Emergence of Thermodynamics from Darwinian Dynamics

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Abstract

Darwinian dynamics is manifestly stochastic and nonconservative, but has a profound connection to conservative dynamics in physics. In this short presentation the main ideas and logical steps leading to thermodynamics from Darwinian dynamics are discussed in a quantitative manner. It suggests that the truth of the second law of thermodynamics lies in the fact that stochasticity or probability is essential to describe Nature.

Keywords: Second law of thermodynamics; Darwinian dynamics; stochastic differential equations

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It's kind of awkward to do the talking seated with face away from the big screen. May I use the podium? (pause) This morning we heard lots of very nice talks. They have, I think, laid out a good foundation for my few minutes. I am grateful for the organizers for giving me the opportunity and honor to speak to the distinguished audience. What I'm going to tell you are a few insights that I got from biology. I will take Darwin and Wallace seriously.

In order to understand thermodynamics, a kind of a static property with no time dependence, the proper way should be that started from a real dynamical structure. What I have learned in biology is that there is already one, which is more than 100 years old, and was from Darwin and Wallace (1). Why should anybody do this demonstration? It is the focus of the present conference, the foundation of thermodynamics and statistical mechanics, which have been under vigorous investigation for more than 100 years (2–9)–J.H. Keenan had thought deeply into this problem (10). It is fair to state that no consensus has been reached.

There are two types of important questions in this perspective. One is of course on the foundation. For example, three major questions have been formulated recently (11):
1) In what sense can thermodynamics be reduced to statistical mechanics?
2) How can one derive equations that are not time-reversal invariant from a time-reversal invariant dynamics?
3) How to provide a theoretical basis for the "approach to equilibrium" or irreversible processes?

With the aid of the evolutionary dynamics of Darwin and Wallace, Darwinian dynamics in short, my answer to 1) is that thermodynamics and statistical mechanics are equivalent. They are the two sides of same coin. The answer to 2) is that additional primitive concepts, such as probability and stochasticity, have to be introduced. Not time-reversal invariant dynamics, while consistent with, is logically independent from a time-reversal invariant one. Thus, the answer to 3) is that Darwinian dynamics provides a natural theoretical basis.

Another type of questions is from a dazzling on the enormous success of thermodynamics and statistical mechanics. It has been wondering that (12),
4) Such success would be irrelevant to inference and decision-making; and
5) were assured by unstated methodological practices of censoring data and selective applying arguments; or
6) is a result of extraordinary good fortune.
It is evident that 4) is not true. The connection between statistical mechanics and inference has been well established (13), two sides of our effort to understand Nature. 5) is not true either. Physicists have not used any arbitrary and selective methodology. Nevertheless, 6) contains certain truth: It has been shown (14) that Darwinian dynamics which is adaptive has a remarkable connection to conservative dynamics. Such a relation between two extreme theoretical frameworks demonstrates the unity of sciences.

You may ask then, what is Darwinian dynamics? Word equation of the evolutionary dynamics discovered by Darwin and Wallace (1) is:

\[
\text{Evolution by Variation and Selection.} 
\]

(0)

For nearly 150 years since its conception, this word equation has been applied to all levels of biology (15). There is no exception yet for its validity. While universal, it is not in the mathematical form as expressions in thermodynamics and statistical mechanics. This word equation needs to be expressed in terms of proper mathematical equations. Two further fundamental concepts in biology are needed for this purpose. The first is the so-called fundamental theorem of natural selection (FTNS) (16) which links the variation to the adaptation and optimization. In the hindsight, it appears to be equivalent to fluctuation-dissipation theorem in nonequilibrium physics (14; 17). The second is the existence of adaptive landscape (18). It is equivalent to the assertion of the existence of potential function or Hamiltonian in an evolutionary process (14).

Intuitively it is evident that evolution is about successive processes: Quantities at a later stage are related to their values at its earlier stage under both predictable (deterministic) and unpredictable (stochastic) constraints. For example, the world population of humans in next 20 years will be surely related to its current one. Hence, the genetic frequency, the probability in the population, of a given form of gene (allele) in the next generation is related to its present value. Here sexual conducts and other reproduction behaviors are treated as means to realize the variation and selection for evolution. We may denote those genetic frequencies as \( \mathbf{q} \) with \( n \) components denoting all possible alleles. Thus \( \mathbf{q}^\tau = (q_1, q_2, ..., q_n) \) is a vector (Here \( \tau \) denotes the transpose). There are huge amount of human traits related to genetics (or genes): height, skin color, size of eye ball, faster runner, gene for liver cancer, gene for smartness, ... . The number \( n \) is then large: it could be as large, and likely larger, as the number of genes in human genome, which is about 20000, if one simply assigns one allele
or a trait to one gene without any combinatory consideration. This number is far larger than
the number of chemical elements, which is about 100, and than the number of elementary
particles, about 30. With a suitable choice of time scale equivalent to an averaging over
many generations, the incremental rate in such an evolutionary process may be represented
by a time derivative, \( \dot{q} = dq/dt \). The deterministic constraint at a given time may be
represented by a deterministic force \( f(q) \). For example, there is a high confidence to predict
the eye color of a child based on the information from his/her parents, but the smartness of
an offspring is not so strongly correlated to that of the parents. The random constraint, the
unknown and/or irrelevant force, is approximated by a Gaussian-white noise term \( \zeta(q, t) \),
with zero mean, \( \langle \zeta \rangle = 0 \) and the \( n \times n \) matrix \( D(q) \):
\[
\langle \zeta(q, t') \zeta^\tau(q, t) \rangle = 2D(q)\theta \delta(t - t').
\]
Here the factor 2 is a convention and \( \theta \) is a positive numerical constant reserved for the role of
temperature in physical sciences. \( \delta(t) \) is the Dirac delta function. With these notations we
are ready to transform the word equation into a precise mathematical equation, which reads
\[
\dot{q} = f(q) + \zeta(q, t).
\] (1)

However, an immediate question arises: while we may represent the variation in evolution
by the matrix \( D \), where is Wright’s adaptive landscape and the corresponding potential
function?

The deterministic force \( f(q) \) in general cannot be related to a potential function in a
straightforward way, because \( f(q) \neq D(q)\nabla \phi(q) \). Here \( \nabla = (\partial/\partial q_1, \partial/\partial q_2, \ldots, \partial/\partial q_n)^\tau \) is
the gradient operation in the phase space formed by \( q \), and \( \phi(q) \) is a scalar function. A
nonequilibrium process typically has further five qualitative characteristics or difficulties:
i) dissipative, \( \nabla \cdot f(q) \neq 0 \); ii) asymmetric, \( \partial f_j(q)/\partial q_i \neq \partial f_i(q)/\partial q_j \) for at least one pair of indices of \( i, j \); iii) nonlinear, \( f(\theta q) \neq \theta f(q) \); and
iv) stochastic with multiplicative noise, \( D(q) \) depending on the state variable \( q \).
v) Possibly singular, that is, \( \det(D(q)) = 0 \).

During the study of the robustness of the genetic switch in a living organism (19; 20)
a constructive method was discovered to overcome this difficulty (21–23): Eq.(1) can be
transformed into the following stochastic differential equation,
\[
[A(q) + T(q)]\dot{q} = \nabla \phi(q) + \xi(q, t),
\] (2)
with $\langle \xi(q, t')\xi^*(q, t) \rangle = 2A(q)\theta \delta(t-t')$ and $T = -T^*$. Here the matrices $A, T$ are determined from $D$ and $f$ by two matrix equations: $[A(q) + T(q)]D(q)[A(q) - T(q)] = A(q)$ and $\nabla \times \{[A(q) + T(q)]f(q)\} = 0$. With this construction done, Wright’s adaptive landscape can be easily identified with the scalar function $\phi$. Darwinian dynamics may then be summarized into three general laws in the Table I (14).

| Table I: Laws of Darwinian dynamics and the F-Theorem |
|------------------------------------------------------|
| Mathematical expressions                      | Alternative names | Comments     |
| First Law                                   | $\{q\} \rightarrow \{q_{\text{attractor}}\}$ | law of Aristotle | determinism |
| Second Law                                  | $[A(q) + T(q)]\dot{q} = \nabla \phi(q) + \xi(q, t)$ | law of Darwin & Wallace | stochasticity |
| F-Theorem                                    | $\langle \xi(q, t')\xi^*(q, t) \rangle = 2A(q)\theta \delta(t-t')$ | FTNS | optimization |
| Third Law                                    | $m \rightarrow 0$ | law of hierarchy | multiple scales |

With above general quantitative formulation we are ready to move from biology to physics. We first point out two immediate consequences of Darwinian dynamics.

Allowing the stochastic drive be negligible, ”temperature” $\theta = 0$, Eq.(2) becomes

$$[A(q) + T(q)]\dot{q} = \nabla \phi(q) .$$

(3)

Because the ascendant matrix $A$ is non-negative and $T$ is anti-symmetric, the system will approach the nearest attractor determined by its initial condition, and stay there if already there. Specifically, Eq.(3) leads to

$$\dot{q} \cdot \nabla \phi(q) \geq 0 .$$

(4)

This equation implies that the deterministic dynamics cannot decrease the evolutionary potential $\phi$. If the ascendant matrix $A$ is positive definite, the potential of the system always increases. Hence, the first law clearly states that the system has the ability to find the local adaptive landscape peak or an attractor represented by the Wright evolutionary potential $\phi$, determined by the initial condition. However, the shifting between different evolutionary peaks would become impossible in this limit, because the transition probability vanishes exponentially. We note that Eq.(11) implies that the Wright evolutionary potential $\phi$ is a Lyapunov function.
Conservative Newtonian dynamics may be regarded as a further limit of the above formulation: zero friction and zero noise limit, $A = 0$. Hence, from Eq.(3), Newtonian dynamics may be expressed as,

$$T(q) \dot{q} = \nabla \phi(q),$$

which is the form similar to Hamilton equation. This suggests a profound connection between biology and physics. Here the value of potential function is evidently conserved during the dynamics since $\dot{q} \cdot \nabla \phi(q) = 0$. The system moves along equal potential contours in the adaptive landscape. This conservative behavior suggests that the rate of approaching to equilibrium is associated with the ascendant matrix $A$, not with the diffusion matrix $D$. There are situations where the diffusion matrix is finite but the ascendant matrix is zero, and thus the dynamics is conservative (24).

Darwinian dynamics can be described by a probabilistic equation, a special form of Fokker-Planck equation. It has been derived from Eq.(2) (23) that the equation for probability distribution function $\rho$ is

$$\frac{\partial}{\partial t} \rho(q,t) = \nabla^\tau [(D(q) + Q(q))\theta \nabla - f(q)] \rho(q,t),$$

with $[D(q) + Q(q)] = [A(q) + T(q)]^{-1}$ and $f(q) = [D(q) + Q(q)] \nabla \phi(q)$. Its steady state distribution is of Boltzmann-Gibbs type, if it exists:

$$\rho(q, t = \infty) = \frac{1}{Z} \exp \left\{ \frac{\phi(q)}{\theta} \right\}.$$ 

Here $Z = \int \prod_{i=1}^{n} dq_i \exp \{ \psi(q)/\theta \}$, the partition function.

We note that three independent parts in a general dynamics are suggested by Eq.(6) and (7): The non-conservative dynamics associated with diffusion matrix $D$, the conservative dynamics with $Q$, and the potential function with $\phi$. Thus, this is a remarkable synthesis between near and far from equilibrium processes, and conservative and non-conservative dynamics. This feature is also true for discrete master equations, though usually a different interpretation is provided (25).

I hope I have made it logically clear that the Boltzmann-Gibbs distribution follows in a natural and consistent manner from Darwinian dynamics. Starting from this distribution it is a relative straightforward procedure to deduce rigorously the second law of thermodynamics (8; 26). I will not waste your time here by going through such process. Instead, I should point out that further new results on stochastic equalities can be obtained from Darwinian
dynamics, such as a generalized Einstein relation, a free energy dynamical equality in the absence of detailed balance (8). I should also point out that among the three universal dynamics known to us, Darwinian dynamics, relativity, and quantum mechanics, only Darwinian dynamics is non-conservative. This may be the reason for the natural emergence of thermodynamics. Thank you very much for your attention.

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