Pattern formation and coexistence domains for a nonlocal population dynamics

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In this Rapid Communication we propose a most general equation to study pattern formation for one-species populations and their limit domains in systems of length L. To accomplish this, we include nonlocality in the growth and competition terms, where the integral kernels now depend on characteristic length parameters α and β. Therefore, we derived a parameter space (α,β) where it is possible to analyze a coexistence curve $\alpha^* = \alpha^*(\beta)$ that delimits domains for the existence (or absence) of pattern formation in population dynamics systems. We show that this curve is analogous to the coexistence curve in classical thermodynamics and critical phenomena physics. We have successfully compared this model with experimental data for diffusion of *Escherichia coli* populations.

Introduction. In recent years the phenomenon of pattern formation has been intensively studied to describe the spatial distribution of species in population dynamics. This amazing behavior of populations, observed under certain conditions, can be modeled by nonlinear equations of reaction and diffusion types [1–7]. Such mathematical models provide a rich structure that includes a variety of intra- or interspecific interactions among species [8,9], and they allow us to describe many forms of effects of dispersal with or without memory effects [10–12].

However, the overwhelming majority of the studies has shown that Fickian-type diffusion [13–15] is unable to describe spreading of species in population equations formulated through reaction-diffusion models. Moreover, this is not the only possible criticism that one can find in the ordinary nonlinear reaction-diffusion approach. In a population dynamics context, it is commonly believed that there is no real justification for assuming that interactions among species are, in fact, local. There are many models in which such an assumption clearly becomes unwarrantable, for example, in the competition of one species in a habitat where the system is rapidly equilibrated or in typical biological interactions where the individuals intercommunicate via chemical means. Of course, these are typical nonlocal effects that should not be overlooked. Other forms of nonlocal growth and interaction effects have also been observed when dealing with a wide variety of biological fields, such as epidemic spread in a network [16–18], embryological development, and bacterial growth [19], where the density of individuals involved is not small and the analysis of local or short-range diffusive flux is not sufficiently accurate to understand the dynamical aspects of these phenomena. In these cases we need to include the contribution of long-range effects and then to analyze the domain limits for the existence of patterns in these systems.

This Rapid Communication is an attempt to build a most general equation to study the effects of pattern formation

in one-species population dynamics. Our starting point is to write an equation that includes nonlocal growth and interaction terms involving long-range effects in the system. This equation can be written as

$$\frac{\partial u(x,t)}{\partial t} = a \int_{\Omega} g_{\alpha}(x - x')u(x',t)\, dx'$$
$$- bu(x,t) \int_{\Omega} f_{\beta}(x - x')u(x',t)\, dx', \quad (1)$$

where $u(x,t)$ describes the population density with growth a and competition b terms. Then we denote by $g_{\alpha}(x - x')$ the correlation growth function, which weights the growth of a population in the domain Ω for a specific growth length parameter α. We call $f_{\beta}(x - x')$ the correlation competition function, which weights the interaction among the constituents of the population for a competition length parameter β in the domain Ω. In order to modeling population dynamics, we have assumed that the kernels are symmetric functions, such that $f_{\beta} \to 0$ and $g_{\alpha} \to 0$ as $|x - x'| \to \infty$. An advantage of Eq. (1) is that it provides a useful concept for describing a great variety of long-range diffusive effects in physical systems by allowing all higher derivatives (diffusion and dissipation terms) to be absorbed in only the integral term. Moreover, this model is then parametrized mainly by α and β quantities, which allows us to theorize on the existence of values (α,β) for which there are pattern formation. Indeed, the relation between these length domains offers the simplest model for dealing with quantitative estimates of experimental data related to the growth dynamics of bacteria, for example. In this case, specific domains that show the existence (or absence) of pattern formation, which incorporates long-range effects as well, are important for the physical description of the spreading of individuals with nonlocal dynamics.

Starting from Eq. (1), we can derive important connections with classical population models by carrying out appropriate limits. For example, if $f_{\beta}(x - x') = g_{\alpha}(x - x') = \delta(x - x')$, we get the logistic equation [15]

$$\frac{\partial u(x,t)}{\partial t} = au(x,t) - bu(x,t)^2. \quad (2)$$

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We can also consider $g_\alpha(x - x')$ with a finite range, such that we can expand the growth term as

$$a \int_\Omega g_\alpha(x - x') u(x',t)\, dx' = \sum_{m=0}^\infty \frac{a \overline{y^{2m}}}{(2m)!} \frac{\partial^{2m}}{\partial x^{2m}} u(x,t), \quad (3)$$

where $y = x - x'$ and the k moments are

$$\overline{y^k} = \int y^k g_\alpha(y)\, dy. \quad (4)$$

Using this procedure with $f_\beta(y) = \delta(y)$ and retaining the first two terms in Eq. (3), we get the ordinary Fisher equation:

$$\frac{\partial u(x,t)}{\partial t} = D \frac{\partial^2 u(x,t)}{\partial x^2} + au(x,t) - bu^2(x,t). \quad (5)$$

Here we show a very important point: The first gain with the nonlocal growth term is the possibility of connecting the growth rate a with the diffusion constant

$$D = \frac{a \overline{y^2}}{2}. \quad (6)$$

Note that this equation shows that a species with a large growth rate has "more need" for diffuse behavior; that is, a large growth rate creates a large pressure proportional to the concentration gradient $D \frac{\partial}{\partial x} u(x,t)$, which increases the diffusion. It shows that the diffusion is intrinsically related to the existence of the nonlocal growth term g_α; that is, it is necessary for a second moment $\overline{y^2} \neq 0$ to exist according to Eq. (4).

The higher-order terms ($m > 1$) in the expansion of Eq. (3) yield the dispersive terms. It is interesting to note that if g_α is not even, the first derivative yields the convective term $v \frac{\partial}{\partial x} u(x,t)$, from which we can obtain the convective velocity as $v = \overline{y} a$. On the other hand, if we have an asymmetric g_α, it corresponds to a convective drift [20]. If we keep the expansion up to second order and $f_\beta(y)$ in the second integral, we get nonlocal Fisher equation:

$$\frac{\partial u(x,t)}{\partial t} = au(x,t) + D \frac{\partial^2 u(x,t)}{\partial x^2}$$
$$- bu(x,t) \int_\Omega f(x - x') u(x,t)\, dx, \quad (7)$$

which has been widely used by many authors to discuss pattern [9]. Note that Eq. (1) is the most general, incorporating all the previous equations.

Perturbative analysis. In the study of pattern formation through a model of population dynamics, it is usual to calculate a quantity known as the growth rate of pattern γ [9,10] that leads to the pattern formation in the system. Therefore, we first shall start with the perturbative analysis through the function

$$u(x,t) = \frac{a}{b} + \epsilon \exp(ikx + \phi(k)t), \quad (8)$$

where a/b is the homogeneous steady-state solution, constant in space and time. The term $\epsilon \exp(ikx) \exp(\phi t)$ is a perturbation to the steady state that will grow or die out, depending on the values of the wave numbers k. Substituting Eq. (8) into Eq. (1) and retaining only the first-order perturbative terms, we find a dispersion relation between the complex pattern growth

rate ϕ and the wave number k, given by

$$\phi(k) = a(\mathcal{F}_c\{g_\alpha(y)\} - \mathcal{F}_c\{f_\beta(y)\})$$
$$+ ia(\mathcal{F}_s\{g_\alpha(y)\} - \mathcal{F}_s\{f_\beta(y)\}), \quad (9)$$

where $\mathcal{F}_c\{\cdot\}$ and $\mathcal{F}_s\{\cdot\}$ are, respectively, the Fourier cosine and sine transforms of the influence functions $g_\alpha(y)$ and $f_\beta(y)$ (assumed to be even). Therefore, only the real part of the complex growth rate $\phi(k) = \gamma(k) + i\xi(k)$, where $\gamma(k) = a[\int_\Omega g_\alpha(y) \cos(ky) dy - \int_\Omega f_\beta(y) \cos(ky) dy - 1]$, i.e., the growth rate of pattern $\gamma(k)$, will be important to determine whether the perturbation with wave number k will die out or will generate a pattern for negative or positive values, respectively. Now, let us consider the simple case of the square interaction influence function given by

$$f_\beta(y) = \frac{1}{2\beta} [\Theta(\beta - y) \Theta(\beta + y)], \quad (10)$$

where Θ refers to the Heaviside function and β is the cutoff range ($0 < \beta < L$, where L is the size of the system). If we consider a similar relation for g_α with cutoff $0 < \alpha < L$, from condition (10), $\gamma(k)$ is given by

$$\gamma(k) = a \left(\frac{\sin(k\alpha)}{k\alpha} - \frac{\sin(k\beta)}{k\beta} - 1 \right). \quad (11)$$

Therefore, we can study self-organization of Eq. (1) considering that the system depends physically on the domain of the functions g_α and f_β. In this case, pattern formation appears when wave numbers k, in the growth rate of pattern, obey the condition $\gamma(k) > 0$. Note that for $\alpha = 0$, $\gamma(k)$ is larger. This will happen for less-diffusive systems with $D \approx 0$.

Equation (11) is plotted in Fig. 1 for different values of the growth length $\alpha = (0.01, 0.03, 0.09, 0.40)$ with competition length parameter $\beta = 0.45$ fixed. In Fig. 1, we verified that when $\alpha < \beta$, we have $\gamma(k) > 0$. If $\alpha \to \beta$, the function $\gamma(k)$ becomes negative. This behavior of $\gamma(k)$ is very important for determining if we have a large or a negligible amplitude of pattern. We show in Fig. 1 that pattern formation appears for values of $\alpha < \beta$ with $\gamma(k) > 0$. This behavior is also verified
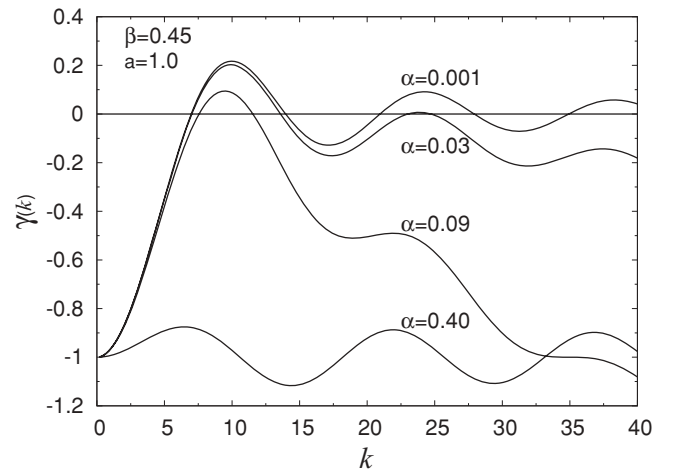

FIG. 1. The real part of growth exponent $\gamma(k)$ as a function of k plotted for different values of the correlation length of growth α with the length interaction of individuals β fixed. The pattern formation appears for those values of k for which γ is positive.

later with numerical results (see Fig. 4) and discussed through experimental values.

Numerical method. To solve Eq. (1) numerically, we applied the operator-splitting method (OSM) [21]. By this method, the operator of a differential equation is split into several parts, which act additively on $u(x,t)$. If we write Eq. (1) as

$$\frac{\partial u(x,t)}{\partial t} = \hat{T}u(x,t), \tag{12}$$

where $\hat{T}$ is the total operator, then

$$\hat{T}u(x,t) = \hat{T}_{\text{grow}}u(x,t) + \hat{T}_{\text{int}}u(x,t), \tag{13}$$

with

$$\hat{T}_{\text{grow}}u(x,t) = a \int_{\Omega} g_{\alpha}(x-x')u(x',t)\,dx' \tag{14}$$

$$\hat{T}_{\text{int}}u(x,t) = -bu(x,t) \int_{\Omega} f_{\beta}(x-x')u(x',t)\,dx'. \tag{15}$$

In Eqs. (14) and (15), $\hat{T}_{\text{grow}}$ and $\hat{T}_{\text{int}}$ are nonlocal growth and nonlocal interaction operators, respectively. In our numerical calculations, we have used periodic boundary conditions $u(x=0,t) = u(x=L,t)$ with spatial period L. For each part of the operator, we apply a known difference scheme for updating the function $u(x,t)$ from step j to step $j+1$.

In Fig. 2 we show the evolution of $u(x,t)$. We start with a distribution of individuals

$$u(x,0) = \frac{1}{\Gamma} \exp\left[-\frac{(x-x_0)^2}{2\sigma^2}\right], \tag{16}$$

where $\Gamma = \sqrt{\frac{\pi}{2}}\sigma[\text{erf}(\frac{x_0}{\sqrt{2}\sigma}) + \text{erf}(\frac{L-x_0}{\sqrt{2}\sigma})]$, and we see the evolution to a state that exhibits pattern. We use $\sigma = 0.3$, $x_0 = 0.5$, and $L = 1.0$. The spatial and time increments are $\delta x = 1 \times 10^{-3}$ and $\delta t = 1 \times 10^{-2}$, respectively. In all simulations we use $a = b = 1.0$. Several numerical experiments show the final state independent of the initial conditions [20]. These simulations are fundamental to showing the pattern formation that appears after a long time of bacterial growth [8–11,22]. Similar simulations are used to compose Figs. 3 and 4.

In Fig. 3, we show the evolution after 60000 time steps, when the density has reached its final form. Each curve

FIG. 3. Snapshots of the stationary state $u(x)$ for several values of the competition length parameter β and growth length parameter α with the correlation competition function and correlation growth function in Eq. (10). Here we consider the growth rate a and competition rate b to be 1.0. For a fixed β, as α increases, the pattern disappears.

is similar to the simulations described in Fig. 2. The left column of Fig. 3 shows $\beta = 0.07$ for (from top to bottom) $\alpha = (0.009, 0.012, 0.019)$. The right column shows $\beta = 0.11$ for (from top to bottom) $\alpha = (0.012, 0.020, 0.030)$. For each β the lower curve represents the height value of α, for which there is no longer pattern formation, i.e., for $\alpha \geqslant \alpha^*$, where we get $u(x,t) = a/b$.

FIG. 4. The phase diagram of tje critical correlation growth length α_c as a function of the critical competition length parameter β_c. The "Pattern" and "No Pattern" regions indicate the separation of large-amplitude patterns and negligible-amplitude patterns for Eq. (16).
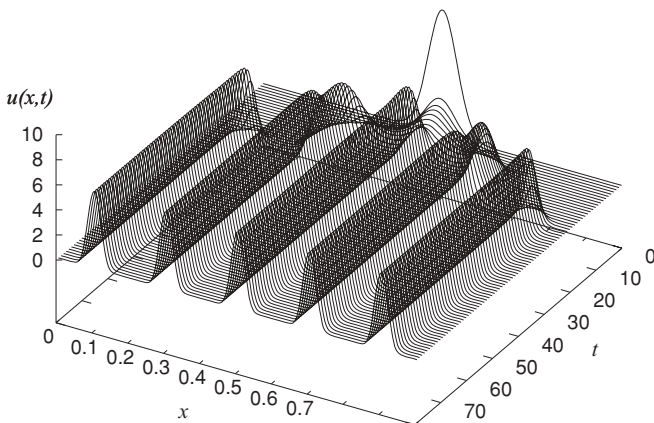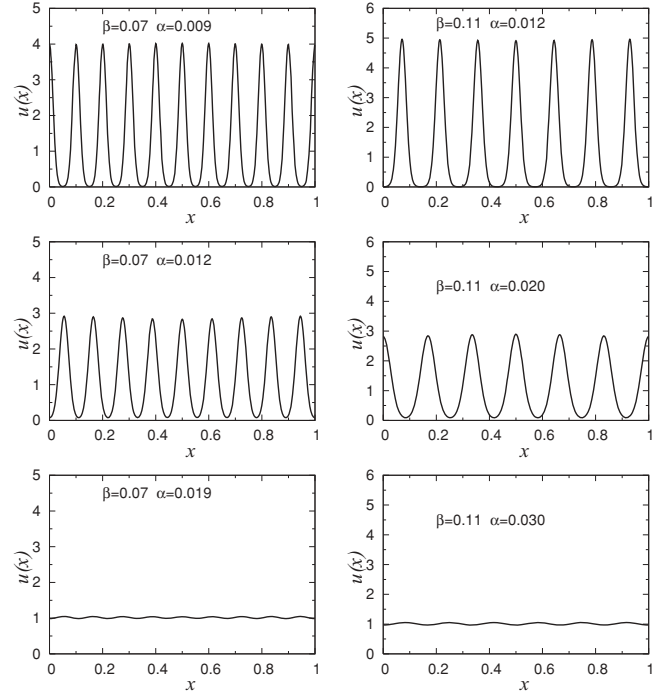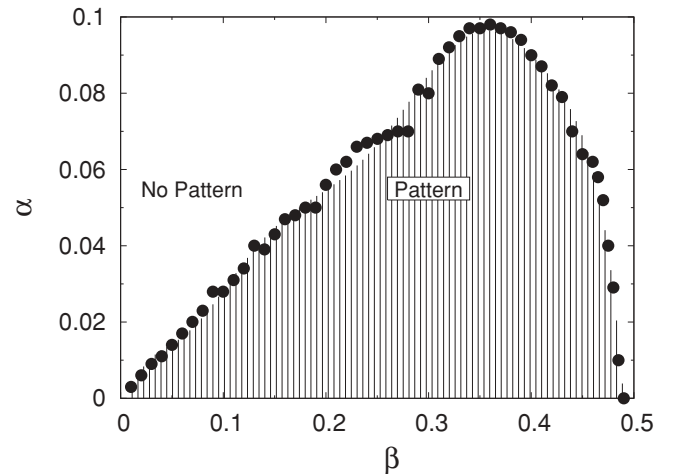

FIG. 2. The typical pattern formation on density $u(x,t)$ as a function of x and t in arbitrary units. The growth rate and interaction rate are $a = b = 1.0$. The competition length parameter $\beta = 0.15$, and the growth length parameter $\alpha = 0.009$.

In Fig. 4, we show the region in the space (α, β) where pattern can exist. For each β the points represent the α^* above which there is no longer pattern, such as described in Fig. 3. The shaded area is limited by the coexistence curve

$$\alpha^*(\beta) = P(\beta)(\beta_c - \beta)^\mu, \qquad (17)$$

which is the best fit of the points. $P(\beta)$ is a polynomial with no roots in the region $0 < \beta < \beta_c$. For $\beta \to \beta_c$ we get from Eq. (10) $\beta_c = 1/2$, i.e., the function $f_\beta(y)$ weights equally the whole space $0 < x < L$, and consequently, we have no pattern formation for $\beta \geqslant \beta_c$. Finally, from the data we have estimated the value $\mu = 0.53 \pm 0.06$ at the vicinity of β_c for the exponent in Eq. (17).

Experimental data. Starting from Eq. (10), we can compute $\overline{y^2} = \alpha^2/3$. By inserting this result into Eq. (6) we get

$$\alpha = \sqrt{\frac{6D}{a}}. \qquad (18)$$

Now, using the experimental values for $a = (2.23 \pm 0.2) \times 10^{-4} \mathrm{s}^{-1}$ and $D = (2.2 \pm 0.2) \times 10^{-5}$ cm^2 s^{-1} obtained by Perry [22], for systems with *Escherichia coli* populations, we can estimate the value of α, given by $\alpha = (7.70 \pm 0.09)$ mm. Then, to form pattern in a finite system of length L, β must be inside the shaded area in Fig. 4. In fact, the value of α as obtained in Eq. (18) is determined by the coefficient of diffusion D of the system, and it establishes a lower referential limit for the presence (or absence) of pattern formation. For $\beta \ll L$, we are in the linear part of Eq. (17), and we get $\alpha = 0.3\beta$; therefore, we have pattern for $\beta > 25.4$ m. In this case, only experimental values of the width of the influence function $\beta > 25.4$ mm permit patterns, which are in concordance with our theoretical and numerical results. Moreover, our formulation allows us to analyze pattern formation as an interplay between two length parameters α

and β. It is important to note that the fact that $0 < \alpha < \beta$ is not just a curiosity of the theory, it is one of its major results. Without a finite value of α, there will be no diffusion, which is fundamental for any species, and so reproduction and propagation are associated. Consequently, one should expect a non-null α. On the other hand, if α is too large, bonds are tight, and they may be difficult to meet and, consequently, to reproduce. The phenomenon described here for pattern formation in a bacterial colony can be observed in large animals with migratory habits, such as deer and wolves, who only travel with family; we call this phenomenon the *faithful sailor travel*.

Conclusion. The presence of memory and nonlocality in time have been used to explain ergodicity violation in particle diffusion [23,24]. Since pattern formation implies ergodicity breaking, one could expect that a nonlocal space kernel would yield that. Consequently, we proposed here a new formulation for population dynamics that includes growth and competitive nonlocal terms. The presence of two kernels $g_\alpha(x)$ and $f_\beta(x)$ demands the existence of a growth length parameter α and a competition parameter β. Particular values for the kernels yield most of the previous formulations of population dynamics. We obtain a domain region $0 < \alpha < \beta$ where patterns may arise, a coexistence curve similar to those in phase transition, and a direct connection between the diffusion constant D, the growth rate a, and the mean-square deviation $\overline{y^2} = \int f_\alpha(y)y^2 dy$, which is a function of α. More results can be obtained from this formulation; however, there are some restrictions, and we need more-detailed dynamical experiments in growth so that we can propose more-elaborate kernels. Those presented here in Eq. (4) give us a rough idea of the dynamics. More-accurate $g_\alpha(x)$ and $f_\beta(x)$ will permit us to get a better description and a generalization for two dimensions.

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