Entropy Maximization as a Holistic Design Principle for Complex Optimal Networks

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A general holistic theory is presented for the organization of complex networks. The theory proposes that complex networks, both human-engineered and naturally evolved, are organized to meet certain design or survival objective(s) for a wide variety of operating or environmental conditions. Using the concepts of "value " of interactions and "satisfaction " in a network as generic performance measures, we show that the underlying organizing principle is to meet an overall performance target for a wide variety of operating environments as the design objective. This design requirement for reliable performance under maximum uncertainty leads to the emergence of power laws as a consequence of the Maximum Entropy Principle. The theory also predicts the emergence of exponential and Poisson distribution regimes as a function of the redundancy of the network, thus explaining all three regimes as different manifestations of the same underlying phenomenon within a unified theoretical framework.
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Introduction

Recently, much attention has been paid to the structure of complex networks found in a wide variety of domains such as biology, ecology, sociology, engineering, and so on.[1-6] The concepts and tools of this important emerging discipline are quite relevant to many problems in engineering in general and chemical engineering in particular. For example, the questions about efficiency, robustness, and reliability in the design of supply chain networks can be productively attacked using the recent results in complex networks.[7] Similarly, in metabolic engineering the optimal design of metabolic networks can benefit from the insights learned recently about the structure of complex networks. In product design, such as in the optimal design of catalysts with desired performance properties, developing a reduced-order model of complex reaction networks is an important subproblem to be solved, which can be addressed using the methodologies of complex networks. However, the recent intellectual excitement about the science of complex networks has not yet seemed to have had much of a following in the chemical engineering community. As pointed out by Ottino[8,9] recently "engineering should be at the centre of these developments, and contribute to the development of new theory and tools." In this paper, we present a novel theory that addresses an important question in this nascent discipline.

One of the central questions in systems biology and in

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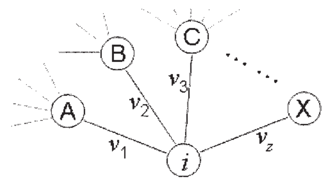

Figure 1. Perceived values of interaction at an arbitrary node *i*.

complex networks organization is how the *local* properties of a network such as the vertex degree of its nodes, which is a property at the individual node level, determine the *global* or system-level properties such as the network's survival or performance. It has been pointed out that these networks, despite the differences in their domain of applications or scale, share some common properties. Perhaps the most striking observation is that many of these networks, but not all, often display a scale-free or power-law behavior of the vertex degree distribution.[1-6] However, recent studies have largely focused on proposing various mechanisms for the emergence of the power-law behavior but not so much on the question of how the local properties of a network are related to the global, system-level, performance measures. In other words, *how do we go from parts to whole* in a complex system? We address this question herein and propose a general holistic design theory for the organization of complex networks. We show that this design theory naturally leads to the emergence of power laws, as well as the emergence of exponential and Poisson regimes, thus explaining all three regimes observed in reality as different manifestations of the same underlying phenomenon within a novel unified theoretical design framework.

Modeling Interactions in a Network: Concepts of Value and Satisfaction

Consider a network of interacting members. This may be a computer network such as the Internet, a network of interacting proteins, a social network of friends, an economic network such as a supply chain, and so on. Such a network is usually represented as a graph, which is a collection of N nodes or vertices and E links or edges. The nodes represent members of the network and the links between nodes represent interactions or relationships between members. Throughout, we use the terms *network* and *graph*, *nodes* and *vertices*, interchangeably. The vertex degree z of a node is the number of edges attached to it.[10] Let us define $n(z)$ as the number of vertices with degree z and $p(z)$ as the probability that any vertex will have degree z. The plot of $n(z)$ vs. z, or $p(z)$ vs. z, known as the vertex degree distribution is of great interest here. This is an important property because it characterizes the overall topology of a network. As noted, for many real-world networks the vertex degree distribution is often found to be a power law, that is, $p(z)$ is proportional to $z^{-\gamma}$, with the exponent γ usually in the range of 2.0–3.0.[1] For random networks it is well known that the degree distribution is Poisson.[10]

In such a network, let each member i receive some *value* v_i from another member via a relationship or an interaction (Figure 1). Further, let each member enter into multiple relationships with other partners contributing and deriving values. We use the notion of "value " in a generic manner. In reality, value may be a design variable such as productivity, money, effort, efficiency, time, CPU, bandwidth, emotional support, and so forth, or some combination of such variables. In addition, there may be various domain-specific constraints on these variables. In general, each such relationship may *cost* the member a certain amount, similar to the expenses associated with creating and maintaining computer lines, roadways, transaction lines, and friendships in real networks. Again, we use "cost " here in a generic manner.

Let us further introduce the notions of *intrinsic value* that a member can contribute in a relationship and *perceived value* as felt by the recipient in that relationship. In general, these two need not be the same. Now consider a member i that is building several relationships with other members to accumulate *value* for itself from the contributions of its interacting partners. Every member is doing this, but we will examine it from the perspective of member i. We now consider three special cases: Case A, where the number of partners of i is *large* and the value contributed by any individual partner to i is much smaller than the cumulative contribution from all the partners to i; Case B, where the number of partners is quite *small* and the individual contributions are a significant portion of the total value accumulated by i; and Case C, where the number of partners is *extremely large*, an extreme version of Case A.

Case A: Large Number of Partners

Let us first consider the situation where the number of partners of i is large. As member i begins to build relationships, the first partner A it picks up is valued highly (that is, the *perceived value* is high). We will call the first partner as a *rank one* partner in this relationship and denote it as $A\{(i, 1)\}$. The second partner $B\{(i, 2)\}$ is valued a little less, the third partner $C\{(i, 3)\}$ even less, and the zth partner $X\{(i, z)\}$ considerably less valued compared with the first partner. Thus, the *perceived value* decreases with every incremental contribution. This is a reasonable situation to consider because such diminishing returns are often encountered in many practical applications when a large number of entities are contributing small amounts each. Let v_m denote the perceived value felt by member i from its partner of rank m. We have not treated the cost of relationships explicitly here. However, it is handled implicitly in the sense the value measure may be treated as the *net value*, after accounting for cost. Although we motivate the notion of rank as the sequential order of a partner in a set of relationships, it need not be restricted to this role alone. In general, the rank of a partner is an indicator of its relative importance in comparison with other partners in a set of relationships.

We call the cumulative sum of all the perceived values the *local satisfaction* measure, S. This measure can be thought of as a *local performance* metric. We postulate this satisfaction measure to be finite as the number of relationships tends to infinity. As noted earlier, this is again a reasonable requirement because, in most real-life situations, there is some kind of a *saturation effect* in such interactions and the notion of diminishing returns is a commonly used principle in many applications. Thus we have the following expression:

$$S_\infty = \nu_1 + \nu_2 + \nu_3 + \cdots = \sum_{m=1}^{\infty} \nu_m < \infty \tag{1}$$

For the sake of simplicity, let all members contribute the same *intrinsic value*. In a very large population of similar members, this is again a reasonable assumption. Thus, everyone contributes the same intrinsic value v, but it is perceived differently by others depending on how many partners they already have, that is, depending on the rank of the relationship. As mentioned earlier, the perceived value of a partner decreases with increasing rank in that particular relationship. This behavior can be modeled as in the following equation, where m is the rank and v_m is the perceived value:

$$\nu_m = v\left(\frac{1}{m^q}\right) \tag{2}$$

Note that the same partner X may be valued differently in different relationships depending on its rank in all those relationships, even though X contributes exactly the same intrinsic value v in all those relationships. Therefore, the satisfaction S for member i from all its z contributing relationships (partners) is given by

$$S_z = \nu \sum_{m=1}^{z} \frac{1}{m^q} \tag{3}$$

Recall that in the limit $z \rightarrow \infty$, we require this sum to converge to a finite value:

$$S_\infty = \nu \sum_{m=1}^{\infty} \frac{1}{m^q} < \infty \tag{4}$$

This implies that the exponent $q > 1$, because the series will otherwise diverge. Although q can take on any number of values that will satisfy this requirement, all those values place additional demands or expectations on the behavior of the function S. The *least restrictive* requirement corresponds to the *threshold* or *limiting case* where $q = 1 + \varepsilon$, where $\varepsilon > 0$, but arbitrarily small. Under this requirement, we have

$$S_\infty = \nu \sum_{m=1}^{\infty} \frac{1}{m^{1+\varepsilon}} < \infty \tag{5}$$

As $\varepsilon \rightarrow 0$, for large but finite z, the resultant harmonic series is approximated by

$$S_z = \nu \sum_{m=1}^{z} \frac{1}{m} \approx \nu[\ln z + 0.577] \tag{6}$$

where 0.577 is an approximation of the Euler's constant. Setting $\varepsilon \rightarrow 0$ may be considered as the *asymptotic limit* of the saturation function S. Because v is an arbitrary quantity, we set $v = 1$ to simplify the analysis. Thus, in the limit $\varepsilon \rightarrow 0$, the cumulative perceived value, that is, the local satisfaction measure S_z for any member, increases approximately as $\ln z$ for large z.

So far we have considered only one member, that is, i. However, every member j in this network tries to accumulate satisfaction given by Eq. 6 such that, in general, we have (letting $v = 1$)

$$S_z^{(j)} = \sum_{m=1}^{z^{(j)}} \frac{1}{m} \approx \ln z^{(j)} + 0.577 \tag{7}$$

where $z^{(j)}$ is the number of partners for member j. Every member tries to increase its local satisfaction to the extent it can, subject to cost and other constraints. Thus, there will be a distribution of local satisfaction measures for the entire network.

From a holistic design perspective, both human-engineered and naturally evolved networks are organized to perform certain overall function(s) well, that is, designed to meet certain performance criteria or survival objectives as a whole. Thus, one is not overly concerned with the local satisfaction or performance of any particular member but with the *overall* satisfaction or performance level in the entire network. A simple intuitive measure of this overall satisfaction level is the average of all the local satisfaction measures. Let us call this average the *global satisfaction measure* (S_G), given by

$$S_G = \langle S^{(j)} \rangle = 0.577 + \langle \ln z^{(j)} \rangle \tag{8}$$

The global satisfaction measure may be thought of as a *performance metric* of the entire network. Thus, from a holistic perspective, the design principle for the organization of the entire network would be to meet a certain level of global satisfaction θ^G, that is, global performance, as the design target, shown in the following expression:

$$S_G = \theta^G = 0.577 + \langle \ln z \rangle = 0.577 + \theta \tag{9}$$

where $\theta = \langle \ln z \rangle$. Therefore, the design of the network—that is, the distribution of relationships or links in the network—will be constrained by the design criterion in Eq. 9.

In addition, there is another design criterion. One would like the network to be designed in such a manner that it can survive and meet its performance target under a wide variety of operating conditions or environments. For example, in the design of computer and communication networks, the design team would try to anticipate a wide variety of communication situations, demand patterns, failure of nodes and edges, addition of new nodes and edges, and so on, and then devise a network that can survive under such varied operating conditions and meet its performance target criteria. A reliable design would not presume that only certain conditions will prevail in the future and thus limit the design to perform well only under those conditions. That is, one would not want to *bias* the design for a specific operating environment, particularly if the nature of future environments is unknown, uncertain, or unpredictable. Thus, the network design should reflect this *inherent uncertainty* about future operating environments and *minimize the bias* or any unwarranted assumptions about them. In other words, a reliable design should accommodate as much uncertainty about the future operating environments as allowed by the constraints, that is, maximum reliability under uncertainty. Thus, we have two global, system-level, design criteria determining the structure of a network: (1) the global satisfaction measure target and (2) reliable performance under *maximum uncertainty*.

Combining these two criteria, the network design problem can now be posed as the following question: *What is the least biased distribution of links in a network such that the constraint $S_G = \theta^G$ or, equivalently, $\langle \ln z \rangle = \theta$ is satisfied?*

Entropy Maximization as a Holistic Design Principle

This question can be answered by applying the Maximum Entropy Principle,[11,12] which states that given some partial information about a random variate, of all the distributions that are consistent with the given information or constraints, the *least-biased distribution* is the one that has the *maximum entropy* associated with it. In the context of the discussion above, maximizing entropy is the same as *maximizing uncertainty* in an information-theoretic sense.[13] By applying the Maximum Entropy formulation to Eq. 9, the least-biased distribution satisfying the constraint $\langle \ln z \rangle$ is a *power law* given by

$$\Pr(Z = z) \approx \frac{1}{\theta} \frac{1}{(z)^{\gamma}} \tag{10}$$

where $\gamma = (1 + \theta)/\theta$ for large z.

We will presently derive this result. Consider a continuous random variate Z. Let $z \geq 1$ and $y = \ln z \geq 0$. Under the constraint $\langle y \rangle = \theta$, for some positive real number θ, it is well known that the maximum entropy formulation yields the exponential probability density function and the cumulative distribution function given respectively below[11,12]:

$$f_Y(y) = \frac{1}{\theta} e^{-(y/\theta)} \qquad \text{and } F_Y(y) = 1 - e^{-(y/\theta)} \qquad \text{for } y \geq 0 \tag{11}$$

However, $F_Z(z) = P(Z \leq z) = P(\ln Z \leq \ln z) = P(Y \leq y) = 1 - e^{-(y/\theta)} = 1 - e^{-(\ln z/\theta)} = 1 - z^{-(1/\theta)}$.

Therefore

$$f_Z(z) = \frac{1}{\theta} \frac{1}{z^{[(1+\theta)/\theta]}} = \frac{1}{\theta} z^{-\gamma}$$

where $\gamma = (1 + \theta)/\theta$.

Using this power-law density, we can also easily show that

$$\gamma = \frac{2\langle z \rangle - 1}{\langle z \rangle - 1} \tag{12}$$

where $\langle z \rangle = \int_1^\infty z f_Z(z) dz$.

Finally, in the practical case where Z is taking values z in the positive integers, the power-law probability density of Eq. 11 can be discretized with the help of Taylor's theorem to yield the discrete power law:

$$\Pr(Z = z) \approx \frac{1}{\theta} \frac{1}{(z)^{\gamma}} \tag{13}$$

where $\gamma = (1 + \theta)/\theta$ for large z.

In the above equation, Z denotes the random variable taking values z in the positive integers.

The importance of Eq. 12 lies in the fact that the mean value of Z is a quantity easily estimated in practice using observed sample averages. To estimate θ from data, the constraint $\langle \ln z \rangle = \theta$ may be used directly. In other words, θ may be estimated as the sample average of $\ln z$ from the data. However, if the sample average of $\ln z$ is not available but the sample average of z is, then Eq. 12 can be used to estimate θ and γ. Nevertheless, it should be noted that if and when the true value of θ is close to one (and the true value of γ is close to 2), then the sample average of z can be an unreliable estimator of its theoretical expectation because the latter can be huge in that case. It is easy to see from Eq. 12 that the bounds on γ for a connected network are $2 < \gamma < 3.02$.

Thus, when one designs a network to meet a certain target global satisfaction or performance measure for a wide variety of operating environments as the design criteria, in the asymptotic limit for large networks, power law emerges as the *optimal* distribution of network connections. It is optimal in the sense that this is the distribution that maximizes the uncertainty about the future operational environments. Thus, it is optimized over all possible future scenarios, where the optimality is with respect to the uncertainty of the assumptions underlying the design. Because the power law emerges under some very general conditions, without any domain specific details or constraints playing a role, it appears to be a *universal behavior* explaining its prevalence in a wide variety of complex systems.

Since Eq. 12 estimates γ in terms of $\langle z \rangle$, we compare this estimation (γ_{est}) with reported results in the literature[1] for a wide variety of networks (Table 1). Because the published data[1] do not separately provide $\langle z_{in} \rangle$ and $\langle z_{out} \rangle$ but only the overall $\langle z \rangle$, γ_{est} is also such an overall value. The subscripts *in* and *out* refer to directed links coming into and going out of a node, respectively. It should also be noted that, because $\langle z \rangle$ is independent of N in Eq. 12, this implies that the estimation of γ is valid for all network sizes, provided they satisfy the general conditions discussed earlier.

We are not surprised by the disagreement with the γ values for food webs (Ythan Estuary and Silwood Park). We believe, and as pointed out by others also,[15] that food webs belong to a different class of complex networks because of the special predator–prey relationship between nodes. In the class of networks addressed in this paper, for every member (node) it is always better to have more partners or relationships (links) because they all contribute value, however small. In food webs, however, each species would like to have *more prey* but *fewer predators*. This conflict makes the situation asymmetric. Thus, we believe the above analysis does not directly apply to food webs.

Case B: Small Number of Partners

In the above analysis, we considered a redundant network where the number of links per node (the link density E/N)—that is, the number of partners—was large. It is quite instructive to explore the theory's predictions in two other limiting cases. One is the scenario where the number of links per node is small, that is, a small number of partners. Since links generally have an associated cost, such a situation is likely to be encountered when the cost per link is very high. Given that in most practical situations one is limited by the total cost one can

Table 1. Comparison of the Estimated and Observed γ Values for Various Networks*

Network	Size	$\langle z \rangle$	γ_{out}	γ_{in}	γ_{est}
WWW	325,729	4.51	2.45	2.1	2.28
WWW	4×10^7	7	2.38	2.1	2.17
WWW	2×10^8	7.5	2.72	2.1	2.15
Internet, domain	3015–4389	3.42–3.76	2.1–2.2	2.1–2.2	2.36–2.41
Internet, router	3888	2.57	2.48	2.48	2.63
Internet, router	150,000	2.66	2.4	2.4	2.60
Movie actors	212,250	28.78	2.3	2.3	2.04
Coauthors, SPIRES	56,627	173	1.2	1.2	2.00
Coauthors, neuro.	209,293	11.54	2.1	2.1	2.09
Coauthors, math.	70,975	3.9	2.5	2.5	2.34
Metabolic, *E. coli*	778	7.4	2.2	2.2	2.16
Protein, S. cerev.	1870	2.39	2.4	2.4	2.72
Ythan Estuary	134	8.7	1.05	1.05	2.13
Silwood Park	154	4.75	1.13	1.13	2.27
Citation	783,339	8.57		3	2.13
Phone call	53×10^6	3.16	2.1	2.1	2.46
Words, cooccurrence	460,902	70.13	2.7	2.7	2.01
Words, synonyms	22,311	13.48	2.8	2.8	2.08

*From Albert and Barabási.[1]

expend on forging links, this would then constrain the total number of links to a small number for a given N. This is the situation where each member would have, on an average, only a small number of relationships. In such a situation, a member then perceives every relationship as more or less equally valuable, quite the opposite of case A. Under this condition, *far below the saturation limit*, the log function $\ln z$ may be approximated linearly as shown in Eq. 14. Thus the cumulative local satisfaction measure may be represented as

$$S_{small} \approx \nu z \tag{14}$$

However, this is not the only condition under which Eq. 14 will be applicable. It would be valid even when the number of relationships/node is relatively high, *provided the satisfaction function is far below the saturation limit*. Thus, the key requirement here is that the satisfaction measure grows at least *approximately linearly* with additional relationships and the diminishing returns regime as modeled by the log function has not set in for any of the nodes in the network. Therefore, the global satisfaction measure is given by (letting $\nu = 1$):

$$S_{G_{small}} = \langle S_{small} \rangle = \langle z \rangle = \theta_{small} \tag{15}$$

Under this constraint, the Maximum Entropy Principle yields the *exponential distribution* as the least-biased distribution as given by

$$f_Z(z) = \frac{1}{\theta_{small}} e^{z/\theta_{small}} \quad \text{and} \quad F_Z(z) = 1 - e^{z/\theta_{small}} \quad z \geq 0 \tag{16}$$

Case C: Extremely large number of partners

Similarly, in the other limit of extremely large number of links per node, we expect the satisfaction measure to saturate much faster than the log function approximation. In this scenario, after some z_{sat} number of relationships have been attained by a member, any additional relationship (link) brings *zero value*. Thus, such links may be placed randomly between any two nodes with equal probability because it does not matter as a result of the zero value contribution, thus leading to a Poisson distribution. Thus, the theory predicts that three distinct classes of networks arise under three different functional behaviors of the local satisfaction measure. Exponential networks correspond to the class where the satisfaction measure grows approximately linearly with additional relationships, power-law networks correspond to the class where the dependency is log-like, and Poisson networks when saturation has set in.

These three classes can also appear as three regimes in a given network as the network moves from a sparsely connected state to reasonably redundant to extremely redundant in the number of links. In such a situation, the exponential regime has a relatively narrow range stemming from the limited validity of the linearity approximation of the log function in Eq. 14. It is more difficult, however, to determine the upper bound for the power-law regime a priori because the rate at which the satisfaction measure saturates may vary from network to network.

The existence of these three regimes as a function of redundancy has been observed in simulations by Guimera et al.[16] and Venkatasubramanian et al.[12] but without a coherent theoretical explanation for their occurrence. Furthermore, exponential degree distribution has been reported to emerge for real networks when the cost constraints of adding new links are particularly severe, as noted by Mossa et al.[17] and Amaral et al.[18] The disappearance of power law also occurs at the other end of the spectrum when the network is extremely redundant in number of links.[3] Barabási and Albert[3] found that starting with N nodes and no links, and adding links incrementally, the power-law scaling was found at early times but was not stationary and eventually disappeared. Because most real-world networks are designed to be reasonably redundant to make them more robust and efficient, they all typically fall in the middle regime and thus the apparent ubiquitous occurrence of power laws and their seeming universality.

Summary

In conclusion, we have presented a general holistic design theory for the organization of complex networks. The theory proposes that complex networks, both human-engineered and naturally evolved, are organized to meet certain design or survival objective(s) for a wide variety of operating or environmental conditions. For a large class of networks, where the interactions between members are of mutual benefit or value, the design objective is to achieve a desired overall network performance as modeled by the average cumulative interaction value. Under some general conditions discussed above, we have shown that for large networks in the asymptotic limit of local performance saturation, the design requirement of reliable performance under maximum uncertainty leads to the emergence of power laws as a consequence of the maximum entropy principle. That is, under these general conditions, a power-law–based organization gives a network the *maximum flexibility* to perform well overall in a wide variety of operating environments. Note that for a particular operating environment, there may exist some other distribution that will outperform the maximum entropy distribution with respect to the global performance target. However, such a *biased* network may fail when the underlying environment is changed, whereas the maximum entropy distribution-based network will continue to survive and perform. Thus, under entropy maximization, the network's performance is *optimized* to accommodate a wide variety of future environments whose nature is unknown, unknowable, and thus uncertain.

In this context, it is interesting to consider the implications of this result for a well known economic phenomenon: the Pareto distribution of wealth. It has been known for nearly a century that the distribution of wealth in many countries follows a power law with $2 < \gamma < 3$ as first observed by the Italian engineer Vilfredo Pareto.[19] The main consequence of this distribution is the inequity in the distribution of wealth, that is, a small number of people hold the majority of the wealth in a society. Although this may seem socially unfair our theory suggests that this is indeed the optimal distribution of wealth for the society at large in the long run. That is, given the design criterion that a society needs to remain economically productive (that is, meet some global productivity or performance target measures) for its survival under a wide variety of future economic environments whose nature is unknown, unpredictable, and thus uncertain, the Pareto distribution is the optimal way of distributing wealth in the face of an uncertain future. Note that this power law result also implies that the local satisfaction measure here, which is a function of a given individual's (that is, node's) accumulated wealth (the proxy for partners), varies as a log function of wealth. Although the log function is not typically used to model wealth effects in economics because it does not saturate in the infinite limit, the point here is that the approximate saturation-like behavior displayed by the log function for large, but not infinite, amount of wealth is a *reasonable enough approximation* in modeling this economic phenomenon that the theory's prediction of a power law as the optimal distribution is observed in reality as the Pareto distribution.

The generality of this theory explains the apparent universality of power laws in many complex systems. The theory also predicts the emergence of exponential and Poisson regimes as a function of the redundancy of a network, thus explaining all three regimes as different manifestations of the same underlying phenomenon within a unified theoretical design framework.

The main contribution of this paper is to present a theoretical design framework to address one of the most important questions in complex networks organization: how the local properties of a network such as the vertex degree are determined by, and conversely determine, the global or system-level properties such as the network performance criteria. This is an important question to resolve because it can pave the way for an integrative perspective on complex networks and systems by relating node or subsystem level properties to system-level ones, going from parts to whole, which has significant implications in a wide variety of domains such as biology, engineering, economics, and sociology. This theory is an attempt to discover the equivalent of the partition function in statistical mechanics, which relates the molecular level properties of a gas to its macroscopic thermodynamic properties. Thus, it has not escaped our notice that the functional form of the satisfaction measure resembles that of entropy and information and that the maximum entropy principle plays such a central role in our theory. It appears that the principle that governs the organization of inanimate physical systems is also at work for the organization of animate biological systems.

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