

11.17.

Anderson, Gracium, Kurtz (preprint).

Microscopic
stochastic
model

X continuous time MC (counts # molecules of each species at time t).

$$X(t) \in \mathbb{Z}_+^n = \mathbb{N}^n, \quad t \geq 0.$$

Q -matrix, $Q = (q_{xx'})$ $x \neq x'$. $q_{xx'}$ = inf rate of going from x to x' .

$$x = x', \quad q_{xx} = - \sum_{x' \neq x} q_{xx'}.$$

Reactions: $v_k \xrightarrow{K_k} v_k', \quad k=1, \dots, K.$

Deterministic model.

$$(*) \quad \dot{c} = f(c) = \sum_k K_k c^{v_k} (v_k' - v_k).$$

Assume $c \in \mathbb{R}_{\geq 0}^n$ is a complex balance equilibrium for $(*)$.

$$\sum_{j \neq i} K_{j \rightarrow i} c^{y(j)} = \sum_{j \neq i} K_{i \rightarrow j} c^{y(i)}, \quad \forall \text{ complex } i.$$

Theorem:

Suppose $\mathbb{Z}_+^n$ is a single communicating class for X .

$$\text{Let } \pi(x) = M \frac{c^x}{x!}, \quad x \in \mathbb{Z}_+^n,$$

M = normalizing constant so that $\sum_{x \in \mathbb{Z}_+^n} \pi(x) = 1$.

$$\pi(x) = M \frac{\prod_{i=1}^n c_i^{x_i}}{\prod_{i=1}^n x_i!}$$

Then π is the unique stationary distribution of X .

Proof: Verify $\pi'Q = 0$.

(Since X does not explode, this will imply π is a stationary distribution for X ; i.e., $\pi'P(t) = \pi \forall t \geq 0$)

$$P_{xx'}(t) = P(X(t) = x' \mid X(0) = x)$$

$$\pi'Q = 0 \Leftrightarrow \sum_{x \in \mathbb{Z}_+^n} \pi(x) q_{xx'} = 0, \quad \forall x' \in \mathbb{Z}_+^n.$$

$$\begin{aligned} \Leftrightarrow \sum_{x \neq x'} \pi(x) q_{xx'} &= \pi(x') (-q_{x'x'}) \\ &= \pi(x') \sum_{x \neq x'} q_{x'x} \end{aligned}$$

$$\begin{aligned} \Leftrightarrow \sum_{k=1}^K \pi(x) R_k \underbrace{\prod_{i=1}^n x_i \cdots (x_i - v_{ik} + 1)}_{\alpha_k(x)} \cdot \mathbb{1}_{\{x = x' - v_k' + v_k, \quad x - v_k \in \mathbb{Z}_+^n\}} \\ = \pi(x') \sum_{k=1}^K R_k \underbrace{\prod_{i=1}^n x_i' \cdots (x_i' - v_{ik} + 1)}_{\lambda_k(x')} \cdot \mathbb{1}_{\{x' - v_k \in \mathbb{Z}_+^n, \quad x = x' + v_k' - v_k\}} \end{aligned}$$

$$\begin{aligned} \Leftrightarrow \sum_{k=1}^K M \frac{e^x}{x!} R_k \prod_{i=1}^n x_i (x_i - 1) \cdots (x_i - v_{ik} + 1) \cdot \mathbb{1}_{\{x = x' - v_k' + v_k, \quad x - v_k \in \mathbb{Z}_+^n\}} \\ = M \sum_{k=1}^K \frac{e^{x'}}{x'!} R_k \prod_{i=1}^n x_i' \cdots (x_i' - v_{ik} + 1) \cdot \mathbb{1}_{\{x = x' + v_k' - v_k, \quad x' - v_k \in \mathbb{Z}_+^n\}} \end{aligned}$$

$$\Leftrightarrow \sum_{k=1}^K R_k \frac{e^{v_k - v_k'}}{(x - v_k)!} \mathbb{1}_{\{x = x' - v_k' + v_k, \quad x - v_k \in \mathbb{Z}_+^n\}}.$$

$$= \sum_{k=1}^K R_k \frac{1}{(x' - v_k)!} \mathbb{1}_{\{x' - v_k \in \mathbb{Z}_+^n\}}, \quad \forall x'.$$

$$\Leftrightarrow \sum_{k=1}^K R_k \frac{e^{v_k - v_k'}}{(x' - v_k')!} \mathbb{1}_{\{x' - v_k' \in \mathbb{Z}_+^n\}}$$

$$= \sum_{k=1}^K R_k \frac{1}{(x' - v_k)!} \mathbb{1}_{\{x' - v_k \in \mathbb{Z}_+^n\}}, \quad \forall x'.$$

$$\Leftrightarrow \sum_{\substack{z \\ \text{complexes}}} \sum_{\substack{\text{reactions } k: \\ z \text{ is a product} \\ \text{i.e.}; v_k \rightarrow z}} R_k \frac{c^{v_k - z}}{(x' - z)!} 1_{\{x' - z \in \mathbb{Z}_+^n\}}$$

$$= \sum_{\substack{z \\ \text{complexes}}} \sum_{\substack{\text{reactions } k: \\ z \text{ is a reactant} \\ \text{i.e.}; z \rightarrow v_k'}} \cancel{R_k} \frac{1}{\cancel{R_k} (x' - z)!} 1_{\{x' - z \in \mathbb{Z}_+^n\}}, \quad \forall x'.$$

\cancel{R_k} \text{ complex } z.

$$\Leftarrow \sum_{v_k \rightarrow z} R_k \frac{c^{v_k}}{(x' - z)!} 1_{\{x' - z \in \mathbb{Z}_+^n\}}$$

$$= \sum_{\substack{k: \\ z \rightarrow v_k'}} \frac{R_k \cdot c^z}{(x' - z)!} 1_{\{x' - z \in \mathbb{Z}_+^n\}}$$

$$\Leftrightarrow \sum_{v_k \rightarrow z} R_k c^{v_k} = \sum_{z \rightarrow v_k'} R_k \cdot c^z$$

This holds because c is a complex balance solution.

□

Diffusion (second-order) approximation to X .

Recall $\bar{X}^r(t) = \frac{X^r(rt)}{r} = \bar{X}^r(0) + \frac{1}{r} \sum_k N_k(r) \int_0^t f_k^r(\bar{X}^r(s)) ds$

(v_k' - v_k)

where $f_k^r(c) = \tilde{R}_k \prod_{i=1}^n c_i (c_i - \frac{1}{r}) \cdots (c_i - \frac{v_{ik}}{r} + \frac{1}{r})$.

$$f_k(c) = R_k \prod_{i=1}^n c_i^{v_{ik}}$$

Suppose $\bar{X}^r(0) \Rightarrow x_0 \in \mathbb{R}_+^n$ as $r \rightarrow \infty$.

Shown $\bar{X}^r \Rightarrow \bar{X}$ as $r \rightarrow \infty$ where $\bar{X}$ is the solution of $\bar{X}(t) = x_0 + \sum_k (\int_0^t f_k(\bar{X}(s)) ds) (v_k' - v_k)$, $t \geq 0$.

Consider

$$\hat{V}^r(t) = \sqrt{r} (\bar{X}^r(t) - \bar{X}(t)).$$

Let $\hat{N}_k(t) = N_k(t) - t$, $t \geq 0$, $\hat{N}_k^r(t) = \frac{\hat{N}_k(\sqrt{r}t)}{\sqrt{r}}$.

$$\hat{V}^r(t) = (\bar{X}^r(0) - \bar{X}_0) \cdot \sqrt{r}$$

$$+ \frac{1}{\sqrt{r}} \sum_k \hat{N}_k^r(r \int_0^t f_k^r(\bar{X}^r(s)) ds) (v_k' - v_k)$$

$$+ \frac{1}{\sqrt{r}} \sum_k r \left(\int_0^t f_k^r(\bar{X}^r(s)) ds \right) (v_k' - v_k).$$

$$- \sqrt{r} \sum_k \left(\int_0^t f_k(\bar{X}(s)) ds \right) (v_k' - v_k).$$

$$\hat{V}^r(t) = \hat{V}^r(0) + \sum_k \hat{N}_k^r \left(\int_0^t f_k^r(\bar{X}^r(s)) ds \right) (v_k' - v_k).$$

$$+ \sqrt{r} \sum_k \int_0^t (f_k^r(\bar{X}^r(s)) - f_k(\bar{X}(s))) ds (v_k' - v_k).$$

(*)

Know $\hat{N}_k^r \Rightarrow W_k$ as $r \rightarrow \infty$ where W_k is standard B.M.

By independence, $(\hat{N}_1^r, \dots, \hat{N}_K^r) \Rightarrow (W_1, \dots, W_K)$ as $r \rightarrow \infty$
independence.

Let $\hat{\Phi}_k^r(t) = \int_0^t f_k^r(\bar{X}^r(s)) ds.$

Showed previously that jointly with (*).

$$(\hat{\Phi}_1^r, \dots, \hat{\Phi}_K^r) \Rightarrow (\Phi_1, \dots, \Phi_K) \text{ where } \Phi_k(t) = \int_0^t f_k(\bar{X}(s)) ds.$$

Can use random time change to conclude that

$$(\hat{N}_1^r(\hat{\Phi}_1^r(\cdot)), \dots, \hat{N}_K^r(\hat{\Phi}_K^r(\cdot)))$$

$$\Rightarrow (W_1(\Phi_1(\cdot)), \dots, W_K(\Phi_K(\cdot))) \text{ as } r \rightarrow \infty.$$

Hence, $\sum_k \hat{N}_k^r \left(\int_0^t f_k^r(\bar{X}^r(s)) ds \right) (v_k' - v_k)$

$$\Rightarrow \sum_k W_k \left(\int_0^t f_k(\bar{X}(s)) ds \right) (v_k' - v_k) \text{ as } r \rightarrow \infty.$$

Assume that $\hat{V}^r(0) \Rightarrow V_0$ as $r \rightarrow \infty$, jointly with above

$$f_k^r(\bar{X}^r(s)) - f_k(\bar{X}(s)) = f_k^r(\bar{X}^r(s)) - f_k(\bar{X}^r(s)) + f_k(\bar{X}^r(s)) - f_k(\bar{X}(s)).$$

$$f_k^r(c) = \tilde{K}_k \prod_{i=1}^n c_i (c_i - \frac{1}{r}) \cdots (c_i - \frac{v_{ik}}{r} + \frac{1}{r}).$$

$$f_k(c) = \tilde{K}_k \prod_{i=1}^n \underbrace{c_i \cdot c_i \cdots c_i}_{v_{ik}}.$$

$$f_k(\bar{X}^r(s)) - f_k(\bar{X}(s)) = \nabla f_k(\bar{X}(s)) \cdot (\bar{X}^r(s) - \bar{X}(s))$$

for some point $\bar{X}^r(s)$ between $\bar{X}^r(s)$ and $\bar{X}(s)$.

Can show $\sqrt{r} \sum_k \int_0^t (f_k^r(\bar{X}^r(s)) - f_k(\bar{X}(s))) ds (v_k' - v_k) \Rightarrow \sum_k \int_0^t \nabla f_k(\bar{X}(s)) \cdot V(s) ds (v_k' - v_k)$

where $V = \lim_{r \rightarrow \infty} \hat{V}^r$ in distribution.

$$V(t) = V(0) + \sum_k W_k \left(\int_0^t f_k(\bar{X}(s)) ds \right) (v_k' - v_k) + \sum_k \int_0^t \nabla f_k(\bar{X}(s)) \cdot V(s) ds (v_k' - v_k).$$

In fact, $\hat{V}^r \Rightarrow V$ as $r \rightarrow \infty$.

$$\sqrt{r}(\bar{X}^r - \bar{X}) \Rightarrow V \text{ as } r \rightarrow \infty.$$

$$\bar{X}^r \approx \bar{X} + \frac{1}{\sqrt{r}} V.$$