

Lecture 5: October 17

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First recall that

$$\bar{X}^r(t) = \bar{X}^r(0) + \sum_{k=1}^K (v'_k - v_k) \frac{1}{r} N_k \left( r \int_0^t f_k^r(\bar{X}^r(s)) ds \right) \quad (1)$$

and

$$f_k^r(\bar{x}^r) = \prod_{i=i}^n \tilde{\kappa}_k \bar{x}^r \left( \bar{x}^r - \frac{1}{r} \right) \cdots \left( \bar{x}^r - \frac{v_{ik} - 1}{r} \right)$$

We want to show that  $\bar{X}^r \Rightarrow \bar{X}$  which is a solution of a system of ODEs (fluid model). We need two steps for the proof:

- (1)  $\{\bar{X}^r\}$  is C-tight (tight and all limit points are almost surely continuous);
- (2) Any limit “point” of  $\bar{X}$  satisfies an ODE (which has a unique solution).

## 5.1 Criterion for C-tightness

$\{\bar{X}^r\}$  is C-tight if for each  $T > 0$ ,  $\varepsilon > 0$ , there is  $K^* = K(\varepsilon, T)$ ,  $\delta^* = \delta(\varepsilon, T)$ ,  $r^* = r(\varepsilon, T)$ , such that for all  $r > r^*$ ,

$$(i) \quad P(\|\bar{X}^r\|_T > K^*) \leq \varepsilon \Leftrightarrow P(\|\bar{X}^r\|_T \leq K^*) \geq 1 - \varepsilon,$$

and

$$(ii) \quad P(w(\bar{X}^r, \delta^*, T) > \varepsilon) < \varepsilon \Leftrightarrow P(w(\bar{X}^r, \delta^*, T) \leq \varepsilon) \geq 1 - \varepsilon$$

(Recall that  $\|x\|_T = \sup_{0 \leq t \leq T} |x(t)|$  and that the modulus of continuity is  $w(x, \delta, T) = \sup_{u, v \in [0, T]; |u-v| \leq \delta} |x(u) - x(v)|$ .) Condition (i) is called compact containment.

*Assumptions on reactions:* Continuous flow stirred tank reactor:

Divide the set of reactions into 3 sets: (1)  $k \in \{1, \dots, K_1\}$ . These reactions will be conservative to some quantities like mass:  $\exists m > 0$  in  $\mathbb{R}^n$  such that  $m \cdot (v'_k - v_k) = 0$ . (E.g.  $S_1 + S_2 = S_3$  then choose  $m = (1, 1, 2)$ .) (2)  $k \in \{K_1 + 1, \dots, K_2\}$ . These reactions are inflows such that  $\emptyset \rightarrow S_i$ . For these  $m \cdot (v'_k - v_k) \geq 0$ . (3)  $k \in \{K_2 + 1, \dots, K\}$ , these reactions are outflows such that  $S_i \rightarrow \emptyset$ . For these  $m \cdot (v'_k - v_k) \leq 0$ .

## 5.2 Show compact containment

First realize that for each  $i$ ,  $0 \leq m_i \bar{X}_i^r(t) \leq |m \cdot \bar{X}^r(t)|$ . If  $\|m \cdot \bar{X}^r\|_T \leq L$  for some  $L$ , we have for all  $i$ ,  $|\bar{X}_i^r(t)| \leq L/m_i$  for  $0 \leq t \leq T$ , therefore

$$\|\bar{X}^r\|_T \leq \sqrt{n} \max_i (L/m_i). \quad (5.1)$$

Now, by the assumptions on the reaction set, we have

$$m \cdot \bar{X}^r(t) \leq m \cdot \bar{X}^r(0) + \sum_{k=K_1+1}^{K_2} m \cdot (v'_k - v_k) \bar{N}_k^r \left( \int_0^t f_k^r(\bar{X}^r(s)) ds \right), \quad (2)$$

(denote  $d_k = m \cdot (v'_k - v_k)$  in the following text) where

$$\bar{N}_k^r(t) = \frac{1}{r} N_k(rt), \quad \forall k, t \geq 0.$$

For  $k = K_1 + 1, \dots, K_2$ ,  $f_k^r(\bar{X}^r(s)) = \tilde{\kappa}_k$ . Therefore the right hand side of (2) becomes

$$m \cdot \bar{X}^r(0) + \sum_{k=K_1+1}^{K_2} d_k \bar{N}_k^r(\tilde{\kappa}_k t).$$

Assume  $\bar{X}^r(0) \Rightarrow x_0$  (which implies that  $m \cdot \bar{X}^r(0) \Rightarrow m \cdot x_0$ ). Along with the convergence of  $\bar{X}^r(0)$ , we have

$$(\bar{N}_1^r(\cdot), \dots, \bar{N}_K^r(\cdot)) \Rightarrow \mathbb{1}(\cdot)$$

with  $\mathbb{1}(t) = (t, \dots, t)$  with length  $K$ . This is from the functional Law of Large Numbers. The argument is as below. Recall that as  $r \rightarrow \infty$ ,

$$\left\{ \frac{N_k(rt) - rt}{\sqrt{r}}, \quad t \geq 0 \right\} \Rightarrow B_k(\cdot).$$

By Skorokhod, without loss of generality, we may suppose this is almost sure convergence uniformly on compact time intervals, which is

$$\sup_{0 \leq t \leq T} \left| \frac{N_k(rt) - rt}{\sqrt{r}} - B_k(t) \right| \rightarrow 0$$

almost surely as  $r \rightarrow \infty$ . Multiply both sides by  $1/\sqrt{r}$ , we get

$$\sup_{0 \leq t \leq T} \left| \frac{N_k(rt) - rt}{r} - \frac{B_k(t)}{\sqrt{r}} \right| \rightarrow 0.$$

This gives, almost surely,  $\bar{N}_k^r(t) - t \rightarrow 0$  uniformly for  $0 \leq t \leq T$ . Since  $T$  is chosen arbitrarily, we are done.

It follows that the right hand side of (2) is converging in distribution to  $\bar{Y}$  given by  $\bar{Y}(t) = m \cdot x_0 + \sum_{k=K_1+1}^{K_2} d_k \tilde{\kappa}_k t$ . Denote  $\bar{Y}^r(t) = m \cdot \bar{X}^r(0) + \sum_{k=K_1+1}^{K_2} d_k \bar{N}_k^r(\tilde{\kappa}_k t)$ . Since  $\{\bar{Y}^r(\cdot)\}$  is converging in distribution to the continuous “process”  $\bar{Y}$ , the sequence  $\{Y^r(\cdot)\}$  is C-tight.

Consequently, given  $T > 0, \varepsilon > 0$ ,  $\exists C(\varepsilon, T), r(\varepsilon, T)$  such that

$$P(\|Y^r\|_T > C(\varepsilon, T)) < \varepsilon, \quad \forall r > r(\varepsilon, T).$$

Then, by (5.1),

$$\begin{aligned} & P(\|m \cdot \bar{X}^r\|_T > C(\varepsilon, T)) < \varepsilon \\ & \Leftrightarrow P(\|m \cdot \bar{X}^r\|_T \leq C(\varepsilon, T)) \geq 1 - \varepsilon \\ & \Rightarrow P(\|\bar{X}^r\|_T \leq \sqrt{n} C(\varepsilon, T) / \min_i m_i) \geq 1 - \varepsilon \end{aligned}$$

### 5.3 Control of oscillations

Let  $f_k(x) = \tilde{\kappa}_k \prod_{i=1}^n x_i^{v_{ik}} = \tilde{\kappa}_k x^{v_k}$ ,  $x \in \mathbb{R}^n$ . Notice that  $f_k^r \rightarrow f_k$  as  $r \rightarrow \infty$ , uniformly on compact sets. Also for all  $r \geq 1$ ,

$$|f_k^r(\bar{x}^r)| \leq f_k(\bar{x}^r), \quad (5.2)$$

in the lattice where  $\bar{x}^r$  takes its values.

Fix  $\varepsilon > 0, T > 0$ , and let  $K^*, r^*$ , be such that  $P(\|\bar{X}^r\|_T \leq K^*) \geq 1 - \varepsilon/2$  for all  $r \geq r^*$ . Let  $G^{\varepsilon, r} = \{\|\bar{X}^r\|_T \leq K^*\}$  (Good set) On  $G^{\varepsilon, r}$ , we have for  $0 \leq t \leq T$ ,

$$\begin{aligned} |f_k^r(\bar{X}^r(t))| &\leq f_k(\bar{X}^r(t)) \quad \text{by (5.2)} \\ &\leq \sup_{x \in \mathbb{R}_{\geq 0}^n, |x| \leq K^*} f_k(x) \\ &\leq M^*. \end{aligned}$$

Here  $M^* = \sup_{k=1, \dots, K} \sup_{x \in \mathbb{R}_{\geq 0}^n, |x| \leq K^*} f_k(x)$ . This implies that  $\|f_k^r(\bar{X}^r(\cdot))\|_T \leq M^*$ ,  $k = 1, \dots, K$ , on  $G^{\varepsilon, r}$ .

Now recall that the right hand side of (1) is

$$\bar{X}^r(0) + \sum_{k=1}^K (v'_k - v_k) \bar{N}_k^r \left( \int_0^t f_k^r(\bar{X}^r(s)) ds \right).$$

Recall that  $(\bar{N}_1^r(\cdot), \dots, \bar{N}_K^r(\cdot)) \Rightarrow \mathbb{1}(\cdot)$  as  $r \rightarrow \infty$ , so it is C-tight. By the second part of C-tight criterion,  $\exists \delta_1^*, r_1^*$ , such that

$$P(w(\bar{N}_k^r(\cdot), \delta_1^*, M^*T) \leq \varepsilon / |d_k| K \quad \forall k) \geq 1 - \varepsilon/2$$

for all  $r \geq r_1^*$ . Denote the event inside the probability bracket as  $\tilde{G}^{\varepsilon, r}$ .

Let  $\bar{\Phi}_k^r(t) = \int_0^t f_k^r(\bar{X}^r(s)) ds$ ,  $k = 1, \dots, K$ . On  $G^{\varepsilon, r}$  we have for each  $k$ ,  $\|\bar{\Phi}_k^r(\cdot)\|_T \leq M^*T$  and also

$$w(\bar{\Phi}_k^r, \delta, T) \leq M^* \delta = \delta_1^*,$$

if we let  $\delta = \delta_1^*/M^*$ .

So for  $r \geq r_1^* \vee r^*$ ,

$$\begin{aligned} &P(w(\bar{N}_k^r(\bar{\Phi}_k^r(\cdot)), \delta_1^*, T) \leq \varepsilon / |d_k| K, \quad \forall k) \\ &\geq P(w(\bar{N}_k^r(\cdot), \delta_1^*, M^*T) \leq \varepsilon / |d_k| K, w(\bar{\Phi}_k^r(\cdot), \delta, T) \leq \delta_1^*, \|\bar{\Phi}_k^r(\cdot)\|_T \leq M^*T, \quad \forall k) \\ &\geq P(G^{\varepsilon, r} \cap \tilde{G}^{\varepsilon, r}) \geq 1 - \varepsilon \end{aligned}$$

This finishes the part 2 of the C-tightness for  $\{\bar{X}^r\}$ . Therefore  $\{\bar{X}^r\}$  is C-tight.