Replicator equations, response functions and entropy measures in science: mathematical background

Y. A. Pykh & I. G. Malkina-Pykh
Research Center for Interdisciplinary Environmental Cooperation (INENCO RAS), Russian Academy of Sciences

Abstract

Replicator dynamics is an evolutionary strategy well established in different disciplines of biological sciences. It describes the evolution of self-reproducing entities called replicators in various independent models of, e.g., genetics, ecology, prebiotic evolution, and sociobiology. Besides this, replicator selection has been applied to problem solving in combinatorial optimization and to learning in neural networks and also in fluid mechanics, game and laser theory. So, the replicator systems arise in an extraordinary variety of modeling situations. In this report we'll consider the new class of generalized replicator equations with nonlinear response functions and construct the Energy Lyapunov function and entropy measures for this system.
Keywords: replicator equations, Lyapunov functions, entropy, distance measure.

1 An overview and introduction

A *replicator* is a fundamental unit in evolutionary processes, representing a population *type*, and characterized by two attributes: $p_i(t)$, its proportion in the population at time t, and its non-negative fitness at time t. A replicator's fitness is a measure of its significance to the future evolution of the population. The proportions of replicators in a population change as a result of their mutual interactions, and their relative fitnesses.

The founding fathers of evolutionary genetics, Fisher, Haldane and Wright used mathematical models to generate a synthesis between Mendelian genetics and Darwinian evolution. Kimura's theory of neutral evolution, Hamilton's kin

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selection and Maynard Smith's evolutionary game theory are all based on mathematical descriptions of evolutionary dynamics. Concepts like fitness and natural selection are best defined in terms of mathematical equations.

The notion of a *replicator* – originally invented by Dawkins [6] – is now used in biology for "*an entity that passes on its structure largely intact in successive replications*" (Vrba [28]). The origin of life is characterized by the emergence of heritable information that, through the interplay of selection and variation, leads to Darwinian evolution.

Very recently the interest in evolutionary dynamical models has increased dramatically, mainly because in the game theoretic literature it is commonly thought that such models can provide a better understanding of the Nash equilibrium solution concept than traditional static game theory, as well as a description of the non-equilibrium behavior of the players. The replicator dynamics, introduced into the literature by Taylor and Jonker [27] for the special case of two player games in the late seventies of our century, is the classical example of such an evolutionary dynamical model.

Throughout last century the formal analogies between the mathematical models in population dynamics and certain models of different physical or chemical processes have been a source of inspiration both for biologists and physicists. As early as in 1911 Sharpe and Lotka [25] made an analogy between the stable age structure of human populations and an acoustical problem.

Autocatalytic reaction networks which in general involve two classes of catalytic processes – autocatalytic instruction for reproduction and additional material and process specific catalysis – were postulated as models for studies of prebiotic and early biological evolution scenarios Eigen, Schuster [7,8]. In the last decade it turned out that they serve also as models in very different fields like molecular biology, population genetics, theoretical ecology or dynamical game theory (Schuster and Sigmund [24]). A variety of self-replicating chemical systems have been constructed and investigated experimentally in the past 25 years since Spiegelman's [26].

Besides this fundamental importance in theoretical biology, replicator selection has been applied to problem solving in combinatorial optimization and to learning in neural networks (Bomze [3], Menon [11]). Recent results show that the same type of differential equations is also obtained by non-linear coordinate transformations from models in fluid mechanics and laser theory (Brenig and Goriely [4]). So, it is clear that replicator systems are a class of first order, nonlinear differential equations, arising in an extraordinary variety of modeling situations.

In this report we'll introduce the new class of generalized replicator equations with nonlinear response functions and construct Energy Lyapunov function and entropy measures for this systems.

2 Generalized replicator equations

First replicator-like equation was introduced by Fisher [9], who immediately recognized certain formal analogies between the mechanistic models introduced by Boltzmann [2] to analyze physical systems, and the selection models proposed by Darwin [5] to explain adaptation in biological systems. By considering the dynamical system which describes the changes in gene frequency of the population which occurs under natural selection, Fisher proved a directionality theorem, which he called the fundamental theorem of natural selection.

The absolute fitness of the zygote A_iA_j, denoted as w_{ij} is defined as the relative or fractional number of offspring per unit time that the genotype will produce that will grow to maturity and themselves reproduce.

The state of the genetical system at time t is simply the vector $p(t)=(p_1(t),\ldots,p_n(t))$, which is clearly constrained to lie in the standard simplex σ in n-dimensional Euclidean space $\mathbb{R}^n$:

$$\sigma = \left\{p \in \mathbb{R}^n : p_i \geq 0, \quad i=1,\ldots,n, \ \mathbf{e}^T p = 1\right\}.$$

Here and in the sequel, the letter **e** is reserved for a vector of appropriate length, consisting of unit entries $\left(\text{hence } \mathbf{e}^T p = \sum_{i=1}^{n} p_i\right)$. The original Fisher's selection equation of haploid genotypes evolution is, then, written as:

$$\dot{p}_i = p_i\left(\sum_{j=1}^{n} w_{ij} p_j - \sum_k \sum_j w_{kj} p_k p_j\right) \quad i=1,\ldots,n \tag{1}$$

where the dot is derivative w.r.t. time. The population state is then given as a point in simplex σ. Fisher took into account only zygote fitness. In this case $w_{ij} = w_{ji}$ i.e. matrix $W=(w_{ij})=W^T$. The difference between symmetric and nonsymmetrical matrices W is crucial. Indeed in the symmetric case the quadratic form $p(t)^T Wp(t)$ is increasing along trajectories of the selection dynamics (1) – this is the Fundamental Theorem of Natural Selection going back to R. A. Fisher.

Theorem 1. (Fisher [9]) *If $W=W^T$ then the function $p(t)^T Wp(t)$ is strictly increasing with increasing t along any non-stationary trajectory $p(t)$ under (1). Furthermore, any such trajectory converges to a stationary point.*□

Fisher claimed that the theorem was an analog of Boltzmann's [2] principle of entropy increase, and thus to be an analog of the Second Law. These claims have later been re-evaluated.

This theorem is tantamount to saying that mean fitness is an Energy Lyapunov function of the dynamical system (1). Let me recall that a single–valued function which is continuous and has continuous partial derivatives is called the Energy Lyapunov function (ELF) for dynamical system if it is monotonically increasing along the trajectories of this dynamical system (Meyer [12]). So, if we know ELF for dynamic system under consideration then we know practically everything about evolution of this system. It was shown by (Pykh [18]) what ELF may be also used as a measure of biodiversity.

In 1969 V.A. Ratner [23] showed that if we take into account also gamete selection when the fitness matrix $G = DW$, where $D = diag(d_i)$ is diagonal matrix with $d_i > 0$ and W is symmetrical matrix. In this case Fisher's theorem is a false. But, it was shown by Pykh [19, 22] that there exists an analog of Fisher's theorem. Let us denote by $\langle \cdot, \cdot \rangle$ the inner product of the two vectors.

Theorem 2. (Pykh [16,17]) *If matrix G has the next form: $G = D_1 B D_2$, where B is symmetrical, D_1 and D_2 are diagonal matrices and matrix $D = D_1^{-1} D_2 > 0$ then the function $E : \sigma \to \mathbb{R}^1$*

$$E(p) = \frac{p^T D_2 B D_2 p}{\langle d, p \rangle^2} \tag{2}$$

is ELF for system (6). □

3 Replicator equations with nonlinear response functions

In this report we'll restrict our consideration with generalized replicator equations Pykh [19] in the next form:

These equations are written as

$$\dot{p}_i = h(p) f_i(p_i) \left(\sum_{j=1}^{n} w_{ij} f_j(p_j) - \theta^{-1}(p) \sum_{j,k=1}^{n} w_{jk} f_j(p_j) f_k(p_k) \right) \quad i = 1, \dots, n \tag{3}$$

Here, f_i are nonlinear response functions satisfying the conditions $f_i(0) = 0$, $\partial f_i / \partial p_i > 0$ $p_i > 0$, and $\partial f_i / \partial p_i \geqslant 0$ for $p_i = 0$; $W = (w_{ij})$ is the matrix of interactions; the function $h : \sigma \to (0, \infty]$ is determined by the particular problem under consideration; $\theta(p) = \langle \mathbf{e}, f(p) \rangle$; and $f(p) = (f_1(p_1), \dots, f_n(p_n))$. Obviously, since $\langle \dot{p}(t), \mathbf{e} \rangle \equiv 0$ and $f_i(0) = 0$, the simplex σ and each of its faces are invariant sets of system (3). Examples of different response functions one can find in Pykh and Malkina-Pykh [22].

To state the main theorem, we need some preliminary results. First, it is convenient to pass to the matrix form of representation. In this form, system (3) becomes

$$\dot{p} = h(p) \mathcal{D}(f) \left(Wf - \mathbf{e} \theta^{-1}(p) \langle f, Wf \rangle \right) \tag{4}$$

where $\mathcal{D}(f) = diag(f_1, \dots, f_n)$.

If the matrix W is nondegenerate, then system (4) has at most one isolated equilibrium point in $\mathrm{Int}\sigma$, which we call nontrivial.

Statement. (Pykh [16,19]). *System (3) has a unique nontrivial equilibrium point $\hat{p} \in \mathrm{Int}\sigma$ if and only if the vector $W^{-1}\mathbf{e}$ is either strictly positive or strictly negative.*□

The coordinates of this equilibrium point are determined from the system

$$\hat{f} \big/ \langle \hat{f}, \mathbf{e} \rangle = W^{-1}\mathbf{e} \big/ \langle \mathbf{e}, W^{-1}\mathbf{e} \rangle \quad (5)$$

where $\hat{f} = \left(f_1(\hat{p}_1), \ldots, f_n(\hat{p}_n)\right)$. Let us introduce the notation $W^{-1}\mathbf{e} = b$; then, for $\hat{p}_i$, we obtain the following system of $(n+1)$ equations:

$$\hat{p}_i = f_i^{-1}(\lambda b_i) \qquad i = 1, \ldots, n, \qquad \sum_{i=1}^{n} \hat{f}_i^{-1}(\lambda b_i) = 1,$$

where λ - is an auxiliary variable similar to the Lagrange multiplier. Obviously, this system has a unique solution if all the b_i are of the same sign.

Theorem 3. (Pykh [19]). *If the matrix W is symmetric, then the function*

$$E(p) = \langle f(p), Wf(p) \rangle \theta^{-2}(p) \quad (4)$$

is a Lyapunov energy function for system (2). □

Corollary. (Pykh [14, 17]). If system (2) has a nontrivial equilibrium point $\hat{p} \in \mathrm{Int}\sigma$, then it is totally stable in $\mathrm{Int}\sigma$ if and only if the matrix W has $(n-1)$ negative characteristic numbers.□

Table 1: Different entropy measures.

Response function	Entropy	Name
Logariphmic $f_i(p_i) = (1 - \ln p_i)^{-1}$	$H_o(p) = \sum_{i=1}^{n} p_i \ln p_i$	Bolzmann entropy
Power-law $f_i(p_i) = p_i^{1-q};\ q \neq 1$	$H_o(p) = \frac{(\sum p_i^q - 1)}{1 - q}$	Tsallis entropy
Logistic $f_i(p_i) = \frac{1}{b + ce^{-\alpha p_i}}$ $b > 0,\ c > 0,\ \alpha > 0$	$H_o(p) = \sum_{i=1}^{n} \ln\left(1 - e^{-\alpha p_i}\right)$	Logistic entropy

4 Entropy measures

Now, we can state the main result

Theorem 4. (Pykh [21]) *If system (4) has a nontrivial equilibrium point* $\hat{p} \in Int\sigma$ *and the matrix* $(W^T + W)$ *has* $(n-1)$ *negative characteristic value, then the function*

$$H_\varepsilon(p) = \sum_{i=1}^{n} \int_{\varepsilon_i}^{p_i} \frac{\hat{f}_i dx}{f_i(x)}$$

where $0 \leqslant \varepsilon_i \leqslant 1, i = 1, ...n$ *are some constant is a Lyapunov energy function for system (4).* □

Based on this theorem we can receive a set of response function for existing entropy measures and construct new entropy and distance measures for any response functions. Short summary of this approach listed in tables 1 and 2.

Table 2: Different distance measure.

Response function	Interaction matrix	«Distance »	Name
Linear $f_i(p_i) = p_i$	Theorem 4	$H_{\hat{p}} = \sum \hat{p}_i \ln \frac{p_i}{\hat{p}_i}$	Relative entropy (Kullback [10])
Linear $f_i(p_i) = p_i$	$W = D_1 B D_2$	$H_{\hat{p}} = \sum_{i=1}^{n} d_i \hat{p}_i \ln \frac{p_i}{\hat{p}_i} - -\langle d, \hat{p} \rangle \ln \langle d, p \rangle$	Weighted relative entropy (Pykh [16,17])
logistic $f_i(p_i) = = \frac{1}{b + ce^{-\alpha p_i}}$ $b > 0, c > 0, \alpha > 0$	Theorem 4	$H_{\hat{p}} = \sum_{i=1}^{n} \hat{f}_i \ln \left(\frac{1 - e^{-\alpha p_i}}{1 - e^{-\alpha \hat{p}_i}} \right)$	Weighted logistic entropy (new)

5 Conclusion

It is seen from the examples given above that, if we consider entropy characteristics, then we should set $\varepsilon_i = 0$ in the expression for $H_\varepsilon(p)$, and if we are interested in "distances" between distributions, then we should take $\varepsilon_i = \hat{p}_i$. We also emphasize that there exists a relation between the derivative of the function $H_\varepsilon(p)$, which can be interpreted as a generalized entropy, and the function $E(p)$, which is often (in particular, in works on the theory of neural networks) considered as an analog of the energy. This relationship for entropy production was established by Pykh [20,21] and has the next form:

$$\dot{H}_\varepsilon = h(p)\theta\hat{\theta}\left(E(\hat{p}) - E(p)\right) \geqslant 0$$

In conclusion, we mention that all results stated above were obtained by formally analyzing systems of generalized replicator equations, which arise in very diverse fields of natural sciences and, therefore, can serve as a basis for finding analogies between these domains of natural sciences.

Also note that it was Ilya Prigogine who the first pointed out [13] the importance of the relationship between Lyapunov functions and entropy.

References

[1] Beck C. and Schlogl F., *Thermodynamics of Chaotic Systems*, Cambridge University Press, Cambridge, UK, 1995.

[2] Boltzmann L., *Vorlesungen űber Gas Theorie*, Leipzig, Germany: Barth, 1896.

[3] Bomze I.M., “Evolution towards the maximum clique”, *Journal of Global Optimization*, no. 10, pp. 143 – 164, 1997.

[4] Brenig L. and Goriely A., “Universal canonical forms for time-continuous dynamical systems”, *Phys. Rev. A*, no. 40, pp. 4119–4122, 1989.

[5] Darwin C., *On the Origin of Species*, London: Murray, 1859.

[6] Dawkins R., *The Selfish Gene*, Oxford University Press, Oxford, 1976.

[7] Eigen M., “Self-organization of matter and the evolution of biological macromolecules”, *Natur-wissenschaften*, no. 58, pp. 465–526, 1971.

[8] Eigen M. and Schuster P., *The Hypercycle. A Principle of Natural Self-organization*, Springer-Verlag, Berlin, 1979.

[9] Fisher R.A., *The Genetical Theory of Natural Selection,* New York: Dover, 1930.

[10] Kullback S. and Leiber R. On information and sufficiency. *Ann. Math. Stat.,* Vol.22, N1, pp. 79-87, 1951.

[11] Menon A., *Replicators and Complementarity: Solving the Simplest Complex System without Simulation*, in: V.N. Alexandrov et.al., eds., ICCS 2001, LNCS 2074, pp. 922–931, 2001.

[12] Meyer K., “Energy functions for Morse-Smale systems”, *Amer. J. Math*., v. 90, no. 4, pp. 1031–1040, 1968.

[13] Prigogine I., Time, structure and fluctuations. Nobel lecture, 8 December, 1977

[14] Pykh Yu. A., *On the Global Stability of Some Ecological Models*, Mathematical Models of Cell Population, Inter-University Collection/Gorky State University, Gorky, pp. 70–74, 1981, (Russian).

[15] Pykh Yu. A., “On monostability of certain equations of population dynamics”, *Biosphere Problems*, no. 2, pp. 71–80, USSR Academy of Sci., Moscow, 1981a (in Russian).

[16] Pykh Yu. A., *Steady-State and Stability in the Models of Population dynamics*, Nauka, Moscow, 1983 (Russian).

[17] Pykh Yu.A., “Lyapunov functions for Lotka-Volterra systems: an overview and problems”, *Proceedings of 5th IFAC Symposium “Nonlinear Control Systems” 2001,* pp. 1655–1660. www.inenco.org/publications

[18] Pykh Yu.A., Liapunov function as a measure of biodiversity: theoretical background. *“Ecological indicators”, 2 (2002) 123-133*

[19] Pykh Yu.A., Energy Lyapunov Function for Generalized Replicator Equations. *Proceedings of International Conference “Physics and Control”,* 2003, pp.271-276 www.inenco.org/publications

[20] Pykh Yu.A., “Construction of entropy characteristics based on Lyapunov energy function”. *Doclady Mathematics. V 69, N 3, 2004, pp.355-358* www.inenco.org/publications

[21] Pykh Yu.A., Construction of the entropy measures on the basis of replicator equation with nonsymmetrical interaction matrix. *Doclady Mathematics,* 2005, in press.
[22] Pykh Yu.A., Malkina-Pykh I.G. *The method of response function in ecology*. WIT Press, 2000, 275 p.
[23] Ratner V.A., *Mathematical Models in the Population genetics: Frequency-Dependent Deterministic Models,* in "Mathematical Models in Biology", VINITI, pp. 88–115, 1969 (Russian).
[24] Schuster P. and Sigmund K., "Replicator dynamics", J. Theor. Biol., no. 100, pp. 533–538, 1983.
[25] Sharpe F.R. and Lotka A.J., "A problem in age-distribution", *Philosophical Mag.*, no. 21, pp. 435–438, 1911.
[26] Spiegelman S., "An approach to the experimental analysis of precellular evolution", *Quarterly Review of Biophysics*, no. 4, pp. 213–251, 1971.
[27] Taylor P. G. and Jonker L., "Evolutionary stable strategies and game dynamics", *Math. Biosci*., no. 40, pp. 145–156, 1978.
[28] Vrba E.S., *Levels of Selection and Sorting with Special Reference to the Species Level*, in Oxford Surveys in Evolutionary Biology, P.H. Harvey and L. Partridge, eds., Oxford University Press, no. 6, pp. 114–115, 1989.