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QUADRATIC STOCHASTIC OPERATORS AS A TOOL IN MODELLING THE DYNAMICS OF A DISTRIBUTION OF A POPULATION TRAIT

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ABSTRACT

Quadratic stochastic operators can exhibit a wide variety of asymptotic behaviours and these have been introduced and studied recently. In the present work we discuss biological interpretations that can be attributed to them. We also propose a computer simulation method to illustrate the behaviour of iterates of quadratic stochastic operators.

INTRODUCTION

The study of nonlinear Markov evolution has become a subject of interest due to its applications which include population and disease dynamics, physics, evolutionary biology and economic and social systems. One of the simplest but still nontrivial examples of nonlinear dynamics is the quadratic one. Quadratic stochastic operators were first introduced by Bernstein [1] to describe the evolution of a distribution of classes of individuals (*i.e.* groups of individuals possessing a particular trait) in a population. Since then the theory has developed in different directions and has the potential to be an important tool in modelling various phenomena.

We begin by defining a quadratic stochastic operator. Let $\mathfrak{X}$ be the Banach space of all absolutely summable or finite real sequences $\underline{x} := (x_j)_{j \geq 1}$ (*i.e.* $\mathfrak{X} = \ell^1$ or $\mathfrak{X} = \ell_d^1 = \mathbb{R}^d$ in the d -dimensional case) equipped with the standard norm $\|\underline{x}\|_1 = \sum_{j=1}^{\infty} |x_j|$. Following [2],

Definition 1. A quadratic stochastic operator $\mathbf{Q}$ is defined as a cubic array of nonnegative real numbers $[q_{ij,k}]_{i,j,k \geq 1}$ (infinite when $\mathfrak{X} = \ell^1$) or $[q_{ij,k}]_{1 \leq i,j,k \leq d}$ (in the d -dimensional case when $\mathfrak{X} = \ell_d^1$) if it satisfies

(D1) $0 \leq q_{ij,k} = q_{ji,k} \leq 1$ for all $i, j, k \geq 1$,

(D2) $\sum_{k=1}^{\infty} q_{ij,k} = 1$ for any pair (i, j) .

The family of all quadratic stochastic operators is denoted by $\mathfrak{Q}$.

Every cubic matrix $\mathbf{Q} \in \mathfrak{Q}$ may be viewed as a bilinear mapping $\mathbf{Q} : \mathfrak{X} \times \mathfrak{X} \rightarrow \mathfrak{X}$ if we set $\mathbf{Q}(\underline{x}, \underline{y})_k = \sum_{i,j=1}^{\infty} x_i y_j q_{ij,k}$ for any $k \geq 1$. Clearly, $\mathbf{Q}$ is monotone (*i.e.* $\mathbf{Q}(\underline{x}, \underline{y}) \geq \mathbf{Q}(\underline{u}, \underline{w})$ whenever $\underline{x} \geq \underline{u} \geq 0$ and $\underline{y} \geq \underline{w} \geq 0$) and bounded as $\sup_{\|\underline{x}\|_1, \|\underline{y}\|_1 \leq 1} \|\mathbf{Q}(\underline{x}, \underline{y})\|_1 = 1$.

Let $\mathcal{D} = \{\underline{x} \in \mathfrak{X} : x_j \geq 0, \sum_{j=1} x_j = 1\}$, i.e. $\mathcal{D}$ is the set of all probabilistic vectors (distributions) $\underline{x} \in \mathfrak{X}$. Clearly, if $\underline{x}, \underline{y} \in \mathcal{D}$, then $\sum_{i,j=1} x_i y_j q_{ij,k} \geq 0$ for any $k \geq 1$ and $\sum_{k=1} \sum_{i,j=1} x_i y_j q_{ij,k} = 1$. Thus, $\mathbf{Q}(\mathcal{D} \times \mathcal{D}) \subseteq \mathcal{D}$. Hence the quadratic stochastic operator $\mathbf{Q}$ has an immediate biological interpretation. By $\underline{x}$ and $\underline{y} \in \mathcal{D}$ we denote the distribution of a discrete trait (e.g. allele) of two different populations. Then $\mathbf{Q}(\underline{x}, \underline{y})$ is the distribution of that trait in the offspring coming from the mating of individuals descending from the different populations. The special case of inbreeding arises when $\underline{x} = \underline{y}$, i.e. a nonlinear mapping $\mathcal{D} \ni \underline{x} \mapsto \mathbb{Q}(\underline{x}) := \mathbf{Q}(\underline{x}, \underline{x}) \in \mathcal{D}$ is being considered. Then $\mathbb{Q}(\underline{x})$ represents the trait distribution in the next generation if $\underline{x} \in \mathcal{D}$ is the trait distribution in the parents' generation. The values $q_{ij,k}$ are sometimes called the heredity coefficients and correspond to probabilities of obtaining an individual of class k as a result of mating two individuals of classes i and j . In this simplified model the iterates $\mathbb{Q}^n(\underline{x})$, where $n = 0, 1, \dots$, describe the evolution of the distribution of a discrete trait in a population.

Direct applications of quadratic stochastic operators are still in their infancy but [3–5] can serve as examples. These works illustrate both the usefulness of quadratic stochastic operators and the complexity of applying them. In [4] a framework for describing a single gene following Mendelian evolution is provided. In [3] (see also [5]) the authors model the heredity of blood groups and the Rhesus factor. The coefficients $q_{ij,k}$ ($i, j, k \geq 1$) of $\mathbf{Q}(\cdot, \cdot)$ are obtained from observing the blood groups of parents and their children but only point estimates are provided. Propagation of statistical uncertainty with the number of generations seems to be an open research direction. It would be interesting to study it as in the above mentioned work some coefficients that should be 0 due to the Mendelian laws of heredity holding for this trait, are slightly greater than 0 (mutations being a possible explanation).

CONVERGENCE OF QUADRATIC STOCHASTIC OPERATORS

One of the fundamental issues is the study of the asymptotic behaviour of iterates of quadratic stochastic operators. Even if we focus on the case of inbreeding, the problem is not easily tractable because of the nonlinearity. It is possible to obtain a linear model by considering nonhomogeneous chains of stochastic operators, i.e. a sequence $(P^{[n,n+1]})_{n \geq 0}$ of positive linear operators $P^{[n,n+1]}$ on $\mathfrak{X}$ preserving $\mathcal{D}$ (simply define $P^{[n,n+1]} := [p_{r,s}^{n,n+1}]_{r,s \geq 1}$, where for any integer number $n \geq 0$, $p_{r,s}^{n,n+1} \geq 0$ and $\sum_{s=1} p_{r,s}^{n,n+1} = 1$ for any $r \geq 1$, and $P^{[n,n+1]}$ acts on $\mathfrak{X}$ by $(P^{[n,n+1]}\underline{x})_s = \sum_{r=1} x_r p_{r,s}^{n,n+1}$). Following [2] we consider

Definition 2. Given a quadratic stochastic operator $\mathbf{Q}$ and any initial distribution $\underline{y} \in \mathcal{D}$, a non-homogeneous Markov chain associated with $\mathbf{Q}$ and a seed $\underline{x} \in \mathcal{D}$ is defined by

$$P_{\underline{x}}^{[n,n+1]} = [p_{\underline{x};j,k}^{n,n+1}]_{j,k \geq 1} = [\mathbf{Q}(\mathbb{Q}^n(\underline{x}), \underline{e}_j)_k]_{j,k \geq 1},$$

where $\underline{e}_j = (\delta_{k,j})_{k \geq 1}$.

It is easy to see that for any $n \geq 0$ we have $P_{\underline{x}}^{[n,n+1]}(\mathbb{Q}^n(\underline{x})) = \mathbb{Q}^{n+1}(\underline{x}) = P_{\underline{x}}^{[0,n+1]}(\underline{x})$, hence the iterates of $\mathbb{Q}$ can be defined as a nonhomogeneous Markov chain with transition probability matrix $[p_{\underline{x};j,k}^{n,n+1}]_{j,k \geq 1}$ at the instant n .

In [2] the authors introduced different types of asymptotic behaviours of a quadratic stochastic operator depending on the mode of convergence of its iterates and expressed them in terms of convergence of the associated (linear) nonhomogeneous Markov chain. This allows us to study the limit properties of a quadratic stochastic operator by applying the theory of nonhomogeneous Markov chains. A detailed study of relevant asymptotic behaviours of nonhomogeneous Markov chains can be found in [6, 7]. Since the contents of [2] are strictly based on mathematical theory and methods, in this paper we give their biological interpretations, as well as illustrating them with computer simulations.

Following [2] we consider

Definition 3. A quadratic stochastic operator $\mathbf{Q}$ is called:

- (1) *norm mixing (uniformly asymptotically stable, uniformly regular)* if there exists a probabilistic vector $\underline{p}^* \in \mathcal{D}$ such that

$$\lim_{n \rightarrow \infty} \sup_{\underline{x} \in \mathcal{D}} \|\mathbf{Q}^n(\underline{x}) - \underline{p}^*\|_1 = 0,$$

- (2) *strong mixing (asymptotically stable, regular)* if there exists a probabilistic vector $\underline{p}^* \in \mathcal{D}$ such that for all $\underline{x} \in \mathcal{D}$ we have

$$\lim_{n \rightarrow \infty} \|\mathbf{Q}^n(\underline{x}) - \underline{p}^*\|_1 = 0,$$

- (3) *strong almost mixing* if for all $\underline{x}, \underline{y} \in \mathcal{D}$ we have

$$\lim_{n \rightarrow \infty} \|\mathbf{Q}^n(\underline{x}) - \mathbf{Q}^n(\underline{y})\|_1 = 0.$$

Notice that different definitions of mixing have different biological interpretations. All notions mentioned above are in a sense related to the case of inbreeding. Norm mixing may be understood as a situation in which the population is completely isolated from other populations and the trait distribution stabilizes with the passage of time. The same interpretation has the property of strong mixing. Even though these two types of mixing are mathematically very different (strong mixing is essentially weaker than norm mixing), biologically they have a similar meaning. However, strong almost mixing describes the evolution of two populations placed in the same environmental conditions (*i.e.* the law of the evolution given by $\mathbf{Q}$ is the same). Each one of them can have an arbitrary initial trait distribution and the difference between these distributions vanishes with the passage of time. Another type of asymptotic behaviour in the class of quadratic stochastic operators can be introduced by using the associated Markov chains as follows (*cf.* [2]):

Definition 4. We say that $\mathbf{Q} \in \mathfrak{Q}$ is *norm quasi-mixing* if

$$\lim_{n \rightarrow \infty} \sup_{\underline{x}, \underline{u}, \underline{v} \in \mathcal{D}} \|P_{\underline{x}}^{[0,n]}(\underline{u}) - P_{\underline{x}}^{[0,n]}(\underline{v})\|_1 = 0.$$

The norm quasi-mixing property has a slightly more subtle biological interpretation. First, let us take a closer look at $P_{\underline{x}}^{[0,n]}(\underline{u})$. Expanding the iterations of the associated Markov operator we get

$$\begin{aligned} P_{\underline{x}}^{[0,n]}(\underline{u}) &= P_{\underline{x}}^{[n-1,n]}(P_{\underline{x}}^{[n-2,n-1]}(\dots(P_{\underline{x}}^{[0,1]}(\underline{u}))\dots)) \\ &= \mathbf{Q}(\mathbf{Q}^{n-1}(\underline{x}), \mathbf{Q}(\mathbf{Q}^{n-2}(\underline{x}), \mathbf{Q}(\dots(\mathbf{Q}(\mathbf{Q}(\underline{x}), \mathbf{Q}(\underline{x}, \underline{u})))\dots))). \end{aligned}$$

Imagine two populations (placed in the same environmental conditions) with initial trait distributions $\underline{x}$ and $\underline{u}$ respectively, living on patches of habitat connected by movement of individuals only from the first patch to the second. Then after one time step we observe inbreeding on the first patch and mixing of two populations on the second patch occurs by mating the individuals from the second location with immigrants coming from the first one. Hence $P_{\underline{x}}^{[0,n]}(\underline{u})$ represents the trait distribution in the n -th generation living on the second patch, whose members are the offspring of immigrants from the first patch (constant inbreeding and trait distribution $\mathbf{Q}^{n-1}(\underline{x})$ at instant $n - 1$) and inhabitants of the second patch (mating with immigrants from the first patch at each time step and trait distribution $\mathbf{Q}(\mathbf{Q}^{n-2}(\underline{x}), \mathbf{Q}(\dots(\mathbf{Q}(\mathbf{Q}(\underline{x}), \mathbf{Q}(\underline{x}, \underline{u})))\dots))$ at instant $n - 1$). Now, to give the interpretation of norm quasi-mixing, let us assume that we observe three populations with initial trait distributions $\underline{x}$, $\underline{u}$ and $\underline{v}$ respectively, living on three patches of habitat connected by movement of individuals only from the first patch to the second and third (no other interaction is allowed). As before, inbreeding on the first patch takes place and we notice mating of individuals from the second and the third patch with immigrants coming from the first patch. Norm quasi-mixing may be understood as a situation in which the difference between the trait

distributions of the populations living on the second and the third patch vanishes with the passage of time. This however does not imply the stabilization (*i.e.* convergence) of these distributions, but solely says that even if these distributions are strongly fluctuating, they will be fluctuating in the same way with the passage of time (the difference between them will be decreasing to zero).

SIMULATING A QUADRATIC STOCHASTIC OPERATOR

Simulating a movement of a particle among its possible states is straightforward (setting aside numerical issues) if it is determined by a linear homogeneous Markov chain. Simply, one updates the current value (state of a particle) according to the probability law that it indicates. The idea of how to simulate the movement of a particle governed by a quadratic stochastic operator is not immediate. A pair of values indicates the probability law generating a single value. The question then becomes how to arrive at two values of the trajectory to generate the new one and how to get the next one. It is much easier to obtain (and to simulate from) the probability distribution on a state space (*i.e.* a space of all possible values or, in a biological approach, a space of all possible phenotypes) at each discrete time moment n . Given an initial distribution $\underline{y} \in \mathcal{D}$, by its trajectory we understand the sequence $(Q^n(\underline{y}))_{n \geq 0}$. Hence, one needs to iterate n times the operator $Q(\cdot)$ and then draw from the resulting distribution. Most of the literature uses the phrase “simulating” a quadratic stochastic operator in this sense (*cf.* [4, 8]). Probability distributions at each generation are found numerically and the trajectory of the initial distribution as a function of time is presented (see *e.g.* Fig. 2). This however is not simulating a trajectory of the process itself. It would be desirable to observe particles behaving according to the quadratic stochastic operator. Therefore we propose a procedure, described in Algorithm 1, to simulate a trajectory of $\underline{y} \in \mathcal{D}$. We would

Algorithm 1 Simulating $Q(\underline{y})$

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Draw  $N$  independent individuals according to the law of  $\underline{y}$  and call them  $P_0$ 
for  $i = 1$  to  $n$  do
   $P_i := \emptyset$ 
  for  $j = 1$  to  $N$  do
    Draw a pair  $(f_j, m_j)$  of individuals from population  $P_{i-1}$ 
    Draw an individual  $Z_j$  according to the law of  $Q(\underline{e}_{f_j}, \underline{e}_{m_j})$ 
     $P_i = P_i \cup \{Z_j\}$ 
  end for
end for
return  $P_0, P_1, \dots, P_n$ 

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expect that at the i -th step of Algorithm 1 the trait in population P_i should be distributed according to $Q^i(\underline{y})$. In fact, if we look at Fig. 1, left panel, this is the case. However, in the right panel we can see an example exception, when Q restricted to $\mathcal{D}$ possesses absorbing distributions. In such a case a trajectory has to (with probability 1) sooner or later fall into one of the absorbing states. The absorbing states of the identity operator considered in Fig. 1 (right panel) are $\underline{e}_1 = (1, 0)$ and $\underline{e}_2 = (0, 1)$. The probability (at iteration 0) that the trajectory will end at $\underline{e}_i$ ($i = 1, 2$) equals y_i , where $\underline{y} = (y_1, y_2)$ is the initial distribution. We can also notice two other properties of the trajectories in Fig. 1: the trajectory rapidly approaches the stationary distribution and also rapidly falls into the absorbing state.

Another interesting example arises in the class of the so-called Volterra operators, *i.e.* the class of such $Q = [q_{ij,k}]_{i,j,k \geq 1} \in \mathfrak{Q}$ that $q_{ij,k} = 0$ if $k \notin \{i, j\}$ for any $i, j, k \geq 1$. On the basis of numerical calculations, S. M. Ulam [9] conjectured that for the Volterra operator Q the limit $\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{k=0}^{n-1} Q^k(\underline{y})$ exists for any $\underline{y} \in \mathcal{D}$. It was shown to be false by Zakharevich in [10]. Namely, he proved that for $Q \in \mathfrak{Q}$ defined on 2-dimensional simplex by $q_{11,1} = q_{22,2} = q_{33,3} = q_{12,1} = q_{23,2} = q_{13,3} = 1$, the Cesàro means diverge for every interior point $\underline{y} \in \mathcal{D}$ (except the

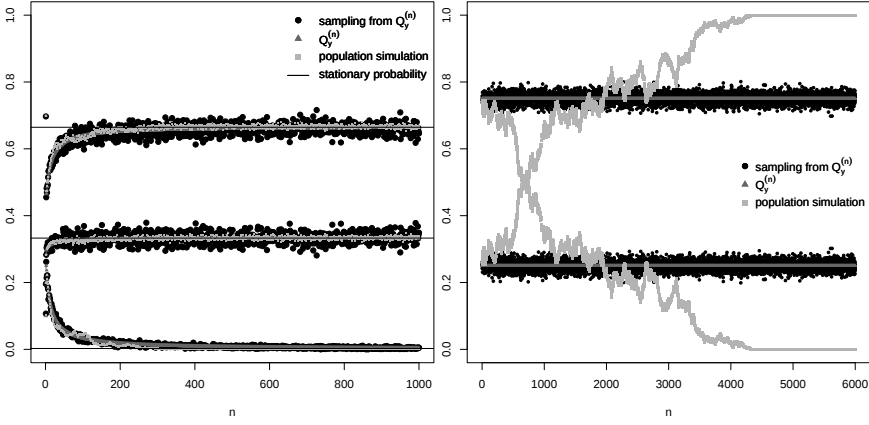


Figure 1. Simulating a quadratic stochastic operator according to Algorithm 1 (“population simulation”, number of individuals $N = 10000$), numerically calculating the distribution (“ $Q_y^{(n)}$ ”) and sampling from $Q_y^{(n)}$ at each generation. Each point of the line “sampling from $Q_y^{(n)}$ ” is an average of 10000 random values drawn from the numerically calculated $Q_y^{(n)}$. Each graph presents all values (3 in the left panel, 2 in the right panel) of the simulated probability vector by the distinct lines.

Left: $\mathbb{Q} \in \Omega$ defined on 3—dimensional space by $q_{11,1} = q_{22,2} = 1$, $q_{13,3} = 1$, $q_{12,1} = q_{23,2} = \frac{3}{4}$, $q_{12,3} = q_{23,3} = \frac{1}{4}$, $q_{33,1} = q_{33,3} = \frac{1}{2}$, $\underline{y} = (0.1, 0.2, 0.7)$, $\underline{p}^* \approx (0.333, 0.003, 0.664)$.

Right: $\mathbb{Q} \in \Omega$ defined on 2—dimensional space by $q_{11,1} = q_{22,2} = 1$, $q_{12,1} = q_{12,2} = \frac{1}{2}$, $\underline{y} = (0.75, 0.25)$. Here $\mathbb{Q}$ is the identity operator and every initial distribution is a fixed point of $\mathbb{Q}$ (hence there is no stationary distribution).

fixed point $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$. This is because the trajectory of any interior initial distribution (different than the fixed point) spirals out approaching arbitrarily close to the boundaries of the simplex, but never reaches it (cf. Fig. 2) and the number of times that it spends close to the consecutive vertices of the simplex increases rapidly (see also [11, 12]). In fact, it was shown in [13] that the iterates of any $\mathbb{Q}((y_1, y_2, y_3)) = (y_1(1 + ay_2 - by_3), y_2(1 - ay_1 + cy_3), x_3(1 + by_1 - cy_2))$, where $-1 \leq a, b, c \leq 1$ are nonzero and have the same sign, possess this property.

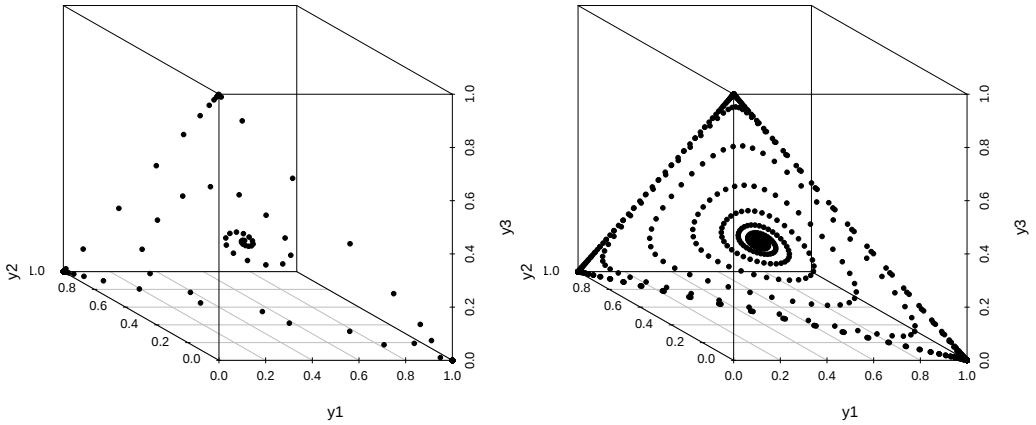


Figure 2. The evolution of the probabilistic vector $\underline{y}$ on a 2 - dimensional simplex according to $\mathbb{Q}((y_1, y_2, y_3)) = (y_1(1 + ay_2 - by_3), y_2(1 - ay_1 + cy_3), x_3(1 + by_1 - cy_2))$.

Left: Zakharevich’s example [10], i.e. $a = b = c = 1$, $\underline{y} = (0.33, 0.33, 0.34)$.

Right: $a = b = c = -\frac{1}{3}$, $\underline{y} = (0.33, 0.33, 0.34)$.

FINAL REMARKS

A practitioner could readily say that the asymptotic descriptions presented here are trivial in the sense that this is how one would expect a sensible reproductive system to behave. Quadratic stochastic operators offer a framework for a formal mathematical description of this behaviour and they could be used to test whether the population is behaving as expected. For example, we would expect that if two populations live in the same environmental conditions, they become similar after a number of generations (strong almost mixing), but they do not. Is this just a result of random fluctuations (due to *e.g.* sample size) or is there some unobserved variable? Similarly, we would expect a population to converge to a given distribution (strong and norm mixing) and one could ask if the deviation is statistically insignificant or if one has missed some factor.

Our work also provides a new direction of study regarding how to effectively simulate particles following a quadratic stochastic operator and what the stochastic properties of Algorithm 1 are. We wrote that we would expect at each iteration the particle population to be distributed according to $\mathbb{Q}^n(y)$. However, the finite population size causes dependencies between pairs (*e.g.* the same pair could be sampled more than once) and this could result in deviations from the theoretical distribution. Another problem is to characterize the behaviour of the population with an absorbing set of distributions.

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