Stochastic Methods for the Lotka-Volterra Model with Migration

Alec Koppel, mentored by Renato Feres

March 21, 2011

Department of Mathematics, Washington University in St. Louis

Abstract

The Lotka-Volterra Model is a classical set of differential equations used to model predator-prey interactions. This model may be generalized in a variety of ways, but does not incorporate any spatial-temporal relationships. We examine the spatial element of the model by expanding the system to contain multiple predator-prey sites in a finite linear chain with migrational interactions between them. Modern numerical techniques from chemical kinetics were employed in our analysis and include ODE solvers, the Gillespie SSA arising from Petri Net representations, and the Estimated-Midpoint Langevin Method motivated by Diffusion and Poisson Approximations of the discrete Petri Net description. With these tools we can examine the differences between some deterministic and stochastic formulations of the system with special interest given to disparities in spatial-temporal relationships, periodicity, and extinction rates.

Contents

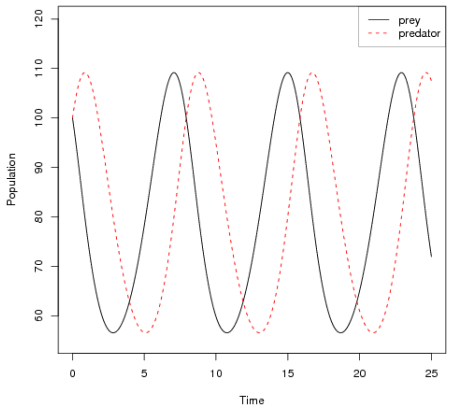
Introduction

Many classical models in population dynamics are deterministic in nature. In order to broaden their applicability, they may be generalized as stochastic processes. We focus on the Lotka-Volterra Model, a set of differential equations meant to describe elementary interactions of cohabiting predator-prey populations. The stochastic theory surrounding the motivation of the Lotka-Volterra Model is firmly rooted in recent developments in chemical kinetics in that modern stochastic methods are required to describe the intricacies of the model and perform well-grounded simulations. To date, few Lotka-Volterra Models explore the spatial distribution of population density over time and even fewer stochastic methods can handle such spatial-temporal components. In adapting modern stochastic methods for a spatially oriented Lotka-Volterra Model (that is, one that incorporates migrational interactions), we may expose some sharp new problems in stochastic theory.

The Lotka-Volterra Model

Predator-prey interactions in nature are key to understanding evolution and population dynamics. Around 1910-1920 Vito Volterra and Alfred J. Lotka simultaneously developed a set of differential equations to represent interacting predator and prey populations. The original motivation for the model came from a noticeable spike in predatory fish in the Adriatic Sea following World War I. In seeking to understand what conditions might be more favorable to the predatory fish, this model was formulated. The model assumes the prey population (for example, rabbits) reproduces and is consumed by the predator at specified rates. Additionally, the predator population (for example, foxes) declines at a certain rate. Their population level changes over time are described by the following equations called the *Lotka-Volterra Model*:

Predator and Prey Population Over Time



Initial conditions: $x_0 = 100$, $y_0 = 100$
$\alpha = 1$, $\beta = 0.05$, $\gamma = 1$, $\delta = 0.05$

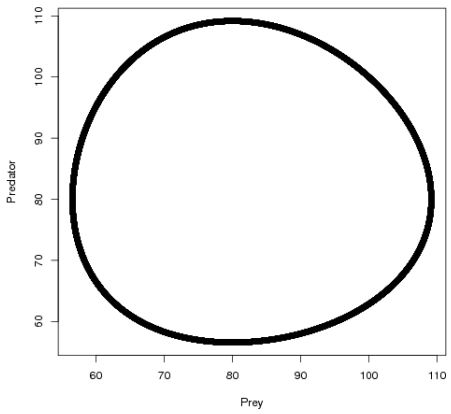
$$\frac{dx}{dt} = x(\alpha - \beta y)$$

$$\frac{dy}{dt} = -y(\gamma - \delta x)$$

where x is the prey population, y is the predator population, and the system is parametrized by α the prey population growth rate, β the prey consumption rate, γ the predator population decline rate, and δ predator population growth rate. The state space for the Lotka-Volterra Model is the set $S = \{(x, y)\epsilon\mathbb{R}^2 : x \geq 0, y \geq 0\}$. The solutions to any dynamical system can be characterized in the following way:

- If $x(t) = \mathbf{x}$ for $\forall t\epsilon\mathbb{R}$ then $\mathbf{x}$ is called a *rest point.*
- If $x(T) = \mathbf{x}$ for some $T\epsilon\mathbb{R}$ but $x(t) \neq \mathbf{x}$ for $\forall t\epsilon(0, T)$ then $\mathbf{x}$ is called a *periodic point* with *period* T.
- If $t \to x(t)$ is an *onto* function, the orbit never crosses itself. It will topologically appear as a line.

Predator-Prey Orbital Relationship



Even a simplistic model like the Lotka-Volterra Model exhibits complicated behavioral patterns and requires careful analysis. The stability points come from setting the states of change to 0. Any solution set to the basic Lotka Volterra Model takes the form:

$$(i)\ x(t) = y(t) = 0$$

$$(ii)\ x(t) = 0,\ y(t) = y(0)e^{-\gamma t}$$

$$(iii)\ x(t) = x(0)e^{\alpha t},\ y(t) = 0$$

The solutions to this model imply a few important facts. For one, if either the prey or predator population at some time is 0 then it remains there for all time. If there are no prey present, the predator population will decay exponentially to 0. Further, if the predator population reaches 0 at any point, the prey population increases to ∞. Clearly the model could use some fine tuning, as several of these assumptions are invalid. This system of differential equations produces a closed orbital pattern relating the predator and prey population levels over time shown in the above figure. Once a deterministic system such as the one shown starts off on a nonzero path, it remains on this orbital path

forever and is said to be *invariant* on S. Also, by our above definitions, this solution is periodic. The x axis and y axis form the other solution sets and clearly are rest states. If one unravels the parametric orbital curve shown over time, periodic oscillations appear. These oscillations are shown based on the same initial conditions as the orbital pattern figure. The parameters determine the form the oscillations take over time. The particularly stable character of this experimental setup derives from the equality of the prey and predator growth rates as well as the equality of the prey and predator decline parameters (which is obviously unrealistic but we mean to emphasize simple periodicity in this example).

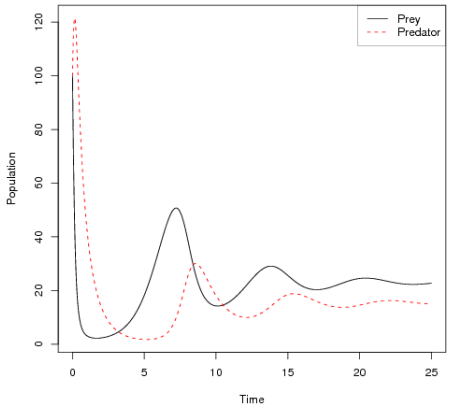
The Lotka-Volterra Model lends itself naturally to many modifications and generalizations. The solutions of the classical Lotka-Volterra model absurdly imply that the prey population will increase toward infinity without any predators present. It's important we bound the increase of the prey in the absence of the predators by some carrying capacity related parameters. This is typically done by assuming a logistic growth form as a result of competition within a species. This takes the form:

$$\frac{dx}{dt} = x(\alpha - \varepsilon x - \beta y)$$

$$\frac{dy}{dt} = -y(\gamma - \delta x + \varsigma y)$$

Here $\varepsilon > 0$ is some value that determines competition within a species (*intraspecies competition*) for the prey, and likewise for $\varsigma \geq 0$ with the predator population. It is less important that $\varsigma > 0$ because the predator population will decline naturally in the absence of food. In the absence of predators, the prey population x will converge to its carrying capacity which is uniquely determined by the parameters. Formally speaking, $x \to \frac{\alpha}{\varepsilon}$ as the predator population $y \to 0$. In standard ecology notation, the carrying capacity is denoted by $K = \frac{\alpha}{\varepsilon}$. The notion of stable periodic conditions in this carrying capacity model become quite labyrinthine, require careful analysis, and are omitted. Qualitatively, the differences in complexity between the carrying capacity model and the standard Lotka-Volterra are readily apparent. Over time we can see the system stabilizing. This

Predator and Prey Population, Adjusted For Carrying Capacity



Initial conditions: $x_0 = 100$, $y_0 = 100$, $\alpha = 1$, $\beta = 0.05$, $\gamma = 1$, $\delta = 0.05$, $\varepsilon = 0.01$, $\varsigma = 0.01$

rest point has been rigorously established to exist under particular conditions of $\omega - limits$ for a given state (see Hofbauer and Sigmund).

We also examine the system's expansion to incorporate additional species. For example, one could imagine the population level of the rabbits as depending on grass. In the most general case, we formulate the multispecies model as

$$\frac{dx_i}{dt} = x_i(\beta_i + \sum_{j=1}^{n} \alpha_{ij} x_j)$$

where β_i is the growth rate of species i and α_{ij} describes the effect of the jth population upon the ith population. We consider $A = [\alpha_{ij}]$ to be the interaction matrix. We assume $\alpha_{ij} > 0$ if it describes a positive effect on a species population growth, and $\alpha_{ij} < 0$ if it describes a growth inhibiting relationship. There are many points of stability such as $x_i(0) = 0$ and $0 = x_i(\beta_i + \sum_{j=1}^{n} \alpha_{ij} x_j)$. This system takes values on $\{(x_1, .., x_n) \epsilon \mathbb{R}^n : x_i \geq 0 \; for \; i = 1, ..., n\}$ and like the simpler models above, if a species population $x_i(0) = 0$ then $x_i(t) = 0$ for all t. Some important results follow from this multispecies formulation. The set of solutions to $0 = x_i(\beta_i + \sum_{j=1}^{n} \alpha_{ij} x_j)$ can have at most one solution in the interior of $\mathbb{R}^n$. That is, for $x_i > 0 \; \forall i$ there is only one solution; however, in the case of det(A)=0 there will be multiple solutions that will be identically rest points. Both modifying the model to include intraspecies competition and to incorporate multiple species are steps in the right direction, but only explore temporal relationships.

In order to broaden the model to incorporate spatial relationships (and spatial-temporal interactions), we modify the classical model to a system of multiple predator-prey "sites" with migratory interactions between each site. One could think of many neighboring ponds and species populations within each pond, or bird and insect populations spread across an archipelago as the natural motivation for this modification. This migratory interaction amounts to two different summations for each species equation, one for departure rates and another for an arrival rates. Each site (L sites in total) consists of a pair $\left(\frac{dx_i}{dt}, \frac{dy_i}{dt}\right)$

$$\frac{dx_i}{dt} = x_i(\alpha_i - \beta_i y_i) - x_i \sum_{j,\, j \neq i} k_{ij} + \sum_{j,\, j \neq i} k_{ji} x_j$$

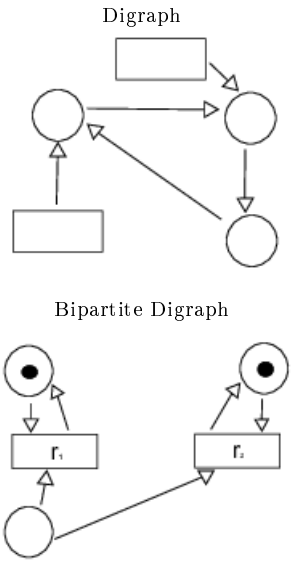
$$\frac{dy_i}{dt} = -y_i(\gamma_i - \delta_i x_i) - y_i \sum_{j,\, j \neq i} c_{ij} + \sum_{j,\, j \neq i} c_{ji} c_j$$

where each k_{ij} ,c_{ij} denote the migration rates from site i to site j for the prey and predator respectively. Note that $i \neq j$ is due to the fact site i cannot migrate to itself. In the most general case, every site is connected with every other site. The most intuitive ideas of distance and spatial relationships are conveyed when we whittle down the number of connections between sites. In that, we will limit ourselves to a finite linear chain of sites in order to observe spatial-temporal

interactions, especially interesting boundary conditions. Also, α_i, β_i, γ_i, δ_i are defined as in the classical Lotka-Volterra Model, so each site may have unique specifications if need be. This model can easily be modified to incorporate additional species at each of the L sites or to incorporate intraspecies competition for each species; however, we will simply consider the migratory modification of the classical system to best understand the spatial-temporal interactions. With the groundwork laid to explore migration, we will focus on the differences that arise when we assume changes in the system occur randomly according to some underlying probability distributions rather than at fixed deterministic rates. To understand exactly what is occurring in such a stochastic migrational model, we need a precise method of visual representation.

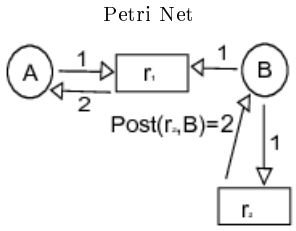
Petri Nets

Carl Adam Petri developed a particular type of graphical network called a Petri Net in 1962 that is very useful for modeling, analysis, and representation of systems of interactions. Petri nets are widely implemented in chemical kinetics, but but we will be using them to describe the Lotka-Volterra model. Every Petri net has an underlying graphical representation that has some key properties. Firstly, every Petri net may be represented by a *digraph*, a set $G = (V, E)$ where V is the set of vertices and $E \subset V \times V$. E is the set of edges of the graph. Every element of E is called an edge and may be represented as an ordered pair (v_1, v_2) where v_1 and v_2 are vertices. If the edge (v_1, v_2) connects v_1 to v_2, we may represent it as $v_1 \to v_2$.



Note the difference in connectivity. Every edge only connects a place to a transition or vice versa.

A digraph is said to be *bipartite* if its set of vertices V can be decomposed into two pairwise disjoint sets P and R, that is, $V = P \cup R$ and $P \cap R = \emptyset$. P denotes the set of *places* (or *species*) and R the set of *transitions* (or *reactions*). This amounts to saying every edge of G may only connect vertices of different types: a place to a transition or a transition to a place. Every edge can be written as $p \to r$ or $r \to p$ for some $r \epsilon R$ and $p \epsilon P$. It is customary to represent *places* (or *species*) as circles and *transitions* (or *reactions*) as rectangles.



The weights given to each edge correspond to the coefficients of the products and reactants.

At any given time, the state of a Petri net is characterized by the number of *tokens* at each place (or bold dots in the diagram). For our purposes it will be instructive to call the amount of tokens at each place the *population size* of a species. We assign a non-negative integer X(p) to represent the population size of a species for each place ($p \epsilon P$). We can think of the state of a Petri Net as the location of the tokens at a given time. For instance, if we have ($X(p_1) = x$,$X(p_2) = y$), we can think of this as a state for two places p_1, p_2. For each edge (p,r) going from a place to a transition, we assign a non-negative integer Pre(p,r) as a weight for the reaction. Similarly, we assign for each edge (r,p) going from a transition to a place a non-negative integer Post(p,r). We may think of Pre(p,r) as the status of the species before reaction r and Post(p,r) as the result of reaction r. The tokens move from place to place depending on the results of the reactions that take place. For example, the following set of reactions for species A and B correspond to the representation in the following figure.

$$r_1 : A + B \to 2A$$

$$r_2 : B \to 2B$$

Then $Pre(r_1, A) = 1$, $Pre(r_1, B) = 1$, $Post(r_1, A_1) = 2$, $Pre(r_2, B) = 1$, and $Post(r_2, B) = 2$. If m is the number of species and n is the number of reactions, we may represent Pre(p,r) and Post(p,r) as m by n matrices. In this example, $Pre(r, p) = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}$ and $Post(r, p) = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$ and X(A), X(B) represent the population sizes of species A, B at some given time. Reactions that in some way are an endpoint are denoted $\emptyset \to A$ or $B \to \emptyset$. These sorts of events may signify birth, death, migration, or some other reaction that absorbs or produces a species. We will be discussing migrational reactions in greater detail later.

Stochastic Petri Nets

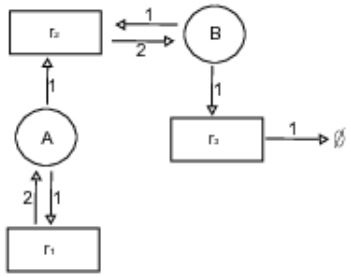
The Petri Net representation lends itself well to describing time-evolving processes. Dynamical systems arising from Petri Net representations may be formulated as stochastic or deterministic; however, we will focus on the stochastic formulation that incorporates the theory of the Poisson Process in that each reaction occurs asynchronously according to independent exponentially distributed

times. In order to describe a dynamical system in this fashion, we need a function to determine how often each reaction event occurs. For n reactions and m species, we define the reaction rate function $h(r_i, X)$ as a function of a reaction r_i and state X. It is not intuitively clear how to describe these reaction rate functions. For i=1,...,n, $h(r_i, X)$ gives the transition rates for the different states of a Petri Net. Through this, we may think of Petri Nets as the transition diagrams for continuous-time Markov Chains. We can describe the general change over time of a Stochastic Petri Net in the following manner with R as the set of reactions:

$$X_{t_1}(p) = X_{t_0}(p) + \sum_{r \epsilon R} \#_r([t_0, t_1])(Post(r,p) - Pre(r,p))$$

The quantity $\#_r([t_0, t_1])$ describes the number of events (reactions) of type r that occurred in the time interval $[t_0, t_1]$. This equation describes the present state as the previous state in addition to the sum of all events that occurred, weighted appropriately by Pre and Post to describe the outcome of each reaction.

Lotka-Volterra Model as a Petri Net



We may describe the change in the system over time but we first must choose appropriate reaction rate functions. For lack of a rigorously established result from mathematical ecology, we somewhat arbitrarily choose our reaction rate functions according to the *Law of Mass Action*, a conventional choice from chemical kinetics. For a given reaction, we define the *order* of a reaction to be $d = \sum_{r \epsilon R} Pre(r,p)$. Most frequently in chemistry reactions of higher order than 2 are made up of a sequence of elementary reactions that in aggregate produce the higher reaction. Thus we will adopt this convention and strictly concern ourselves with elementary reactions. Applying the Petri Net theory built up so far to the Lotka-Volterra Model, we can describe its basic components in terms of elementary reactions where A is the prey population and B is the predator population:

$$A \rightarrow 2A$$

$$A + B \rightarrow 2B$$

$$B \rightarrow \emptyset$$

The order of these reactions is respectively 1, 2, and 1. The first reaction represents the reproduction of a prey, the second reaction denotes the predator reproducing after consuming a prey, and the last reaction represents the death of a predator. These reactions correspond to the following matrices $Pre =$

$\begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix}$ and $Post = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \end{bmatrix}$. From these matrices, we may define a new matrix U the stoichiometric matrix in the following manner: $U = Post - Pre$. In this case,

$$U = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \end{bmatrix} - \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \end{bmatrix}$$

This Lotka-Volterra Petri Net is depicted on the previous page. We assume these reactions occur asynchronously according to some rates $\{c_1, c_2, c_3\}$, or more generally, c_i for each $r_i \epsilon R$. The *Law of Mass Action* gives us a way to formulate the reaction rate functions in terms of the species quantity present at a given place, X(A) and X(B). Thus we have our reaction rate functions:

$$h(r_1, X) = c_1 X(A)$$

$$h(r_2, X) = c_2 X(A) X(B)$$

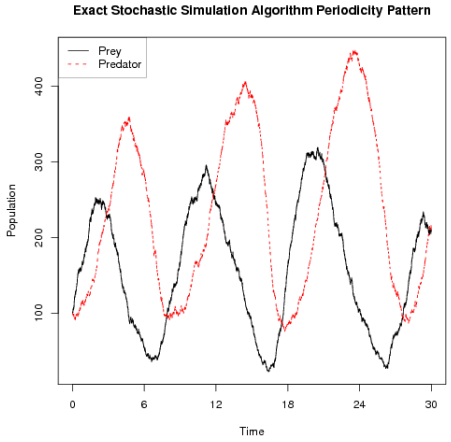
$$h(r_3, X) = c_3 X(B)$$

Generally speaking, for a reaction $r : \ n_1 s_1 + n_2 s_2 + ... + n_m s_m$, we have $h(r, X) = cX(s_1)^{n_1} X(s_2)^{n_2} \cdots X(s_m)^{n_m}$.

Any Petri Net can be fully described in terms of its component parts in the following way: $\mathcal{N}$ = (P, R, Pre, $Post$, h, X). P specifies the set of places (or species) and R specifies the set of transitions (or reactions). Further, Pre gives the place-transition edge weights and described by the set of all edges (p,r); Post gives the transition-place weights and is the set of all edges (r,p). h gives the reaction rate probability rates often chosen according to the Law of Mass Action where we say probability rates rather than probabilities because they are not normalized to sum to 1. Lastly, X denotes the state of the Petri Net at some time and is denoted by a column vector $X(P) = (X(p_1), ...X(p_m))^T$ for m different species and the superscript T denotes the transpose operation. It's important to note that the set of edges is fully encompassed by the specifications of P, R, Post, and Pre so that it is omitted from the explicit description of a Petri Net.

The Petri Net theory can be used to visualize this set of Lotka-Volterra reactions where the each event occurs randomly according to the reaction rate functions $h(r_i, X)$. As previously noted, Petri Nets are widely implemented in chemical kinetics, the field in which the following algorithmic technique arose, known as the Gillespie Stochastic Simulation Algorithm (or simply SSA). This algorithm gives an iterative method for describing the way the interacting populations change over time according to the reaction rates, the weights Pre and Post given by the reactions themselves, and the Poisson Process. We assume a *"well-stirred"* mixture of species in order to preserve the *independence of events* assumed by the Poisson Process and denote X as the vector of species for n different reactions. Note that X has m components, one for each species. We then input the Petri Net $\mathcal{N}$ and the end time T_{max} to simulate the Stochastic Petri Net evolution over the time interval $[0, T_{max}]$.

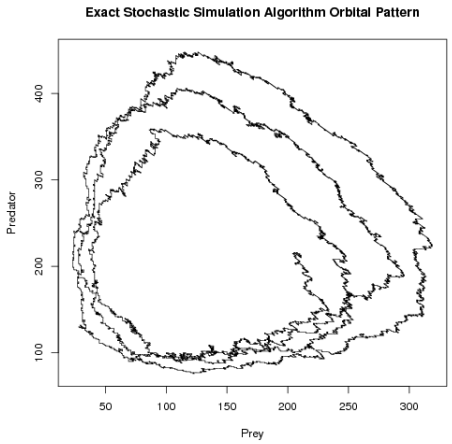
1. Initialize the state vector X at some initial time (typically $t_0 = 0$) and call it X_0.
2. For each reaction r_i, calculate $h(r_i, X)$ for j=1,...,n.
3. Set $h(X) = \sum_i h(r_i, X)$
4. Simulate a sample value of of an exponential random variable with rate $\lambda = h(X)$ and call it s.
5. Set the current time t to $t + s$, and rename it t.
6. Simulate a sample value of index k according to the probability distribution $h(r_k, X)/h(X)$ and call it j.
7. Set the state of the system to $X = X + U_j$ (where U_j is the jth column of the stoichiometric matrix).
8. Save X and t in some list.
9. If $t < T_{max}$,the preassigned stopping point, go back to step 2.



Initial Conditions: $X_0 = 100$, $Y_0 = 100$, $c_1 = 1$, $c_2 = 0.005$, $c_3 = 0.6$ where X_0, Y_0 denote the prey and predator populations respectively at t=0

Some important qualitative results can be discerned from the simulation shown here. As with any stochastic process, this process is nowhere differentiable (due to the spiky nature of the path). The population-time plots illustrate the asymmetric periodicity and uneven amplitudes, as a result of asynchronous events driving the populations rather than deterministic rates of change. Further, the stochastic orbital pattern formed from the predator-prey plot lacks periodic or rest points. Instead of a stable path over time, the system evolves randomly. The stochastic evolution of the Lotka-Volterra System will lead to some extinction: either predator or prey population will reach 0 as $t \to \infty$. Allowing for random fluctuation brings our model closer to reality, but there is additional groundwork we must lay before examining any intricate expansions of the system.

We implement the SSA method to examine how the stochastic formulation of the Lotka-Volterra Model differs from the standard deterministic differential equations. This continuous time stochastic process occurs in a manner that



allows us to see the specific changes in species populations after *every* event. For this reason, the SSA is sometimes called the *Exact* SSA because of its specificity. It is indeed a continuous time process, but each event is a unique event that changes the population by fixed integer amounts (the results of the reactions that occur). Therefore, it may considered a discrete state change description of the model while it is defined as a continuous time process. In very large systems of interactions, this specificity requires storage of huge quantities of data and lengthy computation times. Instead of recording a new data point after every event, we may instead use the Normal Approximation to the Poisson Process and other mathematical tools to approximate the discrete event by event description of the Lotka-Volterra Model by a system of stochastic differential equations.

Stochastic Differential Equations

Traditionally, the rate of change of dynamical systems is described by differential equations. In some cases, a well-defined deterministic path is not appropriate because the rate of change is subject to random fluctuation. We introduce stochastic differential equations to incorporate random variation (or "white noise"). In the following discussion, we'll assume a basic knowledge of random variables, independence, expectation, and variance. To arrive at a stochastic differential form of the Lotka-Volterra model we'll first need to establish some key definitions.

This white noise term will be defined in terms of Brownian Motion. *A standard Brownian Motion* over $[0, T]$ is a random variable $W(t)$ with the following properties:

1. $W(0) = 0$ with probability 1.
2. For $0 \leq s < t \leq T$, over the interval $[s, t]$, the random variable $W(t) -$

$W(s) \sim N(0, t-s)$ where $N(0,1)$ denotes the standard unit normal distribution. This may also be represented by $W(s) \sim \sqrt{t-s}N(0,1)$.

3. For any $0 \leq s < t < u < v \leq T$, $W(t) - W(s)$ and $W(v) - W(u)$ are independent.

We partition the interval [0,T] by setting $\delta t = T/N$ for some $N \epsilon \mathbb{N}$, and set $t_j = j\delta t$. Here $j\epsilon\{0, 1, ..., N\}$and we denote $W_j = W(t_j)$. Notice that every $dW_j \sim \sqrt{\delta t}N(0,1)$ and $W_j = W_{j-1} + dW_j$. This will be essential in the construction of the stochastic integral.

For any scalar valued function h(t) over the interval $[0, T]$, we may approximate the integral $\int_0^T h(t)dt$ by the Riemann sum

$$\sum_{j=0}^{N-1} h(t_j)(t_j - t_{j-1})$$

Notice this is the left endpoint form of the Riemann sum. Similarly, we may approximate the stochastic integral $\int_0^T h(t)dW(t)$ by the left-endpoint Riemann sum

$$\sum_{j=0}^{N-1} h(t_j)(W(t_j) - W(t_{j-1}))$$

noting that $dW(t_j) = W(t_j) - W(t_{j-1})$. For a single time-dependent random variable $X(t)$, it's state at any given time $t\epsilon[0, T]$ is given by

$$X(t) = X_0 + \int_0^t f(X(s))ds + \int_0^t g(X(s))dW(s)$$

We may describe the rate of change by the following differential form of the previous integral equation

$$dX(t) = f(X(t))dt + g(X(t))dW(t)$$

where $f(X(t))$,$g(X(t))$ are any functions of $X(t)$, dt is a standard time differential term, and $dW(t)$ is the needed white noise term, made precise as a *Brownian Motion differential*, the rate of change of a standard Brownian Motion. We do not write $\frac{dX(t)}{dt}$ because a standard Brownian Motion is nowhere differentiable with probability 1 and is shown to have infinite variation. The Brownian Motion differential is also commonly called an *Ito differential* due to the role it plays in stochastic calculus developed by Ito.

The most important information to take away from this stochastic differential form is that the rate of change is partitioned into a deterministic term with rate of change dt and a white noise term defined by the Brownian Motion differential dW(t). It is customary to emphasize the differential form dX(t) over the preceding integral form. This differential equation is known as the *Ito differential equation* and is the limiting case of a left-endpoint Riemann sum

with $\delta t \to 0$ (or as $N \to \infty$) so that [0,T] is partitioned into infinitely small intervals. The Ito formulation of stochastic integration is one of two solution approaches; another approach is the Stratonovich equation which is the limiting case of a midpoint Riemann sum. We will be implementing the Ito form. Using shorthand notation we can rewrite the stochastic differential equation above as $dX_t = f(X_t)dt + g(X_t)dW_t$ where X_t is some time-dependent random variable.

A Stochastic Differential Lotka-Volterra Model

Earlier in the discussion of Stochastic Petri Nets we noted that the explicit event by event evolution of the Stochastic Lotka-Volterra model is given by:

$$X_{t_1}(p) = X_{t_0}(p) + \sum_{r \epsilon R} \#_r([t_0, t_1])(Post(r,p) - Pre(r,p))$$

We adopt the time subscripts t to emphasize the state of the system at a particular time and use this formula to arrive at a nice stochastic differential equation to describe the approximate path of the Lotka-Volterra Model through some careful manipulations and limits.

First rearrange the above equation to be stated as

$$X_{t_1}(p) - X_{t_0}(p) = \sum_{r \epsilon R} \#_r([t_0, t_1])(Post(r,p) - Pre(r,p))$$

which can be written more generally as

$$\Delta X(p) = \sum_{r \epsilon R} \#_r(\Delta t)(Post(r,p) - Pre(r,p))$$

We earlier assumed that our events follow the Poisson Process. Formally speaking, we have $\#_r(\Delta t) \sim Pois(\lambda)$ and $E(\#_r(\Delta t)) = Var(\#_r(\Delta t)) = \lambda$. We apply the Normal Approximation to the Poisson Process as follows:$Z \approx \frac{\#_r(\Delta t) - \lambda \Delta t}{\sqrt{\lambda \Delta t}}$ where $Z \sim N(0,1)$. Then by the transformation properties of the standard normal distribution, rewrite this as $\#_r(\Delta t) \approx \lambda \Delta t + \sqrt{\lambda \Delta t} Z$. The *Chemical Langevin Equation* is obtained by taking the limit as $\triangle t \to 0$ which is known as the *Diffusion Approximation*.

$$\lim_{\triangle t \to 0} \Delta X(p) = \lim_{\triangle t \to 0} \sum_{r \epsilon R} \#_r(\Delta t)(Post(r,p) - Pre(r,p))$$

$$dX_t(p) = \sum_{r \epsilon R} (Post(r,p) - Pre(r,p))(\lambda_r(X_t)dt + \sqrt{\lambda_r(X_t)} dW_t)$$

Thus we have arrived at a stochastic differential equation to describe the evolution of the Lotka-Volterra Model subject to random fluctuation. This differential equation follows the Ito differential form in that the rate of change

is partitioned into a deterministic differential and an Ito differential. With $U = Pre - Post$, $H(X_t) = \begin{bmatrix} h(r_1, X_t) \\ \vdots \\ h(r_n, X_t) \end{bmatrix}$, and $p = \begin{bmatrix} p_1 \\ \vdots \\ p_m \end{bmatrix}$, we can formally define the relationship between the rates λ_r of our Poisson Processes $\#_r(\Delta t)$ and the reaction rate functions in convenient matrix notation.

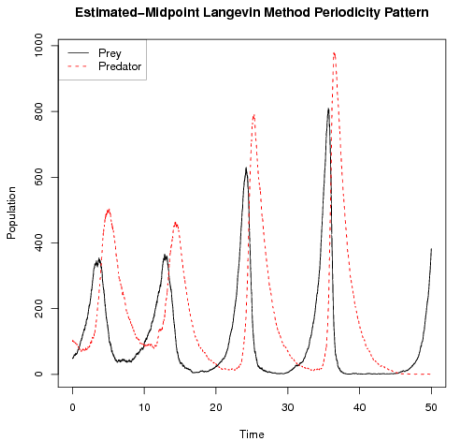
$$dX_t(p) = UH(X_t)dt + \sqrt{U\, diag\{H(X_t)\}U^T}dW_t$$

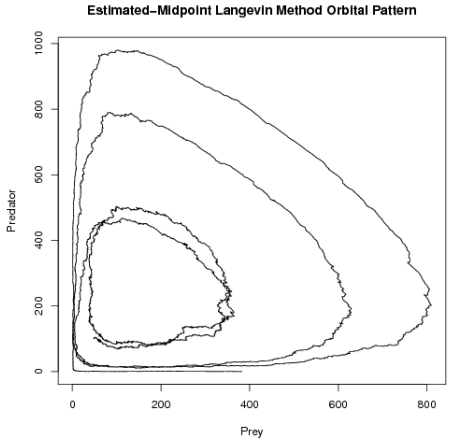
where $diag\{H(X_t)\}$ represents the matrix whose entries on the main diagonal are identical to the matrix $H(X_t)$ and 0 off the main diagonal, and U^T represents the transpose of the stoichiometric matrix U. Researchers in chemical kinetics (such as Gillespie) have established two key criteria for when the Chemical Langevin Equation (obtained via the Diffusion Approximation) can accurately describe the evolution of such a stochastic process.

(i) In a given small time interval dt, the reaction rate functions $h(r_i, X)$ do not change significantly.

(ii) Each reaction r_i occurs many more times than once during such a time interval.

The Gillespie Algorithm or Exact SSA records every event as the process progresses in time. For more elaborate systems of interactions with many reactions and species, this meticulous construction of the system's full history is quite computationally intensive and provides an unnecessarily high level of detail. Fortunately, we can approximate such an elaborate system's approximate path to an acceptable level via the Chemical Langevin Equation. Simulating this stochastic differential system is an intricate problem that has motivated some novel algorithmic solutions. We will be employing a type of $\tau - Leaping$. The central idea behind





Initial Conditions: $X_0 = 50$, $Y_0 = 100$, $c_1 = 1$, $c_2 = 0.005$, $c_3 = 0.6$, $\tau = 0.005$

The amount of data points saved is significantly reduced but the same patterns are apparent in this method of stochastic simulation.

this method is to only record the change in the species populations at fixed time intervals rather than after *every* change. The above criteria for when we can approximate a continuous time Markov Chain by a Markov Jump process are made precise as follows.

1. Leap Condition: Require τ to be small enough so that the overall state change will be minute in any time interval $[t, t+\tau)$. Then none of the reaction rate functions will change significantly in such a time interval. Concisely, we want $H(X_{t+\tau}) \cong H(X_t)$ where as before $H(X_t)$ refers to the matrix whose rows are the vector-valued reaction rate functions $h(r_i, X_t)$. If the Leap Condition is satisfied, each $h(r_i, X_t)$ will give the instantaneous rate for a particular event during any infinitesimally small time interval.

2. $\tau \gg max_i\{\frac{1}{h(r_i,X_t)}\}$ which amounts to requiring that each event occurs multiple times in a given small time interval $[t, t+\tau)$.

We follow the conventional bound for when τ-Leaping (and a system of stochastic differential equations) is more appropriate than the Exact SSA: $\tau \leq \frac{2}{h(r_i,X_0)}$ for all i. This bound can be best explained by noting that if τ is less than a few multiples of the time the Exact SSA requires to transition states, it makes more sense to opt for the explicit rather than approximate description of the system's path. We just as well could relax this second requirement and remain using the rates of the Poisson Processes $\#_r(\Delta t)$ in a more explicit event by event description; however, in our goal to find a nice stochastic differential equation (SDE) to describe the evolution of the Stochastic Lotka-Volterra Model, we must use the Diffusion Approximation. Therefore, we impose condition 2. Simulating the Lotka-Volterra Model following the structure of the Chemical Langevin Equation is subject to errors just as any SDE simulation is. In order to correct for some computational errors inherent in simulation of SDEs, we opt for a Midpoint approach. This *Estimated-Midpoint Langevin Method* will be implemented in later numerical experimentation and is described here. Note that before we can implement such a method, we must choose τ so that the above conditions are satisfied.

1. Compute $\bar{\lambda} = \tau \sum_{i=1}^{n} h(r_i, X_t)U_i$ where as before, U_i is the ith column of the stoichiometric matrix.

2. Set $\tilde{X}_t = X_t + \frac{\bar{\lambda}}{2}$ where $\frac{\bar{\lambda}}{2}$ is the midpoint correction.

3. For each i=1,...,n, generate a random sample value n_i from the standard normal distribution $N(0,1)$.

4. Set $k_i = h(r_i, \tilde{X}_t)\tau + n_i\sqrt{h(r_i, \tilde{X}_t)\tau}$

5. Compute $\lambda = \sum_{i=1}^{n} k_i U_i$

6. Set $t = t + \tau$ and $X_t = X_t + \lambda$.

7. Save t and X_t in some list. If $t < T_{max}$ for some preassigned stopping point, go back to the first step.

This method is only correct provided that we are bounded away from the limit $\tau \to 0$. After significant work, we have an effective simulation method for a system of stochastic differential equations approximating the Lotka-Volterra Model applied to Stochastic Petri Nets. Equipped with this tool, the Gillespie Exact SSA, and some rudimentary ODE solvers to handle the deterministic system, we can effectively explore some numerical possibilities that will shed light on the differences between the stochastic and deterministic formulations of the Lotka-Volterra Model.

Experimentation and Exploration

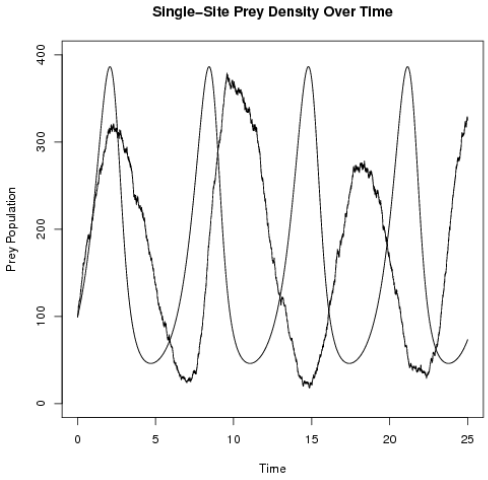
Single-Site Simulations

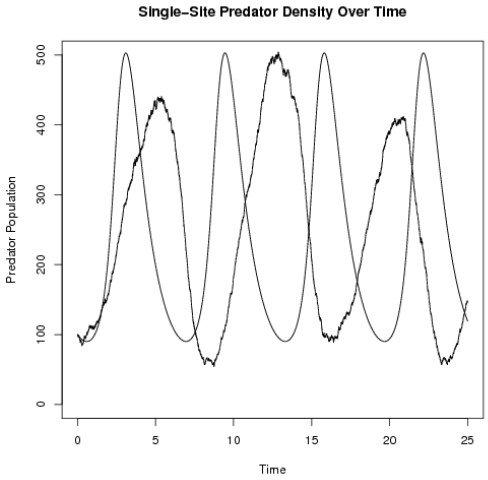
Single site simulations were included in earlier discussions to illustrate realizations of the Lotka-Volterra Model according to different methods. Comparing these realizations is a natural precursor to looking at the migrational expansion of the system. It's important to note that the single site deterministic system requires four parameters: α the prey population growth rate, β the prey predation rate, γ the predator death rate, and δ predator population growth rate. In the preceding stochastic methods, there were only three elementary reactions. That is, the reaction $A + B \to 2B$ describes both the β prey predation rate and δ the population growth rate for the predator in light of having sufficient food to eat. For consistency and greater ease of understanding, we'll set $\beta = \delta$ in our comparison of the stochastic and deterministic models.

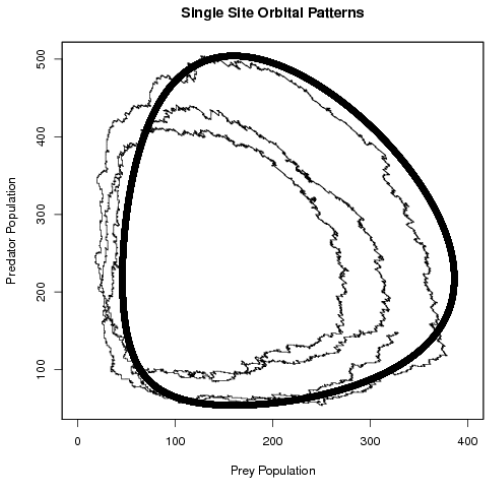
The simulations on the following page present much information solely based on qualitative observation. The deterministic system produces consistent amplitudes and period lengths whereas the stochastic systems do not. Further, from randomness alone both stochastic systems reach lower valleys, supporting the rigorous result that such stochastic systems will necessarily reach an extinction event. Intuitively, the approximate path appears pretty close to the exact path; however, the Exact SSA is much closer to reaching the extrema of the deterministic system, especially the minima. To be precise, the deterministic system's maxima for predator and prey are 504 and 387 respectively. The Exact SSA's simulated maxima are 504 and 379 whereas the Langevin Method's simulated maxima are 431 and 318. As expected, finding an accurate stochastic differential equation that significantly improves on computational time to describe the Lotka-Volterra's evolution in real time remains an open problem. The orbital diagrams reflect these discrepancies in the range of simulated values as well as the lack of stable periodic conditions for the stochastic simulations. Now that we are aware of some possible outcomes of elementary simulations, it is time to explore the Lotka-Volterra Model expanded to include migrational interactions.

Single-Site Comparison of Stochastic Methods to the Deterministic System

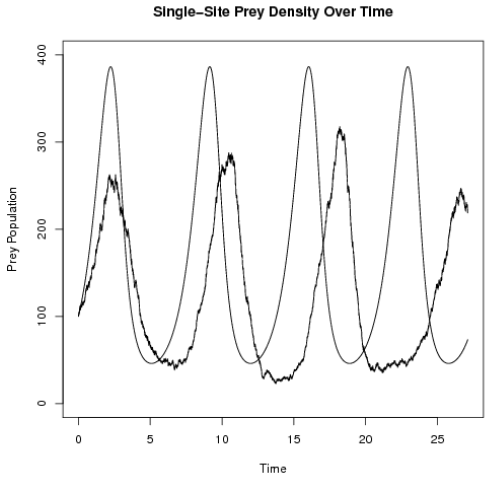
Exact Stochastic Simulation Algorithm

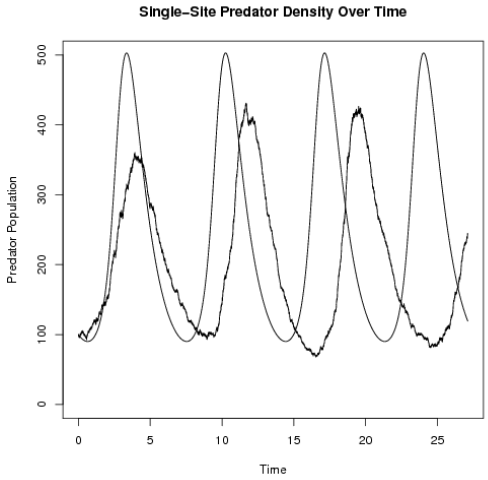


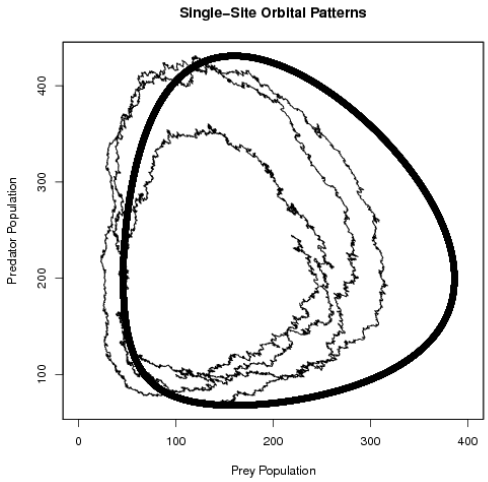




Estimated-Midpoint Langevin Method







Initial conditions: $X_0 = 100$, $Y_0 = 100$,$\alpha = 1.2$, $\beta = 0.005$, $\gamma = 0.8$, $\delta = 0.005$,
$c_1 = 1$, $c_2 = 0.005$, $c_3 = 0.6$

Migrational Simulations

The deterministic Lotka-Volterra Model with migration takes the following form:

$$\frac{dx_i}{dt} = x_i(\alpha_i - \beta_i y_i) - x_i \sum_{j,\, j\neq i} k_{ij} + \sum_{j,\, j\neq i} k_{ji} x_j$$

$$\frac{dy_i}{dt} = -y_i(\gamma_i - \delta_i x_i) - y_i \sum_{j,\, j\neq i} c_{ij} + \sum_{j,\, j\neq i} c_{ji} c_j$$

where each site (L sites in total) consists of a pair $\left(\frac{dx_i}{dt}, \frac{dy_i}{dt}\right)$ and k_{ij},c_{ij} denote the migration rates from site i to site j for the prey and predator respectively. The model will be simplified in a few ways stated below to better discern spatial and temporal relationships in the simulations.

- Set L=10 so that simulations will occur over a manageable system that still has strict "boundary" and "interior" sites.
- $\alpha_i = \alpha_j$, $\beta_i = \beta_j$, $\gamma_i = \gamma_j$, $\delta_i = \delta_j$ for all $i \neq j$. The equality of parameters will remove their dependence from our observations.
- For interior sites, site i is only *connected* (in the sense the migrations occur between the sites in both directions) to site *i+1* and *i-1*. For boundary sites: site *1* is only connected to site *2*; site L is only connected to site *L-1*.

The Lotka-Volterra Model with migration in terms of elementary chemical reactions with the above simplifications reduces to this collection for a single site. The double edged arrows represent the bidirectionality of the migrational reactions.

$(i)\ A_i \to 2A_i$

$(ii)\ A_i + B_i \to 2B_i$

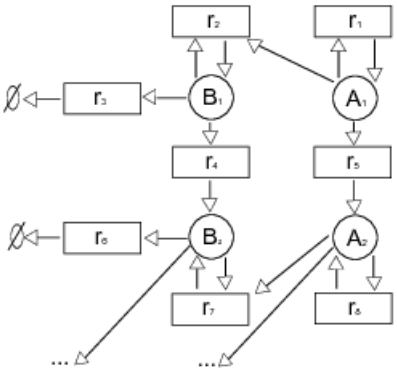
$(iii)\ B_i \to \emptyset$

$(iv)\ B_i \rightleftharpoons B_{i+1}$

$(v)\ A_i \rightleftharpoons A_{i+1}$

$(vii)\ B_i \rightleftharpoons B_{i-1}$

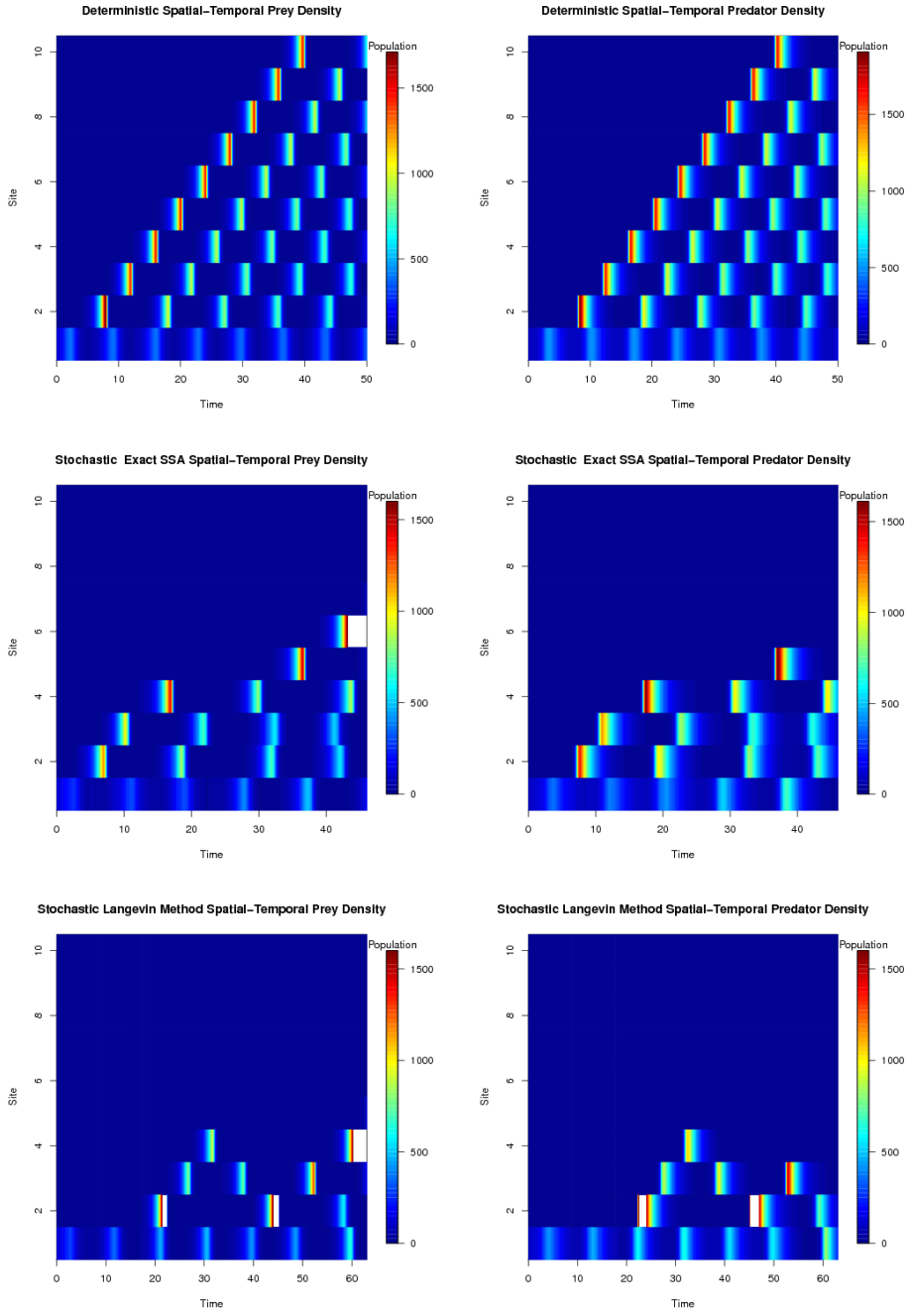
$(vi)\ A_i \rightleftharpoons A_{i-1}$



This set of reactions represents
those of an interior site. For site 1 or site L, remove *(vi),(vii)* or *(iv),(v)* respectively. Recall that each reaction has some specified reaction rate c_i. To remove dependence on these rates, set them equal. That is, each site's reproduction reaction rates will be equal as well as all others (including migration rates). Applying the Petri Net ideas to this expansion, we can view the first and second sites as in the figure. The elipses represents the connection to site 3, and the Petri Net continues as expected. The Exact SSA and the Estimated-Midpoint Langevin Method apply seamlessly to this expansion once we have tailored the Petri Net input appropriately. The stoichiometric matrix U describing this intricate 10 site system has dimensions 20x210 and follows an easily illustrated block-diagonal pattern for the non-migrational portion of the matrix. The migration reactions follow a more complicated pattern.

$$U = \begin{bmatrix} U^{(1)} & 0 & \cdots & & \cdots & 0 & \begin{matrix}1 & -1\\ 0 & 0\end{matrix} & \begin{matrix}0 & 0\\ 1 & -1\end{matrix} & \cdots & & & \\ 0 & U^{(2)} & 0 & & & & \begin{matrix}-1 & 1\\ 0 & 0\end{matrix} & \begin{matrix}0 & 0\\ -1 & 1\end{matrix} & & & & \\ \vdots & 0 & \ddots & \ddots & & & 0 & 0 & \ddots & & & \\ & & \ddots & & & & \vdots & \vdots & & & & \\ \vdots & & & & & 0 & & & & & & \vdots \\ 0 & \cdots & & \cdots & 0 & U^{(10)} & 0 & 0 & \cdots & \begin{matrix}-1 & 1\\ 0 & 0\end{matrix} & \begin{matrix}0 & 0\\ -1 & 1\end{matrix} \end{bmatrix}$$

Here $U^{(i)} = \begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \end{bmatrix}$ and denotes the stoichiometric matrix from the standard Lotka-Volterra Petri Net description. There are 10 such blocks along the main diagonal. The region after the block diagonal matrix consists of all the migrational connections between each site. The two species at each site correspond to two rows in each $U^{(i)}$. Thus for a bidirectional migrational reaction for a *prey* between sites i and j, the block $\begin{bmatrix} 1 & -1 \\ 0 & 0 \end{bmatrix}$ will allign with $U^{(i)}$and the block $\begin{bmatrix} -1 & 1 \\ 0 & 0 \end{bmatrix}$ will allign with $U^{(j)}$. Similarly, the *predator's* bidirectional migrational reaction between sites i and j give the blocks $\begin{bmatrix} 0 & 0 \\ 1 & -1 \end{bmatrix}$ alligned with $U^{(i)}$ and $\begin{bmatrix} 0 & 0 \\ -1 & 1 \end{bmatrix}$ alligned with $U^{(j)}$. The migrational reaction rate functions are constructed in the conventional way using the Law of Mass Action. Now we may examine some numerical results. Typical graphs in $\mathbb{R}^2$ overlaid with all 10 sites are unclear; heatmap-style images lend themselves better to understanding spatial distribution of population densities over time.



Initial conditions: $X_0 = 100$, $Y_0 = 100$,$\alpha = 1.2$, $\beta = 0.005$, $\gamma = 0.8$, $\delta = 0.005$, $c_1 = 1$, $c_2 = 0.005$, $c_3 = 0.6$, all reaction rates set to 0.001

Results and Concluding Remarks

The stochastic simulation produces a spatially assymetric periodic density pattern whereas the deterministic system evolves according to a uniform periodic pattern. That is, the unpredictability of the stochastic process carries over to the spatial component of the model as expected. Additionally, whereas before the stochastic simulations produced comparable amplitudes over time, the spatial interaction compounds their erratic nature. On the other hand, the deterministic system's amplitudes over time decrease predictably and form a uniform "wave" of arrival times across the sites. Qualitatively, the arrival time of a species in the stochastic system is more difficult to discern than that of the deterministic system. Also, the Exact SSA's superior accuracy to the Chemical Langevin Equation becomes readily apparent in the multi-site spatial simulation and redoubles the need for an accurate SDE approximation to the Gillespie Method.

The natural motivation for this expansion of the Lotka-Volterra Model may be seen in archipelagos or other interacting ecological systems. Our ability to describe concrete situations is somewhat limited by the scope of the paper. For example, the parameter choices used in the simulations in this paper are based on experimentation and convention by researchers in the field, not on ecological field observations. With the appropriate theoretical and field background, one might develop observations leading to a more realistic simulation of natural systems, especially in choosing better-suited reaction rate functions than those given by the Law of Mass Action. Several nontrivial open problems were touched upon in this paper such as the formalization of the extinction probabilities at a given site in stochastic Lotka-Volterra Model with Migration. More generally, a concise equation describing the spatial evolution of the Migrational Lotka-Volterra Model in time does not exist. Few digraphical space-time stochastic differential equations may be found in general although many algorithmic approaches have come from chemical kinetics. Additionally, an active area of stochastic research focuses on improving approximations of the Exact SSA (and the Chemical Master Equation) by *highly accurate* stochastic differential equations. With the appropriate tools and visualization methods, it is possible that many intractable situations may become understandable through a correctly formulated model.

References

[1] Bause F., Kritzinger P. (2002). *Stochastic Petri nets : an introduction to the theory.* Wiesbaden.

[2] Gillespie D. (2001), "Approximate Accelerated Stochastic Simulation of Chemically Reacting Systems," Journal of Chemical Physics,115(4):1716-1733.

[3] Gillespie D. (1977), "Exact Stochastic Simulation of Coupled Chemical Reactions," The Journal of Physical Chemistry, 81(25): 2340-2361.

[4] Hofbauer J., Sigmund K. (1998). *Evolutionary Games and Population Dynamics*, Cambridge U Press.

[5] Øksendal B. (2007*). Stochastic Differential Equations: An Introduction with Applications*, Springer-Verlag.

[6] Wilkinson D.J. (2006). "Tutorial on (Computational Systems) Biological Models." SAMSI Kickoff.

[7] Wilkinson D.J. (2006). *Stochastic Modeling for Systems Biology*, Chapman & Hall/CRC Press.