RESEARCH ARTICLE

Natural Networks as Thermodynamic Systems

TUOMO HARTONEN[1] AND ARTO ANNILA[1,2,3]

[1]Departments of Physics and Applied Physics, Aalto University School of Science and Technology, Aalto FI-00076, Finland; [2]Institute of Biotechnology, University of Helsinki, Helsinki FI-00014, Finland; and [3]Department of Biosciences, University of Helsinki, Helsinki FI-00014, Finland

Received July 21, 2012; revised September 6, 2012; accepted September 19, 2012

Natural networks are considered as thermodynamic systems that evolve from one state to another by consuming free energy. The least-time consumption of free energy is found to result in ubiquitous scale-free characteristics. The network evolution will yield the scale-independent qualities because the least-time imperative will prefer attachment of nodes that contribute most to the free-energy consumption. The analysis of evolutionary equation of motion, derived from statistical physics of open systems, reveals that evolution of natural networks is a path-dependent and nondeterministic process. Despite the noncomputability of evolution, many mathematical models of networks can be recognized as approximations of the least-time process as well as many measures of networks can be appreciated as practical assessments of the system's thermodynamic status. © *2012 Wiley Periodicals, Inc. Complexity 00: 000–000, 2012*

Key Words: entropy; evolution; free energy; natural process; noncomputable; power law scaling; scale-free; statistical mechanics; the principle of least action

1. INTRODUCTION

It is a striking observation that diverse networks are all similar in their principal properties, i.e., scale-free characteristics are ubiquitous [1]. Biological networks, e.g., metabolic [2], gene and protein regulatory networks [3], and cognitive [4,5] and population networks [6] just as infrastructures of socioeconomic systems [7–9] display power laws [10]. Likewise, power laws dominate degree distribution of interaction networks of physical systems [11] that range from Bose–Einstein condensates [12] to percolation of galaxies [13].

The universal network characteristics imply to us that proportionate progression by preferential attachment [7,14] could be regarded as a natural process, i.e., a manifestation of the supreme law of nature. This profound principle is not a mystery but known by many names, best as the principle of least action [15] and the second law of thermodynamics [16]. Also the maximum power principle [17], Yule's process for cumulative advantage [18] and evo-

PACS number(s): 89.20.-a, 89.65.-s, 89.70.-a, 89.75.-k
Correspondence to: Arto Annila, Department of Physics, POB 64, University of Helsinki, Helsinki FI-00014, Finland; Email: arto.annila@helsinki.fi

DOI 10.1002/cplx.21428
Published online in Wiley Online Library (wileyonlinelibrary.com)

lution by natural selection [19] can be recognized as accounts of the probable processes that consume free energy in the least time [20,21].

Considering the irrefutable imperative in energy transduction, it is only natural that numerous networks in nature display the scale-free and nondeterministic characteristics of the least-time free energy consumption. Indeed, the principle of least-time has already been used for a long time to describe nature so that its processes will pursue the paths among alternatives which are the most economical in terms of work [22,23]. Yet, when describing complex systems, the variational principle is usually stated in the form of Lagrangian rather than in its original form given by Maupertuis [15]. Lagrange's form describes systems whose energy is conserved whereas Maupertuis' form accounts for evolving systems that either acquire energy from their surroundings or expel energy to their surroundings systems. Consequently, we argue that Maupertuis' form of the equation of motion is the appropriate one to describe evolving natural networks as energy transduction systems.

Objectives of network theory are to model and characterize networks and eventually also to provide quantitative predictions of network evolution [24]. In contrast, our objective is to describe evolving natural networks in thermodynamic terms to understand why certain models and distributions as well as measures that are used in the network theory are so successful in reproducing evolutionary courses and characteristics of natural networks. Specifically, we will analyze the natural law in the form of equation of motion to draw conclusions from where the universal network qualities emerge. In this way, we hope to communicate why the prominent patterns of networks are found throughout nature.

2. NATURAL PROCESSES

The essence of physics is to subsume specific details of distinct systems into universal principles that comply with conservation laws. To this end, the principle of least action, in its holistic form given by Maupertuis [15], describes a system that evolves from one state to another within its surrounding systems by consuming free energy in least time. The old principle states that driving forces of evolution are differences in energy that will level off as soon as possible. This will happen when flows of energy vary their paths and naturally select to direct from highs to lows along the paths of highest throughputs. These least-time paths on curved energy landscapes are known as geodesics [19,21]. The irrevocable least-time consumption of free energy results in sigmoid courses of growth or decline as well as skewed, nearly log-normal distributions [25–28]. Also oscillatory, chaotic and nondeterministic behavior [29–31] as well as power-law scaling and branching are qualities of natural systems [32–37] that emerge from the universal quest for the least-time energy dispersal [38,39].

The notion of a network is a powerful way to portray an energy transduction system. Physically speaking, nodes represent repositories of potential energy and links correspond to paths for flows of energy. We find this association of a physical network with its graphical representation motivated, because all systems must embody at least one quantum to exist. Moreover, the presentation of a network as a physical system ensures that energy is conserved and causality is respected. A flow of energy along a link stems from one node upstream that has opened itself up and expelled at least one quantum. The quantum will eventually be captured by another node downstream as it closes to a new stationary-state action. Thus, according to the adopted physical perspective given in mathematical forms below, natural networks will emerge from and evolve in their surroundings in the quest for the least-time consumption of free energy.

The driving force of evolution composes, in terms of physics, differences in scalar and vector potential, e.g., between chemical potentials and light. From this thermodynamic viewpoint, an evolving network will naturally prefer those attachments that will further the most effective free energy consumption. This least-time imperative, as we will show by analysis below, gives rise to the scale-free characteristics.

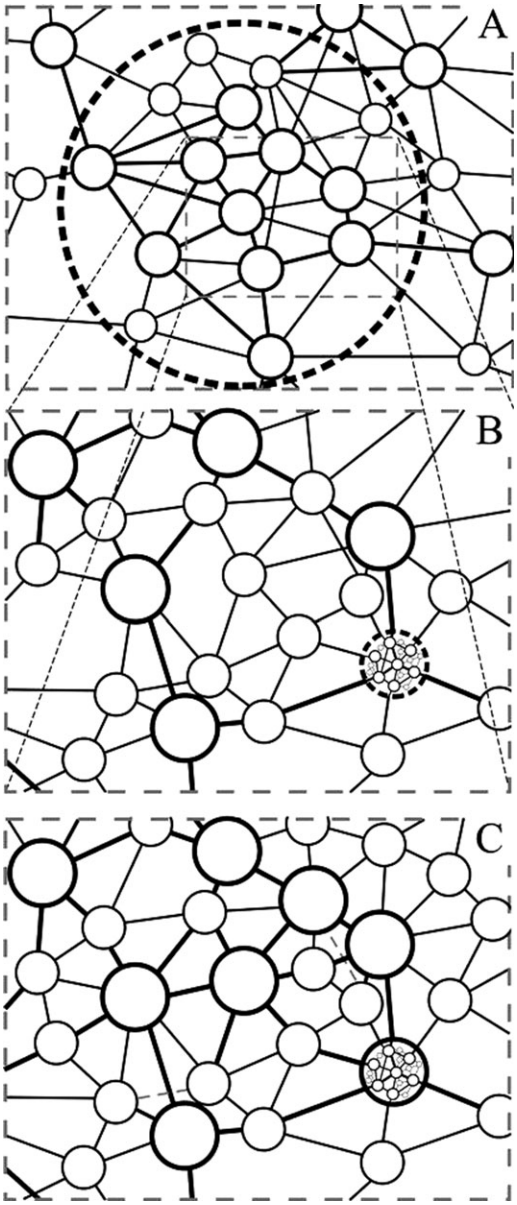
The origin of scale-independent and noncomputable characteristics of natural networks will become apparent when the evolutionary equation of motion for the least-time energy dispersal is formulated and analyzed. To this end following notation is introduced. In the context of network theory, each node of a particular network as well as of any surrounding network is regarded as a quantized repository of energy. In accordance with chemical thermodynamics the node is indexed with j and assigned with energy density $\phi_j = N_j \exp(G_j/k_B T)$, where N_j denotes the number of constituents (quanta) associated with scalar potential G_j relative to the average energy density $k_B T$ per node of the network system [40]. As the components N_j of the j-node are explicitly denoted, the formalism is self-similar. Accordingly, any constituent of a node at a lower level of hierarchy can also be regarded as a node (Figure 1).

The self-similar formalism may not be needed to model a particular network, but it ensures the conservation of quanta, i.e., an accurate account of any network in terms of physics. In other words, for a node to absorb or emit quanta, it must contain some internal structure to accommodate these changes.

During the probable process of network evolution, energy differences between the nodes and their respective surroundings will diminish. The natural process is driven by the consumption of free energy terms $A_{jk} = \Delta\mu_{jk} - i\Delta Q_{jk}$.

DOI 10.1002/cplx

FIGURE 1



(A) Natural network in thermodynamic terms is a self-similar energy transduction system of pathways (links) and repositories of energy (nodes). (B) The expansion exemplifies that within the links there are nodes too. Each node is a thermodynamic system of its own internal interactions between its constituent nodes. (C) The natural network will evolve to diminish differences of energy between the nodes of the network as well as respect those in the surrounding networks. Ensuing net flows of energy will cause changes in the network, e.g., by altering transduction capacity of links as well as attaching new nodes or eventually discarding old less effective connections.

The two components of A_{jk} comprise the mutual differences in scalar potentials, known also as chemical potentials, $\Delta\mu_{jk} = k_B T(\ln\phi_j - \ln\phi_k)$, as well as differences in vector potentials that will manifest themselves in changes of state as dissipation ΔQ_{jk}, such as heat. The imaginary unit is used merely to emphasize that the scalar and vector potentials are orthogonal to each other [41–43]. Moreover, it is noteworthy that at the change of a node's state, at least one quantum will either be absorbed to or emitted from the node. Only a reversible exchange of quanta of equal energy will leave a pair of nodes intact, i.e., stationary. Also in a thermodynamic balance, an exact exchange of quanta with the surroundings will leave the network invariant. The quantized flows of energy between the nodes are literally interactions, because each node is regarded as a physical system characterized by its action and associated symmetry [44,45].

The energetic status of a network system in its surroundings can be formulated by statistical mechanics of open systems [21,39,45]. The additive, hence logarithmic probability P of a system as a product of P_j, the probabilities of subsystems, is known as entropy:

$$S = k_B \ln P = k_B \sum_j \ln P_j \approx k_B \sum_j N_j \left(1 - \sum_k A_{jk}/k_B T\right). \quad (1)$$

It contains the bound $k_B T \Sigma N_j$ and free $\Sigma N_j A_{jk}$ forms of energy. Entropy is an exhaustive measure of the system's thermodynamic status. The Stirling's approximation for indistinguishable combinations $\ln N_j! \approx N_j(\ln N_j - 1)$ implies that $k_B T$ is a sufficient statistic, i.e., $A_{jk}/k_B T << 1$, for the distribution of energy within the network. In other words, the statistical approximation means that the heat capacity of the network is big enough so that absorption or emission of one quantum will not cause a marked change in the average energy density $k_B T$ of the system. A specific node or a link cannot be described in the statistical sense by entropy, when it is about to emerge or to branch out as well as when it is about to vanish [36,46]. At these critical steps, manifesting themselves as bifurcations [36], the system's changing status is best characterized directly by the change dP_j/dt. Moreover, the change of P will be abrupt at a phase transition when the system rapidly reorganizes its entire interaction network to adapt to a change in its surroundings.

According to the variational principle in its original form [15], flows of energy will themselves search for paths and eventually also open new links to consume free energy in the least time [21,47]. Hence, from this variational perspective, the network notion of preferential attachment is subsumed in the natural selection for the least-time dispersal of energy. Consequently, entropy S will not only increase,

DOI 10.1002/cplx

$$\frac{dS}{dt} = k_B L \geq 0\ ; \quad L = -\sum_{j,k} \frac{dN_j}{dt}\frac{A_{jk}}{k_B T} \tag{2}$$

but it will increase in the least time. It is of interest to note that the least-time imperative is equivalent to Newton's second law $\mathbf{F} = d\mathbf{p}/dt = md\mathbf{v}/dt + \mathbf{v}dm/dt$ which says that the change in momentum $\mathbf{p}$ will keep directing along the resultant force $\mathbf{F} = \Sigma\mathbf{F}_j$ [15,47]. Thus, at all times and at all places, the network will naturally select pathways to evolve so that free energy cannot be consumed any faster. In other words, networks evolve by consuming forces to attain balance in their surroundings in the least time. The power law dependence as a ubiquitous characteristic of networks is already apparent from the integrated Newton's second law $\int Fdt/p = \int dv/v + \int dm/m = lnv + lnm$ = constant, which is a straight line on a log–log plot.

The conservation of energy requires that an influx ($\Sigma A_{jk} < 0$) or efflux ($\Sigma A_{jk} > 0$) will force the node to change its constituents at a rate [21]:

$$\frac{dN_j}{dt} = -\sum_k \sigma_{jk}\frac{A_{jk}}{k_B T} \tag{3}$$

proportional to free energy. The coefficient of conductance σ_{jk} is a characteristic of the link between the two nodes, which are indexed with j and k. For example, a city will grow due to an influx of inhabitants as well as of goods arriving via roads, railroads, etc., from surrounding rural areas. According to self-similar formalism, the link itself can be considered as a network of nodes and links (Figure 1). For example, two cities are rarely linked by a nonstop train connection, as the train also stops at other major towns for influx and efflux of passengers and goods. Likewise, when a computational task is distributed, a client and a server do not usually link directly, but instead they link over a network of hubs and connections.

According to the variational principle, energy tends to flow along the least-time links. The least action defines the length s of a geodesic in energetic terms by $2K = \int (ds/dt)^2 dt$ [48]:

$$\left(\frac{ds}{dt}\right)^2 = \frac{d2K}{dt} = T\frac{dS}{dt} = -\sum_{j,k}\frac{dN_j}{dt}A_{jk} = \frac{1}{k_B T}\sum_{j,k}\sigma_{jk}A_{jk}^2 \geq 0 \tag{4}$$

being proportional to the magnitudes of free energy components. Accordingly, when there is no difference in energy between the j- and k-nodes, the two nodes will be indistinguishable from each other; hence, $j = k$ and the particular s_{jj} vanishes (cf. the identity of indiscernibles).

The average of $s = \Sigma s_{jk}$, as a characteristic of network topology, will decrease with the increasing number of jk links between an invariant set of nodes. It is noteworthy that a particular value of the total length s cannot be determined for an evolving network simply because the total energy of the system is changing. Physically speaking, eigenvalues and eigenmodes can, of course, not be determined when they are changing. New network qualities will emerge along with increasing energy as new paths, such as highways, open up for flows of energy [49]. Conversely, old attributes will vanish when the flows of energy redirect along more effective paths of free energy consumption leaving some paths obsolete.

If the transduction rates dN_j/dt were suboptimal, counterforces A_{jk} would rise and redirect the flows of energy back along the most voluminous gradients. In other words, even when a sufficiently statistical network is evolving, its distribution of energy is not expected to depart much from a quasistationary balance known as Le Chatelier's condition [50]:

$$A_j = \sum_k A_{jk} \approx 0 \Leftrightarrow N_j \approx \prod_k \left(N_k e^{-(\Delta G_{jk} - i\Delta Q_{jk})/k_B T}\right) \tag{5}$$

where the product Π_k is over all k-substrates. The product form in Eq. (5) reveals that the j-node emerges from k-multiplicative operations. The multiplicative form is the characteristic of a log-normal distribution [51] whose cumulative curve follows a power law. So we reason that the power-law characteristic of natural networks follows from the least-time consumption of free energy.

The distribution's dependence on the average energy is familiar from the temperature dependence of the Maxwell–Boltzmann velocity distribution and from the black-body radiation spectrum, but it is also recognized in temporal changes during ecological succession [52,53], economic development [54,55], cultural changes [56,57], changes in strategies of behavior [58] as well as when logistic [59] and communication infrastructure are building up [60].

The above thermodynamic description of networks by the natural law is formally simple, yet its analysis [Eq. (2)] reveals that evolution of a network is an intractable process meaning that there is no deterministic solution of its equation of motion describing nonholonomic evolution [61]. Namely, when a particular source of energy, i.e., a node is consumed via two or more links, i.e., degrees of freedom, the flows of energy and the energy difference cannot be separated from each other to solve Eq. (2) by way of integration to a closed form [21,47,61]. This property clarifies why evolution of natural networks are often found impossible to predict precisely.

It is a mere consequence of conservation of energy that an evolutionary step from one state to another is a

DOI 10.1002/cplx

dissipative event. The flow of quanta from the system to its surroundings or vice versa will alter both the system and its surroundings. Because of this intrinsic interdependence among all quantized constituents of the system and its surroundings, evolution is changing its settings, i.e., the energy landscape that directs the natural process. The flow itself will affect conduction by urging an increase in communication capacity or by strengthening lines of communication, such as synapses of neurons. Another familiar example would be a river that will by the mere act of flowing erode the landscape, and thereby affect its own flow. Also similar to an ecological succession where immigrant species will transform the ecosystem, a rural district will change its way of life as new means, such as fertilizers and engine power, of energy transduction enter the community. Accordingly, changes in the surroundings will inflict new forces on the system, e.g., changing urban demands will call for changes in the community's economic structure.

Because of dissipation, the change in momentum is not collinear with the velocity, which is a characteristic of non-Abelian systems. In other words, natural processes are dissipative, path-dependent and hence inherently intractable. It is noteworthy that the nondeterministic nature of network evolution does not stem from network complexity as such, but appears already in the problem of three bodies [62] and other hard problems with two or more degrees of freedom [63–65]. Although evolution of natural network in general is a noncomputable process, certain mathematical models as approximate accounts of network evolution can be solved [66,67].

Finally, the above conclusions derived from the formal analysis of the evolutionary equation of motion [Eq. (2)] do not depend on how one defines a network system. When a definition of a network happens to include nodes that are in imbalance with each other, the development will manifest primarily as a restructuring of the network when internal forces are being consumed. For example, a social system will display this sequence of events during integration processes of immigrants. Likewise, the conservation of energy in bound and free forms of interactions will be respected when a definition of a node happens to subsume nodes. For example, a definition for two cities may seem arbitrary in subsuming some suburban communities while discarding others. Nevertheless, fervent communication between the twin cities will establish a metropolitan area irrespective of its formal boundaries.

3. APPROXIMATE FORMS OF NATURAL DEGREE DISTRIBUTION

The above thermodynamic formulation of networks as open systems can be analyzed to unravel why certain mathematical models account well for the natural networks. In particular, the skewed degree distribution, common to natural networks, can be found as an excellent approximation of the thermodynamic stationary-state condition ($d\ln P = 0$) of Eq. (5),

$$\begin{aligned}\ln N_j &= \ln \prod_k \left(N_k e^{-\left(\Delta G_{jk} - i\Delta Q_{jk}\right)/k_B T}\right) \\ &= j \ln N_1 \sum_{1 \le m,n \le j} -A_{mn}/k_B T \ \propto j \ln N_1,\end{aligned} \tag{6}$$

which is linear on a semi-log scale [28,38]. Here, each j-node in the hierarchy of the network (Figure 1) is expressed as being composed of some basic constituents N_1 (quanta), because all nodes are results of some earlier processes. It follows from this recursive form that the j-node with N_j constituents embodies an energy density

$$\begin{aligned}&\phi_j = N_j e^{G_j/k_B T} = N_1^j e^{j(G_1 + i\Delta Q_1)/k_B T} = e^{j(\ln \phi_1 + i\Delta Q_1/k_B T)} \\ &\quad \Leftrightarrow \ \ln \phi_j = j \ln \phi_1',\end{aligned} \tag{7}$$

where the number of quanta $j\Delta Q_1$ that have been incorporated in the entity whose energy density is denoted with ϕ_j are included in the shorthand notation ϕ_1'. Accordingly, another node with $j + n$ constituents comprises an adjacent energy density

$$\begin{aligned}&\phi_{j+n} = \exp\left[(j+n)\phi_1'\right] = \phi_j \exp\left(n \ln \phi_1'\right) \\ &\quad \Leftrightarrow \ln \phi_{j+n} = (j+n) \ln \phi_1'.\end{aligned} \tag{8}$$

This form reveals that when $n << j$ the distribution of energy densities $\phi_{j\ -\ n \ldots j\ +\ n}$ over a range of nodes $j-\ n \ldots j + n$ about ϕ_j

$$\ln \phi_{j-n \ldots j+n} = \ln \phi_j + \sum_n n \ln \phi_1' \tag{9}$$

is normal according to the central limit theorem. The condition of small variation is effectively the criterion by which the nodes are qualified to the same degree distribution. For example, when a distribution of cities is compiled from a network of population centers, small villages, or suburbs will be excluded. Because of the ubiquitous quest for the least-time free energy consumption, natural distributions will display scale-free, skewed characteristics irrespective of classification criterion.

It is noteworthy that the natural distribution does deviate from the aforementioned log-normality in the way it tails off both at low and high ends [68]. According to thermodynamics, the distribution will tail off when the functional mechanism of a particular class of nodes becomes increasingly ineffective or energetically expensive as a means of energy transformation [39]. For example, powerful energy

DOI 10.1002/cplx

transduction mechanisms that are characteristics of a city such as factories are not supported by small villages. Hence, villages are not considered in the distribution of cities. Conversely, the distribution of cities tails of because an increasingly larger metropolis struggles with increasingly more acute transportation problems that curtail its further growth. Because of these imperatives in energy transduction, the sigmoid cumulative curve will deviate from the power law at both the low and high ends. The low-end cut-off is usually referred to as the finite-size effect [69]. For example, the species–area relationship [25,70–73] is a well-known cumulative curve of ecosystems, which totals from the distributions of species that populate increasing larger areas [74]. It mostly follows a power law, but at the low end, the resources in a small area do not support any species in a particular genus, as well as, toward the high end, no species of that genus is capable of harvesting the large but scattered resources [75–77].

The recursive power-law form of the cumulative probability distribution, as found above to result from the least-time free energy consumption, is closely followed by certain functions. For example, beta distribution for large values of either of its gamma-function arguments is a good approximation of certain natural distributions [78]. Moreover, the scale-free stationary distribution $\Sigma k^{-\alpha}$ is proportional to the Riemann zeta function $\zeta(\alpha)$, which in turn has been associated to the stationary states by the thermodynamic principle [79]. However, these and other mathematical models [18] do rarely account for the entire span of a natural distribution that tails off at both ends due to the mechanistic limitations of energy transduction.

4. KINETIC MODELS OF EVOLVING NETWORKS

Evolution of natural networks mostly follows a power law. This time-dependence can be recognized to result from the maximal energy dispersal when the equation for evolving probability $dP/dt = LP$ [Eq. (2)] is analyzed.

In practice, it is the number of nodes N_j that can be monitored during evolution rather than the associated probability P_j [Eq. (2)]. When N_j of the nascent network is small in comparison with the stationary population of nodes N_j^s of the mature network, the change in the free energy $\Sigma_k \partial A_{jk}/\partial t = \Sigma_k \sigma_{jk}$ is a good approximation independent of the energy flow. This deterministic, zero-order approximation

$$\begin{aligned} &\sum_k \frac{\partial A_{jk}/k_B T}{\partial t} = \frac{dN_j}{dt}\sum_k \frac{\partial A_{jk}/k_B T}{\partial N_j} \approx \sum_k \sigma_{jk} \\ &\Rightarrow \frac{dN_j}{dt} = \sigma_j N_j \ , \ \text{when } A_{jk}(t) \approx A_{jk}(0) \end{aligned} \tag{10}$$

will give the exponentially increasing initial growth $N_j(t) = N_j(0)\exp(\sigma_j t)$ when variables are separated and integrated from 0 to t. Evolution will punctuate off when a transformation mechanism appears in the system for the first time and taps into a nascent reservoir of free energy [25]. For example, the initial growth of a business branch is exponential.

Conversely, the decreasing exponential approximation will be obtained when energy in the maturing population $N_j(t)$ has almost attained $N_j^s(\infty)$ at the stasis where $A_{jk}^s = 0$. Then, the change $\Sigma_k \partial A_{jk}/\partial t = -\Sigma_k \sigma_{jk}$ is nearly constant

$$\begin{aligned} &\sum_k \frac{\partial A_{jk}/k_B T}{\partial t} = \frac{dN_j}{dt}\sum_k \frac{\partial A_{jk}/k_B T}{\partial N_j} \approx -\sum_k \sigma_{jk} \\ &\Rightarrow \frac{dN_j}{dt} = -\sigma_j N_j \ , \ \text{when } A_{jk}(t) \approx A_{jk}^s = 0. \end{aligned} \tag{11}$$

The exponential decrease $N_j(t) = N_j^s - N_j(0)\exp(-\sigma_j t)$ at the late stage will be obtained when variables are separated and N_j is integrated from $N_j(0)$ to N_j^s. Evolution will settle to a stasis when the transformation mechanisms have consumed all free energy. For example, a mature business branch will saturate a market. Thereafter, the balanced operation depends only on the amount of steadily available and renewable potential.

In the intermediate region between the initial increase and the final decrease, the population N_j is given by Eq. (6), which is valid for a sufficiently statistical system. This means that N_j of the quasi-stationary network can be written in terms of multiplicative operations of the basic constituents in numbers N_1,

$$N_j = \prod_k \left(N_k e^{-A_{jk}/k_B T}\right) = N_1^j \prod_{1\le m,n\le j} e^{-A_{mn}/k_B T} = \alpha_j N_1^j, \tag{12}$$

where the constant $\alpha_j = \Pi_{m,n}\exp(-A_{jk}/k_B T)$ is over available m,n-indexed transformation paths. The multiplicative form is recognized as a power law. The typical time course about a quasi-stationary point A_{jk}^{qs} follows from the approximation $\Sigma_k \partial A_{jk}/\partial t = \partial A_j/\partial t = -\sigma_j$

$$\begin{aligned} &\frac{dN_j}{dt} = \frac{dN_j}{dN_1}\frac{dN_1}{dt} = \alpha_j j N_1^{j-1}\frac{dN_1}{dt} = \frac{jN_j}{N_1}\frac{dN_1}{dt} \\ &\Rightarrow \frac{dN_j}{N_j} = \frac{j dN_1}{N_1} \ , \ \text{when } A_{mn} \approx A_{jk}^{qs}. \end{aligned} \tag{13}$$

When the variables are separated, the integration will give $\ln N_j = j\ln N_1 +$ a constant. Hence, the scale invariance, which is a characteristic of natural networks, is apparent from the log–log plot where the curve is a straight line.

The obtained functional form is also familiar from the law of mass action. However, it is noteworthy that it is not the number of nodes but the difference in energy contained between the nodes and relative to their

DOI 10.1002/cplx

surroundings that contributes to the driving force of evolution A_{jk}/k_BT. Consequently, the law of mass action does not comply with conservation of energy. Hence, in that model of network kinetics [80], the forward and backward flow coefficients are erroneously deemed as if they were changing during the course of evolution, whereas, in reality, the free energy is decreasing and the conduction coefficient σ_{jk} in Eq. (3) is a constant. Obviously, new means of transformation may also emerge to facilitate the flows.

Finally, we emphasize that the evolutionary equation [Eq. (2)] is nondeterministic, unlike its mathematical models that can be integrated to closed forms. Often the overall sigmoid course is, to a good approximation, also given by the logistic equation or Gompertz equation both with three arbitrary constants, i.e., the upper asymptote, the tie origin, and the rate constant governing the point of inflection [81]. The above analysis of the evolutionary equation [Eq. (2)] and the associated kinetic [Eq. (3)] and balance equations [Eq. (5)] for the initial, intermediate, and final stages of growth (or decline) reveals that the ubiquitous power law characteristics of networks are consequences of the natural principle of the least-time energy dispersal.

5. GROWTH MODELS OF NATURAL NETWORKS

The preferential attachment model will generate random scale-free networks with skewed degree distributions [7,82,83]. The basic algorithm weights the connection probability $P_j(N)$ of a j-node with its degree N. Hence, new nodes are most likely to make connections with already densely connected nodes. We find that this method mimics the natural process of least-time free energy consumption where interactions among constituents of a larger and denser system form increasingly more effective mechanisms of energy transduction. The basic algorithm will reproduce a power-law region, but not the early punctuation and the late settling to stasis, since the thermodynamic limitations of growth denoted in Eqs. (1) and (2) are not included in P_j. After all, it is not the number of links that drives the growth but the energy influx via links that fuels the expansion.

Weighted networks [84] are better models to account for variation in energy transfer characteristics of natural links. When the j-node is assigned with strength

$$s_j = \sum_k w_{jk} \tag{14}$$

as a weighted sum of links to neighboring k-nodes, the degree distribution $P(N)$ is replaced by a strength distribution $P(s)$. This model can be recognized as an approximation of Eq. (3) when assuming that the driving forces of evolution A_{jk} would be constants and small relative to the overall energy content, i.e., $A_{jk}/k_BT << 1$. Then s_j would be equal to the total conductivity $\sigma_j = \sum\sigma_{jk}$ that links the j-node with its surrounding k-nodes.

When the network algorithm assigns the j-node with probability

$$P_j = s_j/\sum_i s_i \tag{15}$$

to attach to a new k-node [85], the basic idea of the preferential attachment that "rich get richer" will be transcribed for the weighted networks in a form that "busy get busier." For example, when a new highway is constructed between two cities, traffic on older and smaller roads will reduce. Simple weight-driven dynamics will yield scale-free characteristics [86]. As an added link introduces variations to the existing weights across the network, the algorithm conforms to the interdependence among natural nodes, although Eq. (15) does not express P_j in explicit terms of energy as Eq. (1) does.

Normalization by the sum of weights relates to the average energy per node. When P_j is bound, the distribution will be stationary. However, as the net influx powers the growth of the natural network, k_BT will increase during evolution. Hence, there is no firm ground for normalization. When energy is absorbed into a network, approximately logarithmic progression of both the degree and weight of a node i [85] will follow. For example, when a city becomes more prosperous, more and more people will move in and the countryside will become desolate. The urbanization will also result to increase in traffic in and out of the city thus strengthening the important connections between other growing areas. However, growth of degree and weight always requires influx of energy, i.e., insertion of new nodes.

Intriguingly, a seemingly random process of network evolution will also generate scale-free characteristics. Namely, these are obtained by a method that will attach a new node to the network so that the new node will link to those nodes that were selected as termination points of a series of random walks, which were carried out the previous time step [87]. Yet, this method of selecting the nodes, albeit random, captures the path-dependent character of natural processes. In other words, how the network will grow by linking the new node with the existing nodes is not truly arbitrary, but the selection of links depends on the steps that were taken earlier. When the process itself will affect its future state space, it is nonholonomic. This character is expressed by the evolutionary equation of motion given by Maupertuis' principle.

Moreover, the selection by the random walks method is in fact not all immaterial, i.e., energetically inconsequential, because the mere act of marking the end points of random walks is ultimately represented by some form of a physical change in the network description. As only those nodes that differ in energy can be distinguished from each other, the seemingly immaterial and statistical method of

DOI 10.1002/cplx

producing scale-free characteristics by random walks will invariably entail also physical representations that in turn are subject to the laws of thermodynamics.

6. TOPOLOGICAL MEASURES OF NATURAL NETWORKS

In thermodynamic terms, the lengths of least-time paths, i.e., geodesics [Eq. (4)] are informative about the network topology, whereas in network theory, the average length

$$l = \frac{1}{N(N-1)} \sum_{j,k} d_{jk} \tag{16}$$

of a path in a nonweighed graph is defined as the sum of the shortest distances d_{jk} between all combinations of j- and k-nodes in total $N(N-1)$. This useful measure parallels the total geodesic length when normalizing with all conceivable jk-combinations. However, according to the thermodynamic tenet the flows of energy themselves do value a link by its means σ_{jk} and associated driving forces A_{jk}. For example, when a logistic network is structuring itself across a rough terrain, means of transportation and expected returns will matter more when deciding which lines of transportation require upgrading than the actual distances as the crow flies. When weights are applied on the links, reality will be modeled more precisely.

Clustering coefficients are informative about local linkage density and eventually, when reduced to an average figure of merit, also about the average connectivity of the entire network [88]. In thermodynamic terms, the skewed degree distribution as a quasi-stationary partition [Eq. (5)] covers the network of diverse localities. However, this measure is not normalized with all conceivable connections. In general, the statistical mechanics of open systems refrain from normalization because when the total energy content of an evolving system is changing, and even in a nondeterministic manner, there are no grounds for normalization.

Finally, the logarithmic dependence $L \propto \ln N/\ln k$ of the typical distance L between two randomly chosen nodes on the total number of nodes N and the number of neighbors k are related to thermodynamic terms. When a locus is understood as a closed action of scalar potential energy, a distance between two loci will also be understood, e.g., as a difference between one chemical potential $\mu_j \propto \ln N_j$ and the other μ_k. Thus, the typical distance is proportional to the potential of an entire network $\mu \propto \ln N$. Moreover, the typical distance scales down with the logarithm of the number of neighbors in a small-world network, because the nearby high-throughput links hardly contribute to the length of a geodesic [Eq. (5)]. Thus, the total number of nodes is effectively scaled down by the number of neighbors.

Obviously, the numerical values of topological measures will change when the network is evolving, but the thermodynamic tenet emphasizes that evolution is by its nature nondeterministic. This is of course understood in practice, since trends are followed and extrapolated with reservations rather than attempting to make precise predictions.

7. CONCLUSIONS

The physical portrayal of networks as energy transduction systems may appear to some superficial by subsuming numerous mechanistic details in its general concepts. However, the mathematical formalism ensures conservation by enumerating all constituents to a precision of one quantum. Moreover, the ubiquitous scale-free and nondeterministic characteristics of natural networks themselves imply that there is an underlying universal law in action. This law is known by many names, here, mostly referred to as the principle of least action. When it is given as an equation of motion and analyzed, the principle will reveal that network evolution and structure can indeed be modeled by preferential attachment and outlined by certain analytical functions, notably by skewed, log-normal distributions, power laws, as well as logistic and other nonlinear equations. However, these functional forms are reticent in revealing the underlying cause of universality, i.e., that energy differences drive natural networks toward free energy minima in respective surroundings in the least time. Likewise, preferential attachment algorithms or path-dependent protocols of network generation are excellent models of network growth, branching, and clustering, but these models are taciturn about the nondeterministic, dissipative character of natural processes, i.e., that evolution of a network affects its own course by molding the energy landscape.

Undoubtedly, the physical portrayal of natural networks according to the statistical mechanics of open systems does not relate one-to-one with many mathematical models of networks. Therefore, we find no way to provide an exact correspondence, e.g., in a form of a proof, but we were only able to show that many models and measures used in network theory are excellent approximations of the thermodynamic process. Specifically, when network nodes are depicted as identical with each other, there is no energetic bias, i.e., a sufficient reason, that would structure the natural network. Likewise, when links are drawn as having equal capacities, i.e., they are indiscernible, there is no variation for natural selection to prefer a particular attachment. In addition, the notion that probability is physical may appear to some unmotivated and even bizarre, in particular, because artificial neural networks adapt well to various input by adjusting weights. However, all forms of information are embodied in physical presentations, so they are also subjects of

DOI 10.1002/cplx

thermodynamics. Hence, the provided description, when speaking only in energetic terms, is self-consistent.

Finally, we remind that our objective was neither to question the established mathematical models and measures nor conclusions founded on network theory, but to contribute to the discourse on complex systems by communicating that the scale-free and nondeterministic network characteristics follow from the least-time free energy consumption.

Acknowledgments

The authors thank Robert Leigh for valuable comments and corrections.

REFERENCES

1. Strogatz, S.H. Exploring complex networks. Nature 2001, 410, 268–276.
2. Jeong, H.; Tombor, B.; Albert, R.; Oltvai, Z.N.; Barabási, A.-L. The large-scale organization of metabolic networks. Nature 2000, 407, 651–654.
3. Bork, P.; Jensen, L.J.; von Mering, C.; Ramani, A.; Lee, I.; Marcotte, E.M.; Protein interaction networks from yeast to human. Curr Opin Struct Biol 2004, 14, 292–299.
4. Humphries, M.D.; Gurney, K.; Prescott, T.J. Is there a brainstem substrate for action selection? Phil Trans R Soc B 2007, 362, 1627–1639.
5. Willard, L.; Miranker, A. Neural network wave formalism. Adv Appl Math 2006, 37, 19–30.
6. Vuorinen, V.; Peltomaki, M.; Rost, M.; Alava, M. Networks in metapopulation dynamics. Eur Phys J B 2004, 38, 261–268.
7. Barabási, A.-L.; Albert, R. Emergence of scaling in random networks. Science 1999, 286, 509–512.
8. Newman, M.E.J.; Watts, D.J.; Strogatz, S.H. Random graph models of social networks. Proc Natl Acad Sci USA 2002, 99, 2566–2572.
9. Peltomäki, M.; Alava, M. Correlations in Bipartite Collaboration Networks. J Stat Mech: Theory Exp 2006, 0601, P01010.
10. Clauset, A.; Shalizi, C.R.; Newman, M.E.J. Power-law distributions in empirical data. SIAM Rev 2009, 51, 661–703.
11. Newman, M.E.J. Assortative mixing in networks. Phys Rev Lett 2002, 89, 208701.
12. Bianconi, G.; Barabási, A.-L. Bose–Einstein condensation in complex networks. Phys Rev Lett 2001, 86, 5632–5635.
13. Charlton, J.C.; Schramm, D.N. Percolation of explosive galaxy formation. Astrophys J Part 1 1986, 310, 26–39.
14. Armatte, M. Robert Gibrat et la loi de l'effet proportionnel. Mathématiques et sciences humaines, Centre d'analyse et de mathématiques sociales de l'EHESS, 1995, 129, 5–35.
15. de Maupertuis, P.-L.M. Accord de différentes loix de la nature qui avoient jusqu'ici paru incompatibles. Meém Ac Sc Paris 1744, 417–426.
16. Carnot, S. Reflexions sur la Puissance Motrice du Feu et sur les Machines Propres a Developper cette Puissance; Bachelier: Paris, 1824.
17. Lotka, A.J. Natural selection as a physical principle. Proc Natl Acad Sci 1922, 8, 151–154.
18. Yule, G.U. A Mathematical Theory of Evolution, based on the Conclusions of Dr. J.C. Willis, F.R.S. Phil Trans R Soc Lond Ser B 1925, 213, 21–87.
19. Darwin, C. On the Origin of Species; John Murray: London, 1859.
20. Whitfield, J. Survival of the likeliest? PLoS Biol 2007, 5, e142.
21. Sharma, V.; Annila, A. Natural process—Natural selection. Biophys Chem 2007, 127, 123–128.
22. Lanczos, C. The Variational Principles of Mechanics; University of Toronto Press: Toronto, 1952.
23. Georgiev, G.Y. A Quantitative measure, mechanism and attractor for self-organization in networked complex systems in self-organizing systems: 6th IFIP TC 6 International Workshop, IWSOS 2012, Delft, The Netherlands, March 15–16, 2012; Kuipers, F. A.; Heegaard, P. E., Eds. Springer-Verlag, pp 90–95.
24. Strogatz, S.H. Exploring complex networks. Nature, 2001, 410, 268–276.
25. Eldredge, N.; Gould, S.J. In: Models in Paleobiology; Schopf, T.J. M., Ed.; Freeman, Cooper: San Francisco, CA, 1972.
26. Pareto, V. Manuale di economia politica (Manual of Political Economy). Schwier, A. S., Transl.; Kelley: New York, NY, 1971.
27. Rosenzweig, M.L. Species diversity in space and time; Cambridge University Press: Cambridge, UK, 1995.
28. Limpert, E.; Stahel, W.A.; Abbt, M. Log-normal distributions across the sciences: Keys and clues. Bioscience 2001, 51, 341–352.
29. Volterra, V.Variations and fluctuations of the number of individuals in animal species living together. In: Animal Ecology; Chapman, R. N., Transl.; McGraw–Hill: New York, NY, 1931.
30. Belousov, B.P. Sbornik Referatov po Radiatsionni Meditsine (A Periodic Reaction and Its Mechanism); Field, J.; Burger, M., Transl.; Medgiz: Moscow, 1958.
31. Bak, P. How Nature Works: The Science of Self-Organized Criticality; Copernicus: New York, NY, 1996.
32. Kleiber, M. Body size and metabolism. Hilgardia 1932, 6, 315–351.
33. Zipf, G.K. Human Behaviour and the Principle of Least Effort. Addison-Wesley: Reading, MA, 1949.
34. Bejan, A.; Marden, J.H. The constructal unification of biological and geophysical design. Phys Life Rev 2009, 6, 85–102.
35. Schroeder, M. Fractals, Chaos, Power Laws; Freeman: New York, NY, 1991.
36. Strogatz, S.H. Nonlinear Dynamics and Chaos with Applications to Physics, Biology, Chemistry and Engineering; Westview: Cambridge, MA, 2000.
37. Barabási, A.-L.; Albert, R. Emergence of scaling in random networks. Science 1999, 286, 509–512.
38. Grönholm, T.; Annila, A. Natural distribution. Math Biosci 2007, 210, 659–667.

DOI 10.1002/cplx

39. Mäkelä, T.; Annila, A. Natural patterns of energy dispersal. Phys Life Rev 2010, 7, 477–498.
40. Gibbs, J.W. The Scientific papers of J. Willard Gibbs; Ox Bow Press: Woodbridge, CT, 1993–1994.
41. Tuisku, P.; Pernu, T.K.; Annila, A. In the light of time. Proc R Soc A 2009, 465, 1173–1198.
42. Prigogine, I. Laws of nature, probability and time symmetry breaking. Phys A 1999, 263, 528–539.-
43. Poynting, J.H. Collected Scientific Papers; Cambridge University Press: London, 1920.
44. Noether, E.Invariante Variationprobleme Nach. vd. Ges. d. Wiss. zu Goettingen, Mathphys Klasse 1918, 235–257, Invariant variation problems. Tavel, A. M., Transl.; Transp Theory Stat Phys 1971, 1, 183–207.
45. Annila, A. All in action. Entropy 2010, 12, 2333–2358.
46. May, R.M. Simple mathematical models with very complicated dynamics. Nature 1976, 261, 459–467.
47. Kaila, V.R.I.; Annila, A. Natural selection for least action. Proc R Soc A 2008, 464, 3055–3070.
48. Lavenda, B.H. Nonequilibrium Statistical Thermodynamics; Wiley: New York, NY, 1985.
49. Pernu, T.K.; Annila, A. Natural emergence. Complexity 2012, 17, 44–47.
50. Atkins, P.W.; de Paula, J. Physical Chemistry; Oxford University Press: New York, NY, 2006.
51. Aitchison, J.; Brown, J.A.C. The Log-normal Distribution; Cambridge University Press: Cambridge, UK, 1957.
52. Knight, C.B. Basic Concepts of Ecology; Macmillan: New York, NY, 1965.
53. Würtz, P.; Annila, A. Ecological succession as an energy dispersal process. BioSystems 2010, 100, 70–78.
54. Sundrum, R.M. Income Distribution in Less Developed Countries; Routledge: London, UK, 1992.
55. Annila, A.; Salthe, S. Economies evolve by energy dispersal. Entropy 2009, 11, 606–633.
56. Harris, M. Cultural Materialism—The Struggle for a Science of Culture; Random House: New York, NY, 1979.
57. Annila, A.; Salthe, S. Cultural naturalism. Entropy 2010, 12, 1325–1343.
58. Anttila, J.; Annila, A. Natural games. Phys Lett A 2011, 375, 3755–3761.
59. De Montis, A.; Caschili, S.; Chessa, A. Time evolution of complex networks: Commuting systems in insular Italy. J Geogr Syst 2011, 13, 49–65.
60. Huberman, B.A.; Adamic, L.A. Evolutionary dynamics of the world wide web. Nature 1999, 399, 131.
61. Annila, A.; Salthe, S. On intractable tracks. Phys Essays 2012, 25, 232–237.
62. Poincaré, J.H. Sur le problème des trois corps et les équations de la dynamique. Acta Math 1890, 13, 1–270.
63. Sipser, M. Introduction to the Theory of Computation; PWS: New York, NY, 2001.
64. Fraenkel, A.S. Complexity of protein folding. Bull Math Biol 1993, 55, 1199–1210.
65. Annila, A. Physical portrayal of computational complexity. ISRN Comput Math 2011, 321372, 1–15. arXiv:0906.1084.
66. Dorogovtsev, S.N.; Mendes, J.F.F.; Samukhin, A.N. Structure of growing networks with preferential linking. Phys Rev Lett 2000, 85, 4633–4636.
67. Bollobás, B.; Riordan, O.; Spencer, J.; Tusnády, G. The degree sequence of a scale-free random graph process. Model Random Struct Alg 2001, 18, 279–290.
68. Amaral, L.A.N.; Scala, A.; Barthélémy, M.; Stanley, H.E. Classes of small-world networks. Proc Natl Acad Sci USA 2000, 97, 11149–11152.
69. Fisher, M.E.; Barber, M.N. Scaling theory for finite-size effects in the critical region. Phys Rev Lett 1972, 28, 1516–1519.
70. Knight, C.B. Basic Concepts of Ecology; Macmillan: New York, NY, 1965.
71. MacArthur, R.H.; Wilson, E.O. The Theory of Islands Biogeography; Princeton University Press: Princeton, NJ, 1967.
72. Arrhenius, O. Species and area. J Ecol 1921, 9, 95–99.
73. Preston, F.W. Time and space and the variation of species. Ecology 1960, 41, 785–790.
74. Würtz, P.; Annila, A. Roots of diversity relations. J Biophys 2008, doi:10.1155/2008/654672, arXiv:0906.0251
75. Preston, F.W. The canonical distribution of commonness and rarity: Part I. Ecology 1962, 43, 185–215.
76. Kilburn, P.D. Exponential values for the species-area relation. Science 1963, 141, 1276.
77. McGuiness, K.A. Equations and explanations in the study of species-area curves. Biol Rev 1984, 59, 423–440.
78. Simon, H.A. On a class of skew distribution functions. Biometrika 1955, 42, 425–440.
79. Annila, A. Space, time and machines. Int J Theor Math Phys 2012, 2, 16–32. arXiv:0910.2629
80. Jamshidi, N.; Palsson, B.Ø. Mass action stoichiometric simulation models: Incorporating kinetics and regulation into stoichiometric models. Biophys J 2010, 98, 175–185.
81. Winsor, C.P. The Gompertz Curve as a Growth Curve. Proc Natl Acad Sci USA 1932, 18, 1–8.
82. Barabasi, A.-L.; Albert, R.; Jeong, H. Diameter of the world wide web. Nature 1999, 401, 130–131.
83. Barabasi, A.-L.; Albert, R.; Jeong, H. Mean-field theory for scale-free random networks. Phys A 1999, 272, 173–187.
84. Yook, S.H.; Jeong, H.; Barabási, A.-L.; Tu, Y. Weighted evolving networks. Phys Rev Lett 2001, 86, 5835–5838.
85. Barthélemy, M. Barrat, A. Pastor-Satorras, R.; Vespignani, A. Characterization and modeling of weighted networks. Phys A 2005, 346, 34–43.
86. Barrat, A.; Barthélemy, M.; Vespignani, A. Weighted evolving networks: Coupling topology and weight dynamics. Phys Rev Lett 2004, 92, 228701.
87. Saramäki, J.; Kaski, K. Scale-free networks generated by random walkers. Phys A 2004, 341, 80–86.
88. Watts, D.J.; Strogatz, S. Collective dynamics of 'small-world' networks. Nature 1998, 393, 440–442.

DOI 10.1002/cplx