# Lecture 2 - Master equation and system size expansion 

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## Outline

(1) The master equation for time continuous processes.
(2) Birth and death processes - Intro.
(3) Simulating stochastic orbits: the Gillespie algorithm.
(9) Stochastic predictions: the van Kampen system size expansion.
(0) Theory vs. simulations.

## The Master Equation

This is basically the continuous time version of Markov chains.
Derivation from the Chapman-Kolmogorov (CK) equation
The CK equation is

$$
p\left(n, t+\Delta t \mid n_{0}, t_{0}\right)=\sum_{n^{\prime}} p\left(n, t+\Delta t \mid n^{\prime}, t\right) p\left(n^{\prime}, t \mid n_{0}, t_{0}\right) .
$$

Now, we assume that

$$
p\left(n, t+\Delta t \mid n^{\prime}, t\right)=\left\{\begin{array}{cl}
1-\kappa_{n}(t) \Delta t+\mathcal{O}(\Delta t)^{2}, & \text { if } n=n^{\prime},  \tag{1}\\
w_{n n^{\prime}}(t) \Delta t+\mathcal{O}(\Delta t)^{2}, & \text { if } n \neq n^{\prime} .
\end{array}\right.
$$

$w_{n n^{\prime}}(t)$ is the transition rate and is only defined for $n \neq n^{\prime}$
Now, by normalisation,

$$
\begin{aligned}
1 & =\sum_{n} p\left(n, t+\Delta t \mid n^{\prime}, t\right) \\
& =1-\kappa_{n^{\prime}}(t) \Delta t+\mathcal{O}(\Delta t)^{2}+\sum_{n \neq n^{\prime}} w_{n n^{\prime}}(t) \Delta t+\mathcal{O}(\Delta t)^{2}
\end{aligned}
$$

$$
\Rightarrow \kappa_{n^{\prime}}(t)=\sum_{n \neq n^{\prime}} w_{n n^{\prime}}(t) .
$$

Alternatively, switching the indices,

$$
\begin{equation*}
\kappa_{n}(t)=\sum_{n^{\prime} \neq n} w_{n^{\prime} n}(t) \tag{2}
\end{equation*}
$$

Therefore, using (1), we see that the CK equation reads

$$
\begin{aligned}
p\left(n, t+\Delta t \mid n_{0}, t_{0}\right) & =\left(1-\kappa_{n}(t) \Delta t+\ldots\right) p\left(n, t \mid n_{0}, t_{0}\right) \\
& +\sum_{n^{\prime} \neq n} w_{n n^{\prime}}(t) p\left(n^{\prime}, t \mid n_{0}, t_{0}\right) \Delta t+\mathcal{O}(\Delta t)^{2} \\
\Rightarrow & \frac{p\left(n, t+\Delta t \mid n_{0}, t_{0}\right)-p\left(n, t \mid n_{0}, t_{0}\right)}{\Delta t} \\
& =-\kappa_{n}(t) p\left(n, t \mid n_{0}, t_{0}\right)+\sum_{n^{\prime} \neq n} w_{n n^{\prime}}(t) p\left(n^{\prime}, t \mid n_{0}, t_{0}\right)+\mathcal{O}(\Delta t)
\end{aligned}
$$

Now let $\Delta t \rightarrow 0$ :

$$
\frac{d p\left(n, t \mid n_{0}, t_{0}\right)}{d t}=-\kappa_{n}(t) p\left(n, t \mid n_{0}, t_{0}\right)+\sum_{n^{\prime} \neq n} w_{n n^{\prime}}(t) p\left(n^{\prime}, t \mid n_{0}, t_{0}\right)
$$

Using (2), the middle term may be rewritten to find

$$
\frac{d p\left(n, t \mid n_{0}, t_{0}\right)}{d t}=-\sum_{n^{\prime} \neq n} w_{n^{\prime} n}(t) p\left(n, t \mid n_{0}, t_{0}\right)+\sum_{n^{\prime} \neq n} w_{n n^{\prime}}(t) p\left(n^{\prime}, t \mid n_{0}, t_{0}\right)
$$

If we had started, not from the CK equation, but from the first relation which defines Markov processes:

$$
p(n, t+\Delta t)=\sum_{n^{\prime}} p\left(n, t+\Delta t \mid n^{\prime}, t\right) p\left(n^{\prime}, t\right)
$$

then exactly the same sequence of steps would lead to

$$
\frac{d p(n, t)}{d t}=-\sum_{n^{\prime} \neq n} w_{n^{\prime} n}(t) p(n, t)+\sum_{n^{\prime} \neq n} w_{n n^{\prime}}(t) p\left(n^{\prime}, t\right)
$$

This equation could also have been obtained by multiplying the equation for $p\left(n, t \mid n_{0}, t_{0}\right)$ by $p\left(n_{0}, t_{0}\right)$ and summing over all initial states, since

$$
p(n, t)=\sum_{n_{0}} p\left(n, t \mid n_{0}, t_{0}\right) p\left(n_{0}, t_{0}\right) .
$$

Therefore both $p\left(n, t \mid n_{0}, t_{0}\right)$ and $p(n, t)$ satisfy the same equation. We will frequently write it for $p(n, t)$, with the understanding that this could also be thought of as the conditional probability.

The equation is the desired master equation,

$$
\begin{equation*}
\frac{d p(n, t)}{d t}=\sum_{n^{\prime} \neq n} w_{n n^{\prime}}(t) p\left(n^{\prime}, t\right)-\sum_{n^{\prime} \neq n} w_{n^{\prime} n}(t) p(n, t) . \tag{3}
\end{equation*}
$$

The interpretation of the master equation is straightforward. The first term is just the probability of going from $n^{\prime} \rightarrow n$, and the second the probability of going from $n \rightarrow n^{\prime}$.

In words, the rate of change of being in a state $n$ is equal to the probability of making a transition into $n$, minus the probability of transitioning out of $n$.

In applications the $w_{n n^{\prime}}$ are assumed to be given (this specifies the model) and we wish to determine the $p(n, t)$.

## Comments:

- Notice that because of the Markov property, $w_{n n^{\prime}}$ only depends on the current state of the system $\left(n^{\prime}\right)$, and does not depend on previous states (i.e. how the system got to $n^{\prime}$ ).
- In the derivation we have assumed that $w_{n n^{\prime}}$ depends on time (which it does in general, just as for Markov chains), but usually we are only interested in situations where it is time-independent.


## More informal derivations of the master equation

The master equation is essentially a balance equation; the rate of moving into the state $n$ minus the rate of moving out of the same state is the rate of change of $p(n, t)$. That is,

Rate of change of $p(n, t)=$
[ Rate due to transitions into the state $n$ from all the other states $n^{\prime}$ ] [ Rate due to transitions out of the state $n$ into all other states $n^{\prime}$ ]

When expressed this way, and assuming the process is Markov, the master equation

$$
\frac{d p(n, t)}{d t}=\sum_{n^{\prime} \neq n} w_{n n^{\prime}}(t) p\left(n^{\prime}, t\right)-\sum_{n^{\prime} \neq n} w_{n^{\prime} n}(t) p(n, t),
$$

appears very reasonable.

Another derivation, which is also less rigorous than the original, starts from the system described as a Markov chain, and moves to continuous time by taking the duration of the time-step to zero:
So, let us start from

$$
P_{n}(t+1)=\sum_{n^{\prime}} Q_{n n^{\prime}}(t) P_{n^{\prime}}(t)
$$

where the columns of the transition matrix add to unity:

$$
\sum_{n^{\prime}} Q_{n^{\prime} n}(t)=1
$$

So, if we write

$$
P_{n}(t+1)-P_{n}(t)=\sum_{n^{\prime}} Q_{n n^{\prime}}(t) P_{n^{\prime}}(t)-\sum_{n^{\prime}} Q_{n^{\prime} n}(t) P_{n}(t)
$$

then the terms in the sums with $n^{\prime}=n$ can be cancelled to give

$$
P_{n}(t+1)-P_{n}(t)=\sum_{n^{\prime} \neq n} Q_{n n^{\prime}}(t) P_{n^{\prime}}(t)-\sum_{n^{\prime} \neq n} Q_{n^{\prime} n}(t) P_{n}(t)
$$

Now, we take the time step to be $\Delta t$, rather than unity, and divide through by the time step;

$$
\frac{P_{n}(t+\Delta t)-P_{n}(t)}{\Delta t}=\sum_{n^{\prime} \neq n} \frac{Q_{n n^{\prime}}}{\Delta t} P_{n^{\prime}}(t)-\sum_{n^{\prime} \neq n} \frac{Q_{n^{\prime} n}}{\Delta t} P_{n}(t)
$$

Then, it is clear that taking the time step to zero, reduces the left-hand side to a differential of the probability, with respect to time. Furthermore instead of assuming that exactly one sampling event happens per time step, we assume that on average one event happens in the time step. To achieve this set

$$
Q_{n n^{\prime}}(t)=w_{n n^{\prime}}(t) \Delta t+\mathcal{O}(\Delta t)^{2}, \quad n \neq n^{\prime}
$$

So letting $\Delta t \rightarrow 0$ we obtain the master equation:

$$
\frac{d P_{n}}{d t}=\sum_{n^{\prime} \neq n} w_{n n^{\prime}}(t) P_{n^{\prime}}(t)-\sum_{n^{\prime} \neq n} w_{n^{\prime} n}(t) P_{n}(t)
$$

## The birth and death stochastic model


(1) Simple model of population growth.
(2) Individuals enter/exit the community.

- Bacteria dynamics.
- Demography.
- Queueing theory.



## Exact numerical scheme: the Gillespie algorithm

Consider a given chemical equation, $R_{1}$. Assume $S_{i}$, with $i=1,2$, to label the involved reactants (called Substrates in the original paper by Gillespie):

$$
S_{1}+S_{2} \xrightarrow{c} 2 S_{1}
$$

In words: the (individual!) molecule of type $S_{1}$ can combine with an (individual!) molecule of type $S_{2}$ to result into two molecules of type $S_{1}$.

The probability that such a reaction will take place in the forthcoming time interval $d t$ is controlled by:

- the number of molecules of type $S_{1}$ and $S_{2}$ and the number of possible combinations that yield to an encounter between a molecule of type $S_{1}$ and another of type $S_{2}$.
- the average probability that given a pair of molecules $S_{1}$ ed $S_{2}$, the reaction $R_{1}$ takes over.

Assume $n_{1}$ e $n_{2}$ to label the number of molecules of type 1 e 2
respectively. Then, $h=n_{1} n_{2}$ is the number of independent combinations that result in a pair $S_{1}-S_{2}$.
On the other hand $c$ measures the probability per unit of time of reacting. Hence:

$$
P_{1}=c h d t=c n_{1} n_{2} d t
$$

is the probability that the reaction $R_{1}$ takes over in a given time interval $d t$.

So far so good! What is going to happen if we have instead a system of reactions?

How are we going to sort out which reaction is going to happen first?

Let us consider first the case where two reactions are at play, namely $R_{1}$ and $R_{2}$, specified as follows:

$$
\begin{array}{rll}
S_{1}+S_{2} & \xrightarrow{c_{1}} & 2 S_{1} \\
2 S_{1} & \xrightarrow{c_{2}} & S_{3}
\end{array}
$$

Answering to two questions is mandatory at this point:

- When is the next reaction going to occur?
- Which reaction is going to happen?

Focus on the general framework.
Imagine to have $k$ type of molecules partitioned in the following families ( $n_{1}, n_{2}, n_{3} \ldots$ ) and assume that those molecules can react according to $M$ distinct reaction channels, labelled with $R_{i}$ con $i=1, . ., M$.

We need to calculate the quantity:

$$
P(\tau, i) d \tau
$$

i.e. the probability that given the system in the state $\left(n_{1}, n_{2}, n_{3} \ldots\right)$ at time $t$ :

- the next reaction occurs in the time interval from $t+\tau$ to $t+\tau+d \tau$.
- it is the reaction $R_{i}$.

The core of the algorithm is to evaluate the, presently unknown, quantity $P(\tau, i) d \tau$.

The key idea is to split such a probability into two distinct contributions, as outlined below:

- the probability $P_{0}(\tau)$ that, given the state $\left(n_{1}, n_{2}, \ldots\right)$ at time $t$, no reaction would eventually occur in the time interval $(t, t+\tau)$.
- the probability $P_{i}$ that the reaction $i$ occurred in the time interval $(t+\tau, t+\tau+d \tau)$.

The second quantity can be readily evaluated. We know that

$$
P_{i}=c_{i} h_{i} d \tau
$$

where $h_{i}$ refers to the number of possible combinations of the chemicals as specified by reaction $R_{i} . c_{i}$ is instead the average probability per unit of time that the molecules could react and so give birth to the prescribed products.

To evaluate $P_{0}(\tau)$, the probability that no reaction occurs in in $(t, t+\tau)$, imagine to partition the inspected time interval $\tau$ into $K$ sub-intervals, each of size $\epsilon=\tau / K$. The probability that no reaction occurred in the first interval $(t, t+\epsilon)$ is:

$$
\Pi_{j=1}^{M}\left[1-c_{j} h_{j} \epsilon\right]=1-\sum_{j=1}^{M} c_{j} h_{j} \epsilon+O(\epsilon)
$$

On the other hand this is also the probability that no reaction would occur in the next time interval $(t+\epsilon, t+2 \epsilon)$. Since we have $K$ consecutive intervals, one can write:

$$
\begin{aligned}
P_{0}(\tau) & =\left[1-\sum_{j=1}^{M} c_{j} h_{j} \epsilon+O(\epsilon)\right]^{K} \\
& =\left[1-\sum_{j=1}^{M} c_{j} h_{j} \tau / K+O\left(K^{-1}\right)\right]^{K}
\end{aligned}
$$

Perform now the limit for $K \rightarrow \infty$. We eventually obtain:

$$
P_{0}(\tau)=\exp \left(-\sum_{j=1}^{M} c_{j} h_{j} \tau\right)
$$

from which the fundamental result follows:
The sougth probability $P(\tau, i)$

$$
P(\tau, i)=P_{0}(\tau) a_{i}=a_{i} \exp \left(-a_{0} \tau\right)
$$

where we have introduced the compact notation:

$$
a_{i}=c_{i} h_{i}
$$

and

$$
a_{0}=\sum_{j=1}^{M} c_{j} h_{j}
$$

The above expression for $P(\tau, i)$ holds for $0<\tau<\infty$ and $i=1, . ., M$. Starting from this setting one can construct an exact algorithm that enables one to track the dynamics of a large ensemble of microscopic constituents that have to obey to an assigned set of chemical rules (or, equivalently, whose probability $P(n, t)$ has to obey to a given Master equation).

The core idea of the computational scheme (Gillespie algorithm) is to implement a Monte Carlo strategy that is able to simulate the stochastic process represented by $P(\tau, i)$. In the following we discuss the sequential steps that we are going to consider.

- STEP 0. At time $t=0$ assign the initial values to the variables $n_{1}, n_{2}, \ldots$ and to the parameters $c_{i}$. Calculate the quantities $h_{i} c_{i}$ which in practice determine $P(\tau, i)$. One can also define the time of observation $t_{1}<t_{2}<\ldots$ and the stopping time $t_{s}$.
- STEP 1. Make use of a dedicated Monte Carlo technique to generate a random pair $(\tau, i)$, which obeys to the joint probability density function $P(\tau, i)$.
- STEP 2. Make use of the values as generated above to advance the system in time by a quantity $\tau$, while adjusting the values of the population sizes $n_{i}$ implicated in the selected reaction $i$. After this operation is being taken to completion, calculate again the quantities $h_{i} c_{i}$ for those reactions that have experienced a change in the chemicals amount.
- STEP 3. If time $t$ is less than $t_{s}$ or if there are no reactants left into the system $\left(h_{i}=0\right)$ stop the simulations. Otherwise, start again from STEP 1.

Clearly the crucial step is:

- STEP 2. Make use of a dedicated Monte Carlo technique to generate a random pair $(\tau, i)$, which obeys to the joint probability density function $P(\tau, i)$.
to which the following slides are entirely devoted.

We should generate the pair $(\tau, i)$ in accordance with the distribution $P(\tau, i)$, as calculated below. We shall illustrate the so called direct method.

To this end we shall make use of our ability to generate random numbers $r$ obeying to a uniform distribution. Notice that $\tau$ is a continuous variable, while $i$ is discrete.
First let us write:

$$
P(\tau, i)=P_{1}(\tau) P_{2}(i \mid \tau)
$$

The probability $P_{1}(\tau)$ follows from:

$$
P_{1}(\tau)=\sum_{i=1}^{M} P(\tau, i)
$$

Hence, inserting in the preceding relation:

$$
P_{2}(i \mid \tau)=P(\tau, i) / \sum_{i=1}^{M} P(\tau, i)
$$

Recalling the above expression for $P(\tau, i)$ yields:

$$
\begin{aligned}
P_{1}(\tau) & =a_{0} \exp \left(-a_{0} \tau\right) \\
P_{2}(i \mid \tau) & =a_{i} / a_{0}
\end{aligned}
$$

where $0 \leq \tau<\infty$ and $i=1,2, . . M$.

Both probability density functions are normalized in their respective domain of definition.

$$
\begin{aligned}
\int_{0}^{\infty} P_{1}(\tau) & =\int_{0}^{\infty} a_{0} \exp \left(-a_{0} \tau\right)=1 \\
\sum_{j=1}^{M} P_{2}(i \mid \tau) & =\sum_{j=1}^{M} a_{i} / a_{0}=1
\end{aligned}
$$

The idea of the direct method is to generate a random number $\tau$ in agreement with $P_{1}(\tau)$ and then an integer $i$ as dictated by $P_{2}(i \mid \tau)$. The resulting pair $(\tau, i)$ will therefore obey to $P(\tau, i)$.

As we shall outline in the following, it is possible to generate a random quantity $\tau$ which obeys to $P_{1}(\tau)$ : (i) by extracting a random number $r_{1}$ from a uniform distribution and (ii) by calculating:

$$
\tau=\left(1 / a_{0}\right) \log \left(1 / r_{1}\right)
$$

Analogously (no proof given here), one can obtain an integer random $i$ which obeys to $P_{2}(i \mid \tau)$ by extracting a random (real) number $r_{2}$ from a uniform distribution and selecting $i$ as the integer that fulfills the double inequivalence:

$$
\sum_{j=1}^{i-1} a_{j}<r_{2} a_{0}<\sum_{j=1}^{i} a_{j}
$$

Finally, we discuss the origin of the formula for $\tau$. It follows from the inversion technique, a Monte Carlo method which enables one to generate random numbers from a generic pdf, by using uniformly distributed random numbers.

Assume, we wish to generate the random number $x$ distributed as $P(x)$. By definition, $P\left(x^{\prime}\right) d x^{\prime}$ is the probability that $x$ falls in the interval delimited by $x^{\prime}$ and $x^{\prime}+d x^{\prime}$. Consider $F(x)$ defined as:

$$
F(x)=\int_{-\infty}^{x} P\left(x^{\prime}\right) d x^{\prime}
$$

clearly $F\left(x_{0}\right)$ is the probability that $x$ is smaller than $x_{0}$. Function $F(x)$ measures the probability for $x$ to be smaller than $x_{0} . F(x)$ is the probability distribution, distinct from the probability density function $P(x)$.

The inversion method, consists in extracting a uniformly distributed random number $r$ and then select $x$ such that $F(x)=r$, namely:

$$
x=F^{-1}(r)
$$

where $F^{-1}(\cdot)$ is the inverse of the distribution function associated to the pdf $P(\cdot)$.

Calculate in fact the probability that $x$ as generated according the the above prescriptions would fall in the interval $\left[x^{\prime}, x^{\prime}+d x^{\prime}\right]$. By construction, this probability is identical to the probability that $r$ falls in between $F\left(x^{\prime}\right)$ e $F\left(x^{\prime}+d x^{\prime}\right)$. Since $r$ is uniformly distributed, such a probability reads:

$$
F\left(x^{\prime}+d x^{\prime}\right)-F\left(x^{\prime}\right)=F^{\prime}\left(x^{\prime}\right) d x^{\prime}=P\left(x^{\prime}\right) d x^{\prime}
$$

Assume one needs to generate a random number distributed as the pdf:

$$
P(x)=A \exp (-A x)
$$

Then $F(x)=1-\exp (-A x)$ e so, by imposing $F(x)=r$ one readily obtains

$$
x=(1 / A) \log (1 / r)
$$

i.e. the formula evoked before. Notice that in the derivation we have replaced $1-r$ with the statistically equivalent quantity $r$.

## On the implementation: back to the birth-death model

$$
\begin{aligned}
& E \xrightarrow{b} X \\
& X \xrightarrow{d} E
\end{aligned}
$$

- $X$ stands for one individual
- $E$ is one empty space (vacancy)
- $n$ number of element of type $X$
- $n_{E}=N-n$

The initial condition:

```
time=zeros(1,tmax);
nX=zeros(1,tmax);
```

$n L(1,1)=X$;

The main loop:

```
for i=2:tmax,
Calculate the transition probability
a1 = b (N-X)/N;
a2 = d X/N;
a0=a1+a2;
Gillespie recipe
r1=rand(1,1); r2=rand(1,1);
tau=-1/a0*log(r1); r2=a0*r2;
ind=1;
Update the population amount
```

Save the results
end

Recall that to obtain a random integer $i$ which obeys to $P_{2}(i \mid \tau)$ one can extract a random (real) number $r_{2}$ from a uniform distribution and then select $i$ as the integer that fulfills the double inequivalence:

$$
\begin{equation*}
\sum_{j=1}^{i-1} a_{j}<r_{2} a_{0}<\sum_{j=1}^{i} a_{j} \tag{4}
\end{equation*}
$$

In practice the values of $a_{j}$ are summed iteratively until the obtained sum becomes larger than $r_{2} a_{0}$. The corresponding integer $j$ (the number of elements summed up) is the index $i$ we are looking for.

```
while(ind),
prob=a1;
if(r2<prob),
X=X+1; ind=0; break;
end
prob=prob+a2;
if(r2<prob),
X=X-1; ind=0; break;
end
end
```


## Perturbative approach to characterize the fluctuations

The birth and death process introduced above yields the following master equation for the probability $P(n, t)$ :

$$
\begin{aligned}
\frac{d P(n, t)}{d t}= & -T(n-1 \mid n) P(n, t)+T(n \mid n+1) P(n+1, t) \\
& -T(n+1 \mid n) P(n, t)+T(n \mid n-1) P(n-1, t)
\end{aligned}
$$

Here $n$ stands for the (discrete) number of individual of type $X$. The transition probabilities can be readily obtained as:

$$
\begin{aligned}
& T(n-1 \mid n)=d \frac{n}{N} \\
& T(n+1 \mid n)=b\left(1-\frac{n}{N}\right)
\end{aligned}
$$

where $N$ is the total number of microscopic constituents, including the empties.

## Recovering the deterministic (mean field) limit

Focus on the time evolution of the mean quantity:

$$
\frac{\langle n\rangle}{N}=\frac{1}{N} \sum_{n} n P(n, t)
$$

To this end, multiply by $n$ both sides of the Master Equation and sum over all possible states.

## Left hand side

$$
\sum_{n} n \frac{d P(n, t)}{d t}=\frac{d}{d(t / N)} \sum_{n} \frac{n}{N} P(n, t)=\frac{d\langle n\rangle}{d \tau}
$$

where $\tau=t / N$.

## Right hand side (first two terms)

$$
\begin{array}{rl}
\sum_{n} & n(T(n \mid n+1) P(n+1, t)-T(n-1 \mid n) P(n, t)) \\
& =\sum_{n^{\prime}}\left(n^{\prime}-1\right) T\left(n^{\prime}-1 \mid n^{\prime}\right) P\left(n^{\prime}, t\right)-\sum_{n} n T(n-1 \mid n) P(n, t) \\
& =-\sum_{n} T(n-1 \mid n) P(n, t)
\end{array}
$$

Recalling the definition of $T(n-1 \mid n)$ one obtains:

$$
-\sum_{n} d \frac{n}{N} P(n, t)=-d \frac{\langle n\rangle}{N}
$$

Similarly, for the other terms

## Right hand side (last two terms)

$$
\begin{array}{rl}
\sum_{n} & n(T(n \mid n-1) P(n-1, t)-T(n+1 \mid n) P(n, t)) \\
& =\sum_{n^{\prime}}\left(n^{\prime}+1\right) T\left(n^{\prime}+1 \mid n^{\prime}\right) P\left(n^{\prime}, t\right)-\sum_{n} n T(n+1 \mid n) P(n, t) \\
& =\sum_{n} T(n+1 \mid n) P(n, t)
\end{array}
$$

Recalling the definition of $T(n+1 \mid n)$ one obtains:

$$
\sum_{n} b\left(1-\frac{n}{N}\right) P(n, t)=b\left(1-\frac{\langle n\rangle}{N}\right)
$$

Collecting all terms together:

$$
\frac{d\langle n\rangle}{d \tau}=b\left(1-\frac{\langle n\rangle}{N}\right)-d \frac{\langle n\rangle}{N}
$$

and introducing $\phi=\langle n\rangle / N$ :

$$
\frac{d \phi}{d \tau}=b(1-\phi)-d \phi
$$

The above ODE governs the evolution of the (continuum) average distribution. Fluctuations have been dropped by performing the ensemble average. The solution of the ODE is:

$$
\phi(\tau)=\frac{b}{b+d}\left[1-\left(1-\phi_{0} \frac{b+d}{b}\right) \exp [-(b+d) \tau]\right]
$$

The system converges asymptotically to the stable fixed point $\phi^{*}=b /(b+d)$

## Accounting for fluctuations: the

## expansion

The van Kampen ansatz consists in splitting the finite size concentration $\mathrm{n} / \mathrm{N}$ into two contributions:

$$
\frac{n}{N}=\phi+\frac{\xi}{\sqrt{N}}
$$

where $\xi$ is a stochastic variable. The quantity $1 / \sqrt{N}$ is small for large or moderate system sizes $N$ : it hence plays the role of small parameter in a perturbative expansion. Start by re-writing the master equation in the following compact form:

$$
\begin{aligned}
\frac{d P}{d t} & =\left(\mathcal{E}^{+1}-1\right) T(n-1 \mid n) P(n, t) \\
& +\left(\mathcal{E}^{-1}-1\right) T(n+1 \mid n) P(n, t)
\end{aligned}
$$

where $\mathcal{E}^{ \pm 1} f(n)=f(n \pm 1), f(n)$ being an arbitrary function of the discrete variable $n$.

Let us begin by considering the left hand side of the master equation. Introduce $\Pi(\xi, t) \equiv P(n(\phi, \xi), t)$. Hence:

$$
\frac{\partial \Pi}{\partial t}=\frac{\partial P}{\partial t}+\frac{\partial P}{\partial n} \frac{\partial n}{\partial t}
$$

and thus:

$$
\frac{\partial P}{\partial t}=\frac{\partial \Pi}{\partial t}-\frac{\partial P}{\partial n} N \frac{d \phi}{d t}
$$

On the other hand:

$$
\frac{\partial \Pi}{\partial \xi}=\frac{\partial P}{\partial \xi}=\frac{\partial P}{\partial n} \frac{\partial n}{\partial \xi}=\frac{\partial P}{\partial n} \sqrt{N}
$$

Combining the two above expressions:

## Right hand side of ME

$$
\frac{\partial P}{\partial t}=\frac{1}{N} \frac{\partial \Pi}{\partial \tau}-\frac{1}{\sqrt{N}} \frac{d \phi}{d \tau} \frac{\partial \Pi}{\partial \xi}
$$

Consider:
$\mathcal{E}^{+1} f(n)=f(n+1)=f(N \phi+\sqrt{N} \xi+1)=f\left(N \phi+\sqrt{N}\left(\xi+\frac{1}{\sqrt{N}}\right)\right)$
Hence:

$$
\mathcal{E}^{+1} f(N \phi+\sqrt{N} \xi)=f\left(N \phi+\sqrt{N}\left(\xi+\frac{1}{\sqrt{N}}\right)\right)
$$

or equivalently:

$$
\mathcal{E}^{+1} f(\xi)=f\left(\xi+\frac{1}{\sqrt{N}}\right) \simeq f(\xi)+\frac{1}{\sqrt{N}} \partial_{\xi} f+\frac{1}{2 N} \partial_{\xi}^{2} f
$$

and:

$$
\left(\mathcal{E}^{+1}-1\right) f(\xi)=\left(\frac{1}{\sqrt{N}} \frac{\partial}{\partial \xi}+\frac{1}{2 N} \frac{\partial^{2}}{\partial \xi^{2}}\right) f(\xi)
$$

Summing up, the above step-operators $\mathcal{E}^{ \pm 1}$ (as they are called) admits a straightforward expansion with respect to $1 / \sqrt{N}$.

$$
\mathcal{E}^{ \pm 1}=1 \pm \frac{1}{\sqrt{N}} \frac{\partial}{\partial \xi}+\frac{1}{2 N} \frac{\partial^{2}}{\partial \xi^{2}}+\ldots
$$

Hence the first term in the right hand side of the master equation reads:

$$
\begin{aligned}
& \left(\mathcal{E}^{+1}-1\right) T(n-1 \mid n) P(n, t) \\
= & \left(\frac{1}{\sqrt{N}} \frac{\partial}{\partial \xi}+\frac{1}{2 N} \frac{\partial^{2}}{\partial \xi^{2}}\right) d\left(\phi+\frac{\xi}{\sqrt{N}}\right) \Pi(\xi, t)
\end{aligned}
$$

By organizing the various terms in the above expression one gets:

## First terms in the right hand side

$$
\frac{1}{\sqrt{N}}\left[d \phi \frac{\partial}{\partial \xi} \Pi\right]+\frac{1}{N} d\left[\frac{\partial}{\partial \xi}(\xi \Pi)+\frac{1}{2} \phi \frac{\partial^{2}}{\partial \xi^{2}} \Pi\right]+\ldots
$$

up to $1 / N$ contributions. Similarly for the other contribution in the master equation:

Last terms in the right hand side

$$
-\frac{1}{\sqrt{N}}\left[b(1-\phi) \frac{\partial}{\partial \xi} \Pi\right]+\frac{1}{N} b\left[\frac{\partial}{\partial \xi}(\xi \Pi)+\frac{1}{2}(1-\phi) \frac{\partial^{2}}{\partial \xi^{2}} \Pi\right]+\ldots
$$

## At the leading order,

Confronting the terms at the leading order in the master equation one obtains:

$$
\frac{d \phi}{d \tau}=b(1-\phi)-d \phi
$$

namely the equation which rules the dynamics of the examined system in the deterministic limit.

## At the next-to-leading order,

Confronting the terms at the next-to-leading order in the master equation one obtains the following Fokker-Planck equation :

$$
\frac{\partial \Pi}{\partial \tau}=(d+b) \frac{\partial}{\partial \xi}(\xi \Pi)+\frac{1}{2}(d \phi+b(1-\phi)) \frac{\partial^{2}}{\partial \xi^{2}} \Pi
$$

The solution of the above one-dimensional Fokker-Planck equation is a Gaussian whose first and second moments can be readily computed. Multiply both sides of the Fokker-Planck equation by $\xi$ and integrate over the real axis in $d \xi$. A simple calculation yields:

## First moment of $\Pi$

$$
\frac{d\langle\xi\rangle}{d \tau}=-(b+d)\langle\xi\rangle
$$

where $\langle\xi\rangle=\int \xi \Pi d \xi$. The solution reads $\langle\xi\rangle=\langle\xi\rangle_{0} \exp [-(d+b) \tau]$. Asymptotically, $\langle\xi\rangle \rightarrow 0$. Finite size fluctuations are hence described by a Gaussian centered in zero for sufficiently long times.

A similar reasoning applies to the second moment. The latter is defined as $\left\langle\xi^{2}\right\rangle=\int \xi^{2} \Pi d \xi$ and it can be shown to obey to the following differential equation:

## Second moment of $П$

$$
\frac{d\left\langle\xi^{2}\right\rangle}{d \tau}=-2(b+d)\left\langle\xi^{2}\right\rangle+[(d-b) \phi+b]
$$

Assume we are interested in the statistics of the fluctuations around the deterministic equilibrium, when $\phi \rightarrow \phi^{*}=b /(b+d)$. Imposing stationarity $\left(\frac{d\left\langle\xi^{2}\right\rangle}{d \tau}=0\right)$ yields:

$$
\left\langle\xi^{2}\right\rangle_{s t} \equiv \sigma^{2}=\frac{d b}{(d+b)^{2}}
$$

The distribution of fluctuations is hence predicted to be:

$$
\Pi_{s t}(\xi) \frac{1}{\sqrt{2 \pi} \sigma} \exp \left(-\frac{\xi^{2}}{2 \sigma^{2}}\right)
$$

