THE MAXIMUM PRINCIPLE FOR REPLICATOR EQUATIONS

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PREFACE

By introducing a non-Euclidean metric on the unit simplex, it is possible to identify an interesting class of gradient systems within the ubiquitous "replicator equations" of evolutionary biomathematics. In the case of homogeneous potentials, this leads to maximum principles governing the increase of the average fitness, both in population genetics and in chemical kinetics.

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1. Introduction

The notion of adaptive landscape is a familiar one in theoretical biology. Evolution is often pictured as an uphill movement leading to ever increasing fitness under the driving force of selection. We mention Wright [19] and Simpson [18] for explicit descriptions of the concepts of adaptive genotypic and phenotypic landscapes, respectively. The general idea of evolution as progressive optimization is so pervasive, however, that it is difficult to give a precise account of its origin.

The strictest version of an uphill movement is that of steepest ascent. In this case, the adaptive landscape itself determines the path, and the dynamics are given by the gradient of the slope. Gradient systems are well-behaved: in fact, they are often too tame for a realistic description of the antics of biological evolution. Even if random drift and other stochastic influences are excluded, the effects of time-dependence, frequency dependence, developmental constraints, genetic linkage, co-evolutionary interactions, etc. will lead to phenomena incompatible with the existence of a potential function. Nevertheless, gradient systems play an important conceptual role in basic dynamical models, both in micro- and macro-evolution (cf. Akin [1] and Lande [11]). They lead to highly suggestive extremum principles and provide a link between the methods of population genetics and mathematical physics.

In this paper we shall consider gradient systems within the framework of replicator equations. Such equations model a rich diversity of phenotypic and genotypic evolution. The state of the system is described by relative frequencies within a population, and hence by a point on the unit simplex. The basic idea of Shahshahani[17] was to replace the Euclidean metric by a Riemann metric. Gradient systems with respect to this metric occur as important examples of replicator equations, both in classical population genetics and in the chemical kinetics of polynucleotide replication. The corresponding maximum principles have been stated by Kimura [8] and Küppers [9] . Their rigorous proof was an immediate consequence of Shahshahani's introduction of the appropriate metric.

2. Replicator equations

Let

$$S_n = \{\underline{x} = (x_1, \ldots, x_n) \in \mathbb{R}^n : \Sigma x_i = 1,\ x_i \geq 0\}$$

denote the unit simplex and let $\underline{f}$ be a vector field defined in a neighborhood of S_n. We associate with $\underline{f}$ the vector field $\hat{\underline{f}}$ on S_n with coordinates

$$\hat{f}_i(\underline{x}) = x_i(f_i(\underline{x}) - \Phi(\underline{x})) \qquad i = 1, \ldots, n \tag{1}$$

where

$$\Phi(\underline{x}) = \Sigma x_i f_i(\underline{x}) \tag{2}$$

A differential equation of the type

$$\dot{\underline{x}} = \hat{\underline{f}}(\underline{x}) \tag{3}$$

is called a replicator equation. Two simple properties are easily checked:

(a) Both the unit simplex S_n and its faces are invariant under (3);

(b) If $\underline{f}$ and $\underline{g}$ are two equivalent vector fields, then $\hat{\underline{f}} = \hat{\underline{g}}$ on S_n. Here, $\underline{f} \sim \underline{g}$ if $f_i(\underline{x}) - g_i(\underline{x})$ is independent of i for all $\underline{x} \in S_n$.

Replicator equations are very common in mathematical biology. They describe the action of selection on many different levels of biological organization. We refer to Schuster and Sigmund [16] and Hofbauer and Sigmund [6] for surveys on this subject (the second of these is more detailed) and shall only give two of the simplest examples here.

(a) If $\underline{f}$ is constant, then (3) becomes

$$\dot{x}_i = x_i(a_i - \Phi) \tag{4}$$

This equation describes the evolution of gene frequencies for frequency-independent asexual reproduction, and in particular the relative concentrations of self-reproducing macromolecules in the absence of mutations and chemical interactions (see Eigen and Schuster [3] and Küppers [10]).

(b) If $\underline{f}$ is linear, then (3) becomes

$$\dot{x}_i = x_i(\Sigma\, a_{ij}x_j - \Phi) \tag{5}$$

This equation occurs in at least four different fields of evolutionary biology. First of all, it is equivalent to the general Volterra-Lotka equation in mathematical ecology

$$\dot{y}_i = y_i(b_{io} + \sum_{j=1}^{n-1} b_{ij}y_j) \qquad i = 1,\ldots,n-1 \tag{6}$$

with $b_{ij} = a_{ij} - a_{nj}$. This equivalence (obtained by setting $y_i = x_i/x_n$) has been pointed out by Hofbauer [5]. Secondly, (5) describes the evolution of gene frequencies for asexual reproduction, if the fitnesses are (linearly) dependent, and of phenotype frequencies in game-theoretic models of animal behavior (cf. Maynard Smith [14]). Thirdly, it plays an important role in the chemical kinetics of catalytically interacting polynucleotides, hypercycles etc. (see Eigen and Schuster [3]). Finally, (5) describes the action of selection in a one-locus viability model, under the assumption of Hardy-Weinberg equilibrium (cf. Hadeler [4]). In this case, x_i is the frequency of allele A_i in the gene pool and a_{ij} is the probability of survival, from zygote to adult age, of the genotype A_iA_j. This yields a special case of (5), namely

$$\dot{x}_i = x_i(\Sigma a_{ij}x_j - \Phi) \quad \text{with} \quad a_{ij} = a_{ji} \tag{7}$$

(7) is the so-called Fisher-Haldane-Wright selection equation.

It is easy to show that for both (4) and (7), the "average fitness" Φ is always increasing (see [4]). Kimura [8] claimed that the orbits of (7) always point in the direction of maximal increase of Φ, and Küppers [9] stated that this same property of "steepest ascent" holds for (4).

At first glance, this seems to be wrong. Indeed, maximal increase implies that the direction of the orbits is orthogonal to the constant level sets of Φ (as every hiker intuitively knows). This is not the case in general.

It turns out, however, that with another notion of orthogonality the orbits do cross the constant level sets at right angles. Thus the maximum principles become valid if one modifies the notion of inner product (see Shashahani [17] and Akin [1]).

3. Shahshahani gradients

The relevant state space for replicator equations is S_n. We are therefore interested in angles between vectors belonging to $T_{\underline{p}}S_n$, the tangent space to S_n at the point $\underline{p} \in \text{int } S_n$: these vectors are characterized by the property that the sum of their components is 0. For two vectors $\underline{x}$ and $\underline{y}$ in $T_{\underline{p}}S_n$, we define, following Jacquard [7] and Shahshahani [17]:

$$\langle \underline{x}, \underline{y} \rangle_{\underline{p}} = \sum_{i=1}^{n} \frac{1}{p_i} x_i y_i \tag{8}$$

and check that this is indeed an inner product. It differs from the "usual" Euclidean inner product

$$\langle \underline{x}, \underline{y} \rangle = \sum_{i=1}^{n} x_i y_i \qquad (9)$$

by the factors $1/p_i$. The i-th term in the sum gains in importance if p_i is small. (8) leads to a notion of orthogonality which depends on $\underline{p}$, and induces a distance which differs from the Euclidean one by attaching more weight to changes which occur near the boundary of S_n. (We refer to Akin [1] for details).

Let V be a differentiable function from some neighborhood U of S_n (in $\mathbb{R}_n$) into $\mathbb{R}$. For each $\underline{p} \in \text{int } S_n$, the derivative $DV(\underline{p})$ is a linear map from the tangent space into $\mathbb{R}$. There exists a unique vector grad $V(\underline{p})$ such that

$$\langle \text{grad } V(\underline{p}), \underline{y} \rangle = DV(\underline{p})(\underline{y}) \qquad (10)$$

holds for all $\underline{y} \in T_p \mathbb{R}_n$. This "Euclidean" gradient grad $V(\underline{p})$ has components $\partial V(\underline{p})/\partial x_i$. Similarly, there is a unique vector Grad $V(\underline{p})$ such that

$$\langle \text{Grad } V(\underline{p}), \underline{y} \rangle_{\underline{p}} = DV(\underline{p})(\underline{y}) \qquad (11)$$

holds for all $\underline{y} \in T_{\underline{p}} S_n$. This vector is called the Shahshahani gradient of V.

4. Replicator equations and Shahshahani gradients

It is easy to characterize those replicator equations (3) which are Shahshahani gradients:

Theorem: $\qquad \hat{\underline{f}} = \text{Grad } V \quad \text{iff} \quad \underline{f} \sim \text{grad } V$

Indeed, suppose that $\underline{f} \sim$ grad V. We know that $\underline{g} \sim \underline{h}$ implies $\hat{\underline{g}} = \hat{\underline{h}}$ on S_n. We may therefore assume, without loss of generality, that $\underline{f} =$ grad V. For $\underline{y} \in T_{\underline{p}} S_n$, one gets

$$\langle \hat{f}(\underline{p}),\underline{y}\rangle_{\underline{p}} = \Sigma \frac{1}{p_i} p_i(f_i - \Phi) y_i = \Sigma f_i y_i - \Phi \Sigma y_i = \Sigma f_i y_i$$

since $\Sigma y_i = 0$. Thus

$$\langle \hat{\underline{f}}(\underline{p}),\underline{y}\rangle_{\underline{p}} = \Sigma \frac{\partial V}{\partial x_i} y_i = DV(\underline{p})(\underline{y}) \tag{12}$$

Hence, by (11), $\hat{f}$ = Grad V.

If, conversely, $\hat{\underline{f}}$ = Grad V, then (12) implies

$$\Sigma f_i y_i = \frac{\partial V}{\partial x_i} y_i$$

for all $\underline{y} \in T_{\underline{p}} S_n$. With $y_i = 1$, $y_n = -1$ and $y_j = 0$ for all $j \neq i,n$, this implies

$$\frac{\partial V}{\partial x_i}(\underline{p}) - \frac{\partial V}{\partial x_n}(\underline{p}) = f_i(\underline{p}) - f_n(\underline{p}).$$

It follows that

$$\frac{\partial V}{\partial x_i}(\underline{p}) = f_i(\underline{p})$$

does not depend on 1, and hence that $\underline{f} \sim$ grad V.

Thus if $\underline{f}$ is a Euclidean gradient, i.e. if

$$\frac{\partial f_i}{\partial x_j} = \frac{\partial f_j}{\partial x_i}$$

holds (for all i and j) in some small neighborhood U of S_n which is simply connected, then the orbits of $\dot{\underline{x}} = \hat{\underline{f}}(\underline{x})$ are orthogonal, in the Shahshahani sense, to the constant level sets of V (in S_n).

5. Homogeneous potentials

If the potential function V is a homogeneous function of degree $s > 0$, i.e. if

$$V(\alpha x_1, \dots \alpha x_n) = \alpha^s V(x_1, \dots, x_n) \tag{13}$$

holds for all $\alpha \in \mathbb{R}$, then the "average fitness" Φ satisfies (by Euler's theorem)

$$\Phi(\underline{p}) = \Sigma\ p_i f_i(\underline{p}) = \Sigma\ p_i \frac{\partial V}{\partial x_i}(\underline{p}) = s\ V(\underline{p}).$$

Hence Φ increases at a maximal rate, in the Shahshahani sense. The rate of increase is

$$\dot{\Phi}(\underline{x}) = s\ \dot{V}(\underline{x}) = s\ \Sigma \frac{\partial V}{\partial x_i} \dot{x}_i = s \sum_i \frac{\partial V}{\partial x_i} x_i \left(\frac{\partial V}{\partial x_i} - \Sigma\ x_j \frac{\partial V}{\partial x_j}\right)$$

$$= s\left[\sum_i x_i (f_i(\underline{x}))^2 - (\Sigma\ x_i f_i(\underline{x}))^2\right] \geq 0 \tag{14}$$

The rate of increase can be viewed (up to the factor s) as the variance of a random variable taking the value $f_i(\underline{x})$ with probability x_i, $i = 1, \dots, n$.

If, for example, $\underline{f} = \text{grad } V$ with

$$V(\underline{x}) = \Sigma\ a_i x_i \tag{15}$$

then (3) becomes (4) and one obtains the (modified) maximum principle of Küppers. If

$$V(\underline{x}) = \frac{1}{2} \sum_{ij} a_{ij} x_i x_j \tag{16}$$

then

$$\frac{\partial V}{\partial x_i}(\underline{x}) = \frac{1}{2} \sum_j (a_{ij} + a_{ji}) x_j$$

In particular, if $a_{ij} = a_{ji}$, then (3) becomes (7) and one obtains the (modified) maximum principle of Kimura. In this case (14) is just Fisher's Fundamental Theorem of Natural Selection (see, e.g. Hadeler [4]): the rate of increase of the average fitness is proportional to the variance of the fitness in the gene pool.

It is obvious that the orbits of any gradient system converge to the set of fixed points. Does every orbit converge to an equilibrium? This need not always be the case, as Takens has shown. But for (4), it is obviously true. For (7), it is also valid, but demands an elaborate proof (see Akin and Hofbauer [2], and Losert and Akin [12]). It would be interesting to know whether for any Shahshahani gradient system with homogeneous potential function V, every orbit converges to an equilibrium.

If V is not homogeneous, then Φ need not always increase. For example $V = x_1^2 + x_2$ has its minimum at $x_1 = \frac{1}{2}$, but the minimum of the corresponding $\Phi = 2x_1^2 + x_2$ is at $x_1 = \frac{1}{4}$. For a state which has x_1 between $\frac{1}{4}$ and $\frac{1}{2}$, the average fitness decreases.

6. First-order replicator equations and Shahshahani gradients

Let us now characterize those linear replicator equations (5) which are Shahshahani gradients.

<u>Theorem</u> (5) is a Shahshahani gradient iff

$$a_{ij} + a_{jk} + a_{ki} = a_{ji} + a_{ik} + a_{kj} \tag{17}$$

holds for all i,j,k between 1 and n.

Condition (17) states that the sum of the coefficients of the matrix $A = (a_{ij})$ over all three-cycles $i \to j \to k \to i$ of indices is independent of the orientation. The same holds, then, for all p-cycles, $p > 3$, as shown by "triangulation".

Indeed, if (17) holds, one has only to set $c_k = a_{kn} - a_{nk}$ to see that

$$b_{ij} = a_{ij} + c_j$$

satisfies $b_{ij} = b_{ji}$. The equation

$$\dot{x}_i = x_i(\Sigma b_{ij}x_j - \Phi) \tag{18}$$

is therefore a Shahshahani gradient, and so is (5), since it coincides with (18) on S_n.

Conversely, if $\hat{\underline{f}} = \text{Grad } V$, then $\underline{f} = \text{grad } V$, i.e. there is some function Ψ such that

$$f_i(\underline{p}) - \frac{\partial V}{\partial x_i}(\underline{p}) = \Psi(\underline{p})$$

holds for all i (and all $\underline{p} \in S_n$). From this follows

$$\frac{\partial f_i}{\partial x_j}(\underline{p}) - \frac{\partial f_j}{\partial x_i}(\underline{p}) = \frac{\partial \Psi}{\partial x_j}(\underline{p}) - \frac{\partial \Psi}{\partial x_i}(\underline{p}) \tag{19}$$

If $f_i = \sum_i a_{ij}x_j$ then $\frac{\partial f_i}{\partial x_j} = a_{ij}$. Thus

$$a_{ij} - a_{ji} = \frac{\partial \Psi}{\partial x_j}(\underline{p}) - \frac{\partial \Psi}{\partial x_i}(\underline{p}) \tag{20}$$

From this (17) follows immediately.

Let us call two $n \times n$ matrices A and B equivalent ($A \sim B$) if there exist constants c_j s.t. $a_{ij} = b_{ij} + c_j$ for all i and j between 1 and n. A and B are equivalent iff the functions $\underline{x} \to A\underline{x}$ and $\underline{x} \to B\underline{x}$ are equivalent in the sense described in Section 2. The theorem implies that (5) is a Shahshahani gradient iff one of the following conditions is satisfied:

(a) there is a symmetric matrix within the equivalence class of the matrix A;

(b) there exist constants c_i such that $a_{ij} - a_{ji} = c_i - c_j$ for all i and j;

(c) there exist vectors $\underline{u}, \underline{v} \in \mathbb{R}^n$ such that $a_{ij} - a_{ji} = u_i + v_j$ for all i and j.

7. Further remarks

(A) For (5), Φ is homogenous. From this it follows that Φ increases at a maximal rate, in the Shahshahani sense, iff A is symmetric.

If (5) is interpreted as the dynamics of a game (see, e.g., Schuster et al. [15]), this means that the average payoff increases at a maximal rate iff the game is a partnership game.

On the other hand it is easy to check that Φ is an invariant of motion for (5) (i.e. constant along every orbit) iff for all i and j, one has

$$a_{ii} = a_{ij} \quad \text{and} \quad a_{jj} = a_{ji}$$

or

$$a_{ij} + a_{ji} = 2a_{ii} = 2a_{jj} \tag{21}$$

It would be interesting to characterize those equations (5) for which Φ is monotonically increasing along every orbit.

(B) Game dynamics between two populations lead to equations of the type

$$\begin{aligned} \dot{x}_i &= x_i\Big(\sum_{j=1}^{n} a_{ij}x_j + \sum_{j=1}^{m} b_{ij}y_j - \Phi\Big) \quad i = 1,\dots,n \\ \dot{y}_j &= y_j\Big(\sum_{i=1}^{n} c_{ji}x_i + \sum_{i=1}^{m} d_{ji}y_i - \Psi\Big) \quad j = 1,\dots,m \end{aligned} \tag{22}$$

with

$$\Phi = \sum_{ij} a_{ij}x_ix_j + \sum_{ij} b_{ij}x_iy_j \qquad \Psi = \sum_{ij} c_{ji}y_jx_i + \sum_{ij} d_{ji}y_jy_i \tag{23}$$

(see, e.g., Schuster et al. [15]). This equation "lives" on the product space $S_n \times S_m$ of two simplices. One may introduce in an obvious way a Shahshahani-type inner product in the corresponding tangent spaces. Equation (22) is a gradient system with respect to this metric if the matrices (a_{ij}) and (d_{ji}) satisfy (17) and if there exist constants c_i and d_j such that with $g_{ij} = c_{ij} - b_{ji}$

$$g_{ij} = c_i - d_j \tag{24}$$

for $i = 1,\dots,n$ and $j = 1,\dots,m$. This is the case iff

$$g_{sj} + g_{ti} = g_{tj} + g_{si} \tag{25}$$

holds for all indices i,j,s and t. (Condition (17) means that $g_{ij} = a_{ij} - a_{ji}$ satisfies (25)).

(C) As mentioned in Section 2, the first-order replicator equation (5) is equivalent to the Volterra-Lotka equation (6). The mapping

$$(x_1,\dots,y_1) \rightarrow (y_1,\dots,y_{n-1})$$

transforms the Shahshahani inner product on S_n into an inner product on $\mathbb{R}_+^{n-1}$. For $\underline{q} \in \operatorname{int} \mathbb{R}_+^{n-1}$ and two vectors Y and Z in $T_{\underline{q}} \mathbb{R}_+^{n-1}$, this yields

$$\langle Y,Z\rangle_{\underline{q}} = \sum_{i=1}^{n-1} \frac{1}{q_i} Y_i Z_i - (\sum_{i=1}^{n-1} Y_i)(\sum_{j=1}^{n-1} Z_j).$$

A more natural inner product would be

$$\langle Y,Z\rangle_{\underline{q}} = \sum_{i=1}^{n-1} \frac{1}{q_i} Y_i Z_i \tag{26}$$

With this metric,

$$\dot{y}_i = y_i f_i(y_1,\dots,y_{n-1}) \quad i = 1,\dots,n-1$$

is a gradient iff

$$\dot{y}_i = f_i(y_1 \dots y_{n-1})$$

is a gradient with respect to the Euclidean metric. In particular, the Volterra-Lotka equation (6) is a gradient system with respect to the metric defined by (26) iff $b_{ij} = b_{ji}$ for $1 \leq i,j \leq n-1$. Volterra-Lotka equations of this type have been investigated by MacArthur [13].

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