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ENTROPY SATISFYING SCHEMES FOR COMPUTING SELECTION DYNAMICS IN COMPETITIVE INTERACTIONS*

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Abstract. In this paper, we present entropy satisfying schemes for solving an integro-differential equation that describes the evolution of a population structured with respect to a continuous trait. In [P.-E. Jabin and G. Raoul, *J. Math. Biol.*, 63 (2011), pp. 493–517] solutions are shown to converge toward the so-called evolutionary stable distribution (ESD) as time becomes large, using the relative entropy. At the discrete level, the ESD is shown to be the solution to a quadratic programming problem and can be computed by any well-established nonlinear programing algorithm. The schemes are then shown to satisfy the entropy dissipation inequality on the set where initial data are positive and the numerical solutions tend toward the discrete ESD in time. An alternative algorithm is presented to capture the global ESD for nonnegative initial data, which is made possible due to the mutation mechanism built into the modified scheme. A series of numerical tests are given to confirm both accuracy and the entropy satisfying property and to underline the efficiency of capturing the large time asymptotic behavior of numerical solutions in various settings.

Key words. selection dynamics, evolutionary stable distribution, relative entropy, positivity

AMS subject classifications. 35B40, 65M08, 92D15

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1. Introduction.

This paper is motivated by the work of Jabin and Raoul [20], in which a direct competitive selection model was investigated. The model for $x \in X \subseteq \mathbb{R}^d$ is given by

$$\partial_t f(t,x) = \left(a(x) - \int_X b(x,y) f(t,y)dy \right) f(t,x) \quad \text{for } t > 0,\ x \in X, \tag{1.1a}$$

$$f(0,x) = f_0(x), \quad x \in X. \tag{1.1b}$$

This is an integro-differential equation that describes the evolution of a population of density $f(t,x)$ structured with respect to a continuous trait x, and X is a subset of $\mathbb{R}^d$. In this model, the reproduction rate of each individual is determined by its trait and the environment, therefore leading to selection. Existence of regular or measure valued solutions is known, provided that the coefficients have enough regularity (see [13]). We refer the reader to [6] for a theory of well-posedness in measures for some structured population models including (1.1).

The model (1.1a) has been derived from random stochastic models of finite populations (see [7, 8]), with an additional mutation term. And such a model or its

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variation arises not only in evolution theory but also in ecology for nonlocal resources (and x denotes the location there; see, e.g., [3, 17]).

The model without mutation is interesting from the point of view of large time behavior; one expects that the dynamics will concentrate on large time, and several related results can be found in the literature; see [1, 5, 13, 20, 29], for instance. The singular steady-state solutions of the selection model correspond to highly concentrated population densities of the form of well-separated Dirac masses, which have been shown to happen only asymptotically in the model with mutation [2, 10, 23, 25, 26, 28, 30]. More complex models are certainly more realistic, such as random environments, spatial effects, and noncompetitive interactions, which should lead to quite different asymptotic behavior.

It is believed that competition will induce a convergence to the repartition of traits, which corresponds to one of many steady-state solutions for model (1.1). Such a special steady-state solution features a particular sign property characterized by the so-called evolutionary stable distribution (ESD), a notion introduced in [20] that we will follow: the measure $\tilde{f}$ is called an ESD of model (1.1) if

$$\forall x \in \operatorname{supp}\tilde{f}, \quad 0 = a(x) - \int_X b(x,y)\tilde{f}(y)dy, \tag{1.2a}$$

$$\forall x \in X, \quad 0 \geq a(x) - \int_X b(x,y)\tilde{f}(y)dy. \tag{1.2b}$$

The proof of global convergence to the ESD in [20] relies on a Lyapunov functional which has been proved to exist under the condition of positivity of a certain operator. The functional has the following form:

$$F(t) = \int_X \left[\tilde{f}(x) \log \frac{\tilde{f}(x)}{f(t,x)} + f(t,x) - \tilde{f}(x) \right] dx, \tag{1.3}$$

which is dissipating in time and serves as a relative entropy.

For different combinations of model parameters, one can expect to see a uniform trait distribution or patterns produced from the selection dynamics. It is usually difficult to predict between these two alternatives. Hence numerical methods are useful tools to evaluate the model prediction. Indeed, numerical illustration has become an important way to confirm or complement the analytical study; see [13, 25]. Desvillettes et al. [13] show speciation processes for system (1.1) by numerical simulations with the spectral method. Mirrahimi et al. [25] provide two numerical approximations to simulate solutions of the Lotka–Volterra model.

The aim of the present study is to give reliable numerical schemes for (1.1) from the perspective of providing numerical solutions with satisfying long time behavior. A key fact is that it admits a certain entropy structure, and we demand our numerical schemes to satisfy the entropy dissipation property in discrete settings. In addition, positivity for (1.1) is required to be preserved as well. These two requirements together are important for system (1.1), yet they add levels of difficulty to the design of a numerical method of high accuracy. As a preliminary attempt, only simple time-space discretization is discussed in the present paper.

In this work, we shall introduce finite volume schemes for approximating the solution of (1.1) so that numerical solutions provide a satisfying long time selection dynamics. We first present the one-dimensional case and then extend to multidimensional cases. Our task is to construct a proper discretization so that the numerical solution

$$f_\alpha^n \sim \frac{1}{h^d}\int_{I_\alpha} f(n\Delta t, x)dx$$

approximates $f(n\Delta t, x)$ over the cell I_α indexed by $\alpha \in \mathbb{Z}^d$ with $\cup I_\alpha = X$, where Δt is the time step and h the spatial mesh size; and the discrete relative entropy

$$F^n = \sum_\alpha \left(\tilde{f}_\alpha \log\left(\frac{\tilde{f}_\alpha}{f_\alpha^n}\right) + f_\alpha^n - \tilde{f}_\alpha \right) h^d \tag{1.4}$$

satisfies the entropy dissipation inequality (see (3.4))

$$F^{n+1} - F^n \leq -\frac{1}{2}\Delta t \|f^n - \tilde{f}\|_b^2,$$

where the notation $\|\cdot\|_b$ is defined later in (4.8).

Another task of this work is to provide an independent algorithm to compute the discrete ESD so that (1.4) is well defined.

Under reasonable assumptions we are able to prove that the problem of finding the discrete ESD is equivalent to solving a quadratic programming problem:

$$\min_{f\in\mathbb{R}^{N^d}} H$$

$$\text{subject to} \quad f \in \{f \geq 0\},$$

where H is a convex function determined by discrete data obtained from a and b.

For initial data not necessarily positive, the scheme leads only to the ESD restricted on a set of computational cells and zero in the complementary set. To capture the global ESD for general nonnegative initial data we propose a two-step algorithm: the modified scheme for the first step is of the form

$$\frac{f_\alpha^{n+1} - f_\alpha^*}{\Delta t} = f_\alpha^{n+1}\left(\bar{a}_\alpha - h^d \sum_{\beta\in\Lambda} \bar{b}_{\alpha\beta} f_\beta^n\right),$$

where

$$f_\alpha^* = \frac{1}{2^d}\sum_{i=1}^d \left(f_{\alpha+e_i}^n + f_{\alpha-e_i}^n\right),$$

together with proper corrections near boundary cells. We remark that since any strictly positive initial condition implies the convergence of the solution to the global ESD, one may adopt an alternative way to make the initial condition strictly positive, say with a small lift $f_j^0 + \epsilon$. However, in structured population dynamics, the spreading of an initial density is often realized through mutations, which motivated the above two-step algorithm.

We finally test the efficiency of numerical schemes proposed and analyzed herein for positive initial data and initial data not strictly positive, respectively. Numerical results include not only the case that the fittest traits are selected while the others become extinct but also the continuous distribution of traits. For the first case, random initial data, if used, represent all traits appearing in the initial populations in the sense that populations do not possess well-separated traits, but a finite number of subpopulations with well-separated traits will emerge with the evolution of time, namely the appearance of clusters. The results we have obtained are in excellent agreement with the analysis of the schemes proposed and display various patterns produced from the selection dynamics of the model.

The rest of this paper is organized as follows. In section 2, we first recall the known theoretical results for model (1.1) and then present the one-dimensional semidiscrete finite volume scheme and the associated steady states. Section 2.3 is devoted to both existence and uniqueness of the discrete ESD, through the equivalence between the problem of finding the ESD and the associated quadratic programming problem. The efficient computation of the ESD can then be carried out by any well-established quadratic programming solver. With the ESD well defined and efficiently computed, we use the discrete relative entropy to prove that the semidiscrete scheme satisfies the entropy dissipation inequality under some relaxed conditions on the discrete coefficients. Section 3 is devoted to a fully discrete scheme, which derives from a semi-implicit time discretization of the semidiscrete scheme. The scheme is easy to compute and has desired features under an appropriate restriction on the time step. Section 4 consists of a natural extension to multiple dimensions. Moreover, the time-asymptotic trend towards the ESD is rigorously justified for any nonnegative initial data. In this respect, the ESD is restricted to cells in which a initial data are positive. In section 5 we discuss how to obtain the global ESD even when the initial data are not strictly positive. The idea is to use a two-step algorithm: in the first step we process the given data by a modified scheme, in which a certain mutation mechanism plays a role of spreading the data. After all solution values become positive, we return to the original scheme to continue the simulation. Section 6 is devoted to extensive numerical tests of the proposed schemes. Finally, some concluding remarks are presented in section 7.

2. The numerical scheme.

We first review the known theoretical results about problem (1.1) and then present a semidiscrete numerical scheme to solve it.

2.1. Existence and time-asymptotic convergence.

We first recall a general existence result obtained in [13] for problem (1.1): for any nonnegative initial data $f_0 \in L^1(X)$, there exists a unique nonnegative $f \in C([0,\infty); L^1(X))$, provided that X is a compact subset of $\mathbb{R}^d$, and both a and b satisfy

$$a \in L^\infty(X), \quad |\{x; \quad a(x) > 0\}| \neq 0; \tag{2.1a}$$

$$b \in L^\infty(X \times X), \quad \operatorname*{essinf}_{x,x' \in X} b(x,x') > 0. \tag{2.1b}$$

However, the main result in [13] is stated with the stronger assumption that a and b are in $W^{1,\infty}$. As shown by Desvillettes et al. [13], under assumption (2.1) the total population $\int_X f dx$ remains bounded from below and above. The assumption (2.1) can be somewhat relaxed (in particular if X is not compact, for example $X = \mathbb{R}^d$).

In order to investigate the long time dynamics, the authors in [20] impose an additional assumption on b,

$$\forall g \in \mathcal{M}(X)\backslash\{0\}, \quad \int\int b(x,y)g(x)g(y)dxdy > 0, \tag{2.2}$$

where $\mathcal{M}(X)$ denotes the set of Radon measures in X. Note that (2.2) is automatically satisfied for $g \geq 0$ because of assumption (2.1b). However, since there is no sign condition on g in (2.2), it is stronger than (2.1b). Assumption (2.2) together with the boundedness of b in (2.1b) is also justified for a weighted norm

$$\|g\|_b = \left(\int\int b(x,y)g(x)g(y)dxdy\right)^{1/2}$$

in $L^1(X)$ (see [20, page 498]). With this norm and the assumption that $F(0) < \infty$, the solution is shown to converge to an ESD in the above weighted norm as time tends to infinity. However, even for bounded and positive initial data f_0, $F(0) < \infty$ holds only when $\int_X \tilde{f} log \tilde{f} dx < \infty$, which essentially means that $\tilde{f}$ has to be a continuous equilibrium. On the other hand, it has been shown by Gyllenberg and Meszéna [18] that the steady states are generically finite sums of Dirac masses—hence singular ESD. Convergence toward a singular ESD is more complex and has been shown in [20] when some additional symmetry is available on b; for example,

$$\forall x, y \in X, \quad b(x, y) = b(y, x). \tag{2.3}$$

2.2. The scheme formulation. We begin with the one-dimensional setting for $X = [-1, 1]$ to illustrate the main ideas and steps. Partitioning X into subcells $I_j = (x_{j-1/2}, x_{j+1/2})(j = 1, \dots, N)$ of uniform mesh $h = 2/N$ satisfies that $x_{j-1/2} = x_{1/2} + (j-1)h$ with $x_{1/2} = -1$, $x_{N+1/2} = 1$. In order to capture the concentration of the distribution, we consider a finite volume–type approximation. Let $f_j(t)$ denote the approximation of

$$\bar{f}_j(t) = \frac{1}{h} \int_{I_j} f\,(t, x)\, dx;$$

then taking the interval average of (1.1a) over $x \in I_j$ gives the following semidiscrete scheme:

$$\frac{d}{dt} f_j = f_j \left(\bar{a}_j - h \sum_{i=1}^{N} \bar{b}_{ji} f_i \right), \quad j = 1, \dots, N, \tag{2.4}$$

where

$$\bar{a}_j = \frac{1}{h} \int_{I_j} a(x) dx, \quad \bar{b}_{ji} = \frac{1}{h^2} \int_{I_i} \int_{I_j} b(x, y) dx dy. \tag{2.5}$$

For a fixed N, one can think of (2.4) as a Lotka–Volterra ODE system, which has been well studied in the literature. We refer the reader to [9, 19, 31] and the references therein for more details about such systems. As a nonlinear dynamical system, the large time behavior of solutions to (2.4) is closely related to the stationary states $\tilde{f}$ satisfying

$$\tilde{f}_j \left(\bar{a}_j - h \sum_{i=1}^{N} \bar{b}_{ji} \tilde{f}_i \right) = 0, \quad j = 1, \dots, N.$$

Clearly, there are many steady states as such. We are interested in the discrete ESD and the long time behavior of the numerical solution under assumptions (2.1), (2.2), and (2.3). These assumptions with a simple verification lead to the following:

$$|\bar{a}_j| \le \|a\|_{L^\infty}, \quad \{1 \le j \le N, \bar{a}_j > 0\} \neq \emptyset; \tag{2.6a}$$

$$0 \le \bar{b}_{ji} \le \|b\|_{L^\infty} \quad \text{and} \quad \bar{b}_{ji} = \bar{b}_{ij} \quad \text{for } 1 \le i, j \le N; \tag{2.6b}$$

$$\sum_{j=1}^{N} \sum_{i=1}^{N} \bar{b}_{ji} g_i g_j > 0 \quad \text{for any } g_j \text{ such that } \sum_{j=1}^{N} |g_j|^2 \neq 0. \tag{2.6c}$$

Remark 2.1. Assumption (2.6c) is implied by (2.2). Indeed, for $g(x)|_{I_j} = g_j$ we have

$$\int_X \int_X b(x,y)g(x)g(y)dxdy = \sum_{j=1}^N \sum_{i=1}^N g_j g_i \int_{I_i} \int_{I_j} b(x,y)dxdy = h^2 \sum_{j=1}^N \sum_{i=1}^N \bar{b}_{ji} g_j g_i.$$

Note that we do not need $\bar{b}_{ji}$ to be strictly positive at the discrete level.

Remark 2.2. The strong competition assumption (2.2) is directly connected to the stability of the ESD. There is no evidence that (2.2) should be satisfied for any particular biological system. Nevertheless, in section 6 we will use both a Gaussian competition kernel $b(x,y) = e^{-\alpha|x-y|^2}$ and $b(x,y) = \frac{1}{1+|x-y|^2}$ in our numerical simulations since the positivity condition applies to these two cases.

With assumptions (2.6b)–(2.6c), $B = (\bar{b}_{ij})_{N\times N}$ is a symmetric, positive definite matrix. Let $\|\cdot\|$ denote the usual Euclidean norm of a vector; then

$$\sqrt{\lambda_{\min}}\|g\|h \le \|g\|_b \le \sqrt{\lambda_{\max}}\|g\|h, \tag{2.7}$$

where $\lambda_{\min}(\lambda_{\max})$ denotes the smallest (largest) eigenvalue of B and $\|B\|_2 = \lambda_{\max}$. Also we define the l^1 norm by

$$\|g\|_1 = \sum_{j=1}^N |g_j|h$$

and the discrete b-norm by

$$\|g\|_b = \left(\sum_{i,j=1}^N \bar{b}_{ij} g_i g_j h^2\right)^{1/2}. \tag{2.8}$$

Note that we still use $\|\cdot\|_b$ to denote the discrete norm (2.8) since they are same for any piecewise constant function $g(x)|_{x\in I_j} = g_j$. These relations and notation will be used in what follows.

We first investigate the existence and uniqueness of the ESD under assumption (2.6).

2.3. ESD. If initial data $f_j(0) > 0$ for $j = 1, 2, \dots, N$, the corresponding discrete ESD $\tilde{f} = \{\tilde{f}_j\}$ may be defined as

$$\forall j \in \{1 \le i \le N, \tilde{f}_i \neq 0\}, \quad 0 = \bar{a}_j - h\sum_{i=1}^N \bar{b}_{ji}\tilde{f}_i; \tag{2.9a}$$

$$\forall j \in \{1 \le i \le N, \tilde{f}_i = 0\}, \quad 0 \ge \bar{a}_j - h\sum_{i=1}^N \bar{b}_{ji}\tilde{f}_i. \tag{2.9b}$$

Introduce the nonlinear function

$$H(f) = \frac{f^{\mathrm{T}}Bf}{2} - a^{\mathrm{T}}f,$$

with $f = (f_1, f_2, \dots, f_N)^{\mathrm{T}}$ and $a = (\bar{a}_1, \bar{a}_2, \dots, \bar{a}_N)^{\mathrm{T}}/h$, and the feasible set

$$S = \{f, \quad f \ge 0\};$$

then an ESD can be expressed as a solution to the following problem:

$$\partial_{f_i} H(f) = 0 \quad \text{for} \quad f_i > 0 \quad \text{and} \quad \nabla_f H \geq 0 \tag{2.10a}$$

$$\text{subject to} \quad f \in S = \{f \geq 0\}. \tag{2.10b}$$

We can show that this problem is equivalent to the following nonlinear programming problem:

$$\min_{f \in \mathbb{R}^N} H \tag{2.11a}$$

$$\text{subject to} \quad f \in S = \{f \geq 0\}. \tag{2.11b}$$

LEMMA 2.1. *If* (2.6) *holds, then problem* (2.10) *is equivalent to the nonlinear programming problem* (2.11).

Proof. ($\Longrightarrow$) First, if $f^* \in S$ satisfies (2.10), we prove f^* is the solution to (2.11), that is,

$$H(f^* + \alpha) \geq H(f^*)$$

for all $\alpha \in \mathbb{R}^N$ such that $f^* + \alpha \in S$. The Taylor expansion of the form

$$H(f^* + \alpha) = H(f^*) + \alpha \cdot \nabla_f H(f^*) + \frac{1}{2}\alpha^{\mathrm{T}} D^2 H \alpha \tag{2.12}$$

ensures that we need only prove

$$\alpha \cdot \nabla_f H(f^*) + \frac{1}{2}\alpha^{\mathrm{T}} B \alpha \geq 0. \tag{2.13}$$

Note that if $f^* + \alpha \geq 0$, then $\alpha \geq -f^*$; this together with $\nabla_f H(f^*) \geq 0$ yields

$$\alpha \cdot \nabla_f H(f^*) \geq -f^* \cdot \nabla_f H(f^*) = 0.$$

The positivity of the second term in (2.13), i.e., $\frac{1}{2}\alpha^{\mathrm{T}} B \alpha \geq 0$, is guaranteed by the fact that B is a positive definite matrix. Putting this together we prove (2.13).

($\Longleftarrow$) We next prove that $f^* \in S$ satisfies (2.10) if f^* is a solution of (2.11). As argued above, f^* being a minimizer of $H(f)$ in S implies that (2.13) holds true for all $f^* + \alpha \in S$. We claim that this yields

$$\alpha \cdot \nabla_f H(f^*) \geq 0. \tag{2.14}$$

Using this claim we can prove (2.10). If $f_i^* > 0$, we take $\alpha_i = \pm f_i^*$ and $\alpha_j = 0$ for $j \neq i$ so that $\partial_{f_i} H(f^*) = 0$ must hold; if $f_i^* = 0$, we take $\alpha_i = 1$ and $\alpha_j = 0$ for $j \neq i$ so that $\partial_{f_i} H(f^*) \geq 0$. Hence (2.10) is proved.

Finally we prove claim (2.14) by the contradiction argument. Suppose $\alpha \cdot \nabla_f H(f^*) < 0$ then $K = -\frac{\alpha}{|\alpha|} \cdot \nabla_f H(f^*) > 0$ is a fixed number. Define $e_\alpha = \frac{\alpha}{|\alpha|}$, and let $\rho(B)$ denote the maximum eigenvalue of B, which has to be positive because of (2.13) and $K > 0$. If we choose $|\alpha| < \frac{2K}{\rho(B)}$, then (2.13) yields

$$\begin{aligned} 0 &\leq |\alpha|[-K + \tfrac{|\alpha|}{2} {e_\alpha}^{\mathrm{T}} B e_\alpha] \\ &\leq |\alpha|[-K + \tfrac{|\alpha|}{2} \rho(B)] < 0. \end{aligned}$$

This contradiction verifies the desired claim (2.14). The proof of the equivalence of the two problems is thus complete. □

Remark 2.3. The above proof shows that the minimization problem (2.11) may also be replaced by

$$\min_{f\in\mathbb{R}^N} H \tag{2.15a}$$

$$\text{subject to} \quad f \in \{f \geq 0 \ \text{ and } \ \nabla H(f) \geq 0\}. \tag{2.15b}$$

Hence, we can easily establish the solvability of (2.11) (see [12]) and therefore of (2.15).

LEMMA 2.2. *If* (2.6) *is satisfied, then there exists at least one nontrivial vector* $g \in S$ *such that*

$$H(g) = \min_{f\in S} H(f).$$

We next show the existence and uniqueness of the ESD.

THEOREM 2.1. *If* (2.6) *is satisfied, then there exists a unique ESD as defined in* (2.9).

Proof. The existence of an ESD follows from the equivalence result in Lemma 2.1 and the existence result in Lemma 2.2. Here we present a direct proof of the uniqueness by mimicking the proof for the continuous case in [20]. We argue by the contradiction argument. Assume that there are two nonnegative ESDs, $\tilde{f}$ and $\tilde{g}$, satisfying (2.9). Then

$$I := \sum_{j=1}^{N} \tilde{g}_j \left(\bar{a}_j - h \sum_{i=1}^{N} \bar{b}_{ji} \tilde{f}_i \right) + \sum_{j=1}^{N} \tilde{f}_j \left(\bar{a}_j - h \sum_{i=1}^{N} \bar{b}_{ji} \tilde{g}_i \right) \leq 0. \tag{2.16}$$

Meanwhile, according to the definition of ESD,

$$\begin{aligned}
I := & \sum_{\{j,\tilde{g}_j\neq 0\}} \tilde{g}_j \left(h\sum_{i=1}^{N} \bar{b}_{ji}\tilde{g}_i - h\sum_{i=1}^{N} \bar{b}_{ji}\tilde{f}_i \right) + \sum_{\{j,\tilde{f}_j\neq 0\}} \tilde{f}_j \left(h\sum_{i=1}^{N} \bar{b}_{ji}\tilde{f}_i - h\sum_{i=1}^{N} \bar{b}_{ji}\tilde{g}_i \right) \\
= & \; h \sum_{\{j,\tilde{g}_j\neq 0\}} \tilde{g}_j \sum_{i=1}^{N} \bar{b}_{ji}(\tilde{g}_i - \tilde{f}_i) + h \sum_{\{j,\tilde{f}_j\neq 0\}} \tilde{f}_j \sum_{i=1}^{N} \bar{b}_{ji}(\tilde{f}_i - \tilde{g}_i) \\
= & \; h \sum_{j=1}^{N} \tilde{g}_j \sum_{i=1}^{N} \bar{b}_{ji}(\tilde{g}_i - \tilde{f}_i) + h \sum_{j=1}^{N} \tilde{f}_j \sum_{i=1}^{N} \bar{b}_{ji}(\tilde{f}_i - \tilde{g}_i) \\
= & \; h \sum_{j=1}^{N}\sum_{i=1}^{N} \bar{b}_{ji} \left(\tilde{f}_i - \tilde{g}_i\right)\left(\tilde{f}_j - \tilde{g}_j\right) \geq 0;
\end{aligned}$$

this says that I is both nonnegative and nonpositive according to (2.16). Therefore $I = 0$, which indicates $\bar{f}_j = \bar{g}_j$ for $j = 1, 2, \ldots, N$. □

Remark 2.4. If positivity of b is not assumed, i.e., B does not satisfy (2.6c), we can still prove the existence of an ESD using the above approach since any solution to (2.11) is necessarily an ESD even if B does not satisfy (2.6c) (see the second part of the proof of Lemma 2.1). Unfortunately, the nonlinear programming point of view is not helpful for finding one among several possible ESD(s).

2.4. Properties of the semidiscrete scheme. With the obtained ESD $\tilde{f}$, we define the discrete entropy functional as follows:

$$F(t)=\sum_{j=1}^{N}\left(\tilde{f}_j\log\left(\frac{\tilde{f}_j}{f_j(t)}\right)+f_j(t)-\tilde{f}_j\right)h. \tag{2.17}$$

THEOREM 2.2. *Assume* (2.6) *holds, and let* $f_j(t)$ *be the numerical solution to the semidiscrete scheme* (2.4)*. Then the following hold:*

(i) *If* $f_j(0)>0$ *for every* $1\le j\le N$*, then* $f_j(t)>0$ *for any* $t>0$*.*

(ii) F *is nonincreasing in time. Moreover,*

$$\frac{dF}{dt}\le-\|f-\tilde{f}\|_b^2. \tag{2.18}$$

Proof. (i) For scheme (2.4), positivity preserving is a direct consequence from the solution formula

$$f_j\left(t\right)=f_j\left(0\right)e^{\int_0^t\left(\bar{a}_j-h\sum_{i=1}^{N}\bar{b}_{ji}f_i(s)\right)ds}>0. \tag{2.19}$$

Here the equality $f_j(t)=0$ does not hold due to the upper bound $f_j(t)\le f_j(0)e^{\|a\|_{L^\infty}t}$.

(ii) A direct calculation using (2.4) yields

$$\frac{dF}{dt}=\sum_{j=1}^{N}\left(-\tilde{f}_j\times\frac{(f_j)_t}{f_j}+(f_j)_t\right)h=\sum_{j=1}^{N}\left(f_j-\tilde{f}_j\right)\left(\bar{a}_j-h\sum_{i=1}^{N}\bar{b}_{ji}f_i\right)h.$$

Dictated by the definition of the ESD in (2.9) we divide the summation over two subsets $J=\{1\le i\le N,\ \tilde{f}_i>0\}$ and $J^c=\{1\le i\le N,\ \tilde{f}_i=0\}$; then we have

$$\begin{aligned}\frac{dF}{dt}&=\left(\sum_{j\in J}+\sum_{j\in J^c}\right)\left(f_j-\tilde{f}_j\right)\left(\bar{a}_j-h\sum_{i=1}^{N}\bar{b}_{ji}f_i\right)h\\&\le\sum_{j\in J}\left(f_j-\tilde{f}_j\right)\left(h\sum_{i=1}^{N}\bar{b}_{ji}\tilde{f}_i-h\sum_{i=1}^{N}\bar{b}_{ji}f_i\right)h\\&\quad+\sum_{j\in J^c}\left(f_j-\tilde{f}_j\right)\left(h\sum_{i=1}^{N}\bar{b}_{ji}\tilde{f}_i-h\sum_{i=1}^{N}\bar{b}_{ji}f_i\right)h\\&=-\sum_{j=1}^{N}\sum_{i=1}^{N}\bar{b}_{ji}\left(f_i-\tilde{f}_i\right)\left(f_j-\tilde{f}_j\right)h^2\le0,\end{aligned}$$

where we have used the fact that $f_j-\tilde{f}_j=f_j\ge0$ and $\bar{a}_j\le h\sum_{i=1}^{N}\bar{b}_{ji}\tilde{f}_i$ for $j\in J^c$ together with (2.6c). The entropy dissipation property is proved. ∎

3. Time discretization. Positivity and entropy properties are both also desired for the fully discrete scheme. We consider the following scheme:

$$\frac{f_j^{n+1}-f_j^n}{\Delta t}=f_j^{n+1}\left(\bar{a}_j-h\sum_{i=1}^{N}\bar{b}_{ji}f_i^n\right). \tag{3.1}$$

This scheme is semi-implicit and linear in f^{n+1} and hence easy to implement. In addition, the two desired properties still hold under certain conditions on the time step. To proceed, we set the discrete entropy as

$$F^n = \sum_{j=1}^{N} \left(\tilde{f}_j \log \left(\frac{\tilde{f}_j}{f_j^n} \right) + f_j^n - \tilde{f}_j \right) h. \tag{3.2}$$

THEOREM 3.1. *Assume* (2.6) *is satisfied and* $F^0 < \infty$, *and let* f_j^n *be the numerical solution to the fullydiscrete scheme* (3.1) *with time step satisfying*

$$\Delta t \le \frac{\lambda_{\min}}{4\lambda_{\max} \left[\|a\|_{L^\infty} + \|b\|_{L^\infty} \|\tilde{f}\|_1 + \lambda_{\max} S(F^0) \right]}, \tag{3.3}$$

where S *is a monotone, positive function defined in* (3.11). *Then the following hold:*

(i) $f_j^{n+1} = 0$ *for* $f_j^n = 0$, *and* $f_j^{n+1} > 0$ *for* $f_j^n > 0$ *for any* $n \in \mathbb{N}$.

(ii) F^n *is a decreasing sequence in* n. *Moreover,*

$$F^{n+1} - F^n \le -\frac{1}{2} \Delta t \|f^n - \tilde{f}\|_b^2. \tag{3.4}$$

Remark 3.1. Note that in the continuous case $F(0) < \infty$ would exclude the singular ESD. In contrast, in the discrete case, $F^0 < \infty$ does include the case when the ESD is singular, though in such cases $F^0 \sim |\log h|$.

Proof. (i) From (3.3) it follows that

$$\Delta t \le \frac{1}{2\|a\|_{L^\infty}},$$

which together with $f_j^n \ge 0$ and $\bar{b}_{ji} \ge 0$ gives

$$\mu_j^n := 1 - \Delta t \bar{a}_j + h \Delta t (B f^n)_j \ge 1 - \Delta t \|a\|_{L^\infty} \ge \frac{1}{2}. \tag{3.5}$$

Hence (3.1) gives

$$0 \le \frac{f_j^n}{\mu_j^n} = f_j^{n+1} \le 2 f_j^n, \tag{3.6}$$

so we have $f_j^{n+1} = 0$ for $f_j^n = 0$, and $f_j^{n+1} > 0$ for $f_j^n > 0$.

(ii) Using the inequality $\log x \le x - 1$ for any $x > 0$, and the definition of the

ESD, we proceed to estimate $F^{n+1}-F^n$ as follows:

$$\begin{aligned}
F^{n+1}-F^n &= h\sum_{j=1}^N\left(\tilde f_j \log\frac{f_j^n}{f_j^{n+1}} + f_j^{n+1} - f_j^n\right)\\
&\le h\sum_{j=1}^N\left(\tilde f_j \frac{f_j^n - f_j^{n+1}}{f_j^{n+1}} + f_j^{n+1} - f_j^n\right)\\
&= h\sum_{j=1}^N\left(\frac{f_j^{n+1}-f_j^n}{f_j^{n+1}}\right)\left(f_j^{n+1}-\tilde f_j\right)\\
&= \Delta t h\sum_{j=1}^N\left(\bar a_j - h\sum_{i=1}^N \bar b_{ji} f_i^n\right)(f_j^{n+1}-\tilde f_j)\\
&\le \Delta t h\Bigg[\sum_{\{j,\ \tilde f_j=0\}}\left(h\sum_{i=1}^N \bar b_{ji}\tilde f_i - h\sum_{i=1}^N \bar b_{ji} f_i^n\right)(f_j^{n+1}-\tilde f_j)\\
&\quad + \sum_{\{j,\ \tilde f_j>0\}}\left(h\sum_{i=1}^N \bar b_{ji}\tilde f_i - h\sum_{i=1}^N \bar b_{ji} f_i^n\right)(f_j^{n+1}-\tilde f_j)\Bigg]\\
&= -\Delta t h^2\sum_{j=1}^N\sum_{i=1}^N \bar b_{ji}(f_j^{n+1}-\tilde f_j)(f_i^n-\tilde f_i).
\end{aligned}$$

Let $g^n = f^n - \tilde f$; then

$$\begin{aligned}
F^{n+1}-F^n &\le -\Delta t h^2 g^{n+1}\cdot Bg^n\\
&= -\Delta t h^2 (g^n\cdot Bg^n + (g^{n+1}-g^n)\cdot Bg^n)\\
&\le -\Delta t h^2 g^n\cdot Bg^n + \Delta t h^2\|B\|_2\|g^n\|\|g^{n+1}-g^n\|.
\end{aligned} \tag{3.7}$$

Next, we estimate $\|g^{n+1}-g^n\|$. Note that

$$\begin{aligned}
(g^{n+1}-g^n)_j &= \Delta t f_j^{n+1}\left[\bar a_j - h\sum_{i=1}^N \bar b_{ji}(g_i^n+\tilde f_i)\right]\\
&= \Delta t\left[\frac{f_j^n}{\mu_j^n}\left(\bar a_j - h\sum_{i=1}^N \bar b_{ji}\tilde f_i\right) - h\frac{f_j^n}{\mu_j^n}\sum_{i=1}^N \bar b_{ji} g_i^n\right]\\
&= \Delta t\left[\frac{f_j^n-\tilde f_j}{\mu_j^n}\left(\bar a_j - h\sum_{i=1}^N \bar b_{ji}\tilde f_i\right) - h\frac{f_j^n}{\mu_j^n}\sum_{i=1}^N \bar b_{ji} g_i^n\right],
\end{aligned}$$

where we have used the definition of the ESD in the last equality. Thus,

$$\|g^{n+1}-g^n\| \le 2\Delta t\|g^n\|\left(C_1 + h\|f^n\|_\infty\|B\|_2\right),$$

where

$$C_1 = \|a\|_{L^\infty} + \|b\|_{L^\infty}\|\tilde f\|_1,$$

and we have used (3.5).

We claim that there exists a nondecreasing, positive function S such that

$$h\|f^n\|_\infty \le S(F^n). \tag{3.8}$$

Substitution of this into (3.7) gives

$$F^{n+1} - F^n \leq -\Delta t h^2 g^n \cdot B g^n \left[1 - 2\Delta t \|B\|_2 [C_1 + \|B\|_2 S(F^n)] \frac{\|g^n\|^2}{g^n \cdot B g^n}\right]. \tag{3.9}$$

For Δt satisfying (3.3), and noticing that $g^n \cdot B g^n \geq \lambda_{\min} \|g^n\|^2$ and $\|B\|_2 = \lambda_{\max}$, we have

$$F^1 \leq F^0 - \frac{1}{2}\Delta t h^2 g^0 \cdot B g^0$$

according to (3.9) with for $n = 0$. Hence $S(F^1) \leq S(F^0)$ so that

$$4\|B\|_2 [C_1 + \|B\|_2 S(F^1)] \Delta t \leq \lambda_{\min},$$

which ensures

$$F^2 \leq F^1 - \frac{1}{2}\Delta t h^2 g^1 \cdot B g^1.$$

By induction, with $4\|B\|_2[C_1 + \|B\|_2 S(F^n)]\Delta t \leq \lambda_{\min}$, we have

$$F^{n+1} - F^n \leq -\frac{1}{2}\Delta t h^2 g^n \cdot B g^n = -\frac{1}{2}\Delta t \|f^n - \tilde{f}\|_b^2.$$

Finally, we discuss the form of S claimed in (3.8). Set

$$G(\xi, \eta) = \xi \log\left(\frac{\xi}{\eta}\right) + \eta - \xi, \tag{3.10}$$

defined on $\mathbb{R}^+ \times \mathbb{R}^+$; then $G \geq 0$, and G is convex and increasing in η for $\eta \geq \xi$ and convex and decreasing in ξ for $\xi \leq \eta$. Note that

$$\sum_{j=1}^{N} G(h\tilde{f}_j, h f_j^n) = F^n;$$

hence, for $\|f^n\|_\infty = f_{j_0}^n$ we have

$$G(h\tilde{f}_{j_0}, h f_{j_0}^n) \leq F^n.$$

From this we see that either $f_{j_0}^n \leq \|\tilde{f}\|_\infty$ or $f_{j_0}^n \geq \|\tilde{f}\|_\infty$; in the latter case the monotonicity of G in $\xi (\leq \eta)$ leads to

$$G_1(h\|f^n\|_\infty) := G(h\|\tilde{f}\|_\infty, h f_{j_0}^n) \leq G(h\tilde{f}_{j_0}, h f_{j_0}^n) \leq F^n.$$

Hence, we obtain $h\|f^n\|_\infty \leq G_1^{-1}(F^n)$, with the inverse taken in the domain of $[h\|\tilde{f}\|_\infty, +\infty)$. We therefore have (3.8) with

$$S(F^n) := G_1^{-1}(F^n). \qquad \square \tag{3.11}$$

The established entropy dissipation property (3.4) ensures the following time-asymptotic result.

COROLLARY 3.1. *Assume* (2.6) *holds. Let* f_j^n *be the numerical solution generated from scheme* (3.1) *with positive initial data* $f_j^0 > 0$ *for all* $j = 1, \ldots, N$. *Then*

$$\lim_{n \to \infty} \|f^n - \tilde{f}\|_b = 0.$$

Remark 3.2. The above results indicate that the positivity assumption in (2.6c) is crucial to guarantee entropy dissipation properties (2.18) and (3.4), as well as the uniqueness of the ESD as stated in Theorem 2.1. One may imagine that the absence of this positivity property of b should not have much impact on the concentration dynamics of the population density. However, due to nonuniqueness of ESD(s), it is an open question whether the concentration appears as oscillations between different ESDs.

4. Extension to multidimensions and restricted ESD.

4.1. Multidimensional schemes. Let $X = [-1, 1]^d$, with a structured partition by $I_\alpha = I_{\alpha_1} \times I_{\alpha_2} \times \cdots \times I_{\alpha_d}$, where the definition of every $I_{\alpha_i} (i = 1, 2, \ldots, d)$ is the same as the one-dimensional case, and α denotes the multiple index which runs over the following index set:

$$\Lambda := \{\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_d), \quad 1 \le \alpha_i \le N, \quad i = 1, \ldots, d\}. \tag{4.1}$$

Let $f_\alpha(t)$ denote the approximation of the cell average $\frac{1}{h^d}\int_{I_\alpha} f(t,x)dx$. We then obtain the following semidiscrete scheme:

$$\frac{d}{dt} f_\alpha = f_\alpha \left(\bar{a}_\alpha - h^d \sum_\beta \bar{b}_{\alpha\beta} f_\beta \right), \quad \alpha \in \Lambda, \tag{4.2}$$

where

$$\bar{a}_\alpha = \frac{1}{h^d}\int_{I_\alpha} a(x)dx, \quad \bar{b}_{\alpha\beta} = \frac{1}{h^{2d}}\int_{I_\beta}\int_{I_\alpha} b(x,y)dxdy, \quad \alpha, \beta \in \Lambda.$$

In a similar manner, the ESD in the multidimensional case is defined as follows:

$$\forall \alpha \in \{\beta \in \Lambda, \tilde{f}_\beta \neq 0\}, \quad 0 = \bar{a}_\alpha - h^d \sum_\beta \bar{b}_{\alpha\beta} \tilde{f}_\beta; \tag{4.3a}$$

$$\forall \alpha \in \{\beta \in \Lambda, \tilde{f}_\beta = 0\}, \quad 0 \ge \bar{a}_\alpha - h^d \sum_\beta \bar{b}_{\alpha\beta} \tilde{f}_\beta. \tag{4.3b}$$

Choose a way to reorder the index set Λ into the natural order from 1 to N^d; then this order will give the vectors f and $\bar{a}$ from f_Λ and $\bar{a}_\Lambda$, respectively. Correspondingly, this order also generates an $N^d \times N^d$ matrix $B = (\bar{b}_{\alpha\beta})_{N^d \times N^d}$ from $\bar{b}_{\Lambda\Lambda}$. The assumptions (2.1), (2.2), and (2.3) in the multidimensional case also lead to a set of conditions on the discrete coefficients.

$$|\bar{a}_\alpha| \le \|a\|_{L^\infty}, \quad \{\alpha \in \Lambda, \bar{a}_\alpha > 0\} \neq \emptyset, \tag{4.4a}$$

$$0 \le \bar{b}_{\alpha\beta} \le \|b\|_{L^\infty} \text{ for } \alpha, \beta \in \Lambda, \text{ and } B \text{ is symmetric}, \tag{4.4b}$$

$$\sum_\alpha \sum_\beta \bar{b}_{\alpha\beta} g_\alpha g_\beta > 0 \text{ for any } g_\alpha \text{ such that } \sum_\alpha |g_\alpha|^2 \neq 0. \tag{4.4c}$$

In an entirely same way, we can prove the existence and uniqueness of the ESD, as summarized below.

Theorem 4.1. *If* (4.4) *is satisfied, then there exists a unique solution to* (4.3).

Again, (4.4b)–(4.4c) imply that B is a symmetric, positive definite matrix; hence the problem of finding the ESD is equivalent to solving the nonlinear programming problem

$$\min_{f\in\mathbb{R}^{N^d}} H \tag{4.5a}$$

$$\text{subject to} \quad f \in S = \{f \geq 0\}, \tag{4.5b}$$

where

$$H(f) = \frac{f^{\mathrm{T}}Bf}{2} - a^{\mathrm{T}}f,$$

with $(a)_{N^d\times 1} = (\bar{a}_\Lambda/h^d)_{N^d\times 1}$. As in the one-dimensional case, we define the semidiscrete relative entropy by

$$F(t) = \sum_{\alpha\in\Lambda}\left(\tilde{f}_\alpha \log\left(\frac{\tilde{f}_\alpha}{f_\alpha}\right) + f_\alpha - \tilde{f}_\alpha\right)h^d,$$

which is shown to be nonincreasing in time, following the same argument as in the one-dimensional case. For the fully discrete scheme we take

$$\frac{f_\alpha^{n+1} - f_\alpha^n}{\Delta t} = f_\alpha^{n+1}(\bar{a}_\alpha - h^d\sum_\beta \bar{b}_{\alpha\beta}f_\beta^n), \quad \alpha \in \Lambda. \tag{4.6}$$

The entropy satisfying property of the scheme is quantified by the discrete relative entropy of the form

$$F^n = \sum_{\alpha\in\Lambda}\left(\tilde{f}_\alpha \log\left(\frac{\tilde{f}_\alpha}{f_\alpha^n}\right) + f_\alpha^n - \tilde{f}_\alpha\right)h^d. \tag{4.7}$$

In order to present a similar multidimensional entropy property, we use the notation

$$G_d(\eta) := G(h^d\|\tilde{f}\|_\infty, \eta), \quad \eta > 0,$$

where G is given in (3.10) and increasing in η for $\eta \geq h^d\|\tilde{f}\|_\infty$; also $G_d(h^d\|f^n\|_\infty) \leq F^n$ as implied by (4.7). Hence the same iterative argument applies with $S(F^n)$ defined by

$$S(F^n) = G_d^{-1}(F^n),$$

where the inverse is taken in the range of $[h^d\|\tilde{f}\|_\infty, \infty)$. In the multidimensional case, we define

$$\|g\|_b = \left(h^{2d}\sum_{\alpha\in\Lambda}\bar{b}_{\beta\alpha}g_\alpha g_\beta\right)^{\frac{1}{2}}, \quad \|g\|_1 = h^d\sum_{\alpha\in\Lambda}|g_\alpha|, \tag{4.8}$$

with which we present the following result.

THEOREM 4.2. *Assume* (4.4) *holds and* $F^0 < \infty$. *Let* f_α^n *be the numerical solution to* (4.2) *with the time step satisfying*

$$\Delta t \leq \frac{\lambda_{\min}}{4\lambda_{\max}\left[\|a\|_{L^\infty} + \|b\|_{L^\infty}\|\tilde{f}\|_1 + \lambda_{\max}S(F^0)\right]}. \tag{4.9}$$

Then the following hold:

(i) $f_\alpha^{n+1} = 0$ *for* $f_\alpha^n = 0$, *and* $f_\alpha^{n+1} > 0$ *for* $f_\alpha^n > 0$ *for any* $n \in \mathbb{N}$.

(ii) F^n *is a decreasing sequence in* n. *Moreover,*

$$F^{n+1} - F^n \leq -\frac{1}{2}\Delta t\|f^n - \tilde{f}\|_b^2. \tag{4.10}$$

4.2. Restricted ESD. From fully discrete scheme (4.6) it follows that if $f_\alpha^0 = 0$ for some α, then $f_\alpha^n = 0$ for all $n > 0$. This suggests that the time-asymptotic trend to the global ESD is not guaranteed for initial data not strictly positive. In order to extend the previous results to the case with nonnegative initial data, we specify a subset $\Lambda_s \subseteq \Lambda$. We can define the usual ESD $\tilde{f}_\alpha$ for $\alpha \in \Lambda_s$,

$$\forall \alpha \in \{\beta \in \Lambda_s, \tilde{f}_\beta \neq 0\}, \quad 0 = \bar{a}_\alpha - h^d \sum_{\beta \in \Lambda_s} \bar{b}_{\alpha\beta} \tilde{f}_\beta; \tag{4.11a}$$

$$\forall \alpha \in \{\beta \in \Lambda_s, \tilde{f}_\beta = 0\}, \quad 0 \geq \bar{a}_\alpha - h^d \sum_{\beta \in \Lambda_s} \bar{b}_{\alpha\beta} \tilde{f}_\beta. \tag{4.11b}$$

This allows for a discrete entropy over Λ_s,

$$F_s^n = \sum_{\alpha \in \Lambda_s} \left(\tilde{f}_\alpha \log \left(\frac{\tilde{f}_\alpha}{f_\alpha^n} \right) + f_\alpha^n - \tilde{f}_\alpha \right) h^d. \tag{4.12}$$

For all $\alpha \in \Lambda$, we denote

$$\tilde{f}_\alpha^R = \begin{cases} 0 \text{ for } \alpha \notin \Lambda_s, \\ \tilde{f}_\alpha \text{ for } \alpha \in \Lambda_s. \end{cases} \tag{4.13}$$

Clearly, when $\Lambda_s = \Lambda$, the ESD is nothing but the global ESD.

THEOREM 4.3. *Assume* (4.4) *is satisfied on* Λ_s *and* $F_s^0 < \infty$. *If* $f_\alpha^0 > 0$ *for* $\alpha \in \Lambda_s$ *and* $f_\alpha^0 = 0$ *for* $\alpha \notin \Lambda_s$, *then the numerical solution to* (4.6) *converges to* $\tilde{f}^R$ *as* $n \to \infty$ *in the sense that*

$$\lim_{n \to \infty} \| f^n - \tilde{f}^R \|_b = 0. \tag{4.14}$$

Proof. For $\alpha \notin \Lambda_s$, $f_\alpha^0 = 0$, then $f_\alpha^n = 0$ for all $n > 0$ since

$$f_\alpha^{n+1} = \frac{f_\alpha^n}{1 - \Delta t \bar{a}_\alpha + \Delta t h^d \sum_{\beta \in \Lambda} \bar{b}_{\alpha\beta} f_\beta^n}, \tag{4.15}$$

as derived from scheme (4.6). For $\alpha \in \Lambda_s$, $f_\alpha^0 > 0$, then $f_\alpha^n > 0$ for all $n > 0$ as long as the time step is suitably small. Restricted on the set Λ_s, all the results in Theorem 3.1 hold true; hence we have

$$F_s^{n+1} - F_s^n \leq -\frac{1}{2} \Delta t \| f^n - \tilde{f}^R \|_b^2. \tag{4.16}$$

From this inequality we see that F_s^n is a decreasing sequence in n and also bounded from below by (4.12); hence the limit of F_s^n exists when n tends to ∞. Fixed Δt and $h > 0$, when passing to the limit $n \to \infty$, the right-hand side of (4.16) must converge to zero, that is, (4.14). This finishes the proof. ∎

5. A numerical scheme with mutation mechanism. The restricted ESD introduced in the previous section is not necessarily globally stable. The natural question is, How can one capture the asymptotic dynamics towards the global ESD from initial data not strictly positive? Motivated by the effect of mutations, our idea is to process the initial data with another scheme defined by

$$\frac{f_j^{n+1} - f_j^*}{\Delta t} = f_j^{n+1} \left(\bar{a}_j - h \sum_{i=1}^{N} \bar{b}_{ji} f_i^n \right), \tag{5.1}$$

where

$$f_j^* = \frac{f_{j-1}^n + f_{j+1}^n}{2}, \quad 2 \le j \le N-1, \tag{5.2}$$

and

$$f_1^* = \frac{f_1^n + f_2^n}{2}, \quad f_N^* = \frac{f_{N-1}^n + f_N^n}{2}. \tag{5.3}$$

Scheme (5.1), when put in the form

$$\frac{f_j^{n+1} - f_j^n}{\Delta t} = f_j^{n+1}\left(\bar{a}_j - h\sum_{i=1}^{N} \bar{b}_{ji} f_i^n\right) + \frac{h^2}{2\Delta t}\frac{f_{j+1}^n + 2f_j^n + f_{j-1}^n}{h^2}, \tag{5.4}$$

serves to better approximate the following selection-mutation model:

$$\partial_t f(t,x) = \left(a(x) - \int b(x,y) f(t,y)dy\right) f(t,x) + \epsilon^2 \partial_{xx} f(t,x), \tag{5.5}$$

where $\epsilon = \frac{h}{\sqrt{2\Delta t}}$. Note that the choices in (5.3) correspond to the natural flux $\partial_x f = 0$ on the boundary for the reaction-diffusion equation (5.5). Our hope is that we use (5.1) to spread the data, as the usual mutation does; then we return to (3.1).

In summary, for initial data not strictly positive, we follow a two-step algorithm:
Step 1. Run (5.1) up to $n = n_0$ so that $f_j^{n_0} > 0$ for all j.
Step 2. Return to (3.1) to continue the simulation.

In the multidimensional case, we follow the same strategy. That is, we replace f_α^n on the left-hand side of (4.6) by

$$f_\alpha^* = \frac{1}{2^d}\sum_{i=1}^{d}\left(f_{\alpha+e_i}^n + f_{\alpha-e_i}^n\right), \tag{5.6}$$

together with proper corrections near boundary cells, in the way of incorporating the zero flux condition on the boundary, i.e., $\partial_\nu f = 0$, where ν is the unit outward normal vector to the boundary.

Numerical validation of this two-step algorithm will be presented in sections 6.4–6.5.

6. Numerical implementation and examples.

6.1. Computing the discrete ESD. It has been shown previously that computing the ESD could be reduced to solving a quadratic programming (QP) problem, which is the problem of minimizing a quadratic function of several variables subject to linear constraints on these variables. For general QP problems a variety of methods have been proposed in the literature, including the interior-point algorithm, the trust-region algorithm, the conjugate gradient method, and the active-set algorithm (see [4, 11, 14, 15, 16, 24, 27]). We shall use the MATLAB code *quadprog.m* to implement the interior-point-convex algorithm.

We now test the case with

$$a(x) = G(x, \sigma_1), \quad b(x,y) = G(x-y, \sigma_2), \tag{6.1}$$

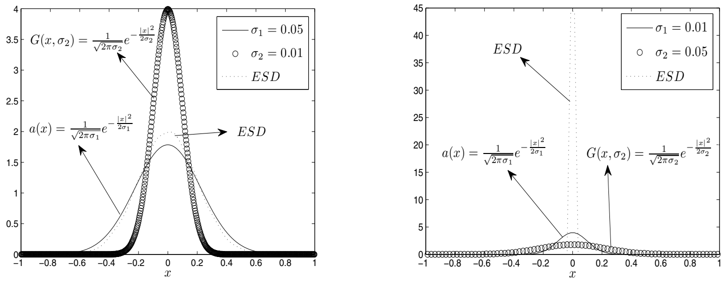

FIG. 1. *ESD profiles for data* (6.1) *on uniform meshes with* $N = 80$.

where

$$G(x,\sigma) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{x^2}{2\sigma}}.$$

This corresponds to widely used standard forms of the input parameters because of their statistical meaning. Kimura [21] was probably the first to derive a Gaussian function as an equilibrium for a structured population model. It is proved by Mirrahimi et al. [25] that for $\sigma_1 > \sigma_2$ there is a smooth steady state which is given by

$$f_{eq} = G(x,\sigma), \quad \sigma = \sigma_1 - \sigma_2.$$

For $\sigma_1 < \sigma_2$, the Dirac mass is a stable steady state. This implies that the ESD is either a Gaussian of form $G(x,\sigma)$ or a Dirac mass of form $\bar{\rho}\delta(x)$. This is numerically confirmed by using the quadratic programming algorithm as stated above.

We use a 3-point Gaussian quadrature rule to generate the discrete data $\bar{a}_j$ and $\bar{b}_{ji}$.

The numerical results are shown in Figure 1, which indicates that the ESD is a Gaussian function for $\sigma_1 = 0.05 > \sigma_2 = 0.01$ but a Dirac mass concentrating on 0 for $\sigma_1 = 0.01 < \sigma_2 = 0.05$. These are in excellent agreement with the theoretical results in [25, Proposition 3.1].

6.2. One-dimensional tests with positive initial data. This section presents several numerical tests to illustrate both the accuracy and the capability of the scheme (3.1).

Recall that the positivity of b in (2.2) when $b(x,y) = K(x-y)$ is equivalent to the positivity of the Fourier transform of K; see [20, page 502]. In addition to the Gaussian kernel, we also use $K = \frac{1}{1+x^2}$. In fact, with a simple calculation using the Cauchy integral formula in the complex plane, one obtains

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{e^{-ix\xi}}{1+x^2} dx = \sqrt{\frac{\pi}{2}} e^{-|\xi|} > 0.$$

Therefore, the b used in (6.2), (6.5), and (6.7) satisfies the positivity condition (2.2) as required.

Example 1 (accuracy and entropy test). Following the setting used in [22], we consider

$$a(x) = 10(x-1)^2(x-0.1005)^2(x+1)^2, \quad b(x,y) = \frac{1}{1+(40(x-y))^2}, \tag{6.2}$$

TABLE 1
Errors and the convergence orders of the numerical solution on uniform meshes of N cells.

	$f_0(x) = 0.5(sin(100x) + 2)$			
N	L^∞ error	order	L^1 error	order
40	3.8705	-	1.4926	-
80	3.2206	0.2652	0.9241	0.6917
160	1.7710	0.8627	0.4799	0.9453
320	0.8569	1.0475	0.2422	0.9868
640	0.3685	1.2173	0.1205	1.0073

TABLE 2
The change of the relative entropy (3.2) *with* $N = 80$ *and* $\Delta t = 0.01$.

T	0	5	10	50	200	400
F^n	41.2743379	0.9227154	0.3781511	0.0493885	0.0048953	9.0692435e-004

which when combined with the 3-point Gaussian quadrature rule gives the needed discrete data, $\bar{a}_j$ and $\bar{b}_{ji}$. For initial data given by

$$f_0(x) = 0.5(\sin(100x) + 2), \tag{6.3}$$

the initialization is by its cell average,

$$f_j^0 = \frac{1}{h}\int_{I_j} f_0(x)dx, \quad j = 1, \dots, N.$$

This evaluation is also carried out by the 3-point Gaussian quadrature rule. Let f_j^n denote the numerical solution with N cells, and let $\tilde{f}_i^n$ denote the reference solution with mN cells. The L^∞ error and the L^1 error are defined as

$$\max_{1\le j\le N}\max_{1\le l\le m} \mid f_j^n - \tilde{f}^n_{m(j-1)+l} \mid, \quad \sum_{j=1}^{N}\sum_{l=1}^{m} \mid f_j^n - \tilde{f}^n_{m(j-1)+l} \mid \frac{h}{m},$$

respectively. In our simulation, the numerical solution of 2560 cells is taken as the reference solution. Let the final time $T = n\Delta t$; the accuracy of numerical scheme (3.1) at $T = 1.0$ with time step $\Delta t = 0.01$ is given in Table 1, which confirms first-order accuracy. Here the choice of Δt may be determined according to the bound in Theorem 3.1. Actually, Δt can be taken slightly larger as long as time-asymptotic convergence is obtained. Table 2 gives the temporal change of the relative entropy (3.2). This entropy dissipation illustrates that numerical solutions with data (6.2) and initial data (6.3) converge to the ESD as time becomes large.

Example 2 (large time behavior with positive $a(x)$). In addition to initial data (6.3), we also test with another positive initial data of the form

$$f_0(x) = \begin{cases} 2(\cos(2\pi(x-0.1)) + 1) + 0.5, & |x - 0.1| \le 0.03, \\ 0.5 & \text{else.} \end{cases} \tag{6.4}$$

The comparison of the time-asymptotic trend to the ESD is shown in Figure 2. Clearly, the asymptotic convergence is faster with initial data (6.4), which is less oscillatory.

Example 3 (large time behavior with Gaussian data (6.1)). For a, b given in (6.1), we test the time-asymptotic convergence to equilibrium with random initial data. The results given in Figure 3 are as expected, modulo a rather slow convergence for the

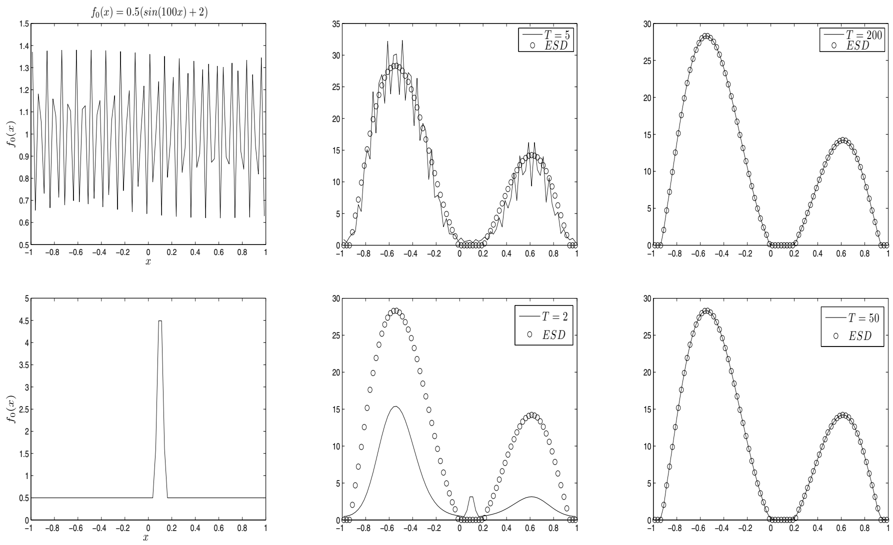

Fig. 2. *Numerical solutions to* (3.1) *converge to the ESD for data* (6.2) *with* $N = 80$ *and* $\Delta t = 0.01$*, the first row: for initial data* (6.3)*; the second row: for initial data* (6.4)*.*

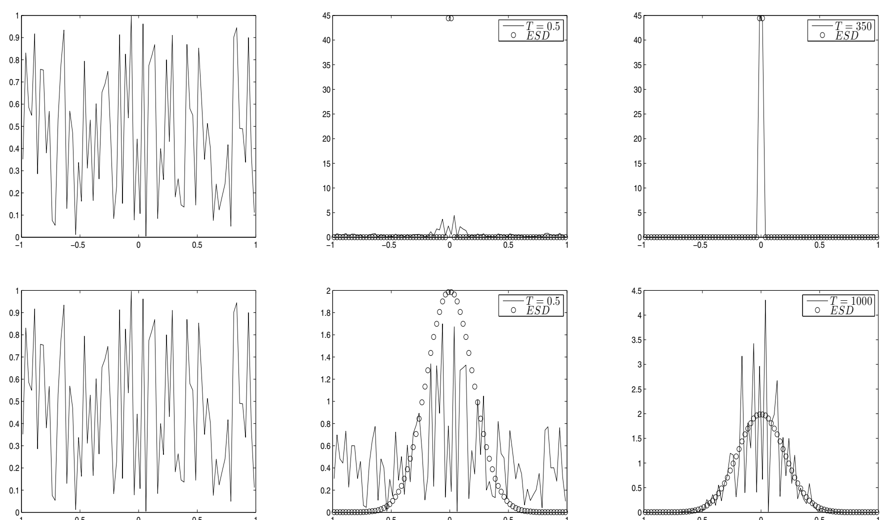

Fig. 3. *Numerical solutions to* (3.1) *converge to the ESD,* $N = 80$*, and* $\Delta t = 0.01$*, the first row:* $\sigma_1 = 0.01 < \sigma_2 = 0.05$*; the second row:* $\sigma_1 = 0.05 > \sigma_2 = 0.01$*.*

case of $\sigma_1 > \sigma_2$. Indeed, in [20, Proposition 1.7] the authors proved the convergence rate of $\frac{logt}{t}$ for some a, b including (6.1) with $\sigma_1 > \sigma_2$.

Example 4 (large time behavior with data (6.5)). We consider a, b of the form

$$a(x) = A - x^2, \quad b(x, y) = \frac{1}{1 + (x - y)^2}. \tag{6.5}$$

This choice was investigated in [13] to illustrate both the speciation process and the branching phenomena, depending on the range of A.

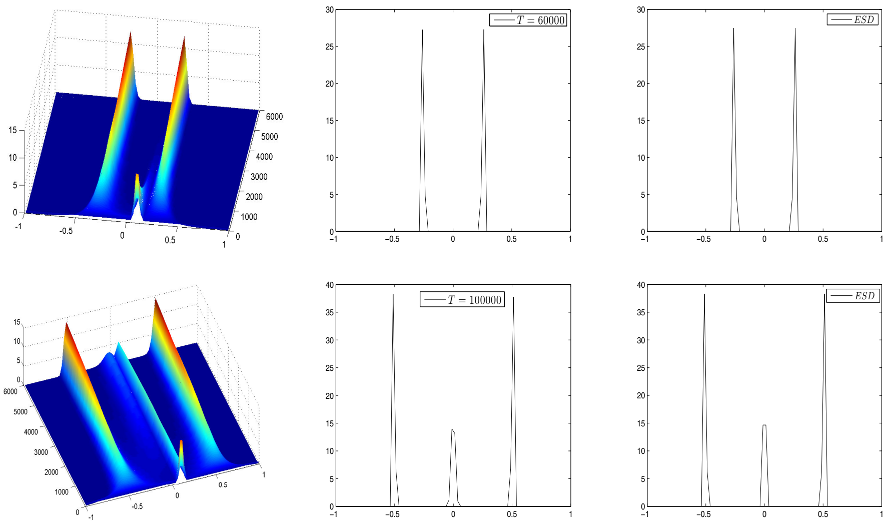

FIG. 4. *Numerical solutions to* (3.1) *tend to the ESD,* $N = 80$, *and* $\Delta t = 0.05$. *The first row: for* $A = 1.5$, $T \in [0, 6000]$ *(left);* $T = 60000$ *(middle); ESD (right). The second row: for* $A = 2.5$, $T \in [0, 6000]$ *(left);* $T = 100000$ *(middle); ESD (right).*

The numerical results with initial data (6.4) show that the initial data branch into two subspecies for $A = 1.5$. When $A = 2.5$, the initial data first branch into two subspecies, and subsequently a new trait appears in the middle which is not induced from any branching. We can also see from Figure 4 that numerical solutions tend to the ESD after sufficiently long time simulation. These results, which may be interpreted as a "speciation process," are in excellent agreement with the theoretical and numerical results obtained in [13].

Example 5 (large time behavior with a general fitness). In this example we consider a general a of changing sign and Gaussian function b as follows:

$$a(x) = 20(x-1)^2(x-0.1005)^2(x+1)^2 - 1, \quad b(x, y) = G(x-y, 0.05). \tag{6.6}$$

The time-asymptotic behavior with random initial data is illustrated in Figure 5, from which we see that the ESD is always zero at points where $a(x) \le 0$, and the numerical solutions asymptotically tend to the ESD, which is the sum of the finite Dirac masses. This indicates the concentration of subpopulations.

6.3. Two-dimensional tests with positive initial data. For $1 \le \alpha_i \le N$ and $1 \le \beta_i \le N$ $(i = 1, 2)$, we relabel the index $\alpha = (\alpha_1, \alpha_2)$ and $\beta = (\beta_1, \beta_2)$ as $j = (\alpha_1 - 1)N + \alpha_2$ and $i = (\beta_1 - 1)N + \beta_2$ so that the coefficients are calculated by

$$\bar{a}_j = \frac{1}{2^2} \sum_{l=1}^{3} \sum_{p=1}^{3} \omega_l \omega_p a(x_{\alpha_1} + 0.5hc_l, x_{\alpha_2} + 0.5hc_p),$$

$$\bar{b}_{ji} = \frac{1}{2^4} \sum_{l_1, l_2, l_3, l_4 = 1}^{3} \omega_{l_1} \omega_{l_2} \omega_{l_3} \omega_{l_4} b(x_{\alpha_1} + 0.5hc_{l_1}, x_{\alpha_2} + 0.5hc_{l_2}, y_{\beta_1}$$
$$+0.5hc_{l_3}, y_{\beta_2} + 0.5hc_{l_4}),$$

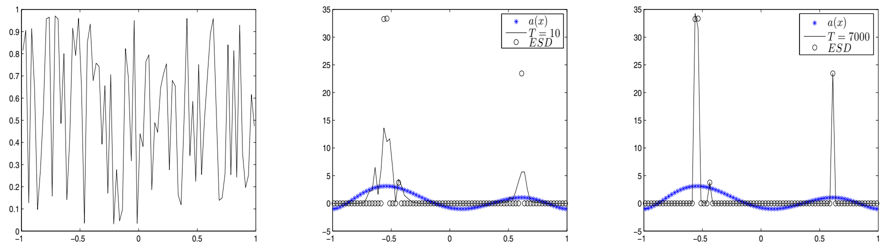

FIG. 5. *Random initial data (left); the ESD and numerical solutions to* (3.1) *at* $T = 10$ *and* $T = 7000$*, with* $N = 80$ *and* $\Delta t = 0.01$.

and the initial data is similarly generated from the cell average,

$$f_j^0 = \frac{1}{2^2}\sum_{l=1}^{3}\sum_{p=1}^{3}\omega_l\omega_p f_0(x_{\alpha_1} + 0.5hc_l, x_{\alpha_2} + 0.5hc_p),$$

such that $(\bar{a})_{N^d\times 1}$ and $(f^0)_{N^d\times 1}$ are column vectors, and $(\bar{b})_{N^d\times N^d}$ is a matrix. Here ω_l and c_l $(l = 1, 2, 3)$ are the weights and abscissae of 3-point Gaussian quadrature rule, respectively.

For $b(x, y)$ of the form

$$b(x, y) = \frac{1}{1 + (x_1 - y_1)^2 + (x_2 - y_2)^2}, \tag{6.7}$$

we test the time-asymptotic convergence to the ESD for different $a(x)$, which is shown in Figures 6–7.

We first consider

$$a(x) = 2.5 - ((x_1)^2 + (x_2)^2), \tag{6.8}$$

which is positive for all $x \in [-1, 1]^2$. For random initial data, we compute numerical solutions to scheme (4.6) and observe the time-asymptotic trend to the ESD, which is the sum of finite Dirac masses.

We then consider

$$a(x) = (x_1)^2 - (x_2)^2, \tag{6.9}$$

which is a saddle surface, and $a(x) < 0$ for some $x \in [-1, 1]^2$. For coefficients (6.7) and (6.9), we test numerical solutions with random initial data and the ESD in Figure 7, which shows time-asymptotic trend to the ESD, which concentrates on $(1, 0)$ and $(-1, 0)$ where a is peaked.

6.4. One-dimensional tests with nonnegative initial data. For data (6.2) and nonnegative δ-like initial data,

$$f_0(x) = \begin{cases} 2(\cos(2\pi(x - 0.1)) + 1), & |x - 0.1| \le 0.03, \\ 0 & \text{else.} \end{cases} \tag{6.10}$$

If we use only scheme (3.1), numerical solutions will tend to the restricted ESD, instead of the global ESD; see Figure 8.

In order to observe the time-asymptotic convergence to the global ESD with initial data which is not strictly positive, we first use scheme (5.1) and then use scheme (3.1) to simulate this process. It can be seen from Figure 9 that numerical solutions with initial data (6.10) tend to the ESD. Here we choose $n_0 = 400$.

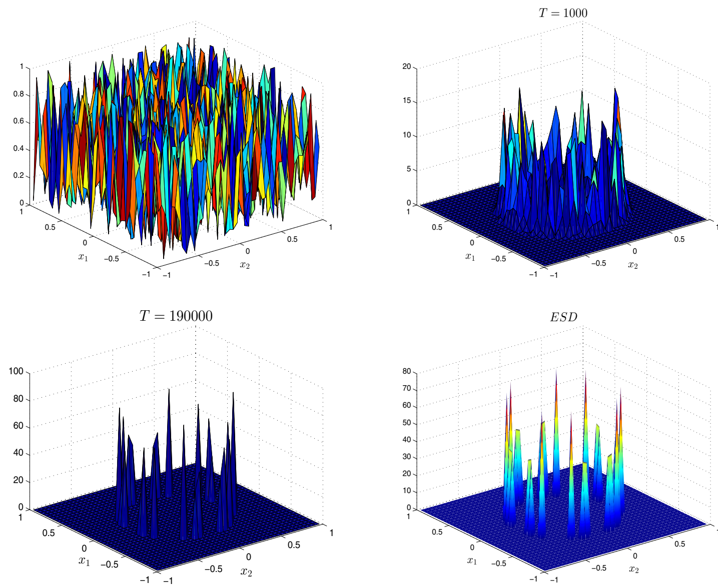

FIG. 6. *Numerical solutions to* (4.6) *with random initial data at* $T = 1000$ *and* $T = 190000$*, as well as the ESD,* $N = 40$*, and* $\Delta t = 0.05$.

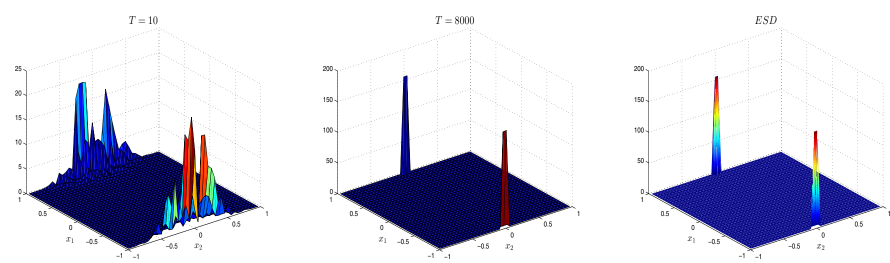

FIG. 7. *Numerical solutions to* (4.6) *until* $T = 8000$ *and the ESD,* $N = 40$*, and* $\Delta t = 0.05$.

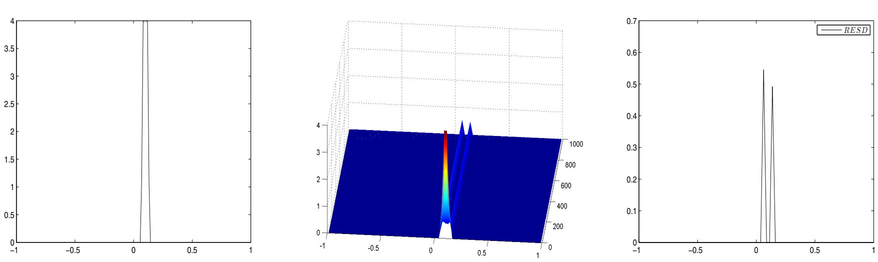

FIG. 8. *Initial data* (6.10) *(left); numerical solutions to* (3.1) *for* $0 \leq T \leq 1000$ *with* $N = 80$ *and* $\Delta t = 0.01$ *(middle); the restricted ESD (right).*

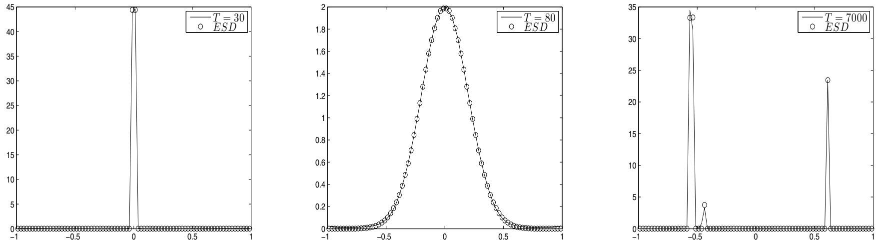

FIG. 9. *Numerical solutions and ESD with* $N = 80$ *and* $\Delta t = 0.01$*, for data* (6.1) *with* $\sigma_1 = 0.01 < \sigma_2 = 0.05$ *(left); for data* (6.1) *with* $\sigma_1 = 0.05 > \sigma_2 = 0.01$ *(middle); for data* (6.6)*(right).*

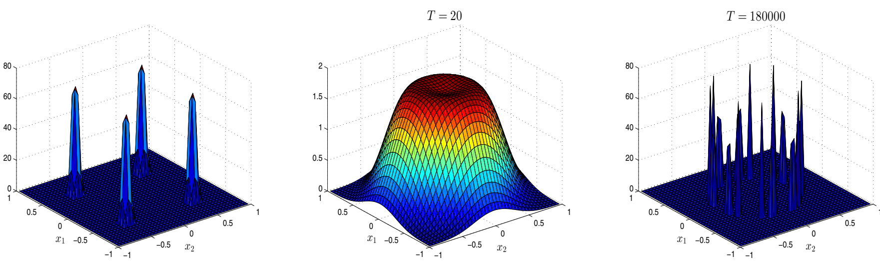

FIG. 10. *Numerical solutions at* $T = 0, 20$ *and* $T = 180000$*,* $N = 40$*, and* $\Delta t = 0.05$*.*

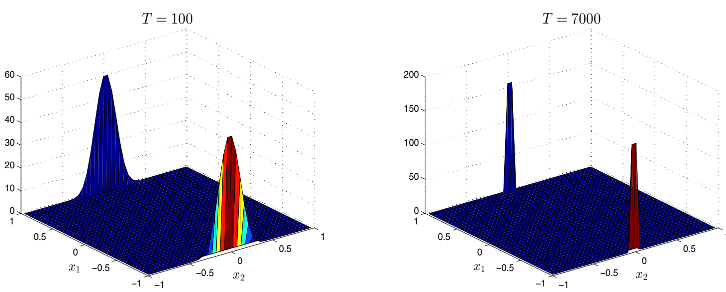

FIG. 11. *Numerical solutions at* $T = 100$ *and* $T = 7000$*,* $N = 40$*, and* $\Delta t = 0.05$*.*

6.5. Two-dimensional tests with nonnegative initial data. We consider the δ-like initial data concentrating at four points:

(6.11)
$$f_0(x) = \begin{cases} 25g(x_1)g(x_2) \text{ in four squares centered at } (\pm 0.5, \pm 0.5) \text{ of area } 0.01; \\ 0 \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{elsewhere,} \end{cases}$$

where $g(s) = -\cos(10\pi s) + 1$. We test by using scheme (5.6) until $n_0 = 200$, followed by (4.6) for two cases. First, for coefficients (6.7) and (6.8), the asymptotic trend to the ESD is shown in Figure 10.

The test for coefficients (6.7) and (6.9) is given in Figure 11.

7. Summary. In this work, we have developed entropy satisfying numerical schemes for solving a nonlocal competition model that describes the evolution of a population structured with respect to a continuous trait. The schemes are easy to implement and feature two desired properties: positivity preserving and entropy satisfying. Some highlights are the following are the following:

- It is shown that finding the discrete ESD is equivalent to solving a QP problem.
- With the ESD on the restricted set of computational cells where the initial data are positive, the relative entropy is well defined and further used to prove that numerical solutions to the fully discrete scheme asymptotically converge to the ESD as n becomes large.
- In order to capture the global ESD for general nonnegative initial data, we adopt a two-step algorithm, which in the first step the initial data is processed by a modified scheme, which contains a certain mutation mechanism.

A series of numerical results have confirmed both the accuracy and the entropy satisfying property of the numerical schemes. The obtained numerical results are compatible either in the case when a uniform trait distribution is produced by the model or when concentrations are obtained. It is usually difficult to predict between these two alternatives. The simple numerical schemes presented in this work may be useful in the model prediction.

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