Computational Modelling
Moment closures and central limit approximation

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Stochastic approximation in a MESOSCOPIC SYSTEM

FLUID APPROXIMATION
|||
THERMODYNAMIC LIMIT

Outline

1. Fluid Equation and Moments
2. System-Size Expansion
3. Linear Noise Approximation

MOMENT CLOSURE.

FLUID + GAUSSIAN NOISE

④ LANGEVIN / DIFFUSION APPROXIMATION SDE

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 take the point of view of perturbation theory, Taylor-expanding the Kolmogorov equation around the mean (Kramers-Moyal expansion).
- Finally, we will look at another kind of expansion, the linear noise, that will bring us to the central limit theorem (Gaussian Process approximation).

Outline

AVERAGE OF CTMC MODEL

$$\frac{dP(x,t)}{dt} = \boxed{\sum_\eta P(x-v_\eta,t)\,r_\eta(x-v_\eta) - \sum_\eta P(x,t)\,r_\eta(x)}$$

$$E_t[X] = \sum_{x\in S} x\cdot P(x,t) \Rightarrow \frac{dE_t[X]}{dt} = \sum_x x\,\frac{dP(x,t)}{dt}$$

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:

$$= \sum_x F(x)\cdot P(x,t) \qquad \boxed{F(x) = \sum_\eta v_\eta\, r_\eta(x)}$$

X - linear
X² - non linear
xy - non linear

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

mass action
X+Y→C ? NO
C→X+Y !
X→Y ? SI
Y→X
order ≤ 1

$E_t[X] : W(t)$

$$\frac{dW(t)}{dt} = F(W(t)) \Rightarrow \text{FLUID EQUATION}$$

APPROXIMATIONS

S+I→2I
I→R

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 τ, 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.

ODE FOR THE AVERAGE

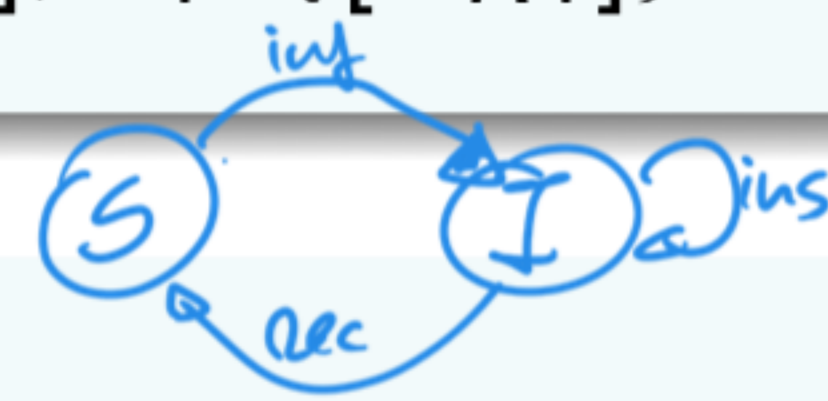
BRUTAL APPROXIMATION

$E_t[F(X)] \approx F(E_t[X])$ (I order)

SIMPLE SHARED RESOURCE MODEL

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

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



$S + I \xrightarrow{k_1 h_1} 2I$

$I \xrightarrow{k_2} S$

SYNCHRONIZATION BY RATE PRODUCT

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

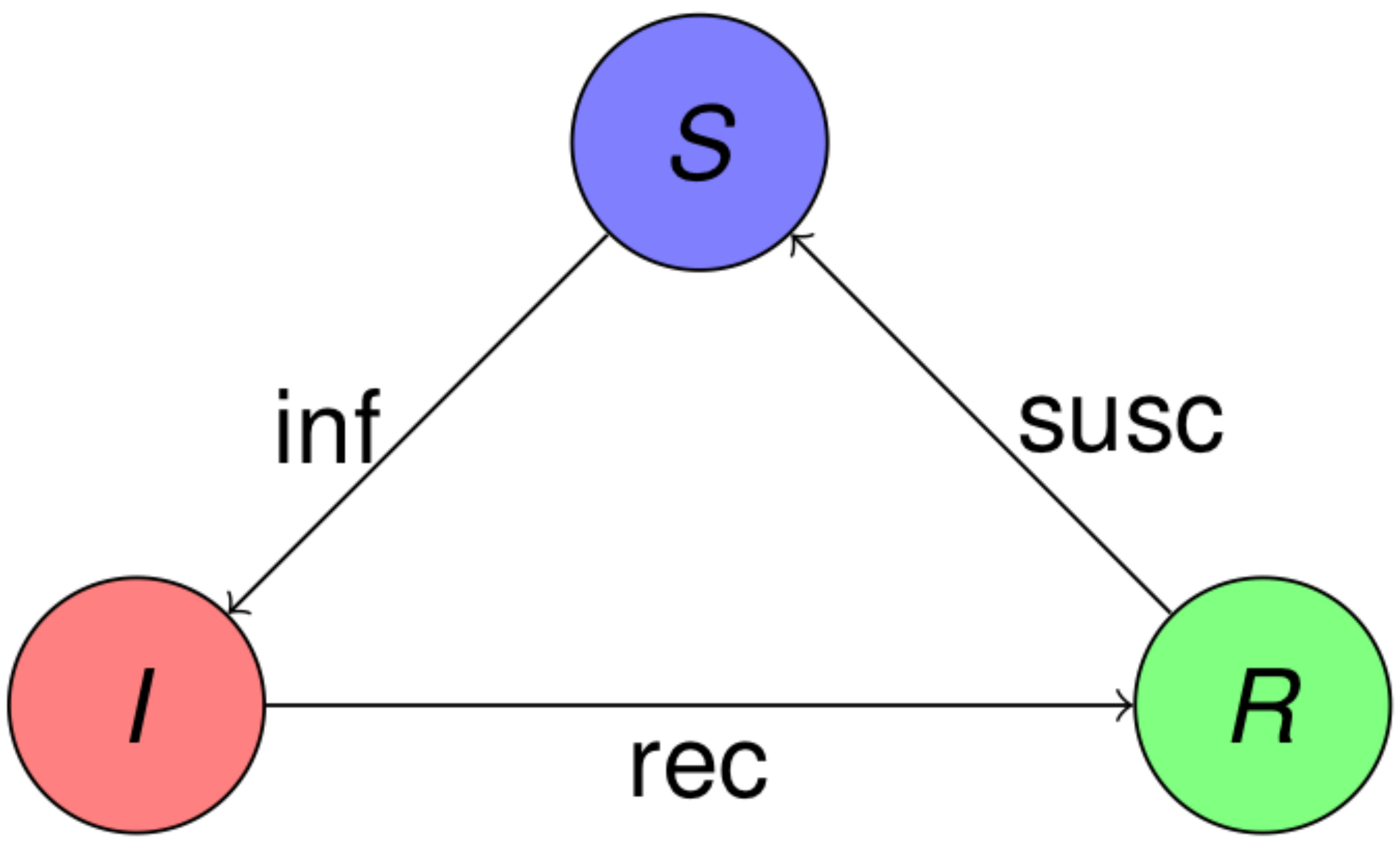
$cov(X_S, X_I) + E[X_S]E[X_I]$

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

$cov(X_S, X_I) = 0$

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

$$\frac{dE_t[g(X)]}{dt} = E_t\left[\sum_\mu f_\mu(X)\left[g(X+v_\mu)-g(X)\right]\right]$$

$$= E_t[\mathcal{L}g(x)]$$

Dinkin's Formula for non-centred moments

$m = (m_1, \dots, m_n)$

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

$g(X) = X_1^{m_1}\cdots X_n^{m_n}$

SIR model example

SIR

$S + I \to 2I$

$I \to R$

$\boxed{R \to S}$

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

$$= k_I/N\mathbb{E}_t[X_S X_I] - 2k_I/N\mathbb{E}_t[X_S^2 X_I] + 2k_S\mathbb{E}_t[X_S X_R] + k_S\mathbb{E}_t[X_R]$$

$$\frac{dE_t[X_S^2]}{dt} = E_t\Big[k_I/N\cdot X_S X_I\big((X_S-1)^2 - X_S^2\big) + k_S X_R\big((X_S+1)^2 - X_S^2\big)\Big]$$

$\cancel{X_S^2} + 2X_S + 1 - \cancel{X_S^2}$

$+ k_S \cdot E[2X_S X_R + X_R]$

$2k_S E[X_S X_R] + E[X_R]$

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

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

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

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

SIR MODEL EXAMPLE

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

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

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

SIR model example

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

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

For the SIR model, the equation for a moment of order k 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 k 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_τ 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.

→ LOW-DISPERSION MOMENT CLOSURE (ASSUMING CUMULANT MOMENTS OF ORDER K+1 ON EQUAL TO ZERO)

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:

$\{1, 1, 2, 3\}$ $(1,1),(2,3)$ — $(1,2),(1,3)$ $\times 2$ —

- 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

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

$E[X_1^2 X_2 X_3]$ — --

$VAR(X) = E[X^2] - E[X]^2$

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

$COV(X,Y) = E[XY] - E[X]E[Y]$

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

$E[(X_S - \mu_S)^2(X_I - \mu_I)] = 0$ $\quad E[X_S^2 X_I] + \cdots\cdots = 0 \Rightarrow$ —

Outline

LOW DISPERSION

CUMULANT MOMENTS.

MOMENT-GENERATING FUNCTION

$$M_x(t) = \mathbb{E}[e^{tX}] \qquad t \in \mathbb{R}$$

$$e^{tX} = 1 + tX + \frac{t^2}{2} X^2 + \dots + \frac{t^n}{n!} X^n + \dots$$

$$\mathbb{E}[e^{tX}] = 1 + t \cdot E[X] + \frac{t^2}{2} E[X^2] + \dots + \frac{t^n}{n!} \mathbb{E}[X^n] + \dots$$

$$\Rightarrow \frac{d^n}{dt^n} M_x(0) = \boxed{E[X^n]}$$

POISSON(λ)

$$M_x(t) = e^{\lambda(e^t - 1)}$$

NORMAL

$$M_x(t) = e^{t\mu + \frac{1}{2}\sigma^2 t^2}$$

CUMULANT GENERATING FUNCTION

$$K(t) = \log \mathbb{E}[e^{tX}] = \log M_x(t)$$

$$K(t) = \sum_{n=1}^{n} k_n \frac{t^n}{n!}$$

k_n = nth cumulant moments

$$k_n = \frac{d^n}{dt^n} K(0)$$

$\kappa_1 = E[X]$

$\kappa_2 = VAR[X]$

$\kappa_3 = SKEW[X]$

κ_4: KURTOSIS

NORMAL

$K(t) = t\mu + \frac{1}{2}\sigma^2 t^2$

LOW DISPERSION of ORDER K

$\Rightarrow$ Set cumulant moments to zero from $K+1$ on.

$\mu_1 = \kappa_1$

$\mu_2 = \kappa_2 + \kappa_1^2$

$\mu_3 = \kappa_3 + 3\kappa_2\kappa_1 + \kappa_1^3$

$\mu_4 = \kappa_4 + 4\kappa_3\kappa_1 + 3\kappa_2^2 + 6\kappa_2\kappa_1^2 + \kappa_1^4$

$\mu_n = E[X^n]$

BELL POLYNOMIAL

$$\mu_n = \sum_{k=1}^{n} \underbrace{B_{n,k}(\kappa_1, \ldots, \kappa_{n-k+1})} \rightarrow \sum_{j_1, \ldots, j_{n-k+1}} \frac{n!}{j_1! \cdots j_{n-k+1}!} \left(\frac{x_1}{1!}\right)^{j_1} \left(\frac{x_2}{2!}\right)^{j_2} \cdots \left(\frac{x_{n-k+1}}{(n-k+1)!}\right)^{j_{n-k+1}}$$

1) There are implementations of M.C.

2) WARNING: # of EQUATIONS FOR ORDER K IS $O(n^K)$

n = number of species / dimensions

exponential in K. => keep K ~~[illegible]~~ low

(up to ~~4~~, or up to 8/16 for a low-ish one)

3) for ~~K~~ large, equations often are ~~[illegible]~~ STIFF

(numerically unstable)

- DISTRIBUTION APPROXIMATION (MAXIMUM ENTROPY)
- PARAMETER ESTIMATION → MOMENT MATCHING }
  → Generalized METHOD OF MOMENTS }