Final paper outline

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Introduction

Reaction-diffusion models are a type of partial differential equation (PDE) that have long been used by ecologists to analyze the migration and population dynamics of invasive species (Cosner, 2008). Recent work has led to innumerable modifications on the original formulations by Fisher (1937) and Skellam (1951). Beyond the fundamental processes of growth and spread, extensions of reaction-diffusion models can be applied to age- and size-structured populations (Neubert and Caswell, 2000), and incorporate environmental heterogeneity, interspecies interactions (competition, predation, mutualism, etc.), Allee effects, invasion control efforts, and long-distance dispersal. For an introduction to the use of PDEs to represent dispersal in a population ecology context, the reader is directed to Holmes et al. (1994) and the seminal papers referenced therein. For an accessible review of recent advancements in modeling invasion using reaction-diffusion equations and integro-difference equations, see Hastings et al. (2005); for a comprehensive treatment, see the textbooks by Shigesada and Kawasaki (1997) or Lewis et al. (2016).

Here, we use a simple two-dimensional reaction-diffusion model to represent the spread of the invasive ascidian *Botrylloides violaceus* in the Gulf of Maine. Colonial tunicates (or ascidians) are compound organisms formed by a mass of small zooids organized within a common gelatinous matrix. These colonies often form visible crusts on rocks, vessel hulls, and other artificial floating structures and submerged objects. Colonial tunicates also commonly grow on macroalgae and bivalves such as shellfish and oysters, making them a nuisance for the low-trophic aquaculture industry.

In New England, economic impacts from biofouling are estimated to be NUMBER. Add additional background about impact of *Botrylloides violaceus* on kelp and oyster aquaculture in the GOM here.

Botrylloides violaceus has a complex life cycle, including a cyclical growth pattern dependent on both sexual and asexual reproduction. The growth and reproduction of colonial tunicates can be highly variable based on a number of environmental factors, including food availability, temperature, salinity, sediment load, and water pollution (Carver et al., 2006). The microscale mechanisms behind tunicate dispersion are therefore very complicated, and a fully-resolved spatiotemporal model of *B. violaceus* spread would need also to incorporate local hydrodynamic conditions, human-mediated transport, competition, and predation.

However, simple reaction-diffusion models can accurately capture population spread without replying on many assumptions and often unknown information about organism-level behavior. The value of these models is derived from their tremendous utility in ecological applications, despite abstracting many biological details (Andow et al., 1990). By eliminating unnecessary complexity and noise, simple reaction-diffusion models present a tangible method of connecting the mathematical theory of partial differential equations to observed data on invasive species, with implications for real-world ecological and economic problems.

Model Development & Theory

Here, we follow the derivation method of Lewis et al. (2016) to justify our use of the following equation to represent the rate of spread of *B. violaceus*:

$$V = \sqrt{4rD} \tag{1}$$

where $V > 0$ is the velocity (distance/time) of the advancing front of the invasive population and D and r are positive constants representing the diffusion coefficient and maximum per capita growth rate, respectively.

Since *B. violaceus* has overlapping generations and can be considered to be continuously reproducing, it is appropriate to represent the invasion dynamics using a continuous-time PDE rather than a discrete integrodifference equation. We represent the the population density of *B. violaceus* at time t and spatial coordinate x as $u(t, x)$.

Assume that the population initially occupies a finite section of the New England coastline of length L and that the initial population distribution is compact.

$$u(0, x) = \begin{cases} \phi(x) > 0 & 0 < x < L \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

The reaction-diffusion model describing the population dynamics takes the form

$$\frac{\partial u}{\partial t} = D\frac{\partial u^2}{\partial x^2} + F(u) \tag{3}$$

Determining the correct form of the population growth term in (3) is challenging. Colonial ascidians generally display indeterminate growth, meaning that colony area tends to increase exponentially with time (Jackson, 1977). If we assumed simple linear population growth, our PDE would take the form

$$\frac{\partial U}{\partial t} = D\frac{\partial U^2}{\partial x^2} + rU \tag{4}$$

This is the simplest version of the general reaction-diffusion model, for a homogeneous, unstructured population growing exponentially and dispersing in a uniform, one-dimensional environment (Andow et al., 1990; Skellam, 1951). However, it is unlikely that colony-scale dynamics would apply over much larger spatial scales. Leaving $F(u)$ as an unspecified function allows for the possibility of logistic growth, as in the Fisher-KPP equation:

$$\frac{\partial u}{\partial t} = D\frac{\partial u^2}{\partial x^2} + r(1 - \frac{u}{K}) \tag{5}$$

The use of nonlinear reaction diffusion models in a biological context is well-established (see Cherniha and Davydovych, 2017). However, note that for biologically reasonable choices of $F(u)$, the growth function will be bounded by the linear function, such that $F(u) \le ru$. Thus,

$$D\frac{\partial u^2}{\partial x^2} + F(u) \le D\frac{\partial U^2}{\partial x^2} + rU \tag{6}$$

Now, note that for compact initial conditions like (2), there exist positive constants G and σ such that we bound the initial distribution from above by a Gaussian distribution:

$$U(x, 0) = \frac{G}{\sqrt{4\pi\sigma^2}} \exp\left(-\frac{x^2}{4\sigma^2}\right) \tag{7}$$

$$\text{such that} \quad u(0, x) \le U(0, x) \quad \text{for all } x \tag{8}$$

From (6) and (8), we use the comparison theorem for PDEs to find that the solution to the linear equation in (6) provides an upper bound to the solution of the potentially nonlinear equation (3).

A detailed derivation of the solution of (4) can be found in Lewis et al. (2016). In brief, we utilize the change of variables $U(t,x) = W(t,x)e^{rt}$, reducing (4) to the standard diffusion equation for W. We then apply Fourier and inverse Fourier transforms to the new PDE and the initial condition (7) to find that

$$W(t,x) = \frac{G}{\sqrt{4\pi(\sigma^2 + Dt)}} \exp\left(-\frac{x^2}{4(\sigma^2 + Dt)}\right)$$

Converting back to our original variable, we conclude that the solution to (4) with the initial condition (7) is a normal distribution:

$$U(t,x) = \frac{G}{\sqrt{4\pi(\sigma^2 + Dt)}} \exp\left(-\frac{x^2}{4(\sigma^2 + Dt)} + rt\right) \tag{9}$$

Now, we can quantify the spatial spread of the population by considering how quickly a level set $U(x,t) = U_c$ moves in space, where U_c could be considered a threshold of detection. In other words, below U_c it is so difficult to find the invasive organisms that for practical purposes they are not present. By rearranging (9), we can get the following expression

$$\left(\frac{x}{t}\right)^2 = 4rD + \frac{4r\sigma^2}{t} - \frac{4(\sigma^2 + Dt)}{t^2} \ln\left(\frac{U_{cr}\sqrt{4\pi(\sigma^2 + Dt)}}{G}\right)$$

As t becomes large, this formula simplifies to $\frac{|x|}{t} \to \sqrt{4rD}$. Thus, the asymptotic rate of spread is $V = \sqrt{4rD}$, as we initially sought to show.

This relationship between V, r, and D holds true for nonlinear forms of $F(u)$, can be extended to higher dimensions, and does not need to rely on the idea of a threshold of detection— in fact, true advancing fronts with asymptotic speeds given by () form (Skellam, 1951, Okubo and Levin, 2001). For invasion of a two-dimensional homogeneous habitat described by the reaction-diffusion equation

$$\frac{\partial u(x,y)}{\partial t} = D\left[\frac{\partial u^2}{\partial x^2} + \frac{\partial u^2}{\partial y^2}\right] + F(u), \tag{10}$$

the radius of the species range should increase linearly with time, with the slope of the increase given by $\sqrt{4rD}$. This theory has been tested for numerous ecological systems and often agrees well with the empirical relationship between measured spread rates, per capita growth rates, and diffusion coefficients. Microscale observations can be used to parameterize () and predict the spreading rate for a given species at a geographic scale. Such spreading-speed analyses have been conducted for a number of terrestrial animal species, including the muskrat, cereal leaf beetle, small cabbage white butterfly, grey squirrel (Andow et al., 1990; Gorsholz, 1996)

Spreading speed theory has also been applied to numerous aquatic species, including the brown trout, green crab, hermit crab, periwinkle, barnacle, mussels, and molluscs (MacDonald et al., 2022; Grosholz, 1996; Marculis and Lui, 2016; Gharouni et al., 2015). Possibly the only application of this method to a tunicate was performed by Grozholz (1996) for *B. leachi*. His estimates of $r = 1.8$ and $D = 1,800$ yielded a predicted rate of spread of 114 km/year, much faster than the observed rate of 16 km/year. In addition to providing insight on the spread of a specific invasive species of commercial concern, comparing the accuracy of our estimation for *B. violaceus* to the previous results for *B. leachi* could allow for broader conclusions to be drawn regarding the applicability of this approach for colonial tunicates in general.

Application

Population growth rate was estimated from Grey (2011) to range from 0.8-1.9.

Discussion

This model attempted to predict the macro-scale dispersal of an invasive tunicate using a simple reaction-diffusion model.

Multiple avenues are apparent for future work modeling the spread of *B. violaceus* using diffusion-type equations. First, there exist many other possible formulations for the term representing population growth. The Fisher-KPP equation, which assumes logistic rather than exponential growth, has been well-studied from a mathematical perspective and has seen widespread application across ecological contexts (SOURCES). Other diffusion models incorporate Allee effects, an ecological phenomenon characterized by decreased individual fitness (lower per capita growth rates) at small population sizes. Accounting for Allee effects in continuous reaction-diffusion models or analogous discrete integrodifference models can alter predictions about the potential success or failure of an invasion, rates of spread, and plausible ranges of an invasive species (Keitt et al., 2001; Kot et al., 1996; Liu and Kot, 2019).

The model from which () was derived assumes a uniform environment and isotropic dispersal. In reality, invasive species are more likely to disperse into more favorable habitats, so assuming that the rate of spread does not vary based on the direction of movement is not realistic. For example, the growth and reproduction of *B. violaceus* generally increase with warmer temperatures, so in a relatively cold climate, southward dispersal may be more likely than northward dispersal.

B. violaceus can disperse naturally by rafting on eelgrass and other floating vegetation or debris (Carver et al., 2006; Worcester, 1994). Human-mediated introduction via hull fouling on recreational or commercial watercraft and aquaculture activities are also major pathways by which invasive tunicates are introduced to new locations (Carver et al., 2006). Although *B. violaceus* has a relatively low attachment strength, the small drag coefficient associated with their low profile means that its displacement velocity is above the top speeds of sailboats, barges, and other slower-moving vessels (Murray et al., 2012).

Future work could utilize discrete integrodifference equations with leptokurtic dispersion kernels to account for transport via hull fouling and other potential vectors of long-distance dispersal. The potential for long-distance dispersal events via natural or human-mediated pathways often prompts the use of integrodifference equations for diffusion models of invasive populations (Lewis et al., 2016; Neubert and Caswell, 2000; Kot and Neubert, 2008). These models assume that growth and dispersal occur in distinct and asynchronous stages (Kot and Neubert, 2008). The ability of *B. violaceus* to utilize multiple forms of reproduction and the fact that both larvae and post-larvae can contribute to the colonization of new habitat potentially violates the assumption of temporally separated growth and dispersion. However, stratified models that separate spatially continuous short-distance dispersal from discrete long-distance dispersal can be valuable tools to reconstruct realistic invasion dynamics (e.g., Gilioli et al., 2013) and their potential for modeling the spread of *B. violaceus* merits further investigation.

Recent work coupling deterministic models with a stochastic component has led to major improvements in the biological realism of PDE-based invasion models. These stochastic models can account for both process and observation error, incorporating the randomness inherent in natural systems. For example, Roques et al. (2011) used a "statistical-reaction–diffusion approach" to analyze the expansion of the pine processionary moth based on moth nest presence/absence data. Using a "mechanistic-statistical" diffusion model assuming logistical growth and imperfect species observation data, Louvrier et al. (2020) was able to forecast the expanding distribution of the grey wolf in France. Applying similar methods to data on *B. violaceus* would be valuable for developing useful predictions of potential future invasions.

Finally, competition-diffusion models that represent the population growth and spread of two competing species in the same habitat admit similar traveling front solutions to those described above for the simple reaction-diffusion equation (Carrère, 2018). It is often interesting to investigate the stability and long-term behavior of a system of competition-diffusion models for different parameter values, including varying the propagation speeds of the two organisms or the differential impacts of the competitive interactions on each species (Carrère, 2018; Ducrot et al., 2014). Experimental evidence suggests that *B. violaceus* colonies can outcompete *Botryllus schlosseri*, a different invasive tunicate that has been equally or more problematic for the New England aquaculture industry (Gittenberger and Moons, 2011; Dijkstra et al., 2007). However,

these studies have been limited to small-scale experiments conducted on a single substrate (e.g., an oyster cage, SOURCE). Our single-species reaction diffusion model could be extended to a system of competition-diffusion equations to examine the potential impacts of competition between *B. violaceus* and *B. schlosseri* on the spread of these two species on a broader scale.