Solving Master Equations. A simple tutorial.

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Organisation of the Tutorial

1. Master Equations: notation, basic facts, and examples
2. Steady State
3. Generating Function Approach
4. Gardiner's Poisson Representation

References

1. Feller, W. (1968) **An introduction to Probability Theory and Its Aplications**, vol.I & II, (3rd ed.). New York: John Wiley & Sons (old but still one of the best references for probabilistis)
2. Gardiner, C. W. (2009). **Stochastic Methods: A Handbook for the Natural and Social Sciences** (4th ed.). Berlin: Springer. (quick and dirty)
3. Van Kampen, N. G. (2007). **Stochastic Processes in Physics and Chemistry** (3rd ed., p. 464). North Holland. (Stochastic processes the "physicist's way")
4. Norris, J. R. (1998). **Markov Chains** (p. 254). Cambridge: Cambridge University Press. (Elegant and tourough)

Markov Processes

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$\mathscr{F}$: the sets of events

Formally σ-algebra on Ω that satisfies:

1. $\varnothing, \Omega \in \mathscr{F}$
2. If $A \in \mathscr{F}$ then $A^{\complement} \in \mathscr{F}$ (negation of events).
3. $\forall \{A_i\}_{i=0}^{\infty} : A_i \in \mathscr{F}, \bigcup_{i=0}^{\infty} A_i \in \mathscr{F}$

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π a (probability) measure

It must satisfy *Kolmogorov's Axioms*:

1. $\forall A \in \mathscr{F}, \pi(A) \in \mathbb{R}$ and $\pi(A) \geq 0$ (positivity)
2. $\pi(\Omega) = 1$ (unitarity or normalisation)
3. $\forall A_i \in \Omega : \forall i \neq j,\ A_i \cap A_j = \emptyset,\ \pi\left(\bigcup_{i=0}^{\infty} A_i\right) = \sum_{i=0}^{\infty} \pi(A_i)$

Stochastic Variable

Intuitively it is a function that takes different values according to the outcome of the system.

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Induced probability

The probability measure induces a probability on the stochastic variable $A \in \mathscr{E}$:

$$p_X(A) = \Pr(X(\omega) \in A) = \pi(X^{-1}(A)) = \int_{\omega} 1_{X^{-1}(A)} \, d\pi$$

Moments

On a stochastic X variable one can define a set of quantities that are called moments. The most commonly used are:

- **Mean :** $\mathbb{E}[X] = \int_\Omega X(\omega)\,\mathrm{d}\pi(\omega) = \int_{X(\Omega)} x\,\mathrm{d}p_X(A)$;
- **Variance :** $\mathrm{Var}(X) = \mathbb{E}[(X - \mathbb{E}[X])^2]$;
- **Covariance :** $\mathrm{Cov}(X) = \mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])]$ if Y is another stochastic variable on the same space.

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A stochastic process is a collection of $(E, \mathscr{E})$ stochastic variables on a probability space $(\Omega, \mathscr{F}, \pi)$ "indexed" by time i.e.

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Natural Filtration

We define a set of events $\mathscr{F}_t$ called *Natural Filtration* a σ-algebra on Ω such that:

1. $\mathscr{F}_t \subset \mathscr{F}$
2. $s < t \rightarrow \mathscr{F}_s \subset \mathscr{F}_t$
3. $\{X_s^{-1}(A) : s \leq t, A \in \mathscr{E}\} \subset \mathscr{F}_t$ **(Adaptivity)**
4. $\mathscr{F}_t$ is the *coarsest* among

Markov Processes

To describe a system you need the joint probabilities for any choice of times for any set $A_{t_n} \subset \mathscr{E} \ldots A_0 \subset \mathscr{E}$:

$$\Pr(X_{t_n} \in A_{t_n} \ldots X_{t_0} \in A_{t_0}) = \Pr(X_{t_n} \in A_{t_n} | X_{t_{n-1}} \in A_{t_{n-1}} \ldots X_{t_0} \in A_{t_0}) \Pr(X_{t_{n-1}} \in A_{t_n} \ldots X_{t_0} \in A_{t_0})$$

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Markov Property

For any $A, B \in \mathscr{E}$ for any $s, t \in T, \; s < t$

$$\Pr(X_t \in A \mid \mathscr{F}_s) = \Pr(X_t \in A \mid X_s \in B)$$

The knowledge of the one point functions $p(A, t) = \Pr(X_t \in A)$ and two point functions $p(A, t \mid B, s) = \Pr(X_t \in A \mid X_s \in B)$ (transition probabilities).

Markov Property: a natural scientist's perspective

Let's assume from now on that $E = \mathbb{R}^k$ or $E = \mathbb{Z}^k$ and the measures can be writen in term either of a density or a discrete probability distribution.

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Markov Property : Discrete time

For a discrete time Markov Chain (i.e. $T = \mathbb{N}$), For all $A_i \in \mathscr{E}$ the markov property reads:

$$\Pr(X_n \in A \mid X_{n-1} \in A_{n-1}, \cdots X_0 \in A_0) = \Pr(X_n \in A_n \mid X_{n-1} \in A_{n-1})$$

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Simplified Markov Property for conuous time

For ant set $t_n, \ldots, t_o \in T$, $t_n > \cdots t_0$ we have:

$$\Pr(X_{t_n} \in A_{t_n} \mid X_{t_{n-1}} \in A_{t_{n-1}}, \cdots X_{t_0} \in A_{t_0}) = \Pr(X_{t_n} \in A_{t_n} \mid X_{t_{n-1}} \in A_{t_{n-1}})$$

Consequences of Markovianity

Any stochastic processes must satisfy consistency requirements. **In particular $n-1$ point functions must be obtained by marginalising an n point functions.**

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In a Markov Process this can be translated in a consistency requirement for transition probabilities.

Champman-Kolmogorov equation for Markov processes

$$p(x,t \mid y,s) = \int_{X_0(\Omega)} p(x,t|z,t')p(z,t' \mid y,s)\,\mathrm{d}z\,, \quad \forall t' \;:\; t > t' > s$$

Markov Jump processes. Continuous time Markov Chains

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$$P(\omega, t + \mathrm{d}t|\omega', t) = \delta_{\omega\omega'} + Q_{\omega\omega'}\,\mathrm{d}t + o(\mathrm{d}t)$$

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Master Equation (Kolmogorov Forward Equation)

A differential version of C–K equation.

$$\partial_t P(\omega', t \mid \omega, s) = \left[\sum_\xi Q_{\omega\xi} P(\xi, t \mid \omega', s)\right] - \left[\sum_\xi Q_{\xi\omega}\right] \cdot P(\omega, t \mid \omega', s)$$

$$P(\omega, s \mid \omega' s) = \delta_{\omega'\omega}$$

Master Equations

The Master Equation can be written in a matricial form:

$$\partial_t P(t, 0) = P(t, 0)Q$$
$$P(s, s) = I$$

where $P(t, 0)_{\omega\omega'} = P(\omega t|\omega' 0)$.

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$$\sum_{\omega'} Q_{\omega\omega'} = 0$$

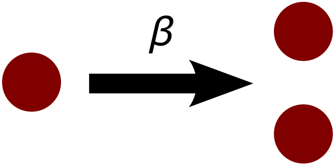
As a consequence

$$Q_{\omega\omega} = -\sum_{\omega'\neq\omega} Q_{\omega\omega'} = 0$$

Birth-Death processes

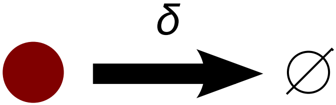
Birth Process

$$\lambda_n = \lambda \cdot n$$



Death Process

$$\delta_n = \delta \cdot n$$



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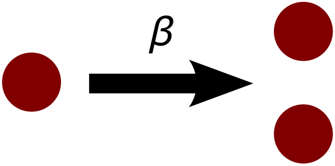

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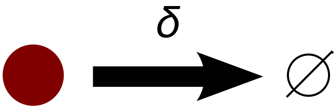
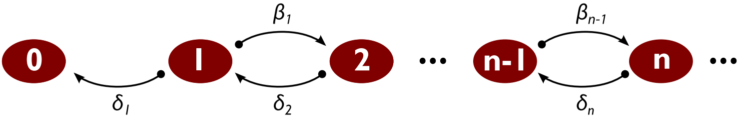
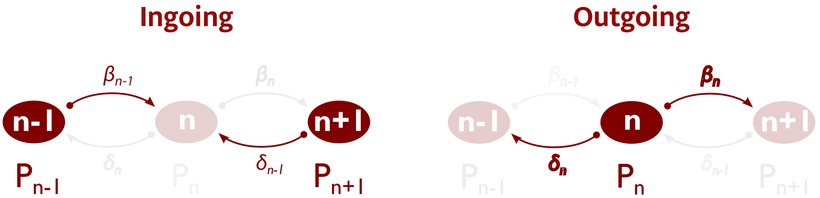




Master Equation for Birth-Death processes



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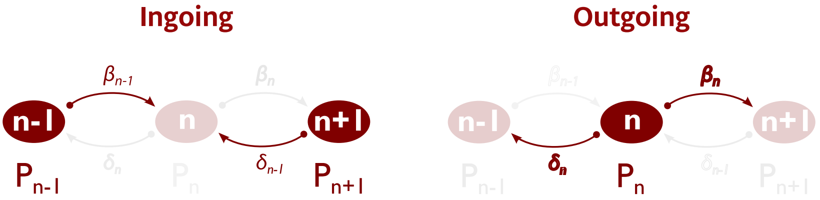

$$\partial_t P_n(t) = \delta \cdot (n+1) P_{n+1}(t) + \beta \cdot (n-1) \cdot P_{n-1}(t) - (\beta + \delta) n P_n(t)$$

Generalised birth-death processes

Accounts for interactions:

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- $n \rightarrow n-1$, δ_n

$$\partial_t P_n(t) = \delta_{n+1} P_{n+1}(t) + \beta_{n-1} P_{n-1}(t) - (\beta_n + \delta_n) P_n(t)$$

Special cases

- $\delta_i = 0$ pure birth process
- $\beta_i = 0$ pure death process
- $\beta_i = \beta, \delta_i = 0$ Poisson process

Contact Processes: *SIS* model.

In a population of size N.

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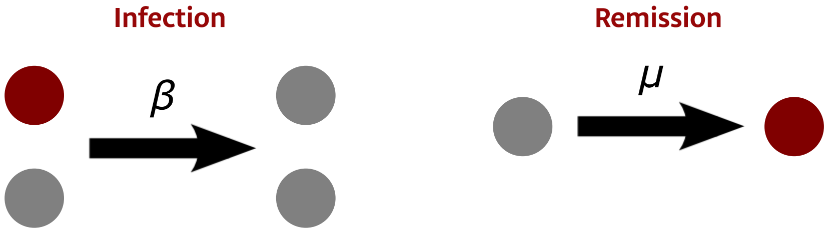

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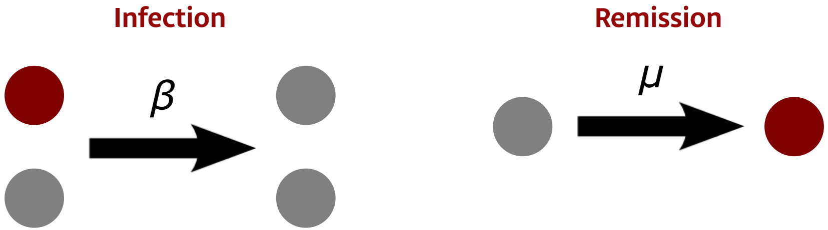

$$\partial_t P(S, I; t) = \beta \frac{I-1}{N}(S+1)P(S+1, I-1; t) + \mu(I+1) \cdot P(I+1, S-1; t) - \left(\beta \frac{I}{N} S + \mu I\right) P(S, I; t)$$

Remember $S + I = N$

Long (long) Run

Invariant distribution

Master Equation defines an evolution operatore for probabilities Π_t such that:

$$\Pi_t : P(\cdot; 0) \longrightarrow P(\cdot; t)$$

Invariant distribution

An invariant distribution $\pi(\cdot)$ satisfies

$$\Pi_t(\pi(\cdot)) = \pi(\cdot)$$

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- If the states space is not finite this is not sure : Explosions.

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- If the states space is not finite this is not sure : Explosions. (e.g. Diffusion on a lattice).

Structure of State space

Transient Space

A subset $T \subset \Omega$ is said to be *transient* if for all $\tau \in T$ there exists a state $\omega \in \Omega$ such for finite $t > s$, $P(\omega t \mid \tau s) > 0$ and for any $t > s$, $P(\tau, t \mid \omega, s) = 0$. An invariant distribution π must satisfy $\pi\,|_T = 0$.

Irreducible Subspace

A subset $I \subset \Omega$ is said *irreducible* if for any two states $\omega_0, \omega' \in I$ there exists a finite sequence $\{\omega_1, \omega_n\}$ such that $Q_{\omega_0\omega_1} \cdot \ldots \cdot Q_{\omega_n\omega'} > 0$ and $Q_{\omega_0\omega_1} \cdot \ldots \cdot Q_{\omega_n\omega'} > 0$

Ergodic Subspace

An irreducible subset is *ergodic* if it is *positive recurrent*: i.e. the expected return time for any state is finite. If the state space is finite any irreducible subset is ergodic.

Finding the Invariant distribution: Detailed balance

The invariant distributions satisfies:

$$\left[\sum_{\xi} Q_{\omega\xi} P(\xi, t \mid \omega', s)\right] - \left[\sum_{\xi} Q_{\xi\omega}\right] \cdot P(\omega, t \mid \omega', s) = 0$$

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detailed balance

A simplified condition. Implies time invariance thus equilibrium **Reversibility**.

$$Q_{\omega'\omega}\pi(\omega') = Q_{\omega\omega'}\pi(\omega)$$

Example: birth-death

Absorbing State

When $\beta_0 = 0$, the subset $E = \{N = 0\}$ is clearly ergodic. It is called **absorbing state** and the stationary distribution $\pi_n = \delta_{0n}$ is clearly an invariant distribution.

In general we should solve the equation:

$$P_{n+1}\delta(n+1) - P_n(\beta+\delta)n + \beta(n-1)P_{n-1} = 0, \;\; n \geq 1$$
$$\delta P(1) = 0$$

Clearly, the absorbing solution is the only invariant solution.

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Clearly, the absorbing solution is the only invariant solution.

Question: does the system always reach the equilibrium solution?

Answer: It depends on the dynamics and the initial state!

Example: generalized birth death process

In this case it depends on the rate. Since the space is irreducible one should check that it is also recurrent. Applying detailed balance we get:

$$P_k = P_0 \prod_{i=0}^{n-1} \frac{\beta_i}{\delta_i}$$

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Ergodicity Condition

If all $\beta_i \neq 0$ and $\delta_i \neq 0$

$$\sum_n \prod_{i=0}^{n-1} \frac{\beta_i}{\delta_i} < +\infty$$

Which thus gives an extinction probability of:

$$P_0 = \frac{1}{1 + \sum_n \prod_{i=0}^{n-1} \frac{\beta_i}{\delta_i}}$$

Example: SIS

If we write $S = N - I$ we can rewrite the master equation os SIS:

$$\partial_t P(I;t) = \beta \frac{I-1}{N}(N - I + 1)P(I-1;t) + \mu(I+1) \cdot P(I+1;t) - \left(\beta \frac{I}{N}(N-I) + \mu I\right) P(I;t), \qquad 0 < I \leq N$$

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finite state-space: The system always converge to a stationary solution

- $E = \{I = 0\}$ Is clearly ergodic (absorbing state).
- The set $T = \{0 < I \leq N\}$ is *transient*, i.e. there is a finite probability of reaching the absorbing state thus. Since the state space is finite $\lim_{t\to\infty} P(t) = \delta_{I0}$

Long run: recap.

- Look at the state space, find the ergodic subspaces to know how many invariant distribution you may expect.
- Try Detailed balance;
- Try to solve the general recurrence;

Generating function Method

Genereting Function theorems

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Probability Generating Function

$G(t;\vec{z}) = \mathbb{E}[\vec{z}^{X_t}]$ **Mellin Transform**

Probability Generating Function: properties (univariate)

Generates Probabilities

$$\left.\frac{1}{n!}\partial_z^n G(t;z)\right|_{z=0} = P_n$$

Normalisation

$$G(t;\vec{1}) = \sum_n P_n(t) = 1$$

Moments

$$\left.(z\partial_z)^k G(t;z)\right|_1 = \sum_{n=1}^{\infty} n^k P_n(t) = \mathbb{E}[X_t^k]$$

Probability generating function for Birth-death

$$G(t,z) = \sum_{k=0}^{\infty} z^k P_k(t).$$

Plugging it in the master equation

$$\sum_n z^n \partial_t P_n(t) = \sum_{n\geq 1} \beta\,(n-1) z^n P_{n-1}(t) + \sum_{n\geq 0} \delta (n+1) z^n P_{n+1}(t) - (\beta+\delta)\; n z^n P_n(t)$$

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- $\sum_{n\geq 0} (\beta+\delta) n z^n P_n \longrightarrow z(\beta+\delta)\partial_z G(t;z)$

Generating function equations

We thus mapped Master equation in :

$$\partial_t G(t;z) = [\beta z^2 - (\beta + \delta)z + \delta]\partial_z G(t;z)$$

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Method of Characteristics

$z \longrightarrow Z(s)$ and $t \longrightarrow T(s)$.

$$\frac{\mathrm{d}G(T(s);Z(s))}{\mathrm{d}s} = \partial_z G(T(s);Z(s))\frac{\mathrm{d}Z}{\mathrm{d}s} + \partial_t G(T(s);Z(s))\frac{\mathrm{d}T}{\mathrm{d}s}$$

You transform it in a set of ODE

$$\begin{cases} Z'(s) = -(\beta Z^2 - Z(\beta + \delta) + \delta) \\ T'(s) = 1 \\ G' = 0 \end{cases}$$

Solution

- $T'(s) = 1$ implies $s = t$,
- $G' = 0$ implies $G(z,t) = G(z_0, 0) = G_0(z) = \sum_n z^n P_n(0)$;
- for a $P_k(0) = \delta_{kN_0}$ implies $G_0(z_0) = (z_0)^{N_0}$.
- $z_0 = \dfrac{\frac{\delta}{\beta} + \frac{e^{-t(\beta-\delta)}\left(z - \frac{\delta}{\beta}\right)}{1-z}}{1 + \frac{e^{-t(\beta-\delta)}\left(z - \frac{\delta}{\beta}\right)}{1-z}}$

$$G(z,t) = G_0\left[\frac{\frac{\delta}{\beta} + \frac{e^{-t(\beta-\delta)}\left(z - \frac{\delta}{\beta}\right)}{1-z}}{1 + \frac{e^{-t(\beta-\delta)}\left(z - \frac{\delta}{\beta}\right)}{1-z}}\right] = \left[\frac{\frac{\delta}{\beta} + \frac{e^{-t(\beta-\delta)}\left(z - \frac{\delta}{\beta}\right)}{1-z}}{1 + \frac{e^{-t(\beta-\delta)}\left(z - \frac{\delta}{\beta}\right)}{1-z}}\right]^{N_0}$$

Active/Absorbing transition

$$P_0(\infty) = \begin{cases} 1 & \text{if } \frac{\beta}{\delta} \leq 1 \\ \left(\frac{\delta}{\beta}\right)^N & \text{otherwise} \end{cases}$$

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$$Var[N(t) = z\partial_z G(z,t) + z^2\partial_z G_{z,t} - z^2(\partial_z G(z,t))^2 \mid_{z=1} = \frac{N(\beta+\delta)e^{t(\beta-\delta)}\left(e^{t(\beta-\delta)}-1\right)}{\beta-\delta}$$

Recap.

- Choose your generating function (different Generating function originates difference
- Transform the system in a PDE
- Solve it!
- Retrieve the Pdf or the moments.

Gardiner’s Poisson representation

Main ideas

- Many process are “close to poissonianity”
- The main idea is to average it out and find equations for the non Poissonian part
- It is a transform of the pdf.

The method

Poisson Transform

$$P_n(t) = \int_0^\infty f(a,t) \frac{e^{-a} a^n}{n!} \, da$$

with the condition: $\int_0^\infty f(a,t) = 1$

Master Equation $\Rightarrow$ PDE for $f(a,t)$

Advantages

- You can calculate easily the moments:

$$\mathbb{E}[N_t] = \int \sum_n \left[\frac{n a^n}{n!} e^{-a} \right] f(a,t)\, \mathrm{d}a = \int_0^\infty a f(a,t)\, \mathrm{d}a$$

$$\mathbb{E}[N_t^2] = \int \sum_n \left[\frac{n^2 a^n}{n!} e^{-a} \right] f(a,t)\, \mathrm{d}a = \int_0^\infty (a^2 + a) f(a,t)\, \mathrm{d}a$$

- A continuous limit **for free**

Example: birth-death

- $\partial_t P_{n-1}(t) = \int_0^\infty \partial_t f(a,t) \frac{e^{-a} a^n}{n!} \, da$
- $(\beta+\delta) n P_n = -(\beta+\delta) \int_0^\infty [(1-a) f(a,t) + a \partial_a f(a,t)] \frac{e^{-a} a^n}{n!} \, da$
- $\delta(n+1) P_{n+1} = \delta \int_0^\infty a f(a,t) \frac{e^{-a} a^n}{n!} \, da$
- $\beta(n-1) P_{n-1} =$
  $\beta \int_0^\infty \left[\beta(a-2) + 2(a-1)\partial_a f(a,t) + a \partial_a^2 f(a,t)\right] \frac{e^{-a} a^n}{n!} \, da$

Poisson Representation for Birth-Death processes

$$\partial_t f(a,t) = \partial_a \left[(\delta - \beta) a f(a,t) + \frac{1}{2} \partial_a \big(2\beta a f(a,t) \big) \right]$$

Thank you!