are neither extensive nor intensive. We examine their behavior and verify that they are able to identify the hectic phases, qualitatively differentiating the bursts from the metastable periods. This is an evidence of punctuated equilibrium as composite dynamics, typical of complex systems.

Finally, by further exploring this thermodynamic association we address a possible mechanism for speeding the formation of quasi-stable periods. We suppose the system somehow can induce itself into an annealing-like (Kirkpatrick et al., 1983) condition.[2] In the TNM, this is accomplished by increasing the mutation rate according to a time-dependent protocol. The results clearly show that control of the mutation rate can improve the effective exploration of the genotype space, accelerating the finding of cooperative pairs (or larger combinations) when compared to a constant mutation rate. As we will discuss, this agrees with the empirical evidence that changes in the mutation rate of bacteria do occur when the population is adapting to a new environment (Sniegowski et al., 1997; Giraud et al., 2001) or when the organisms are subjected to adverse conditions (Earl and Deem, 2004), such as the stress of climate change.

2. Methods

Statistical mechanics—originally viewed as the microscopic theory supporting macroscopic thermodynamics (Viswanathan et al., 2014)—is concerned with systems having a large number of interacting parts. Its goal is to describe global emergent patterns through sets of rules governing only the individual units (an example being spin glasses, a simple system with many applications (Stein and Newman, 2013). The resemblance of macroevolution 'motifs' to typical problems in statistical mechanics has inspired distinct models connecting micro (the single constituent) to macro (the whole structure) evolution. The Bak and Sneppen model (Bak and Sneppen, 1993) is popular in the literature for producing an emergent self-organized state with avalanches of extinctions alternating with coevolution of species, the hallmark of punctuated equilibria. The so-called NKC model of Kauffman and Johnsen (1991) introduces the concept of a dynamically evolving fitness landscape that also gives rise to punctuated equilibria. Both the NKC and the Bak–Sneppen models extend complex-system ideas to ecological processes and are frequently taken as the basis for developing new models of evolution (for a review see Drossel, 2001 and references therein).

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[1] This suggests that interaction networks are themselves subject to evolutionary pressure. Presumably the resultant architecture is one that allows recovery – maintaining a significant degree of biodiversity – once the system falls into a state of low diversity (Sun and Kim, 2011; Barraclough, 2015).

[2] From a statistical physics point of view, annealing is the procedure of increasing system temperature followed by gradual lowering, so that it can more easily make an excursion in phase space, escaping from local high entropic barriers. In real macroscopic thermodynamic systems, annealing can lead to homogenization and stabilizing of certain phases of matter.