# Uncertainty Quantification Using Polynomial Chaos in Spatial Population Dynamics System

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# Outline

# Introduction 1

- Population dynamics in natural systems are usually modelled by differential equations.
- One of the most important mathematical models is given by :

$$\frac{du}{dt} = ru\left(1 - \left(\frac{u}{K}\right)^{\theta}\right), u(0) = u_0$$

- This model describes the population growth $u$ over time (temporally) in a deterministic environment.
- However, natural populations grow over spatial regions subject to stochasticity due to various reasons or sources.

# Introduction 2

- Generally, the existing models make room for stochasticity due to environmental conditions or demographic variations.
- Typically general modelling approach gives a diffusion equation given by :

$$du = ru\left(1 - (\frac{u}{K})^{\theta}\right) dt + \sigma(u)dw_t,$$

  where the red portion is the deterministic part and the blue portion is the stochastic part of the model.
- In essence, the red portion implies that the existing model parameters are assumed to be constants and the blue portion implies that the parameters may vary randomly due to some unknown sources.

# Our Contribution

We plan to model the uncertainty in the population size $u(x, y, t)$'s, distribution by studying it's mean and variance in a spatial domain over time, where the uncertainty is introduced due to randomly varying model parameter.

# Problem Statement

We consider a population growing logistically in a spatial domain governed by :

$$\frac{\partial}{\partial t} u(x, y, t) = u(x, y, t) r \left(1 - \left(\frac{u(x, y, t)}{K}\right)^{\theta}\right) + d \left(\frac{\partial^2}{\partial x^2} u(x, y, t) + \frac{\partial^2}{\partial y^2} u(x, y, t)\right), \tag{1}$$

where

- $u(x, y, t)$ is the population density.
- $K$ is the maximum carrying capacity of the system.
- $d$ is the diffusion coefficient.
- $r$ is the intrinsic growth rate, which we have taken to be a random variable following a known distribution. This makes the population density $u(x, y, t)$ a random variable.
- We have built and solved the system for $\theta = 1$.

**Goal** : To solve the equation 1 for $u(x, y, t) := u$. Essentially to characterise the distribution of $u$ at different times.

# Method 1: Polynomial Chaos Expansion

**Idea**: We express an unknown or complicated random variable $Y$ following and unknown distribution $F_Y$ as a function of known random variable $X$. That is:

$$Y = c_0 + c_1\psi_1(X) + c_2\psi_2(X) + \cdots$$

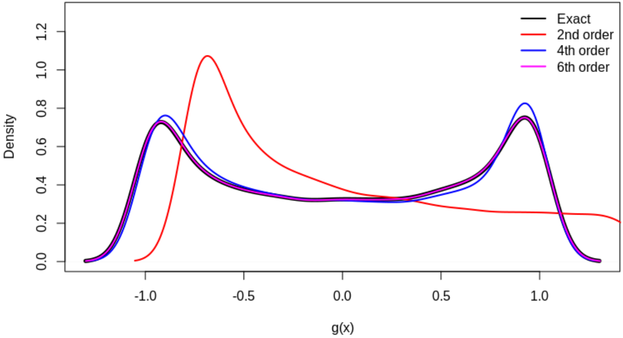
- We now have to find the unknown deterministic constants $\{C_i\}_{i=0}^{\infty}$.
- If the functions $\{\psi_i(X)\}_{i=0}^{\infty}$ are orthogonal polynomials, we have a computational advantage.

This is the basic idea of Polynomial Chaos Expansion, to express an unknown random variable $Y$ as a linear combination of orthogonal polynomials of a known random variable $X$.

# PCE: An Illustrative Example

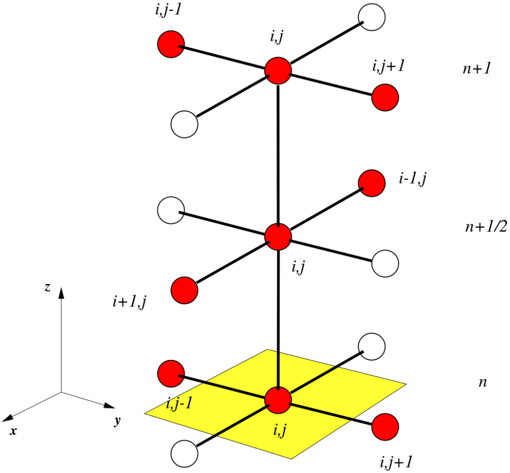
We consider a known random variable $X$, following uniform distribution in this case and approximate the density of it's function $cos(X)$ using PCE. [8]

Figure 1: Approximation of Cos(X)



# Method 2: Alternate Direction Implicit Method

Figure 2: ADI



# Solution to the problem 1

We express the population density:

$$u(x, y, t) = \sum_{i=0}^{\infty} u_i \psi_i(\xi) \tag{2}$$

The equation 2 is the Polynomial chaos expansion(PCE) of $u$.

- $\xi$ is a vector of orthonormal random variables, $\psi(\xi)$ are known orthogonal polynomials. These orthogonal polynomials have a weight function that is precisely the density function of $\xi$.
- The choice of $\xi$ and $\psi$ is free and can be chosen by the type of system.
- As it is not feasible to actually consider an infinite series, we truncate the expansion to P+1 terms with

$$P + 1 = \frac{(N + K)!}{(N!)(K!)}$$

where N is the number of random variables in the vector and K is the highest degree of the polynomial.[5]

# Solution to the problem 2

The truncated PCE of $u$ is:

$$u(x, y, t) = \sum_{i=0}^{P} u_i \psi_i(\xi) \tag{3}$$

Substituting equation 3 in equation 1 we have:

$$\frac{\partial}{\partial t} \sum_{i=0}^{P} u_i \psi_i(\xi) = \xi \sum_{i=0}^{P} u_i \psi_i(\xi) \left(1 - \left(\frac{\sum_{i=0}^{P} u_i \psi_i(\xi)}{K}\right)\right) + d\nabla^2 \sum_{i=0}^{P} u_i \psi_i(\xi) \tag{4}$$

- $r$ is the intrinsic growth rate which is a random variable $\xi$ following Uniform distribution in $[-1, 1]$, and so the polynomials $\psi_i(\xi)$ are the set of Legendre polynomials.
- We denote $\psi_i(\xi) := \psi_i$.
- $\nabla^2$ is the Laplacian operator.

# Mathematical Formulation 1

We take inner product with $\psi_k, \forall k = 0, 1, \cdots, P$ in equation 4. By exploiting orthogonality we obtain a simpler expression:

- $$< \psi_k^2, 1 > (u_k)_t = \sum_{l=0}^{P} (u_i) < \psi_i(\xi), \psi_k > - \frac{1}{K} \sum_{l=0}^{P} (u_i)^2 < \psi_i^2(\xi), \psi_k > - \frac{2}{K} \sum_{m=1}^{P} \sum_{l=0}^{m-1} (u_l u_m) < \psi_l \psi_m(\xi), \psi_k > + d\left((u_k)_{xx} + (u_k)_{yy}\right) < \psi_k^2, 1 >, k = 0, 1, \cdots, P \tag{5}$$

where $(u_k)_t = \frac{\partial}{\partial t} u(x, y, t, \omega), (u_k)_{xx} = \frac{\partial^2}{\partial x^2} u(x, y, t, \omega), (u_k)_{yy} = \frac{\partial^2}{\partial y^2} u(x, y, t, \omega)$

# Mathematical Formulation 2

- A system has been developed for $\theta = 1$ using the ADI method.
- The partial derivatives are approximated using difference schemes.
- We have employed appropriate linearisation techniques.
- There are two systems for each time step.
- The mean and variance of the population size are [5]:

$$E[U(x, y, t)] = U_0$$

$$Var(U(x, y, t)) = \sum_{i=1}^{P} U_K^2 < \psi_K, \psi_K >$$

# Difference Schemes for Partial Derivatives and Linearisation

- We choose grid spacing $\Delta x, \Delta y$ in x and y directions and $\Delta t$ time spacing. We discretise time derivative using forward differencing and the Laplacian using central differencing scheme.

$$\frac{\partial}{\partial t} u_{(i,j)}^{(n+1)} = \frac{u_{(i,j)}^{(n+1)} - u_{(i,j)}^{(n)}}{\Delta t/2}, \textit{Time Derivative Approximation}$$

$$\frac{\partial^2}{\partial x^2} u_{(i,j)}^{(n)} = \frac{u_{(i-1,j)}^{(n)} - 2u_{(i,j)}^{(n)} + u_{(i-1,j)}^{(n)}}{(\Delta x)^2}, \textit{Space Derivative Approximation}$$

- In the first direction, we move in x direction keeping y same in first half time step $(n, n + \frac{1}{2})$.
- In the next direction along y keeping x constant in time interval $(n + \frac{1}{2}, n + 1)$.
- The linearisation has been done in the following way :
  $(u_l) = ((u_l)^{(n+1/2)} + (u_l)^{(n)})/2$
  $(u_l)^2 = ((u_l)^{(n+1/2)}(u_l)^{(n)})$

# The systems

- On substituting the PCE in both directions and rearranging terms, we get the following two systems. The first system gives one column of values of $U_k^{(n+0.5)}$ and the second a row of $U_k^{(n+1)}$.
- We have

$$A1_{k,j}U_{k,j}^{(n+0.5)} = R1_{k,j}^{(n)}$$

  for the first direction and

$$A2_{k,i}U_{k,i}^{(n+1)} = R2_{k,i}^{T\,(n+0.5)}$$

  for each $k = 0, 1, 2, ..., P; n = 0, 1, ..., N - 1$, which is a system of P+1 equations each and j indexes the columns while i indexes the rows.
- $A1_{k,j} and A2_{k,i}$ are matrices of order $(N_x + 1)x(N_x + 1)$ and $(N_y + 1)x(N_y + 1)$ respectively, where $N_x$ and $N_y$ are the number of intervals x and y space directions are discretised in respectively.

# Matrices 1

- $$A1_k = \begin{pmatrix} b_{k(0,j)} & a_0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ a_0 & b_{k(1,j)} & a_0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & a_0 & b_{k(3,j)} & a_0 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & a_0 & b_{k(N_x-2,j)} & a_0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & a_0 & b_{k(N_x-1,j)} & a_0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & a_0 & b_{k(N_x,j)} \end{pmatrix}$$

$$A2_k = \begin{pmatrix} -f_{k(i,0)} & c_0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ c_0 & -f_{k(i,1)} & c_0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & c_0 & -f_{k(i,2)} & c_0 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & c_0 & -f_{k(i,N_y-2)} & c_0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & c_0 & -f_{k(i,N_y)} & c_0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & c_0 & -f_{k(i,N_y)} \end{pmatrix}$$

# Matrices 2

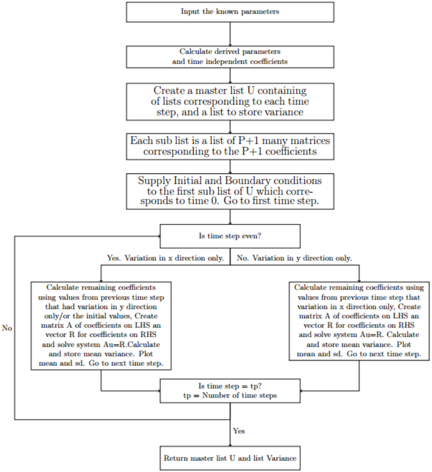
- $U_{k,j}^{(n+0.5)} = \begin{pmatrix} u_{k(0,j)}^{(n+1/2)} \\ u_{k(1,j)}^{(n+1/2)} \\ u_{k(2,j)}^{(n+1/2)} \\ \vdots \\ u_{k(N_x-2,j)}^{(n+1/2)} \\ u_{k(N_x-1,j)}^{(n+1/2)} \\ u_{k(N_x,j)}^{(n+1/2)} \end{pmatrix}$, $U_{k,i}^{(n+1)} = \begin{pmatrix} u_{k(i,0)}^{(n+1)} \\ u_{k(i,1)}^{(n+1)} \\ u_{k(i,2)}^{(n+1)} \\ \vdots \\ u_{k(i,N-2)}^{(n+1)} \\ u_{k(i,N_y-1)}^{(n+1)} \\ u_{k(i,N_y)}^{(n+1)} \end{pmatrix}$
- $R1_{k,j} = \begin{pmatrix} rhs1_{0(0,j)} \\ rhs1_{1(1,j)} \\ rhs1_{2(2,j)} \\ \vdots \\ rhs1_{N_x-2(N_x,j)} \\ rhs1_{N_x-1(N_x,j)} \\ rhs1_{N_x(N_x,j)} \end{pmatrix}$, $R2_{k,i}^{T} = \begin{pmatrix} rhs2_{0(i,0)} \\ rhs2_{1(i,1)} \\ rhs2_{2(i,2)} \\ \vdots \\ rhs2_{N_y-2(i,N_y-2)} \\ rhs2_{N_y-1(i,N_y-1)} \\ rhs2_{N_y(i,N_y)} \end{pmatrix}$

# Coefficients

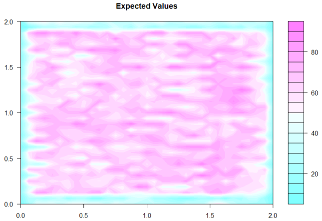
- $a_k = \frac{-d}{(\Delta x)^2}$
- $b_{k_{(i,j)}} = \frac{2<\psi_k^2,1>}{\Delta t} - \frac{<\psi_k(\xi),1\psi_k>}{2} + \frac{(u_k)_{(i,j)}^n}{K} < \psi_k^2(\xi), \psi_k > + \frac{1}{K}\sum_{l=0,l\neq k}^{P}(u_l)_{(i,j)}^n < \psi_l\psi_k(\xi), \psi_k >$ $+ \frac{2d}{(\Delta x)^2} < \psi_k^2, 1 >$
- $c_k = \frac{d}{(\Delta y)^2} < \psi_k^2, 1 >$
- $d_{k_{(i,j)}} = \frac{2<\psi_k^2,1>}{\Delta t} + \frac{<\psi_k(\xi),\psi_k>}{2} - \frac{1}{K}\sum_{l=0,l\neq k}^{P}(u_l)_{(i,j)}^n < \psi_l\psi_k(\xi), \psi_k > - \frac{2d<\psi_k^2,1>}{(\Delta y)^2}$
- $e_{k_{(i,j)}} = \sum_{l=0,l\neq k}^{P}(u_l)_{(i,j)}^n < \psi_l(\xi), \psi_k > - \sum_{l=0,l\neq k}^{P}(u_l^2)_{(i,j)}^n < \psi_l^2(\xi), \psi_k >$ $- \frac{2}{K}\sum_{m=1,m\neq k}^{P}\sum_{l=0,l\neq k}^{m-1}(u_l u_m)_{(i,j)}^n < \psi_l\psi_m(\xi), \psi_k >$
- $f_{k_{(i,j)}} = \frac{2<\psi_k^2,1>}{\Delta t} - \frac{<\psi_k(\xi),\psi_k>}{2} + \frac{(u_k)_{(i,j)}^{(n+1/2)}}{K} < \psi_k^2(\xi), \psi_k > + \frac{1}{K}\sum_{l=0,l\neq k}^{P}(u_l)_{(i,j)}^{(n+1/2)} < \psi_l\psi_k(\xi), \psi_k >$ $+ \frac{2d}{(\Delta y)^2} < \psi_k^2, 1 >$
- $g_{k_{(i,j)}} = \frac{2<\psi_k^2,1>}{\Delta t} + \frac{<\psi_k(\xi),\psi_k>}{2} - \frac{1}{K}\sum_{l=0,l\neq k}^{P}(u_l)_{(i,j)}^{(n+1/2)} < \psi_l\psi_k(\xi), \psi_k > - \frac{2d<\psi_k^2,1>}{(\Delta x)^2}$
- $h_{k_{(i,j)}} = \sum_{l=0,l\neq k}^{P}(u_l)_{(i,j)}^{(n)+1/2} < \psi_l(\xi), \psi_k > - \sum_{l=0,l\neq k}^{P}(u_l^2)_{(i,j)}^n < \psi_l^2(\xi), \psi_k >$ $- \frac{2}{K}\sum_{m=1,m\neq k}^{P}\sum_{l=0,l\neq k}^{m-1}(u_l u_m)_{(i,j)}^n < \psi_l\psi_m(\xi), \psi_k >$
- $rhs1_{k_{(i,j)}} = c_k(u_k)_{(i,j-1)}^{(n)} + d_{k_{(i,j)}}(u_k)_{(i,j)}^{(n)} + c_k(u_k)_{(i,j+1)}^{(n+1/2)} + e_{k_{(i,j)}}.$
- $rhs2_{k_{(i,j)}} = a_k(u_k)_{(i-1,j)}^{(n+1/2)} - g_{k_{(i,j)}}(u_k)_{(i,j)}^{(n+1/2)} + a_k(u_k)_{(i+1,j)}^{(n+1/2)} - h_{k_{(i,j)}}.$

# Flowchart of Algorithm

Figure 3: Algorithm



# Results 1

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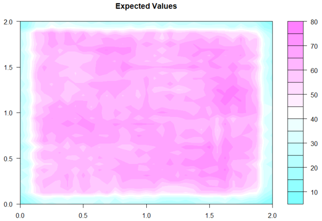


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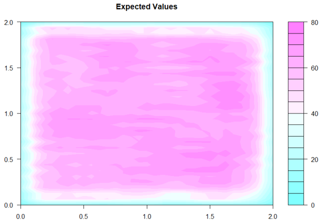


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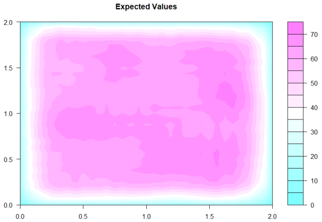
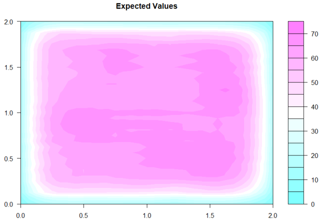



[t=4]

# Results 2

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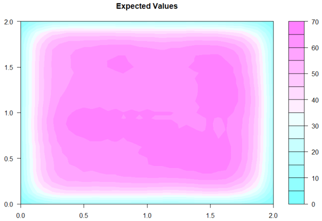


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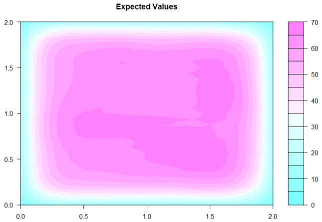


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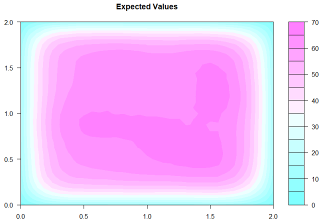
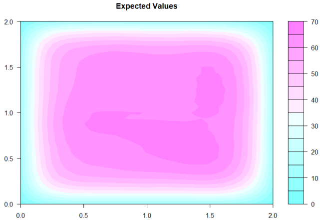



[t=8]

# Results 3

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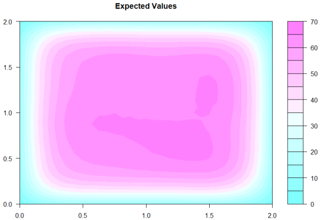


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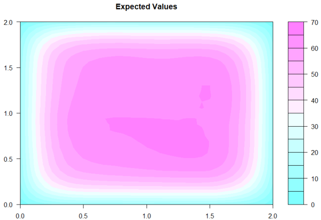


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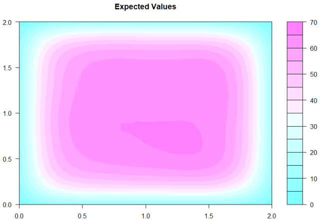


[t=12]

# Future Work

- Full implementation of $\theta$ logistic model for different values of $\theta$.
- Further study concepts to be able to develop system incorporating non-constant random variable in time and space.
- Making code as general and accessible for use as possible.

We expect this method to provide accurate confidence intervals for population predictions.
We sincerely hope that this work will be useful to practitioners and researchers in understanding the natural population growth.
The entire system is solved completely in R. All functions used have been written by us.
Please mail me for the full program at : **kshitijanandpatil@gmail.com**

# Thank you for your time

# References


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