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# Convergence and simulation of centred kernel quadratic stochastic operators

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In this work, we consider a class of centred kernel quadratic stochastic operators. We prove that in this class a centred kernel quadratic stochastic operator convergences almost surely and in  $L^2$  with an exponential  $L^2$ -rate to its limit distribution. We propose an approximation scheme for this class of quadratic stochastic operators and describe three algorithms for simulating them. We consider in detail an example where the kernel is a Guassian one.

*Key words and phrases:* asymptotic stability, mixing nonlinear Markov process, nonhomogeneous Markov operator, quadratic stochastic operator, simulation.

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# Introduction

The theory of quadratic stochastic operators has its origins in the work of S.N. Bernstein [6]. Such operators were introduced to describe the evolution of a discrete probability distribution of a finite number of biotypes in a process of inheritance. Since then the theory has developed in many different directions. A comprehensive overview of results and open problems in this domain can be found in [9, 10].

Quadratic stochastic operators may be considered as a first step in the generalization of (classical) linear Markov chains. In comparison to linear operators, the long-term behaviour of the iterates of the nonlinear ones, is not well understood. Many works were devoted to the study of asymptotic behaviour of quadratic operators (see, e.g., [1, 2, 12, 14]). In [2], weak stability of the so-called centred quadratic stochastic operators was considered. Some exemplary sufficient conditions for the existence of a weak limit were given. In this work, we complement [2] with a study of a subclass of centred kernel quadratic stochastic operator, where we have above the weak convergence (we refer the reader to e.g. [7] for background on weak convergence), almost sure (a.s.) and  $L^2$  convergence to its limit distribution. Furthermore, we are able to make precise statements about the rate of convergence. Finally, we provide three algorithms for simulating the behaviour of its iterates.

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### **1** Basics on quadratic stochastic operators

Given a separable metric space (X, A), where A stands for the Borel  $\sigma$ -field, let  $\mathcal{M} = \mathcal{M}(X, A, \|\cdot\|_{TV})$  denote the Banach lattice of all signed measures on X with finite total variation, where the norm is given by

$$||F||_{TV} := \sup\left\{ \left| \int_X f(x)dF(x) \right| : f \text{ is } \mathcal{A}\text{-measurable, } \sup_{x \in X} |f(x)| \le 1 \right\}.$$

By  $\mathcal{P} := \mathcal{P}(X, \mathcal{A})$ , we denote the convex set of all probability measures on  $(X, \mathcal{A})$ .

**Definition 1.** A bilinear symmetric operator  $\mathbf{Q} \colon \mathcal{M} \times \mathcal{M} \to \mathcal{M}$  is called a quadratic stochastic operator on  $\mathcal{M}$  (QSO on  $\mathcal{M}$  for short) if for all  $F_1, F_2 \in \mathcal{M}, F_1, F_2 \ge 0$ , and any  $A \in \mathcal{A}$  we have

 $\mathbf{Q}(F_1,F_2)(A) \ge 0$  and  $\|\mathbf{Q}(F_1,F_2)\|_{TV} = \|F_1\|_{TV} \|F_2\|_{TV}.$ 

The QSO **Q** on  $\mathcal{M}$  is called a *kernel quadratic stochastic operator* if there exists an  $\mathcal{A} \otimes \mathcal{A}$ -measurable doubly-indexed family  $\mathcal{G} = \{G(\cdot; x, y) : (x, y) \in X^2\} \subset \mathcal{M}$  of probability measures on  $(X, \mathcal{A})$  such that for  $F_1, F_2 \in \mathcal{M}, G \in \mathcal{G}$  we have

$$\mathbf{Q}(F_1,F_2)(A) = \int_{X \times X} G(A;x,y) dF_1 \times F_2(x,y) \quad \text{for all } A \in \mathcal{A}.$$

The family  $\mathcal{G}$  is called the kernel of  $\mathbf{Q}$ .

Clearly any QSO **Q** is bounded, as  $\|\mathbf{Q}(F_1, F_2)\|_{TV} \leq \|F_1\|_{TV} \|F_2\|_{TV}$  for all  $F_1, F_2 \in \mathcal{M}$ . Moreover,  $\mathbf{Q}(\mathcal{P} \times \mathcal{P}) \subseteq \mathcal{P}$ . Let  $\mathcal{M}_0 = \mathcal{M}(\mu)$  be the Banach sublattice of  $\mathcal{M}$  of all finite Borel measures on  $(X, \mathcal{A})$ , absolutely continuous with respect to a fixed positive  $\sigma$ -finite measure  $\mu$ , and let  $\mathcal{P}_0$  be the set of probability measures in  $\mathcal{M}_0$ , i.e.  $\mathcal{P}_0 = \mathcal{P} \cap \mathcal{M}_0$ . Hence  $\mathcal{M}_0 = L^1(\mu)$  and  $\mathcal{P}_0$  is the convex set of all probability densities with respect to  $\mu$ . We notice that if **Q** is a kernel QSO with  $G(\cdot; x, y) \ll \mu$  for all  $x, y \in X$ , then  $\mathbf{Q}(\mathcal{P} \times \mathcal{P}) \subseteq \mathcal{P}_0$ .

QSOs play an important role in evolutionary biology. Roughly speaking, the set *X* is understood as the space of random values of traits in a population and elements of  $\mathcal{P}$  represent the admitted single generation probability distribution of the trait. The model of heritability is constructed with the use of QSOs in the following way. If  $F_1, F_2 \in \mathcal{P}$  describe the trait distributions in two different populations, then  $\mathbf{Q}(F_1, F_2) \in \mathcal{P}$  describes the distribution of this trait in the next generation coming from the mating of independent individuals, one from each of the two populations. Special attention is paid to a nonlinear mapping  $\mathcal{P} \ni F \mapsto \mathbf{Q}(F) := \mathbf{Q}(F, F) \in \mathcal{P}$ . Here  $\mathbf{Q}(F)$  represents the probability distribution of the offspring's trait, when *F* is the law of the parents. In this simplified model the iterates  $\mathbf{Q}^n(F)$ , where  $n = 0, 1, 2, \ldots$ , represent the evolution of the probability distribution. The reader is referred to [2] for a detailed explanation of the model.

The long-term behaviour of QSOs has become a subject of study. Different types of strong asymptotic stability of kernel QSOs were introduced and intensively examined in [5] on  $\ell^1$  space and then extended to the  $\mathcal{M}_0$  space in [4]. In [2], special attention was paid to weak convergence of QSOs.

**Definition 2** ([2]). Given a complete separable metric space (X, A), where A stands for a Borel  $\sigma$ -field, let  $\mathcal{M}$  denote the Banach lattice of all finite Borel measures on (X, A) and let  $\mathcal{P}$  be the convex set of all probability measures on (X, A). A QSO  $\mathbf{Q}$  on  $\mathcal{M}$  is said to be weakly asymptotically stable at  $F \in \mathcal{P}$  if the weak limit of the sequence of values of the iterations of the diagonalized operators  $\mathbf{Q}$  at F exists in  $\mathcal{P}$  (we use the notation w-lim<sub> $n \to \infty$ </sub>  $\mathbf{Q}^n(F) \in \mathcal{P}$ ).

#### 2 Centred kernel quadratic stochastic operators

For further analysis, we restrict our attention to a subclass of the so-called *centred* QSOs. Let  $X = \mathbb{R}$ . Consider the Banach lattice  $\mathcal{M} := \mathcal{M}(\mathbb{R}, \mathcal{B}(\mathbb{R}))$  of all Borel measures on  $\mathbb{R}$  with finite total variation and denote by  $\mathcal{P}$  the convex set of all probability measures on  $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ .

**Definition 3** ([2]). Let  $G \in \mathcal{P}$ . A kernel quadratic stochastic operator  $\mathbf{Q}_G$  with the kernel

$$\mathcal{G}_G = \left\{ G(\cdot; x, y) = G\left( \cdot - \frac{x + y}{2} \right) : (x, y) \in \mathbb{R} \times \mathbb{R} \right\}$$

is called a centred kernel quadratic stochastic operator (CKQSO for short) with perturbation G.

For the convenience of the reader in what follows we recall some useful results from [2], which are fundamental for our further considerations. This brief introduction also serves to fix notation. First, we give the formula for the density function of the CKQSO.

**Corollary 1** ([2]). Let  $F_1, F_2 \in \mathcal{P}$  and let  $G \in \mathcal{G}_G$ . If  $F_1, F_2$  and G are all absolutely continuous with respect to the Lebesgue measure  $\lambda$ , then their densities are  $f_1 := \frac{dF_1}{d\lambda}$ ,  $f_2 := \frac{dF_2}{d\lambda}$ ,  $g := \frac{dG}{d\lambda} \in L^1$  and we can write the density associated with the CKQSO  $\mathbf{Q}_G$  as

$$\frac{d}{d\lambda}\mathbf{Q}_{G}(F_{1},F_{2})(z) = \int_{\mathbb{R}^{d}} \int_{\mathbb{R}^{d}} f_{1}(x)f_{2}(y)g\left(z-\frac{x+y}{2}\right)dxdy, \quad z \in \mathbb{R}.$$
(1)

The density (1) corresponds (see [2, Proposition 1]) to a random variable that can be represented as

$$Z=\frac{X_1+X_2}{2}+Y,$$

where  $X_1 \sim F_1$ ,  $X_2 \sim F_2$  and  $Y \sim G$  (simplifying notation, by *G*, we mean the "canonic" distribution  $G(\cdot, 0, 0) \in \mathcal{G}_G$ ). As mentioned before, we pay special attention to the corresponding nonlinear mapping

$$\mathcal{M} \ni F \mapsto \mathbb{Q}_G(F) := \mathbb{Q}_G(F, F) \in \mathcal{M}.$$

Once again we emphasize the meaning of  $Q_G$  in modelling the heritability of traits of an inbreeding or hermaphroditic population. The formula (1) justifies the interpretation, that  $Q_G$  describes the probability distribution of the offspring's trait that is equal to the additively randomly perturbed arithmetic mean of the parents' traits, when the mating individuals are chosen independently. We hence focus on the iterates  $Q_G^n$ , where n = 0, 1, 2, ..., which represent the *discrete* time evolution of probability distributions of the trait.

Let  $F \in \mathcal{P}$ ,  $G \in \mathcal{G}_G$ . Denote  $H^{(n)} := \mathbb{Q}_G^n(F)$ . We are interested in the asymptotic stability of the CKQSO  $\mathbb{Q}_G$  at F. We write  $H^{(\infty)} := \text{w-lim}_{n\to\infty} H^{(n)}$ , whenever the weak limit of  $H^{(n)}$  exists in  $\mathcal{P}$ . We also use  $\xrightarrow[n\to\infty]{a.s.}$  and  $\xrightarrow[n\to\infty]{L^2}$  to indicate a.s. and  $L^2$  convergence, respectively.

**Theorem 1 ([2]).** Let  $F \in \mathcal{P}$  and  $G \in \mathcal{G}_G$ . Let  $X_1, X_2, X_3, \ldots$  and  $Y_1^{(0)}, Y_1^{(1)}, Y_2^{(1)}, Y_1^{(2)}, \ldots, Y_4^{(2)}, \ldots, Y_1^{(j)}, \ldots, Y_{2j}^{(j)}, \ldots$  be independent sequences of random variables such that  $X_1, X_2, X_3, \ldots$  are independent identically distributed (i.i.d. for short) according to F and  $Y_1^{(0)}, Y_1^{(1)}, Y_1^{(1)}, Y_2^{(1)}, Y_1^{(2)}, \ldots, Y_2^{(1)}, Y_1^{(2)}, \ldots, Y_1^{(j)}, \ldots, Y_{2j}^{(j)}, \ldots$  are i.i.d. according to G. Then, for every  $n \in \mathbb{N}_+$ , we

have that  $H^{(n)} := \mathbb{Q}^n_G(F)$  is the probability distribution of the random variable

$$Z^{(n)} := X^{(n)} + Y^{(n)}, \tag{2}$$

where

$$X^{(n)} := \frac{X_1 + X_2 + \ldots + X_{2^n}}{2^n}, \qquad Y^{(n)} := \sum_{j=0}^{n-1} \frac{Y_1^{(j)} + Y_2^{(j)} + \ldots + Y_{2^j}^{(j)}}{2^j}.$$

The following theorem gives example sufficient condition for the weak asymptotic stability of CKQSO.

**Theorem 2** (special case of [2, Theorem 3]). Assume that the expected value and variance associated with  $F \in \mathcal{P}$  are  $m < \infty$  and  $v_F < \infty$ , respectively, and the expected value and variance associated with  $G \in \mathcal{G}_G$  are 0 and  $v_G < \infty$ , respectively. Then

$$H^{\bigotimes} := w - \lim_{n \to \infty} H^{(n)}.$$

As mentioned above, the iterates of centred kernel quadratic stochastic operators can be associated with a random variable that has an explicit representation as a sum of an exponential number of independent random variables. This allows for exact simulation from their laws, controlled approximate simulation from their and the limit laws and control over rates of convergence. We focus on the "diagonal" CKQSO, i.e. assuming that  $F_1 = F_2 = F$ . We further assume that both F and G have finite second moments, with variances  $v_F$  and  $v_G$ , respectively (while finite second moments are sufficient for weak convergence to hold, they are not necessary, an alternative sufficient conditions are considered in [2]). We are interested in the convergence of the distribution  $H^{(n)} := (\mathbb{Q}_G)^n(F)$  to  $H^{(\infty)} := \text{w-lim}_{n\to\infty}(\mathbb{Q}_G)^n(F)$ . But in fact, in the following theorem, we strengthen Theorem 2 to a.s. and  $L^2$  convergence of random variables associated with the QSO  $(\mathbb{Q}_G)^n(F)$ . We will use the notation for functions f, g that  $f \in \Theta(g)$  if f/g = constant > 0.

**Theorem 3.** Assume that the expected value and variance associated with  $F \in \mathcal{P}$  are  $m < \infty$  and  $v_F < \infty$ , respectively, and the expected value and variance associated with  $G \in \mathcal{G}_G$  are 0 and  $v_G < \infty$ , respectively. Let  $Z^{(n)} \sim H^{(n)}$ , be the random variable associated with  $H^{(n)}$  from the representation given in Theorem 1. Then,  $Z^{(n)} \xrightarrow[n \to \infty]{a.s.,L^2} Z^{(\infty)}$ , where  $Z^{(\infty)} \sim H^{(\infty)}$ , and the convergence rate is  $\Theta(2^{-n/2})$  in the  $L^2$  metric.

*Proof.* By the strong law of large numbers we have that

$$X^{(n)} \xrightarrow[n \to \infty]{a.s.} m,$$

where  $E[X^{(n)}] = m$  and  $Var[X^{(n)}] = 2^{-n}v_F$ . For convenience, for j = 0, 1, 2, ..., we introduce the sequence of random variables

$$U_j := \left(Y_1^{(j)} + Y_2^{(j)} + \ldots + Y_{2^j}^{(j)}\right) / 2^j,$$

and we have that  $E[U_j] = 0$ ,  $Var[U_j] = 2^{-j}v_G$ . As both  $\sum E[U_j]$  and  $\sum Var[U_j]$  are finite, we have almost sure convergence (cf. [11, Theorem 2])

$$\sum_{j=0}^{n-1} U_j = Y^{(n)} \xrightarrow[n \to \infty]{a.s.} Y^{(\infty)} := \sum_{j=0}^{\infty} U_j,$$

with

$$\operatorname{Var}\left[Y^{(n)}\right] = v_G \sum_{j=0}^{n-1} 2^{-j} = \left(2 - 2^{-(n-1)}\right) v_G \to 2v_G.$$

Hence,

$$Z^{(\widehat{n})} \xrightarrow[n \to \infty]{a.s.} Z^{(\widehat{\infty})} := m + \sum_{j=0}^{\infty} U_j,$$

and we can represent

$$Z^{\bigotimes} = X^{(n)} + Y^{(n)} + \epsilon_n^m + \epsilon_n^U,$$

where  $\epsilon_n^m = m - X^{(n)}$ , and  $\epsilon_n^U = \sum_{j=n}^{\infty} U_j$ . We look at the  $L^2$  metric and, as both  $\epsilon_n^m$  and  $\epsilon_n^m$  are mean zero and independent, we have

$$\mathbf{E}\left[\left|Z^{\bigotimes}-Z^{(n)}\right|^{2}\right]=\mathbf{E}\left[\left|\epsilon_{n}^{m}+\epsilon_{n}^{U}\right|^{2}\right]=\mathbf{E}\left[\left|\epsilon_{n}^{m}\right|^{2}\right]+\mathbf{E}\left[\left|\epsilon_{n}^{U}\right|^{2}\right]$$

Calculating each term separately we have

$$\mathbf{E}\left[\left|\epsilon_{n}^{U}\right|^{2}\right] = \operatorname{Var}\left[\epsilon_{n}^{U}\right] = \sum_{j=n}^{\infty} \operatorname{Var}\left[U_{j}\right] = v_{G}\sum_{j=n}^{\infty} 2^{-j} = v_{G}2^{-(n-1)}$$

and

$$\mathrm{E}\left[\left|\epsilon_{n}^{m}\right|^{2}\right]=v_{F}2^{-n}$$

Taken together the  $L^2$  distance will be

$$d_{L_2}^2\left(Z^{(n)}, Z^{(m)}\right) = (v_F + 2v_G)2^{-n}.$$

**Remark 1.** In [2], only weak convergence of measures was considered. Here, we have a simulation oriented perspective, and hence the pointwise and L<sup>2</sup> convergence with rates are of more interest. However, we can notice that from the proof of Theorem 3 we can immediately obtain convergence in the Wasserstein-2 distance

$$d_{W_2}^2\left(H^{(n)}, H^{(m)}\right) = \inf \int_{\gamma \in \Gamma\left(H^{(n)}, H^{(m)}\right)} |x - y|^2 d\gamma(x, y),$$

where  $\Gamma\left(H^{(n)}, H^{(m)}\right)$  is the set of all couplings between  $H^{(n)}$  and  $H^{(m)}$ . We notice that due to the a.s. convergence the coupling  $Z^{(n)}$  and  $Z^{(n)} + \epsilon_n^m + \epsilon_n^U$  will be the optimal one and

$$d_{W_2}^2\left(H^{(n)}, H^{(m)}\right) = \mathbb{E}\left[\left|Z^{(m)} - Z^{(n)}\right|^2\right] = (v_F + 2v_G)2^{-n}.$$

Convergence in the Wasserstein-2 distance will imply w-lim<sub> $n\to\infty$ </sub>  $H^{(n)} = H^{(\infty)}$  (cf. [8]).

Using the notation introduced in the statement and the proof of Theorem 3 we easily get the following result.

**Theorem 4.** Let  $N = N(\alpha, \delta)$  be the required number of iterations so that for any *n* with probability  $\alpha$  the random variable

$$W^{\widehat{N}} := m + \sum_{j=0}^{N-1} U_j$$

deviates from  $Z^{(n)}$  and  $Z^{(\infty)}$  by at most  $\delta$ . We have the upper bound

$$N(\alpha, \delta) \leq \log\left(\frac{4\max(v_F, 2v_G)}{\delta^2 \alpha}\right).$$

*Proof.* For a given *n*, take N < n. Using Chebyshev's inequality we directly obtain

$$P\left(\left|X^{(n)}-m\right| > \delta/2\right) \le \frac{4v_F}{\delta^2} 2^{-n} < \frac{4v_F}{\delta^2} 2^{-N}$$

and

$$P\left(\left|\sum_{j=N}^{n-1} U_{j}\right| > \delta/2\right) \le \frac{8v_{G}}{2\delta^{2}} (2^{-N} - 2^{-n}) < \frac{8v_{G}}{2\delta^{2}} 2^{-N}$$

Solving for a given probability  $\alpha$  we obtain

$$N(\alpha, \delta) \leq \log\left(\frac{4\max\{v_F, 2v_G\}}{\delta^2 \alpha}\right).$$

Notice that for the approximation described in Theorem 4 to be valid one needs *n* to be large. The " $X^{(n)}$ " component of  $Z^{(n)}$  is approximated by the constant *m*, i.e. the initial population is assumed to be constant at its mean.

### 3 A Gaussian CKQSO example

We will consider here in detail a CKQSO  $Q_{\mathcal{N}}$  with a Gaussian kernel  $\mathcal N$  defined by its density

$$\frac{d\mathcal{N}}{d\lambda}(\cdot;x,y) = \frac{1}{\sqrt{\pi}} \exp\left(-\left(\cdot - (x+y)/2\right)^2\right), \quad (x,y) \in \mathbb{R} \times \mathbb{R}.$$
(3)

The resulting CKQSO  $\mathbf{Q}_{\mathcal{N}}$  in its density representation (1) is

$$\frac{d}{d\lambda}\mathbf{Q}_{\mathcal{N}}(F_1,F_2)(z) = \int_{\mathbb{R}} \int_{\mathbb{R}} f_1(x)f_2(y)\frac{1}{\sqrt{\pi}}\exp\left(-\left(z-(x+y)/2\right)^2\right)dxdy, \quad z \in \mathbb{R}, \quad (4)$$

where  $F_1, F_2 \in \mathcal{P}$  and  $f_1 := \frac{dF_1}{d\lambda}, f_2 := \frac{dF_2}{d\lambda}$ .

**Theorem 5.** For any initial, finite mean and variance  $F \in \mathcal{P}$ , the CKQSO  $\mathbf{Q}_{\mathcal{N}}$  of the form (4) converges to a Gaussian distribution with the same expected value as the one associated with *F* and unit variance.

*Proof.* By Theorem 3 we know that  $Z^{(n)}$  converges a.s. and in  $L^2$  to  $Z^{(\infty)}$ . Therefore, convergence of the characteristic functions will suffice for finding  $H_N^{(\infty)}$ . Denote  $\varphi_N(s) := e^{-s^2/4}$  (the "canonic" distribution in  $\mathcal{G}_N$ ), and then the characteristic function of the limit of the CKQSO  $\mathbf{Q}_N$  with kernel  $\mathcal{N} \in \mathcal{P}, \varphi_{H_N^{(\infty)}}(s)$ , is

$$\varphi_{H_{\mathcal{N}}^{\bigotimes}}(s) = e^{ims} \prod_{j=0}^{\infty} \left( \varphi_{\mathcal{N}} \left( \frac{s}{2^{j}} \right) \right)^{2^{j}}, \quad s \in \mathbb{R}.$$

The product form comes from [2, Corollary 1]. The first part of the product,  $e^{ims}$  comes from the strong law of large numbers applied to  $X^{(n)}$ , and the second, infinite product, is proved in [2, Theorem 3]. Exploiting that the kernel is normal, i.e. the form of  $\varphi_N$ , we obtain

$$\varphi_{H_{\mathcal{N}}^{\bigotimes}}(s) = e^{ims} \prod_{j=0}^{\infty} \left( \varphi_{\mathcal{N}}\left(\frac{s}{2^{j}}\right) \right)^{2^{j}} = e^{ims} \prod_{j=0}^{\infty} \left( e^{-\frac{1}{4}s^{2}/2^{2j}} \right)^{2^{j}} = e^{ims-\frac{1}{2}s^{2}}, \quad s \in \mathbb{R},$$

which is the characteristic function of a normal  $\mathcal{N}(m, 1)$  random variable.

**Corollary 2.** If both  $F_1 \in \mathcal{P}$  and  $F_2 \in \mathcal{P}$  are Gaussian with finite means ( $m_1$  and  $m_2$ , respectively) and variances ( $\sigma_1^2$  and  $\sigma_2^2$ , respectively), then  $\mathbf{Q}_{\mathcal{N}}(F_1, F_2)$  will also be Gaussian with mean value ( $m_1 + m_2$ ) /2 and variance ( $\sigma_1^2/4 + \sigma_2^2/4 + 1/2$ ).  $\mathbb{Q}_{\mathcal{N}}$  is mean preserving. Any unit variance normal distribution  $F \in \mathcal{P}$  given by

$$\frac{dF}{d\lambda}(x) = f(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-(x-\mu)^2/2\right), \quad x \in \mathbb{R},$$

is a fixed point distribution of  $Q_N$ .

*Proof.* The characteristic function of  $\mathbf{Q}_{\mathcal{N}}(F_1, F_2)$ , where  $\varphi_{F_2}$ ,  $\varphi_{F_2}$  stand for the characteristic functions of  $F_1$  and  $F_2$ , respectively, is (see [2, Proposition 1])

$$\varphi_{\mathbf{Q}_{\mathcal{N}}(F_1,F_2)}(s) = \varphi_{F_1}\left(\frac{s}{2}\right)\varphi_{F_2}\left(\frac{s}{2}\right)\varphi_{\mathcal{N}}(s), \quad s \in \mathbb{R}.$$

Using that  $F_1$ ,  $F_2$  and N are all Gaussian, for  $s \in \mathbb{R}$  we obtain

$$\varphi_{\mathbf{Q}_{\mathcal{N}}(F_{1},F_{2})}(s) = e^{im_{1}s/2 - \sigma_{1}^{2}s^{2}/8}e^{im_{2}s/2 - \sigma_{2}^{2}s^{2}/8}e^{-s^{2}/4} = e^{i\left((m_{1}+m_{2})/2\right)s - \left(\sigma_{1}^{2}/4 + \sigma_{2}^{2}/4 + 1/2\right)s^{2}/2}$$

This is the characteristic function of an  $\mathcal{N}((m_1 + m_2)/2, (\sigma_1^2/4 + \sigma_2^2/4 + 1/2))$  random variable. One can directly verify that  $\mathbb{Q}_N$  is mean retaining. If we take *F* to be  $\mathcal{N}(m, 1)$ , then from the above it follows that  $\mathbb{Q}_N(F)$  is also  $\mathcal{N}(m, 1)$ . Hence for any  $m < \infty$  we have that  $\mathcal{N}(m, 1)$  is a fixed point of  $\mathbb{Q}_N$ .

We know from Theorem 3 that, for any initial distribution F,  $Z_N^{(i)} \sim H_N^{(i)}$  will converge exponentially fast to the Gaussian limit. As Theorem 3 provides an exact  $L^2$  convergence rate, exploiting the Gaussian form of the kernel will not improve this. However, it will allow for exact derivations in other metrics — the  $L^1$  and Hellinger distances.

**Theorem 6.** Assume that *F* is a normal  $\mathcal{N}(m, v_F)$  distribution. Then in the Hellinger distance  $d_H$  we have

$$d_H\left(H_{\mathcal{N}}^{(n)},H_{\mathcal{N}}^{(m)}\right) \sim \frac{1}{4} \left|v_F - 1\right| 2^{-n}$$

and in the  $L_1$  distance

$$\left\|h_{\mathcal{N}}^{(n)} - h_{\mathcal{N}}^{(\infty)}\right\|_{1} = 2\left|v_{F} - 1\right|\left(\Phi(1) - \frac{1}{2}\right)2^{-n} + \Theta\left(2^{-2n}\right),$$

where  $h_{\mathcal{N}}^{(n)}$ ,  $h_{\mathcal{N}}^{(\infty)}$  are the densities of the normal distributions, and  $\Phi$  stands for the standard normal cumulative distribution function.

*Proof.* We know that  $H_{\mathcal{N}}^{(n)}$  is  $\mathcal{N}\left(m, 1-\frac{1}{2^n}+v_F2^{-n}\right)$  and  $H_{\mathcal{N}}^{(\infty)}$  is  $\mathcal{N}(m, 1)$ . We first consider the Hellinger distance between the two normal distributions with the same mean (see, e.g., [13, p. 46 and 51])

$$d_H^2\left(\mathcal{N}(\mu,\sigma_1^2),\mathcal{N}\left(\mu,\sigma_2^2\right)\right) = 1 - \sqrt{\frac{2\sigma_1\sigma_2}{\sigma_1^2 + \sigma_2^2}}$$

and then in our case  $d_H^2\left(H_N^{(i)}, H_N^{(i)}\right)$  becomes

$$1 - \sqrt{\frac{2\sqrt{1 - \frac{1}{2^n} + v_F 2^{-n}}}{1 + 1 - \frac{1}{2^n} + v_F 2^{-n}}} = 1 - \left(\frac{2^{2n+2} \left(1 + (v_F - 1) 2^{-n}\right)}{2^{2n+2} \left(1 + (v_F - 1) 2^{-(n+1)}\right)^2}\right)^{\frac{1}{4}} = 1 - \left(1 - \left(\frac{(v_F - 1)}{2^{n+1} + (v_F - 1)}\right)^2\right)^{\frac{1}{4}}$$

and using the Taylor expansion around 1 we further obtain

$$d_H^2\left(H_{\mathcal{N}}^{(n)}, H_{\mathcal{N}}^{(m)}\right) \sim 1 - 1 - \frac{1}{4}\left(1 - \left(\frac{(v_F - 1)}{2^{n+1} + (v_F - 1)}\right)^2 - 1\right) \sim \frac{(v_F - 1)^2}{16} 2^{-2n},$$

and hence

$$d_H\left(H_{\mathcal{N}}^{(n)},H_{\mathcal{N}}^{(m)}\right)\sim \frac{|v_F-1|}{4}2^{-n}$$

If we consider now the  $L^1$  norm, we first need to find the point  $t_0 > 0$  such that  $h_N^{(n)}(t_0) = h_N^{(\infty)}(t_0)$ . Due to symmetricity around m, there will be two such points, and we take the one greater than m. Without loss of generality we take m = 0, as the mean is just responsible for the location, and will not affect convergence. Denoting  $\sigma_n = \sqrt{1 + (v_F - 1)2^{-n}}$ , we write

$$e^{-t_0^2/2} = \frac{1}{\sigma_n} e^{-t_0^2/(2\sigma_n^2)}$$

then transform

$$t_0^2 = \left(1 - \frac{1}{\sigma_n^2}\right)^{-1} 2\log\sigma_n,$$

and finally obtain

$$t_0 = \pm \sqrt{(1 + (v_F - 1)^{-1} 2^n) \log (1 + (v_F - 1) 2^{-n})}.$$

Now, denoting by  $\Phi_n$  the cumulative distribution function of  $H_N^{(n)}$ , plugging in the above value for  $t_0$ , and denoting  $\zeta_n := (v_F - 1)^{-1} \log (1 + (v_F - 1)2^{-n})$ , we get

$$\begin{split} \left\| h_{\mathcal{N}}^{(\underline{n})} - h_{\mathcal{N}}^{(\underline{n})} \right\|_{1} &= 2 \left| \Phi_{n}(t_{0}) - \frac{1}{2} - \Phi(t_{0}) + \frac{1}{2} + 1 - \Phi(t_{0}) - 1 + \Phi_{n}(t_{0}) \right. \\ &= 4 \left| \Phi\left( \sqrt{\frac{(1 + (v_{F} - 1)^{-1}2^{n})\log\left(1 + (v_{F} - 1)2^{-n}\right)}{(1 + (v_{F} - 1)2^{-n})}} \right) \right. \\ &- \Phi\left( \sqrt{(1 + (v_{F} - 1)^{-1}2^{n})\log\left(1 + (v_{F} - 1)2^{-n}\right)} \right) \right| \\ &= 4 \left| \Phi\left( \sqrt{2^{n}\zeta_{n}} \right) - \Phi\left( \sqrt{2^{n}\left(1 + (v_{F} - 1)2^{-n}\right)\zeta_{n}} \right) \right|. \end{split}$$

The standard normal cumulative distribution function can be Taylor expanded as

$$\Phi(t) = \frac{1}{2} + \frac{1}{\sqrt{2\pi}} e^{-t^2/2} \sum_{j=0}^{\infty} \frac{t^{2j+1}}{(2j+1)!!}.$$

Using this we write that  $\left\|h_{\mathcal{N}}^{(n)} - h_{\mathcal{N}}^{(\infty)}\right\|_{1}$  equals

$$\begin{aligned} \frac{4}{\sqrt{2\pi}} \left| e^{-\frac{1}{2}2^{n}\zeta_{n}} \sum_{j=0}^{\infty} \frac{\left(2^{n}\zeta_{n}\right)^{\frac{2j+1}{2}}}{(2j+1)!!} - e^{-\frac{1}{2}\left(2^{n}\left(1+\left(v_{F}-1\right)2^{-n}\right)\zeta_{n}\right)} \sum_{j=0}^{\infty} \frac{\left(2^{n}\left(1+\left(v_{F}-1\right)2^{-n}\right)\zeta_{n}\right)^{\frac{2j+1}{2}}}{(2j+1)!!} \right| \\ &= \frac{4}{\sqrt{2\pi}} e^{-\frac{1}{2}2^{n}\zeta_{n}} \left| \sum_{j=0}^{\infty} \frac{1}{(2j+1)!!} \left( \left(2^{n}\zeta_{n}\right)^{\frac{2j+1}{2}} - e^{-\frac{1}{2}\left(v_{F}-1\right)\zeta_{n}} \left(2^{n}\left(1+\left(v_{F}-1\right)2^{-n}\right)\zeta_{n}\right)^{\frac{2j+1}{2}}\right) \right|. \end{aligned}$$

We notice that

$$2^{n}\zeta_{n} = 1 - (v_{F} - 1)2^{-(n+1)} + O\left(2^{-2n}\right) = 1 + \Theta\left(2^{-n}\right)$$

as by Taylor's theorem

$$t \log(1+1/t) = 1 - 1/(2t) + O(t^{-2}), \quad t \to \infty,$$

and also (as for *n* large enough we have  $|(v_F - 1)2^{-n}| < 1$ )

$$\zeta_n = 2^{-n} - (v_F - 1)2^{-2(n+1)} + O\left(2^{-3n}\right).$$

This allows us to write  $\left\| h_{\mathcal{N}}^{(i)} - h_{\mathcal{N}}^{(i)} \right\|_{1}$  as

$$\frac{4}{\sqrt{2\pi}}e^{-\frac{1}{2}(1+\Theta(2^{-n}))}\left|\sum_{j=0}^{\infty}\frac{1}{(2j+1)!!}\left(\left(1+\Theta(2^{-n})\right)^{\frac{2j+1}{2}}-e^{-\frac{1}{2}(v_F-1)(2^{-n}+\Theta(2^{-2n}))}(1+\Theta(2^{-n}))^{\frac{2j+1}{2}}\right)\right|,$$

which asymptotically behaves as

$$\begin{split} \left(\frac{4}{\sqrt{2\pi}}e^{-\frac{1}{2}}\left(\sum_{j=0}^{\infty}\frac{1}{(2j+1)!!}\right) + \Theta(2^{-n})\right) \left|1 - e^{-\frac{1}{2}(v_F-1)\left(2^{-n} + \Theta(2^{-2n})\right)}\right| \\ &= \left(4\left(\Phi(1) - \frac{1}{2}\right) + \Theta\left(2^{-n}\right)\right) \left|1 - e^{-\frac{1}{2}(v_F-1)\left(2^{-n} + \Theta(2^{-2n})\right)}\right| \\ &= \left(2|v_F-1|\left(\Phi(1) - \frac{1}{2}\right)\right) \left(2^{-n}\right) + \Theta\left(2^{-2n}\right) \in \Theta\left(2^{-n}\right). \end{split}$$

We have obtained an exact constant  $2|v_F - 1| \left(\Phi(1) - \frac{1}{2}\right)$  in front of the leading exponential term of  $\mathbb{Q}_{\mathcal{N}}$ 's convergence in the  $L^1$  norm.

**Remark 2.** A very important case is when the initial population is distributed according to  $\delta_{x_0}$ . This is actually biologically relevant as very often a new population starts off from a small number of individuals with very little variability between them. This can be caused by a mutation in some individuals that makes them distinct from the whole population and makes them a new species or allows them to fill up a new environmental niche [15]. From the perspective of Theorem 6 this means setting  $v_F = 0$  and gives  $Z_N^{(n)} \sim \mathcal{N}\left(x_0, 1 - \frac{1}{2^n}\right)$ , and  $Z_N^{(\infty)} \sim \mathcal{N}(x_0, 1)$ , resulting in

$$\left|h_{\mathcal{N}}^{(n)} - h_{\mathcal{N}}^{(\infty)}\right|_{1} = 2\left(\Phi(1) - \frac{1}{2}\right)2^{-n} + \Theta\left(2^{-2n}\right)$$

 $d_H\left(H_{\mathcal{N}}^{(\!\!\!n)},H_{\mathcal{N}}^{(\!\!\!\infty)}
ight)\sim 2^{-(n+2)},$ 

### 4 Simulating QSOs

A "diagonal" QSO can be viewed as a model describing the evolution of a hermaphroditic population. Hence, sampling from the laws described by the QSOs is useful both for illustrative purposes and Monte Carlo analyses of the systems. In principle, one could calculate what  $Q^n(F)$  is and sample from the resulting law. Unless there are special cases, where each iterate of the QSO can be analytically found, one would have to resort to numerical methods. These are subject to rounding errors, that can accumulate as *n* increases. Hence, in [3], a "populationtype" approach was proposed, see Algorithm 1 below for any (on  $L_1 \times L_1$  or  $\ell_1 \times \ell_1$ ) kernel QSO.

```
Algorithm 1 Simulating Q(g)
```

Draw *N* independent individuals according to the law of *g* and call them  $P_0$ for i = 1 to *n* do  $P_i := \emptyset$ for j = 1 to *N* do Draw a pair  $(x_j, y_j)$  of individuals from population  $P_{i-1}$ Draw an individual  $z_j$  according to the law of  $\mathbf{Q}(\delta x_j, \delta y_j) = q(x_j, y_j, \cdot)$   $P_i = P_i \cup \{z_j\}$ end for return  $P_0, P_1, \dots, P_n$ 

In [3], Algorithm 1 was explored for QSOs acting on  $\ell_1 \times \ell_1$ . An observed problem was that if there are multiple invariant distributions, then the population started from an invariant distribution can easily switch (to the proximity) of another one. A particular striking example in [3] was the identity operator. No matter what the initial value  $\vec{x}$  was, each trajectory would end in a state, where exactly only one coordinate of the  $Q^n(\vec{x})$  had non-zero probability. Taking multiple repeats could alleviate the problem, but our point is that looking at a single, even very

long, trajectory from Algorithm 1 can be misleading of the properties of the QSO, especially when the aim is to characterize the limit.

Notice that Algorithm 1 only assumes that the QSO is a kernel one. A more effective algorithm can be proposed if more is known about the QSO. In particular, the sum representation of (2) for a CKQSO allows for direct simulation from its law, by drawing an appropriate (exponential in terms of *n*) amount of independent random variables distributed according to the laws of *F* and *G*. We describe this in Algorithm 2.

**Algorithm 2** Exact sampling from  $\mathbb{Q}_G^n(F)$ 

Draw  $2^n$  random values from the law of *F* and denote this set  $\{X_1, \ldots, X_{2^n}\}$  $X^{(n)} = \frac{1}{2^n} (X_1 + \ldots + X_{2^n})$ for j = 0 to n - 1 do Draw 2<sup>*j*</sup> random values from the law of *G* and denote this set  $\{Y_1, \ldots, Y_{2j}\}$  $U_j := \frac{1}{2^j} (Y_1 + \ldots + Y_{2^j})$ end for return  $X^{(n)} + \sum_{j=0}^{n-1} U_j$ 

Even though exact, the procedures in Algorithm 2 requires an exponential number of random variables, which can be prohibitive. Furthermore, it does not allow for sampling form the limit  $\mathbb{Q}^{\infty}_{G}(F)$ , as this would require an infinite number of values to be drawn. However, Theorem 3 assures us of exponential convergence, hence we can hope for reasonable approximations with only a few iterations. In fact, based on Theorem 4, that explicitly takes advantage of the a.s. convergence of  $Z^{(n)}$ , we can propose Algorithm 3 (we use a marginally better upper bound for *N* that can be extracted from the proof of Theorem 4).

Algorithm 3 Approximate drawing from  $\mathbb{Q}^n_G(F)$  $N := \left\lceil \log\left(\max\left\{\frac{4v_F}{\delta^2 \alpha}, \frac{8v_G}{\delta^2 \alpha + 2^{3-n}v_G}\right\}\right) \right\rceil$ for j = 0 to N - 1 do Draw  $2^{j}$  random values from the law of *G* and denote this set  $\{Y_1, \ldots, Y_{2^{j}}\}$  $U_j := \frac{1}{2^j} \left( Y_1 + \ldots + Y_{2^j} \right)$ end for **return**  $m + \sum_{j=0}^{N-1} U_j$ 

**Remark 3.** If Algorithm 3 is used with the purpose of sampling a population of K individuals from  $\mathbb{Q}^n_G(F)$  ( $\mathbb{Q}^\infty_G(F)$ ), then it does not suffice to choose a small  $\alpha$  independently of K. This is akin to the multiple testing problem: with K large enough just by chance we will observe an event of probability  $\alpha$ . Therefore one way is a "Bonferroni" correction: if on the individual level we want an error with probability  $\alpha$ , then in Algorithm 3 we need to take  $\alpha/K$ instead of  $\alpha$ .



**Figure 1.** Simulation using Algorithms 2, 3, and 1 with the CKQSO's kernel given by (3). Initial population size N = 1000 (Algorithm 1), and the histograms are for iteration n = 20. Algorithm 3 used  $\delta = 0.01$  and  $\alpha = 0.01$ , resulting in 16 iterations (or 20 without Bonferroni correction). Initial populations are drawn from:

in top row: exponential distribution with mean values (left to right): 0.1, 1 and 10;

- in middle row: normal distribution with mean value 0;
- in bottom row: normal distribution with mean value 1.

In the case of the middle and bottom rows the variances are (left to right): 0.1, 1 (fixed point) and 10.

In Figure 1, we illustrate the behaviour of Algorithms 1, 2, and 3 on the Gaussian CKQSO of (4). Then, in Table 1, we present the first and second moment of the simulated samples. We consider both normal and exponential initial distributions, with variances lesser than, equal and greater than the "stationary" variance 1. We take a sample of 1000 and look at generation 20 (more will start to be prohibitive for Algorithms 2 and 3). In all cases we can see that the mean is close to the mean of the initial distribution, and that variance is close to 1. We can clearly see that Algorithm 1 fares the worst (given the sample size and generation). The sample density is the furthest away from the exact one, which visually resembles  $\mathcal{N}(0, 1)$ . This is most

F	Algorithm 2			Algorithm 3			Algorithm 3+B			Algorithm 1		
	т	V	pKS	т	V	pKS	т	V	pKS	т	V	pKS
Exp(10)	0.09	1.07	0.67	0.11	0.98	0.99	0.08	0.92	0.76	0.19	1.02	0.03
Exp(1)	1	0.96	0.97	1.07	1.05	0.07	1.02	1.05	0.16	1.01	0.98	0.84
Exp(0.1)	9.96	1.07	0.59	10.03	1.02	0.51	9.99	1	0.71	10.41	0.95	0
$\mathcal{N}(0, 0.1)$	0.04	1.04	0.1	0.01	1.01	0.64	0.01	1.03	0.9	0.11	1	0
$\mathcal{N}(0,1)$	-0.03	0.93	0.2	0.02	1.04	0.58	0.02	1.02	0.58	0.15	1.12	0
$\mathcal{N}(0,10)$	-0.01	0.96	0.91	-0.01	0.89	0.7	0.03	0.98	0.41	-0.45	1.04	0
N(1, 0.1)	1.02	0.96	0.82	0.95	0.95	0.11	1	1.04	0.76	1.02	1.02	0.74
$\mathcal{N}(1,1)$	0.98	0.97	0.62	0.94	1.03	0.01	1.02	0.97	0.53	0.92	1.01	0.01
$\mathcal{N}(1,10)$	0.97	1.07	0.62	1.03	1.1	0.04	0.99	1.02	0.72	1.02	0.97	0.79

**Table 1.** Moments of the simulation by Algorithms 1, 2, and 3 with the CKQSO's kernel given by (3) at generation n = 20. Algorithm 3+B means that the "Bonferroni" correction was used. The column *m* is the sample mean, *V* is the sample variance, and *pKS* is the *p*-value of the *KS* test. The true variance at generation n = 20 is approximately 1.

clearly seen in the *p*-values of the Kolmogorov-Smirnov (*KS*) test (*ks.test()* in R) presented in Table 1. The population's distribution was compared with  $\mathcal{N}(\mu, 1)$ , where  $\mu$  is the expectation of the initial distribution *F* and hence of the distribution at each generation. In most cases, the sample distribution by Algorithm 1 differs significantly from the asymptotic, unit variance, Gaussian, distribution. All the runs by the other algorithms have *p*-values greater than 0.05. Two simulation runs have a *p*-value of 0.08, however, with so many independent simulations this can be explainable just by chance.



**Figure 2.** Illustration of accumulating bias in Algorithm 1's simulation, under the CKQSO with (3) as its kernel and initial distribution  $\mathcal{N}(0, 1)$  (fixed point).

*Left:* sample average as function of the generation.

*Centre: p*-value of the *KS* test vs.  $\mathcal{N}(0, 1)$ .

*Right: p*-value of the *KS* test vs.  $\mathcal{N}(\overline{x}, 1)$ , where  $\overline{x}$  is the population average.

Both approximate Algorithms 1 and 3 have their advantages and disadvantages. The main advantage of the latter is speed (provided the required n does not become prohibitive). One just has to simulate i.i.d. values from a known distribution G. This is as we approximate the initial distribution by its mean value, indicating that this will work only when n is large,

i.e. many iterations have passed and only information on the expectation of the seed remains. On the other hand, we can control the required *n* very precisely as we know *F* and *G*. In Theorem 4 we used Chebyshev's inequality. Based on Theorem 3 we can only hope for improvement in constants for specific pairs of distributions. We also have exponential convergence in distribution (Theorem 3) as iterations of the operator cause an exponential growth of the number of "independent components" describing the law of  $\mathbb{Q}_G^n(F)$ . The leading constants are not large and the example simulations showed that (in these cases) a small number of generations suffices for approximations that are not significantly (by the *KS* test) different from the limit.

Algorithm 1 allows one to simulate a whole population evolving. This is an advantage if one wants to visualize the evolution. On the other hand, if one is just interested in the law of  $\mathbb{Q}_{G}^{n}(F)$  or  $\mathbb{Q}_{G}^{\infty}(F)$ , then the need to simulate a whole history can be overly lengthy. This algorithm does not require the drawing of a large number of random variables but has another problem which we can see in Figure 2, larger and larger deviations from the true distribution. In a computer simulation we cannot have an infinite population size, only a finite number of individuals is admissible. This means that after iterations of mixing, more and more dependencies will be appearing in the population. In fact, we can see in Figure 2 that the sample average resembles a random walk, with larger and larger deviations from the theoretically true expectation. Already in Table 1 we can see for starting Gaussian populations with unit variance (that are invariant under our  $\mathbb{Q}_{N}$ ) in the last column that even with 20 generations, the *KS* test notices significant deviations.

One can actually think that all of the above issues, especially the exponential number of "independent components", illustrate or rather characterize the complexity of the structure of quadratic stochastic operators. Fortunately, one can start quantifying this complexity as we did with Chebyshev's bound and our results show rapid convergence for finite variance initial and kernel distributions. On the other hand we restricted ourselves to a very specific class – centred kernel quadratic stochastic operators. In the full set of quadratic stochastic operators we should expect many more interesting dynamics.

### Code availability

The GitHub repository https://github.com/krzbar/QSO\_CTA contains R scripts, random seeds and simulation outputs used in this work.

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У цій роботі ми розглядаємо клас центрованих квадратичних стохастичних операторів з ядрами. Ми доводимо, що в цьому класі центрований квадратичний стохастичний оператор з ядром майже напевно збігається в  $L^2$  з експоненціальною швидкістю до свого граничного розподілу. Ми пропонуємо схему апроксимації для цього класу квадратичних стохастичних операторів і описуємо три алгоритми для їх моделювання. Розглянуто детально приклад, де ядро є гуасівським.

Ключові слова і фрази: асимптотична стійкість, змішаний нелінійний процес Маркова, неоднорідний оператор Маркова, квадратичний стохастичний оператор, моделювання.