Partial Differential Equations to Diffusion-Based Population and Innovation Models

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Abstract: - Multiple instances and diffusion mechanisms in biological and economic modeling involve partial differential equations (PDEs). Functional PDEs (with time delays) may be even more adequate to real world problems. In the modeling process, PDEs can also formalize behaviors, such as the logistic growth of populations with migrations, and the adopters' dynamics of new products in innovation models. In biology, these events are then related to the variations in the environment, the population densities and overcrowding, the migrations and spreading of humans, animals, plants and other cells and organisms. In economics and management science, the diffusion processes of technological innovations in the marketplace (e.g. the mobile phone) is a major subject. Moreover, these innovation diffusion models refer mainly to epidemic models. This contribution introduces to this modeling process with PDEs and reviews the essential features of the dynamics in biological, ecological and economic modeling. The computations are carried out by using the software Wolfram*MATHEMATICA*® 7.

Key-Words: Diffusion process, partial differential equation, reaction-diffusion equation, traveling wave solution, critical patch size, population dynamics, innovation diffusion.

1 Introduction

This introductive paper is dedicated to diffusion processes as they occur in population dynamics studies of biological and ecological domains[1] and in adopter's dynamics of new products in the marketing area[2]. The importance of this subject is reflected in the vast literature since the seminal article of (Skellam, 1951) on the random population dispersal in linear and two-dimensional habitat.

2 Diffusion Process Modeling

2.1 Partial Differential EquationsModels

Migrations in population dynamics and innovation diffusion of new products can be modeled by using the same partial differential equation (PDE): the diffusion equation. PDEs allow for modeling state variables which variations depend on more than one independent variable such as time and space. The advection and the diffusion are two different PDE based transport mechanisms[3]. The advection equation describes the bulk movement of particles in a transporting environment (e.g. a swarm of insects in the air or pollutants in a river).

The one dimension advection equation[4] takes the form $a_t = -c\, a_x$ and describes the advection of a scalar field $a(x,t)$ carried along by a flow of constant speed[5] c. The solution is $a(x,t) = f(x-ct)$, where f is deduced from the initial condition $a(x,0) = f(x)$. The

[1] A brief history of mathematical diffusion in ecology is presented by (Okubo, 1980).

[2] (Michalakelis & Sphicopoulos, 2012)introduce to the basic deterministic and stochastic innovation diffusion models.

[3] A convection combines these two kinds of transport.

[4] This equation is closely related to the hyperbolic wave equation $u_{tt} = c^2 u_{xx}$, where u is the displacement and c the wave speed. Such a PDE is derived from a fundamental conservation law.

[5] This equation may be rewritten as $a_t / a_x = -c, a_x \neq 0$ so that the level curves $a(x,t)$ are straight lines of slope c and so that the general

diffusion equation is a parabolic PDE[6] for describing the random motion of particles. A. physical propagation problem (diffusion) is an initial value problem (IVP). The IVP may be a parabolic PDEof the form[7] $u_t = \alpha u_{xx}, x \in (0, L)$ with the initial condition $u(x,0) = f(x), f \in C^1$.

2.2 Reaction-Diffusion Equations

PDEs that model population growth with a simple random diffusion are reaction-diffusion (RD) equations. The vector form of RD equations is

$$\mathbf{u}_t = f(\mathbf{u}) + \mathcal{D}\, \nabla^2 \mathbf{u}$$

where $\mathbf{u} = \mathbf{u}(x,t)$ are the dependent variables, $f(\mathbf{u})$ and $\mathcal{D}$ the diffusion matrix (Britton, 1986).

Let $N(x,t)$ be the density of population at time $t \in [0, \infty)$ and position $x \in \Omega$. A simple RD is[8](Allen L. J., 2007, pp. 309-316)

$$N_t = f(N) + \mathcal{D} N_{xx},$$

where $f(N)$ denotes the reaction rate and $\mathcal{D} N_{xx}$ the diffusion rate. For one species population growth[9], we may have an exponential growth with $f(N) = rN$ (Malthusian populations), a logistic growth[10]with $f(N) = rN(1 - N/K)$, the negative logistic for population decay by Skellam $f(N) = -g^2 N(1 - N/K)$ or the asymmetric Gompertz $f(N) = rN \ln(K/N)$

Suppose the RD equation with exponential growth

$$N_t = rN + \mathcal{D} N_{xx}, x \in (L, 0),$$

with the initial condition $N(x,0) = \varphi(x)$ $x \in [L, 0]$ and the boundary conditions $N(0,t) = N(L,t) = 0$. The change of variable $P(x,t) = N(x,t)e^{-rt}$ leads to the following IBVP: $P_t = \mathcal{D} P_{xx}$ with the conditions $P(x,0) = \varphi(x),\ x \in [L, 0]$ and $P(0,t) = P(L,t) = 0$. The solution to $N(x,t)$ is the solution to $P(x,t)$ multiplied by e^{rt}. Hence, we have

$$N(x,t) = \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi x}{L}\right) e^{\left\{r - \mathcal{D}\left(\frac{n\pi}{L}\right)^2\right\}t}, \quad B_n = \frac{2}{L}\int_0^L N_0(x) \sin\frac{n\pi x}{L} dx \tag{1}$$

In this model the additional growth term increases the density locally and fasters the spatial spread in the population.

2.3 Delay Reaction-Diffusion Equation

Delay partial differential equations (DPDEs) may better fit to the realworld modeling of the population dynamics[11]. The parabolic DPDE is

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solution takes the form $\varphi(ct - x)$ for an arbitrary C^1 function φ.

[6]Recall that a parabolic PDE is one instance (besides ‘hyperbolic’ and ‘elliptic’ PDEs) of a discriminant-based classification for PDEs in two independent variables. For more independent variables, the same instances proceed from an eigenvalue based classification.

[7]Additional boundary conditions (BCs) such as $u(0,t) = u(L,t) = 0,\ t > 0$ transform the model into an initial boundary value problem (IBVP). This physical problem represents the heat conduction in a rod for which the ends are at a zero temperature while the initial temperature at any other point is given by $f(x)$ (Kythe, Puri, & Schäferkotter, 2003, p. 127).

[8]An extension to the local population density $N(x, y, t)$ with spreading in a two-dimensional uniform space is of the form $N_t = f(N) + \mathcal{D}(N_{xx} + N_{yy})$.

[9]Other specifications of the population growth rate and two-species population are given by (Allen L. J., 2007, pp. 310-311).

[10]Biological applications for the deterministic and stochastic logistic growth are in (Allen L. J., 2011, pp. 421-424)

[11]The dynamics and control of time-delay differential systems are studied in (Keller, 2010) with applications to

$$u_t = a(t)u_{xx} - q(t)u(x,t-\tau)$$

where τ denotes a constant positive delay. The temporal Wazewska-Czyzeska & Lasota equation describes the survival of red blood cells in animals. This equation may be extended by incorporating a spatial component as in (Zhang & Zhou, 2007, p. VII). The spatio-temporal delay RD equation becomes

$$p_t = d\ p_{xx} - \delta p(x,t) + qe^{-ap(x,t-\tau)}$$

where $\Omega \subset \mathbb{R}$ is a bounded domain and $(x,t) \in \Omega \times (0,\infty)$. The state variable $p(x,t)$ denotes the number of red blood cells located at x attime t. Theconstant time-delay $\tau > 0$ denotes the time needed to produce blood cells. The parameter δ is the death rate of red blood cells. The parameters q and a are related to the generation of red blood.

3 Population DispersalModel

An RD equation such as Fisher-KPP equation [12] for population models, admits two main properties: firstly, the solution is traveling through the spatial domain at a finite rate of speed and secondly conditions on the spatial domain are determined for a population persistence. These two problems are known as 'the traveling wave solutions' and 'the critical patch size'.

3.1 Fisher-KPP Equation

The Fisher-KPP equation is the parabolic PDE[13]

$$N_t = rN(1-N) + \mathcal{D}N_{xx},\ x \in \Omega \subset \mathbb{R} \qquad (2)$$

where $N(x,t)$ is for the population density at spatial position x at time t>0 with $N(x,0) = N(x)$. The reaction term is the logistic term $rN(1-N)$ and the diffusion rate or random motion is $\mathcal{D}N_{xx}$.

3.2 Traveling Wave Solutions

DefinitionA traveling wave solution of (2) is a solution that can be expressed in terms of the scalar $z = x - vt$ where the constant v is the wave speed. We may write $N(z) = N(x-vt)$

Let $dN/dz = -P$, we obtain the system of first-order ordinary differential equations (ODEs)

$$\begin{cases} \dfrac{dN}{dz} = -P \\ \dfrac{dP}{dz} = -\dfrac{v}{\mathcal{D}}P + \dfrac{r}{\mathcal{D}}N(1-N) \end{cases} \qquad (3)$$

We also impose the following restrictions to the solution $N(z)$: $N(z) \in [0,1]$, $N(z) \to 1$ as $z \to -\infty$ and $N(z) \to 0$ as $z \to \infty$. The phase plane dynamics[14] is illustrated in Figure 1, for $r = v = \mathcal{D} = 1$.The equilibrium point $E(0,0)$ is locally asymptotically stable[15].

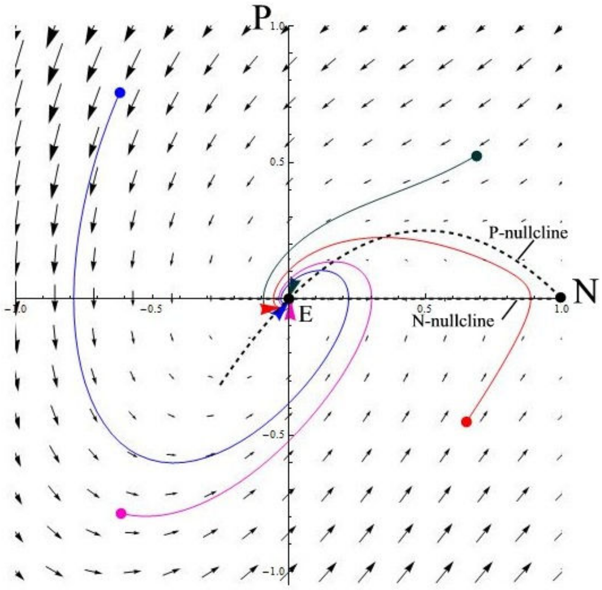

Figure 1. Phase plane dynamics of system (3) of ODEs with parameter values $r = v = \mathcal{D} = 1$.

economics. Time lags in biological models are notably presented in (MacDonald, 1978).

[12]The Fisher's equation was simultaneously introduced by (Fisher, 1937) and (Kolmogorov, Petrovskii, & Piscounov, 1991) for phase transition problems in combustion,physiology, ecology, etc.

[13]The generalization of the Fisher's equation by (Kaliappan, 1984)is $u_t = \mathcal{D}u_{xx} + u - u^k$, for which an exact analytical solution is proposed for traveling waves.

[14] For more cases and details, see (Allen L. J., 2007, pp. 321-324).

[15]Figure 1 has been produced by using the Mathematica graphical interface 'EquationTrekker for specifying initial conditions and plotting the resulting numerical solution to the system of ODEs.

3.3 Critical patch size

What is the minimal size of the spatial domain needed for a population survival? This problem has been studied by (Kierstead & Slobodkin, 1953) for an RD equation with exponential growth[16]. The IBVP is $N_t = rN + \mathcal{D}N_{xx}, x \in (0, L)$ with the homogeneous Dirichlet BCs: $N(0,t) = N(L,t) = 0$ and $N(x,0) = N_0(x)$. The conditions on the spatial domain so that the solutions (1) approaches zero is $r < \mathcal{D}\left(\frac{\pi}{L}\right)^2$ (Allen L. J., 2007, pp. 319-321). The reversed inequality then defines the minimal patch size for the population to survive. Solving the equality for L yields the critical patch size $L_c = \pi\sqrt{\frac{\mathcal{D}}{r}}$. Thus, the population size increases if $L > L_c$ and decreases to zero if $L < L_c$.

4 Innovation Diffusion Model

Innovation diffusion models describe the process by which innovation products (or idea or practice) are communicated over time through certain channels and expand through a population of adopters. The typical time path of the cumulative adopter distribution (e.g. for mobile phone) is a sigmoidal S-shaped time curve: few adopters at the beginning (mainly professionals), then more and more adopters and finally diffusion to public at large. The market is saturated at the upper limit. Modeling the innovations has an extensive literature in marketing. Analogies are with models of epidemics.

4.1 BasicInnovationDiffusion Model

A general diffusion model of new product acceptance is composed of $M(t)$ participants to the market, of $N(t)$ adopters of the new product and m the maximum of potential customers (Mahajan & Muller, 1979). There are three distinct segments of the market: the current market $N(t)$, the potential market $m - N(t)$ and the untapped market $M(t) - m$. The typical diffusion model is

$$\frac{dN}{dt} = g(t)\left(m - N(t)\right) \qquad (4)$$

where $N(t)$ is the cumulative numbers of prior adopters, $m - N(t)$ the potential adopters and $g(t)$ the diffusion coefficient or probability ofadoption[17]. The marketing problem is: how many of the potential adopters will buy the new product at time t ?

4.2 Stochastic Innovation Diffusion

The innovation diffusion process may be disturbed by random impacts from the environment (e.g. socioeconomic factors) as well from the system itself.Uncertainties are inherent in the marketing approach due to changing consumer tastes, technology conditions, etc. These uncertainties can be modeled by using normally distributed parameters (Eliashberg, Tapiero, & Wind, 1983)or by formulating an adapted Itô's stochastic differential equation (SDE)[18]. The stochastic Bass' innovation model by (Skiadas & Giovanis, 1997)is reformulated as[19]

$$dN = \left(p(m - N) + \frac{q}{m}(m - N)N\right)dt + c\left(\frac{p}{q} + \frac{N}{m}\right)dW$$

where W is a Wiener process and c the noise parameter. The mean value (first moment) of the solution is[20]

[16]The application of this study is the growth of phytoplankton (the bottom of the marine food chain). The conditions for population persistence and extinction have also been for a diffusive logistic equation and different types of domains.

[17] In that case, the rate of diffusion at time t equals the expected number of adopters.

[18]Population biology models with time-delay in a noisy environment are studied in (Keller, 2011). The population dependent diffusion model by (Michalakelis & Sphicopoulos, 2012) incorporates a stochastic component.

[19] Different notations are used in (Skiadas & Giovanis, 1997).

[20]The model is solved by reducing the nonlinear SDE to a linear form (Skiadas & Giovanis, 1997). The same method is used by (Giovanis & Skiadas, 1999) to solve a stochastic logistic innovation diffusion model for Greece and USA.

$$E[N] = \frac{m\,e^{(p+q)t}}{\frac{1}{\frac{p}{q}+\frac{N_0}{m}} + \frac{q}{p+q}\left(e^{(p+q)t}-1\right)} - \frac{mp}{q}$$

4.3 Spatial Innovation Diffusion

How innovations are diffusing in different geographical spaces? (Mahajan & Peterson, 1979)integrate the space and time dimensions in the diffusion process. The Bass' model becomes the PDE

$$N_t = \left(p(x) + q(x)N\right)\left(m(x) - N\right),$$

where $N(x,t)$ denotes the cumulative number of adopters in domain x at time t. The innovation dynamics shows a characteristic wavelike set of S-shaped curves.

Recently, the spatial dimension of innovation diffusion is introduced into the classical imitation-innovation Bass' dynamicsby (Hashemi, Hongler, & Gallay, 2012). The resulting multi-agent imitation model generates spatio-temporal patterns. The imitation interactions of agents (agent' observations of their neighbors) can explain the existence of swarms[21] of bacteria, insect swarms, fish schools, etc.

5 Conclusion

This presentation concerned with the dynamics of population dispersal in biology and the spatial diffusion of new products in marketing. The importance of reaction-diffusion equations has been shown with a variety of population growth specifications. Basic one-dimensional diffusion model have been considered. The dynamics of such models have been mainly on traveling wave solutions and on the critical patch size. Appendices allow to specify some technical aspects of the modeling process: the random move based diffusion equation, the basic physical diffusion equation, the characteristic method for solving PDEs, and the reference Bass' model.

Further developments and applications may extend this introductive presentation. The models can be generalized to multi-agent models, to multiple species. The space dimension may be extended. Other specifications of the population growth may be chosen as an alternative, such as a predator-prey specification for multiple species, such as with the diffusional Lotka-Volterra system (Britton, 1986, pp. 21-23). Other domains of the population biology, ecologyand of economics. Constant and variable time-delays may be more systematically introduced.

[21]The dynamics of animal grouping is notably presented in (Okubo, 1980, pp. 110-131)

Appendix A.Random Move-Based Diffusion Equation

A collection of particles moves randomly on the real line $\mathbb{R}$, with steps Δx every time unit τ (Edelstein-Keshet, 1988, pp. 404-406). The time domain $[0,\infty)$ is divided into intervals of length Δt. The probabilities of moving to the left or to the right are respectively λ_l and λ_r. The problem is to determine the equation that describes the change in the number of particles at position x. The number of particles $N(x,t+\tau)$ at time $t+\tau$ is determined by $N(x,t)$ at the previous time, plus the expected arrivals from the left and from the right, minus the expected departures to the left and to the right. We obtain

$$N(x,t+\tau) = (1-\lambda_l-\lambda_r)N(x,t) + \lambda_l N(x+\Delta x,t) + \lambda_r N(x+\Delta x,t)$$

Using Taylor-series expansion for these terms, supposing that $\lambda_l = \lambda_r = 1/2$ and dividing the expression by τ yields

$$N_t + \frac{1}{2}N_{tt}\tau + \cdots = N_{xx}\frac{\Delta x^2}{2\tau} + N_{xxxx}\left(\frac{\Delta x^2}{2\tau}\right)^2 + \cdots$$

Taking $\frac{(\Delta x)^2}{2\tau} = \mathcal{D}$, a limiting form of the equation for $\tau \to 0, \Delta x \to 0$ yields the diffusion equation[22] $N_t = \mathcal{D}N_{xx}$, where $\mathcal{D}$ denotes a constant diffusion coefficient.

Appendix B. Basic Physical Diffusion Equation

Let the Cauchy problem (Allen L. J., 2007, pp. 312-313):

$$N_t = \mathcal{D}N_{xx},\ t \in (0,\infty) \qquad (5)$$

[22]Also the parabolic heat conduction equation.

for which the initial condition is $N(x,0) = N_0(x), x \in \mathbb{R}$ A Fourier transform of $N(x,t)$ in x is defined by

$$\mathcal{F}[N] \equiv \mathcal{N}(s,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} N(x,t)\, e^{isx} dx .$$

Applying Fourier transforms to (5) yields[23]

$$\mathcal{N}_t(s,t) = -\mathcal{D}\, s^2 \mathcal{N}(s,t),\ s \in \mathbb{R}$$

for which the transformed Dirichlet initial condition is $\mathcal{N}_0(s)$. The inverse Fourier transform $\mathcal{F}^{-1}[\mathcal{N}(s,t)]$ and the convolution theorem of Fourier[24] yield the solution

$$N(x,t) = \frac{1}{2\sqrt{\mathcal{D}\pi t}} \int_{-\infty}^{\infty} N_0(v)\, e^{-\frac{(x-v)^2}{4\mathcal{D}t}} dv .$$

Appendix C. Integrating PDEs by Using the Characteristic Method

Let the general PDE

$$F(x_0, x_1, \ldots, x_n, u, p_0, \ldots, p_n) = 0,$$

where $p_i = u_{x_i}, i = 0, \ldots, n$. If we consider that the x_i's and p_i's are functions of the parameter s, the characteristic system[25]of ODEs takes the form

$$\left\{ \frac{dx_i}{ds} = F_{p_i}, \frac{dp_i}{ds} = F_{x_i} - p_i F_u, \frac{du}{ds} = \sum_{j=0}^{n} p_j F_{p_j} \right\},$$

for $i = 0, 1, \ldots, n$. Along the characteristic curves, the solutions of the ODEs are also solutions of the PDE (Zwillinger, 1998, pp. 325-330).

[23]The Fourier transform is obtained by using the properties $\mathcal{F}[\partial N / \partial x] = -is\mathcal{N}(s,t)$ and $\mathcal{F}[\partial^2 N / \partial x^2] = -s^2 \mathcal{N}(s,t)$, assuming that $N \to 0$ and $N_x \to 0$ as $x \to \pm\infty$.

[24]The convolution theorem of Fourier states that

$$\mathcal{F}^{-1}[\mathcal{X}(s)\mathcal{Y}(s)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} X(v) Y(x-v)\, dv$$

[25]The characteristics consist in general equations which are represented by the curves of intersection of two families of integral surfaces defined by $x - ce^t = 0$ and $u = c_1 e^{-t^2/2}$.

Example.Let the following IVP in which the PDE is linear with variable coefficients

$$x u_x + u_t = -tu, u(x,0) = \cos(x).$$

The solution by using the method of characteristics (Allen L. J., 2007, pp. 305-306) is

$$u(x,t) = \cos\left(xe^{-t}\right) e^{-t^2/2}$$

This solution is depicted for $x \in [-20, 20]$ and $t \in [0, 2]$ in Figure 2,by using *MATHEMATICA* for which the primitive NDSolve allows to find numerical solutions to PDEs[26].

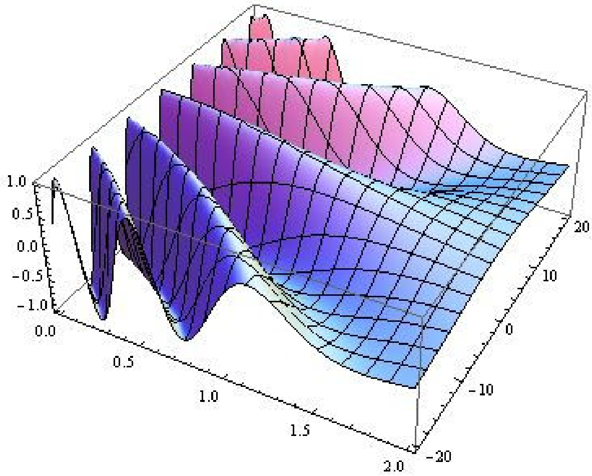

Figure 2. 3D plot of the two-dimensional resulting interpolating function

Appendix D. Bass' Innovation DiffusionModel

The deterministic Bass' model (Bass, 1969) is based on an aggregate differential diffusion model of new product acceptance. The nonlinear dynamics of this model is governed by the ratio of two control parameters p and q, respectively the innovation and the imitation rates. The evolution of the adopters may be the differential equation(4). Suppose that $g(t)$ takes the linear specification[27]

[26]The Mathematica® primitive yields

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NDSolve[{x D[u[x, t], x] + D[u[x, t], t] + t u[x, t] == 0,
  u[x, 0] == Cos[x]}, u, {t, 0, 2}, {x, -20, 20}]

{{u → InterpolatingFunction[{{-20., 20.}, {0., 2.}}, <>]}}
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[27](Mahajan & Peterson, 1985, pp. 12-26)analyse separately the dynamics of the external (innovation) and internal (imitation) effects. The generalized von Bertalanffy's model is also shown to have flexible

$g(t) = p + q\frac{N(t)}{m}$ and define $X(t) = N(t)/m$, the Bass' model is the logistic equation

$$\frac{dX}{dt} = (p + qX(t))(1 - X(t)) \quad (6)$$

Integrating (6) by parts, the time path is

$$X(t) = \frac{1 - e^{-(p+q)t}}{1 + (q/p)e^{-(p+q)t}}$$

The maximum diffusion rate is obtained for $d^2X/dt^2 = 0$ (at the inflexion point of the time path), where $\hat{X} = \frac{1}{2} - \frac{p}{2q}$. To find the time $\hat{t}$, when $X(\hat{t})$ is a maximum penetration rate, we solve $X(t) = \hat{X}$ in time t and obtain $\hat{t} = -\frac{\ln(p/q)}{p+q}$.

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properties w.r.t the symmetry and point of inflexion of the integral diffusion curves.

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