# Stochastic Modelling and Simulation
# Moment closure and central limit approximation

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# Outline


1. Fluid Equation and Moments

2. Linear Noise Approximation

# OVERVIEW

We will look at the relationship between the fluid equation and a Markov population model from the point of view of the average of the stochastic process.

- We will start from an heuristic argument.
- We then look at it more carefully and show a method to get ODE for the moments (mean, variance, and so on) of the process.
- Next, we will look at another kind of expansion, the linear noise, that will bring us to the central limit theorem (Gaussian Process approximation).

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# AVERAGE OF CTMC MODEL

## ODE FOR THE AVERAGE

Sometimes we are interested only in the (transient) average behaviour of the CTMC.
From Kolmogorov equations, we can derive an ODE for the average state $\mathbb{E}_t[\mathbf{X}]$ of the CTMC:

$$\frac{d\mathbb{E}_t[\mathbf{X}]}{dt} = \mathbb{E}_t[F(\mathbf{X})] = \sum_{\tau \in \mathcal{T}} \mathbf{v}_\tau \mathbb{E}_t[f_\tau(\mathbf{X})].$$

## APPROXIMATIONS

If it holds that $\mathbb{E}_t[F(\mathbf{X})] = F(\mathbb{E}_t[\mathbf{X}])$, i.e. $\mathbb{E}_t[f_\tau(\mathbf{X})] = f_\tau(\mathbb{E}_t[\mathbf{X}])$ for all $\tau$, then the previous equation boils down to the fluid ODE.
But this can be done exactly only if $F(\mathbf{X})$ is a linear function.
Otherwise, one can resort to an approximation of the ODE for the true average.

# ODE FOR THE AVERAGE

## SIMPLE SHARED RESOURCE MODEL

$$\frac{d\mathbb{E}_t[X_{P1}]}{dt} = k_2\mathbb{E}_t[X_{P2}] - \mathbb{E}_t[\min\{k_1 X_{P1}, h_1 X_{R1}\}]$$

$$\frac{d\mathbb{E}_t[X_{P1}]}{dt} \approx k_2\mathbb{E}_t[X_{P2}] - \min\{k_1\mathbb{E}_t[X_{P1}], h_1\mathbb{E}_t[X_{R1}]\}$$

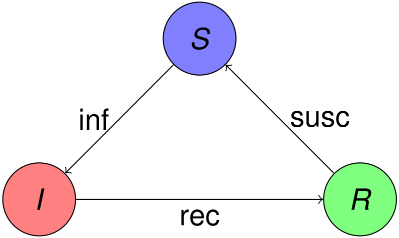
## SYNCHRONIZATION BY RATE PRODUCT

$$\frac{d\mathbb{E}_t[X_{P1}]}{dt} = k_2\mathbb{E}_t[X_{P2}] - k_1 h_1\mathbb{E}_t[X_{P1}X_{R1}].$$

$$\frac{d\mathbb{E}_t[X_{P1}]}{dt} \approx k_2\mathbb{E}_t[X_{P2}] - k_1 h_1\mathbb{E}_t[X_{P1}]\mathbb{E}_t[X_{R1}].$$

In this case, the equation for the true average depends on higher order moments.

# EXAMPLE: SIR EPIDEMICS




We obtain the same equation of the fluid approximation!

$$
\begin{cases}
\frac{d\mathbb{E}[X_S]}{dt} = k_S\mathbb{E}[X_R] - k_I\mathbb{E}[X_I]\mathbb{E}[X_S] \\
\frac{d\mathbb{E}[X_I]}{dt} = k_I\mathbb{E}[X_I]\mathbb{E}[X_S] - k_R\mathbb{E}[X_I] \\
\frac{d\mathbb{E}[X_R]}{dt} = k_R\mathbb{E}[X_I] - k_S\mathbb{E}[X_R]
\end{cases}
$$

# MOMENT CLOSURE

## DINKIN'S FORMULA FOR NON-CENTRED MOMENTS

$$\frac{d\mathbb{E}_t[X_1^{m_1}\cdots X_n^{m_n}]}{dt} = \sum_{\tau\in\mathcal{T}} \mathbb{E}_t\left[f_\tau(\mathbf{X})\left(\prod_{j=1}^{n}(X_j + \mathbf{v}_{\tau,j})^{m_j} - X_1^{m_1}\cdots X_n^{m_n}\right)\right].$$

## SIR MODEL EXAMPLE

$$\begin{aligned}\frac{d\mathbb{E}_t[X_S^2]}{dt} &= \mathbb{E}_t[k_I/N\cdot X_S X_I((X_S-1)^2 - X_S^2)] + \mathbb{E}_t[k_S\cdot X_R((X_S+1)^2 - X_S^2)] \\ &= k_I/N\mathbb{E}_t[X_S X_I] - 2k_I/N\mathbb{E}_t[X_S^2 X_I] + 2k_S\mathbb{E}_t[X_S X_R] + k_S\mathbb{E}_t[X_R]\end{aligned}$$

The equation for the variance of $X_S$ depends on third order moments.

For the SIR model, the equation for a moment of order $N$ depend on moments of order $k+1$, due to quadratic non-linearity.

If we have polynomial rates of maximum degree $m$, then moments of order $N$ depend on moments of order $k+m-1$.

# MOMENT CLOSURE

## DINKIN'S FORMULA FOR NON-CENTRED MOMENTS

$$\frac{d\mathbb{E}_t[X_1^{m_1}\cdots X_n^{m_n}]}{dt} = \sum_{\tau\in\mathcal{T}} \mathbb{E}_t\left[f_\tau(\mathbf{X})\left(\prod_{j=1}^{n}(X_j+\mathbf{v}_{\tau,j})^{m_j} - X_1^{m_1}\cdots X_n^{m_n}\right)\right].$$

If rate functions $f_\tau$ are polynomial the previous equation depends only on non-centred moments. However, equations for moments of order $k$ generally depend on moments of higher order: the system of ODE is not closed (infinite dimensional).
For smooth rate functions, one can approximate the rate with a Taylor polynomial.

# Moment Closure

## Dinkin's Formula for non-centred moments

$$\frac{d\mathbb{E}_t[X_1^{m_1}\cdots X_n^{m_n}]}{dt} = \sum_{\tau\in\mathcal{T}} \mathbb{E}_t\left[f_\tau(\mathbf{X})\left(\prod_{j=1}^{n}(X_j+\mathbf{v}_{\tau,j})^{m_j} - X_1^{m_1}\cdots X_n^{m_n}\right)\right].$$

## Closing the equations

Equations can be closed by replacing higher order moment with non-linear functions of lower order moments.
One example is normal moment closure (assume that moments from third on satisfy relation of a normal distribution).
Another example is log-normal moment closure.

# NORMAL MOMENT CLOSURE

## MOMENTS OF MULTIVARIATE NORMAL DISTRIBUTION

The central moments have a relatively simple form. The $k$-th centred moment, $k \geq 3$, is:

- zero, if $k$ odd.
- Let $i_1, \ldots, i_k$ be indices in $\{1, \ldots, n\}$, non necessarily distinct, and let $\mathcal{L}$ be an allocation of $i_1, \ldots, i_k$ into $k/2$ unordered pairs. Then

$$\mathbb{E}[(X_{i_1} - \mu_{i_1}) \cdots (X_{i_k} - \mu_{i_k})] = \sum_{\mathcal{L}} \prod_{(j,h) \in \mathcal{L}} COV(X_{i_j}, X_{i_h})$$

Example: $\mathbb{E}[(X_1 - \mu_1)^2 (X_2 - \mu_2)(X_3 - \mu_3)] =$
$VAR(X_1, X_1) COV(X_2, X_3) + 2 COV(X_1, X_2) COV(X_1, X_3)$.

To close the equation for the second order moment of $X_S$, we can expand the definition of the third centred moment and use
$\mathbb{E}[X_S^2 X_I] = 2\mathbb{E}[X_S]\mathbb{E}[X_S X_I] + \mathbb{E}[X_S^2]\mathbb{E}[X_I] - 2\mathbb{E}[X_S]^2 \mathbb{E}[X_I]$.

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# THE LINEAR NOISE ANSATZ

Fluctuations around the counting process are of order $N^{\frac{1}{2}}$. We assume that the PCTMC at level $N$ fluctuates around the solution of the fluid equation:

$$\mathbf{X}^{(N)}(t) \approx N\mathbf{x}(t) + N^{\frac{1}{2}}\xi,$$

where $\xi$ is a continuous random variable. This means that

$$\hat{\mathbf{X}}^{(N)}(t) \approx \mathbf{x}(t) + N^{-\frac{1}{2}}\xi$$

# DERIVING THE EQUATIONS

One proceeds as follows

1. Write the master equation in terms of normalized variables;
2. Apply the Ansatz
3. Expand probability and propensity functions around $\mathbf{x}(t)$. This makes sense if $N^{-\frac{1}{2}}\xi$ is small.
4. Introduce a new probability density $\Pi(\mathbf{x}, t)$ for the noise term $\xi$
5. Collect terms in order $\frac{1}{2}$ of $N$ to get the fluid equation for $\mathbf{x}(t)$, and in order 0 of $N$ to get the PDE equation for $\Pi$.

# LINEAR NOISE APPROXIMATION

## DRIFT, JACOBIAN, DIFFUSION MATRIX

$$F(\mathbf{x}) = \sum_{\eta \in \mathcal{T}} \mathbf{v}_\eta f_\eta(\mathbf{x})$$

$$J_{ij}(t) = \sum_{\eta \in \mathcal{T}} \mathbf{v}_\eta[i] \partial_j f_\eta(\mathbf{x}(t))$$

$$D_{ik}(\mathbf{x}) = \sum_{\eta \in \mathcal{T}} \mathbf{v}_\eta[i] \mathbf{v}_\eta[k] f_\eta(\mathbf{x})$$

## NOISE: LINEAR FOKKER-PLANK EQUATION

$$\frac{\partial \Pi(\mathbf{x}, t)}{\partial(t)} = \sum_{i,j} J_{i,j}(t) \partial_i(\xi_j \Pi(\mathbf{x}, t)) + \frac{1}{2} \sum_{i,j} D_{ij} \partial_{ij} \Pi(\mathbf{x}, t).$$

# Linear Noise Approximation

## Linear Fokker-Plank equation

Linear Fokker-Plank equations have solutions which are Gaussian Processes! We can obtain the equations for average and variance from $\Pi$, and solve them to fully determine the noise term $\xi(t)$.

## Average

$\frac{d\mathbb{E}[\xi(t)]}{dt} = J\mathbb{E}\left[\xi(t)\right]$, So if $\mathbb{E}\left[\xi(0)\right] = 0$, then $\mathbb{E}\left[\xi(t)\right] = 0$.

## Covariance matrix $C$

$$\frac{dC}{dt} = JC + CJ^T + D$$

## Solution to the system

$\hat{\mathbf{X}}^{(N)}(t) \approx \mathbf{x}(t) + N^{-\frac{1}{2}}\xi(t)$ is a Gaussian Process.
At time $t$, it is a multivariate Gaussian distribution with mean $\mathbf{x}(t)$ and covariance $N^{-1}C$.

# Central limit theorem

We can look at the linear noise approximation from a limit theorem point of view.

$$\mathbf{X}^{(N)}(t) = N\mathbf{x}(t) + N^{\frac{1}{2}}\xi^{(N)}(t),$$

where we defined

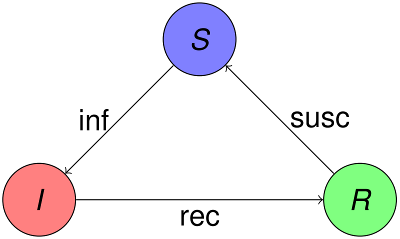
$$\xi^{(N)}(t) = N^{-\frac{1}{2}}(\mathbf{X}^{(N)}(t) - N\mathbf{x}(t))$$

## Central Limit Theorem (Kurtz)

If rate functions are of class $C^1$, then

$$\xi^{(N)} \Rightarrow \xi \text{ (weakly)}$$

# EXAMPLE: SIR EPIDEMICS




Three variables: $X_S$,$X_I$,$X_R$.
State space:
$\mathcal{D} = \{(n_1, n_2, n_3) \mid n_1 + n_2 + n_3 = N\} \subset \{0, \ldots, N\}^3$.

Transitions:

- $(inf, \top, (-1, 1, 0) k_I \frac{X_I}{N} X_S)$
- $(rec, \top, (0, -1, 1), k_R X_I)$
- $(susc, \top, (1, 0, -1), k_S X_R)$

# EXAMPLE: SIR EPIDEMICS

## REDUCE THE SYSTEM DIMENSION

As $X_R = N - X_S - X_I$, we can reduce to two dimensions: $x_S = x$ and $x_I = y$. Call also $u = VAR(\xi_S)$, $v = VAR(\xi_I)$, $c = COV(\xi_S, \xi_I)$

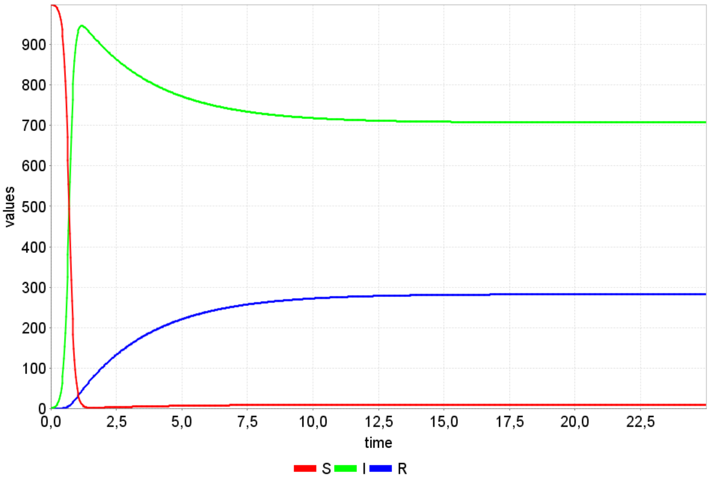
## AVERAGE: FLUID EQUATIONS

$$\frac{dx}{dt} = -k_I xy + k_S(1 - x - y)$$
$$\frac{dy}{dt} = k_I xy - k_R y$$

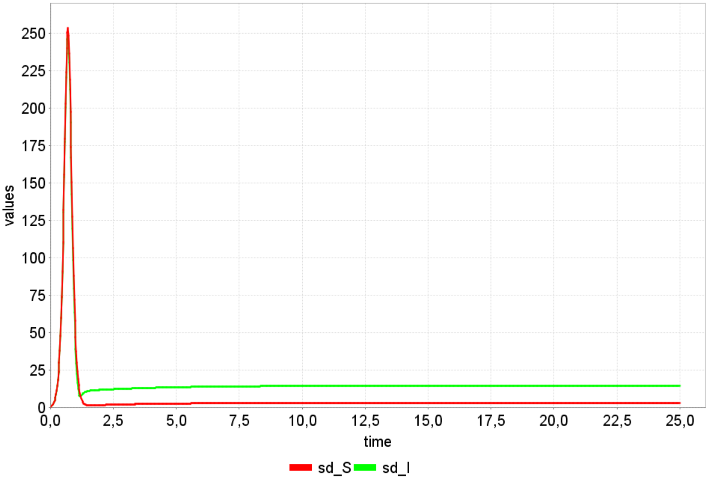
## VARIANCE $u$ OF $x$, $v$ OF $y$, COVARIANCE $c$

$$\frac{du}{dt} = -2u(k_i y + k_s) - 2c(k_i x + k_s) + k_i xy + k_s(1 - x - y)$$
$$\frac{dv}{dt} = 2c(k_i y) + 2v(k_i x - kr) + kixy + k_r y$$
$$\frac{dc}{dt} = -c(k_i y + k_s) - v(k_i x + k_s) + k_i yu + c(k_i x - k_r) - k_i xy$$

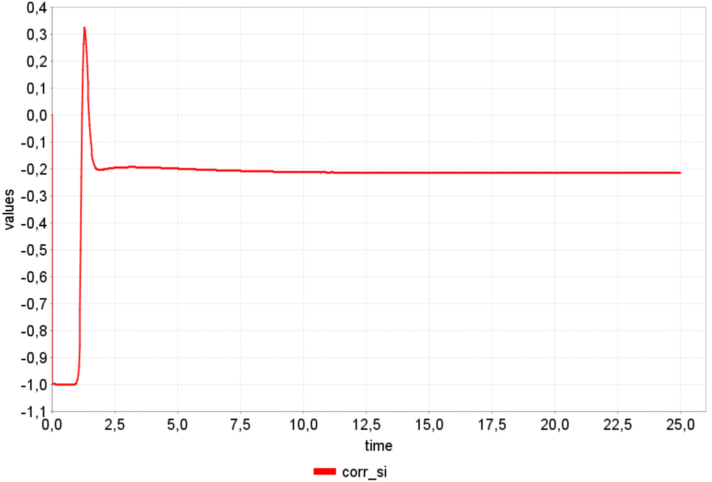
# SIR EPIDEMICS: FLUID EQUATIONS



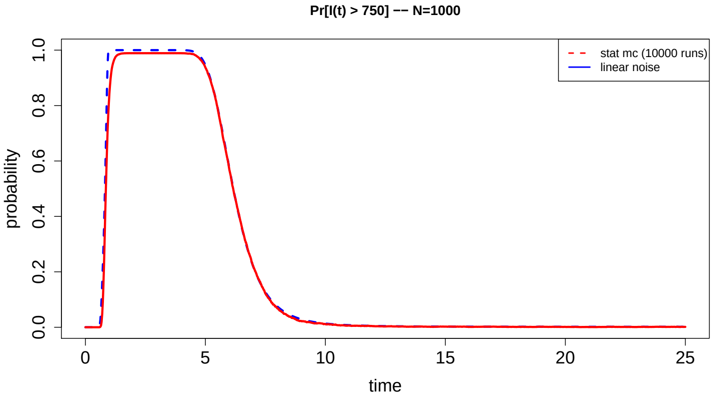
# SIR EPIDEMICS: LN ESTIMATED STANDARD DEVIATION OF $S$ AND $I$



# SIR EPIDEMICS: LN ESTIMATED CORRELATION OF $S$ AND $I$



# SIR EPIDEMICS: LN ESTIMATED $\mathbb{P}\{I(t) \geq 750\}$



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