Path Integrals for Continuous-Time Markov Chains

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AUSTRALIAN RESEARCH COUNCIL
Centre of Excellence for Mathematics and Statistics of Complex Systems
A population process

Simulation of a population

Population density $X(t)$

Time $t$ (years)
A population process

Simulation of a population

Threshold $\gamma = 0.13$
Total cost

Let $X(t)$ be the population density at time $t$.

Let $c(x)$ be the cost per unit time of maintaining the population when its density is $x$ units above a threshold $\gamma$.

Then, if $\tau$ is the time to extinction,

$$
\int_0^\tau c(X(t) - \gamma)1\{X(t) > \gamma\} \, dt
$$

is the total cost over the life of the population.
A population process

\[ \tau = 21.7 \text{ (years)} \]

\[ \int_{0}^{\tau} N(X(t) - \gamma) 1_{\{X(t) > \gamma\}} \, dt = 11.8 \]
Ingredients

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- A set of states \(A\)
- The (random) time \(\tau\) to first exit from \(A\)
- The cost (per unit time) \(f_x\) of being in state \(x\)
- The “path integral”

\[
\Gamma = \int_0^\tau f_X(t) \, dt,
\]

the total cost incurred before leaving \(A\) (also random)
Consider a dam with finite capacity $V$, and let $X(t)$ be the water level at time $t$.

We might wish to estimate the total time for which the level was below a given value $\gamma$,

$$\Gamma = \int_0^\tau 1\{X(t) < \gamma\} \, dt,$$

where $\tau$ is (say) the time to reach capacity or to empty (whichever occurs first).
Dam

Water level in a dam

Level $X(t)$

Time $t$ (weeks)

$67$

$66.5$

$66$

$65.5$

$65$

$64.5$

$64$

$63.5$

$63$
Water level in a dam

Level $X(t)$ vs. Time $t$ (weeks)
Dam

Water level in a dam

Level $X(t)$

Time $t$ (weeks)
Water level in a dam

Level $X(t)$

Time $t$ (weeks)

500 550 600 650 700 750 800 850 900
$\tau = 3546.8 \text{ (weeks)}$

$\int_0^\tau 1_{\{X(t) < 20\}} \, dt = 224.2 \text{ (weeks)}$
Other examples

Let \((S(t), I(t))\) be the number of susceptibles and infectives in an epidemic at time \(t\).

If \(\tau\) is the period of infection and \(f_{(s,i)} = i\), then \(\Gamma\) is the total amount of infection:

\[
\Gamma = \int_{0}^{\tau} I(t) \, dt.
\]
The progress of an infection

S(t) susceptible cells

I(t) infected cells
Epidemic

The progress of an infection

\( \tau = 144.5 \text{ (days)} \)
Epidemic

The progress of an infection

\[ \tau = 144.5 \text{ (days)} \]

\[ \Gamma = \int_0^\tau I(t) \, dt = 7591 \text{ (cell days)} \]
The problem

Our problem is to determine the expected value, and the distribution of the total cost

\[ \Gamma = \int_0^{\tau} f_{X(t)} \, dt, \]

where recall that \( \tau \) is the time to first exit from a set \( A \) and \( f_x \) is cost per unit time of being in state \( x \).

For simplicity, suppose that \( X(t) \) takes values in \( S = \{0, 1, \ldots \} \).

For example, \( X(t) \) might be the number in a population at time \( t \), and \( A = \{1, 2, \ldots \} \), so that \( \tau \) is the time to extinction.
Let $T_j$ be the total time that the process spends in state $j$ during the period up to time $\tau$ and let $N_j$ be the number of visits to $j$ during that period. Then,

$$\Gamma = \sum_{j \in A} f_j T_j$$
Let $T_j$ be the total time that the process spends in state $j$ during the period up to time $\tau$ and let $N_j$ be the number of visits to $j$ during that period. Then,

$$
\Gamma = \sum_{j \in A} f_j T_j \quad \text{and} \quad T_j = \sum_{n=1}^{N_j} X_{jn},
$$

where $X_{jn}, \ n = 1, 2, \ldots,$ are the successive occupancy times for state $j$. 

A first attempt at evaluating $E(\Gamma)$
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Let \( T_j \) be the total time that the process spends in state \( j \) during the period up to time \( \tau \) and let \( N_j \) be the number of visits to \( j \) during that period. Then,

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\Gamma = \sum_{j \in A} f_j T_j \quad \text{and} \quad T_j = \sum_{n=1}^{N_j} X_{jn},
\]

where \( X_{jn}, n = 1, 2, \ldots, \) are the successive occupancy times for state \( j \). Then, under mild conditions,

\[
E(\Gamma) = \sum_{j \in A} f_j E(N_j) \mu_j, \quad \text{where} \quad \mu_j \text{ is the mean occupancy time for state } j.
\]
Markovian models

We will assume that \((X(t), t \geq 0)\) is a **Markov chain** with **transition rates**

\[ Q = (q_{ij}, i, j \in S), \]

so that \(q_{ij}\) represents the rate of transition from state \(i\) to state \(j\), for \(j \neq i\), and \(q_{ii} = -q_i\), where

\[ q_i := \sum_{j \neq i} q_{ij} \quad (< \infty) \]

represents the total rate out of state \(i\).
Markovian models

An example is the *birth-death process*, which has

\[ q_{i,i+1} = \lambda_i \]  \hspace{1cm} \text{(birth rates)}

\[ q_{i,i-1} = \mu_i \]  \hspace{1cm} \text{(death rates)},

with \( \mu_0 = 0 \) and otherwise 0 (\( q_i = \lambda_i + \mu_i \)):

\[
Q = \begin{pmatrix}
-\lambda_0 & \lambda_0 & 0 & 0 & \cdots \\
\mu_1 & -(\lambda_1 + \mu_1) & \lambda_1 & 0 & \cdots \\
0 & \mu_2 & -(\lambda_2 + \mu_2) & \lambda_2 & \cdots \\
\vdots & \vdots & \vdots & \ddots & \ddots
\end{pmatrix}
\]
Example

The *Stochastic Logistic Model* (simulated earlier) is a birth-death process on \( S = \{0, 1, \ldots, N\} \), with

\[
\lambda_i = \frac{\lambda}{N} i (N - i) \quad \text{and} \quad \mu_i = \mu i,
\]

where \( \lambda, \mu > 0 \).
These birth and death rates can be written

\[ \frac{\lambda_i}{N} = \lambda \left( \frac{i}{N} \right) \left( 1 - \frac{i}{N} \right) \quad \text{and} \quad \frac{\mu_i}{N} = \mu \left( \frac{i}{N} \right) \]

**Intuition:** for large \( N \) the population density \( X(t)/N \) becomes more deterministic (non-random):

\[ \frac{dx}{dt} = \lambda(x) - \mu(x), \]

where

\[ \lambda(x) = \lambda x (1 - x) \quad \text{and} \quad \mu(x) = \mu x. \]
Interlude

Soit $p$ la population : représentons par $dp$ l’accroissement infiniment petit qu’elle reçoit pendant un temps infiniment court $dt$. Si la population croissait en progression géométrique, nous aurions l’équation $\frac{dp}{dt} = mp$. Mais comme la vitesse d’accroissement de la population est retardée par l’augmentation même du nombre des habitants, nous devrons retrancher de $mp$ une fonction inconnue de $p$ ; de manière que la formule à intégrer deviendra

$$\frac{dp}{dt} = mp - \varphi(p).$$

L’hypothèse la plus simple que l’on puisse faire sur la forme de la fonction $\varphi$, est de supposer $\varphi(p) = np^2$. On trouve alors pour intégrale de l’équation ci-dessus

$$t = \frac{1}{m} \left[ \log p - \log (m-np) \right] + \text{constante},$$

et il suffira de trois observations pour déterminer les deux coefficients constants $m$ et $n$ et la constante arbitraire.
En résolvant la dernière équation par rapport à \( p \), il vient

\[
p = \frac{np'\ e^m}{np'\ e^m + m - np'} \quad \cdots \cdots (1)
\]

en désignant par \( p' \) la population qui répond à \( t = 0 \), et par \( e \) la base des logarithmes népériens. Si l'on fait \( t = \infty \), on voit que la valeur de \( p \) correspondante est \( P = \frac{m}{n} \). Telle est donc la limite supérieure de la population.

Au lieu de supposer \( np = np' \), on peut prendre \( np = np^2 \), \( a \) étant quelconque, ou \( np = n \log p \). Toutes ces hypothèses satisfont également bien aux faits observés; mais elles donnent des valeurs très différentes pour la limite supérieure de la population.

J'ai supposé successivement

\[
\varphi p = np^2, \ \varphi p = np^3, \ \varphi p = np^4, \ \varphi p = n \log p
\]

et les différences entre les populations calculées et celles que fournit l'observation ont été sensiblement les mêmes.
Interlude

This is from ...


We learn that

\[ p(t) = \frac{mp_0}{np_0 + (m - np_0)e^{-mt}}, \quad t \geq 0. \]

For us,

\[ \frac{X(t)}{N} \sim \frac{(1 - \rho)x_0}{x_0 + (1 - \rho - x_0)e^{-\lambda(1-\rho)t}}, \quad \text{where } \rho = \frac{\mu}{\lambda}. \]
A population process

Stochastic Logistic Model

Population density \( X(t)/N \)

Time \( t \) (years)

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Example

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where \( \lambda, \mu > 0 \).
Example

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\]

where \( \lambda, \mu > 0 \).

The *epidemic model* mentioned earlier is a two-dimensional Markov chain with transition rates

\[
q(s\ i),(s+1\ i) = \alpha s, \quad q(s\ i),(s\ i-1) = \gamma i,
\]

\[
q(s\ i),(s-1\ i+1) = \beta s i,
\]

where \( \alpha, \gamma, \beta > 0 \) are the *splitting, removal* and *infection* rates.
The expected value of $\Gamma$

Returning to our general Markov chain, let
\[ e_i = E_i(\Gamma) := E(\Gamma | X(0) = i), \]
and condition on the time of the first jump and the state visited at that time, to get

\[
E_i(\Gamma) = \int_0^\infty \sum_{k \neq i} \left( \frac{f_i}{q_i} + E_k(\Gamma) \right) \frac{q_{ik}}{q_i} q_i e^{-q_i u} \, du,
\]

which leads to

\[
q_i e_i = f_i + \sum_{k \neq i} q_{ik} e_k,
\]

so that

\[
\sum_k q_{ik} e_k + f_i = 0.
\]
The expected value of $\Gamma$

We can do better:

**Theorem 1** $e = (e_i, i \in A)$, where $e_i = E_i(\Gamma)$, is the *minimal* non-negative solution to

$$\sum_{k \in A} q_{ik} z_k + f_i = 0, \quad i \in A,$$

in the sense that $e$ satisfies these equations, and, if $z = (z_i, i \in A)$ is any non-negative solution, then $e_i \leq z_i$ for all $i \in A$. 
The expected value of $\Gamma$

So, we solve a system of linear equations to obtain the vector of expected total costs starting in the various states:

$$Qz = -f$$
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Transition rates restricted to \( A \) (the model)
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Transition rates restricted to $A$ (the model)

Unit costs
The expected value of $\Gamma$

So, we solve a system of linear equations to obtain the vector of expected total costs starting in the various states:

$$Qz = -f$$

1. **Transition rates restricted to $A$ (the model)**
2. **Unit costs**
3. **Expected total cost (minimal solution)**
Let’s apply this to *birth-death processes*:

\[
Q = \begin{pmatrix}
-\lambda_0 & \lambda_0 & 0 & 0 & \cdots \\
\mu_1 & -(\lambda_1 + \mu_1) & \lambda_1 & 0 & \cdots \\
0 & \mu_2 & -(\lambda_2 + \mu_2) & \lambda_2 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}
\]

Assume that the birth rates \((\lambda_i, i \geq 1)\) and the death rates \((\mu_i, i \geq 0)\) are all strictly positive, except that \(\lambda_0 = 0\). So, all states in \(A = \{1, 2, \ldots\}\) intercommunicate, and 0 is an absorbing state (corresponding to population extinction).
Birth-death processes

Define \( (\pi_i, \ i \geq 1) \) by \( \pi_1 = 1 \) and

\[
\pi_i = \prod_{j=2}^{i} \frac{\lambda_{j-1}}{\mu_j}, \quad i \geq 2,
\]

and assume that

\[
\sum_{i=1}^{\infty} \frac{1}{\mu_i \pi_i} = \infty,
\]

a condition that corresponds to extinction being certain.
On applying Theorem 1 we get:

**Proposition**  The expected cost up to the time of extinction, starting in state $i \ (\geq 1)$, is given by

$$E_i(\Gamma) = \sum_{j=1}^{i} \frac{1}{\mu_j\pi_j} \sum_{k=j}^{\infty} f_k \pi_k,$$

this being finite if and only if $\sum_{k=1}^{\infty} f_k \pi_k < \infty$. 
In the finite state-space case \( S = \{0, 1, \ldots, N\} \), we get

\[
E_i(\Gamma) = \sum_{j=1}^{i} \frac{1}{\mu_j \pi_j} \sum_{k=j}^{N} f_k \pi_k, \quad i = 1, 2, \ldots, N.
\]

For the Stochastic Logistic Model,

\[
E_i(\Gamma) = \frac{1}{\mu} \sum_{j=1}^{i} \frac{N-j}{(N-1)!} \sum_{k=0}^{j} \left( \frac{1}{N \rho} \right)^k \frac{f_{j+k}}{j+k} \frac{(N-j)!}{(N-j-k)!},
\]

where \( \rho = \mu / \lambda \). If \( \rho < 1 \) (the interesting case),

\[
E_i(\Gamma) \sim \frac{\rho}{\mu(1-\rho)} \left( \frac{e^{-(1-\rho)}}{\rho} \right)^N \sqrt{\frac{2\pi N}{N}} \sum_{j=1}^{i} f_j \rho^j \quad \text{as} \quad N \to \infty.
\]
Can we evaluate the distribution of $\Gamma$, that is,

$$\Pr(\Gamma \leq x | X(0) = i)$$
The distribution of $\Gamma$

Can we evaluate the distribution of $\Gamma$, that is,

$$\Pr(\Gamma \leq x | X(0) = i)$$

I will explain how to evaluate $y_i(\theta) = E_i(e^{-\theta \Gamma})$, the Laplace-Steiltjes Transform (LST) of the distribution:

$$y_i(\theta) = \int_0^\infty e^{-\theta x} \, d\Pr(\Gamma \leq x | X(0) = i).$$
An argument similar to that used to evaluate $E_i(\Gamma)$ leads to:

**Theorem 2**    For each $\theta > 0$, $\mathbf{y}(\theta) = (y_i(\theta), i \in S)$ is the *maximal* solution to

$$\sum_{k \in S} q_{ik} z_k = \theta f_i z_i, \quad i \in A,$$

with $0 \leq z_i \leq 1$ for $i \in A$ and $z_i = 1$ for $i \notin A$. 
A catastrophe process

Assume that the transition rates have the form

\[ q_{ij} = \begin{cases} 
  i\rho a, & i \geq 0, \ j = i + 1, \\
  -i\rho, & i \geq 0, \ j = i, \\
  i\rho d_{i-j}, & i \geq 2, \ 1 \leq j < i, \\
  i\rho \sum_{k \geq i} d_k, & i \geq 1, \ j = 0, 
\end{cases} \]

with all other transition rates equal to 0. Here \( \rho \) and \( a \) are positive, \( d_i \) is positive for at least one \( i \) in \( A = \{1, 2, \ldots\} \) and \( a + \sum_{i=1}^{\infty} d_i = 1 \).

Clearly 0 is an absorbing state for the process and \( A \) is a communicating class.
A catastrophe process

We will consider only the subcritical case, where the drift \( D \), given by \( D = a - \sum_{i=1}^{\infty} id_i \), is strictly negative and extinction is certain.

Let \( b(s) = d(s) - s \), where \( d \) is the probability generating function \( d(s) = a + \sum_{i=1}^{\infty} d_i s^{i+1}, |s| < 1 \).

There is a unique solution, \( \sigma \), to \( b(s) = 0 \) on the interval \( 0 < s < 1 \).
We can evaluate $E_i(e^{-\theta \Gamma})$ for specific choices of $f$.

For example, take $f_i = i$.

We seek the maximal solution to

$$\sum_{j=0}^{\infty} q_{ij} z_j = \theta i z_i, \quad i \geq 1,$$

satisfying $0 \leq z_i \leq 1$ for $i \geq 1$ and $z_0 = 1$. 
A catastrophe process

We can evaluate $E_i(e^{-\theta \Gamma})$ for specific choices of $f$.

For example, take $f_i = i$.

We seek the maximal solution to

$$\rho a z_{i+1} - \rho z_i + \rho \sum_{j=1}^{i-1} d_{i-j} z_j + \rho z_0 \sum_{j=i}^{\infty} d_j = \theta z_i, \quad i \geq 1,$$

satisfying $0 \leq z_i \leq 1$ for $i \geq 1$ and $z_0 = 1$. 
A catastrophe process

Multiplying by $s^{i-1}$ and summing over $i$ gives

$$\sum_{i=1}^{\infty} E_i (e^{-\theta \Gamma}) s^{i-1} = \frac{1}{1 - s} - \frac{\theta (\gamma_\theta - s)}{(1 - \gamma_\theta)(1 - s)(\rho b(s) - \theta s)},$$

where $\gamma_\theta$ is the unique solution to $\rho b(s) = \theta s$ on the interval $0 < s < \sigma$, where $\sigma$ itself is the unique solution to $b(s) = 0$ on the interval $0 < s < 1$. 
In the case of “geometric catastrophes” \((d_i = d(1 - q)q^{i-1}, i \geq 1, \text{ where } d > 0 \text{ satisfies } a + d = 1, \text{ and } 0 \leq q < 1)\), we get

\[
E_i(e^{-\theta \Gamma}) = \frac{\beta(\theta) - q}{1 - q} (\beta(\theta))^{i-1}, \quad i \geq 1,
\]

where \(\beta(\theta)\) is the smaller of the two zeros of

\[
a \rho s^2 - (\rho(1 + qa) + \theta)s + \rho(d + qa) + q\theta.
\]
Workshop

ARC Centre of Excellence for Mathematics and Statistics of Complex Systems

Workshop on Metapopulations

The University of Queensland
Thursday 2nd September 2004

Invited speakers: Andrew Barbour (University of Zürich)
Ben Cairns, Phil Pollett, Hugh Possingham, Tracey Regan,
Joshua Ross, Severine Vuilleumier and Chris Wilcoxon
(University of Queensland).