<4> Derivation of state equations & transition rate matrix for the Markov Models:

Let Δt be a positive number so small that we can disregard the possibility of more than one transition in a time interval of length Δt

Based on the Chapman-Kolmogorov equation (P_3), we have

$$P_{ij}(t+\Delta t) = \sum_{k=0}^{r} P_{ik}(t)\cdot P_{kj}(\Delta t)$$

$$= \sum_{\substack{k=0 \\ k\neq j}}^{r} P_{ik}(t)\cdot P_{kj}(\Delta t) + P_{ij}(t)\cdot P_{jj}(\Delta t)$$

According to property P_2 on slide #5 $\left(\sum_{i=0}^{r} P_{ji}(t)=1\right)$, we have

$$P_{jj}(\Delta t) = 1 - \sum_{\substack{k=0 \\ k\neq j}}^{r} P_{jk}(\Delta t)$$

Thus, $P_{jj}(\Delta t)$ is the probability that the process does not leave state j in a time interval of length Δt.

So,

$$P_{ij}(t+\Delta t) = \sum_{\substack{k=0\\k\neq j}}^{r} P_{ik}(t)\cdot P_{kj}(\Delta t) + P_{ij}(t)\left[1-\sum_{\substack{k=0\\k\neq j}}^{r} P_{jk}(\Delta t)\right]$$

$$\Rightarrow P_{ij}(t+\Delta t) - P_{ij}(t) = -P_{ij}(t)\sum_{\substack{k=0\\k\neq j}}^{r} P_{jk}(\Delta t) + \sum_{\substack{k=0\\k\neq j}}^{r} P_{ik}(t)\cdot P_{kj}(\Delta t)$$

After dividing by Δt, letting $\Delta t \to 0$, we have

$$\lim_{\Delta t\to 0}\frac{P_{ij}(t+\Delta t)-P_{ij}(t)}{\Delta t} = \frac{dP_{ij}(t)}{dt} = \dot{P}_{ij}(t) = -P_{ij}(t)\lim_{\Delta t\to 0}\sum_{\substack{k=0\\k\neq j}}^{r}\frac{P_{jk}(\Delta t)}{\Delta t} + \lim_{\Delta t\to 0}\sum_{\substack{k=0\\k\neq j}}^{r} P_{ik}(t)\left(\frac{P_{kj}(\Delta t)}{\Delta t}\right)$$

$$= -P_{ij}(t)\sum_{\substack{k=0\\k\neq j}}^{r}\alpha_{jk} + \sum_{\substack{k=0\\k\neq j}}^{r} P_{ik}(t)\cdot\alpha_{kj} \quad\text{—————}\quad \text{(eq \#1 — state equations)}$$

Note: Defn of transition rate:

$$\alpha_{ij} = \lim_{\Delta t\to 0}\frac{P\{X(t+\Delta t)=j \mid X(t)=i\}}{\Delta t} = \lim_{\Delta t\to 0}\frac{P_{ij}(\Delta t)}{\Delta t} \quad \text{(slide \#6)}$$

Assume the process is in state i at time $t=0$, i.e. $X(0)=i$. This can be expressed as:

$$\left.\begin{aligned} P_i(0) &= P\{X(0)=i\} = 1 \\ P_k(0) &= P\{X(0)=k\} = 0 \qquad k\neq i \end{aligned}\right\} \text{ initial condition}$$

From now on we'll assume that the initial state is known. Then we can simplify the notation of eq #1 by omitting the index i:

eq#1 → eq#2:

Eq#2
$$\begin{cases} \dot{P}_j(t) = -P_j(t) \overbrace{\sum_{\substack{k=0 \\ k\neq j}}^{r} \alpha_{jk}}^{\alpha_{jj}} + \sum_{\substack{k=0 \\ k\neq j}}^{r} P_k(t)\cdot\alpha_{kj} \\ P_i(0)=1 \quad P_k(0)=0 \quad \text{for } k\neq i \end{cases}$$

The transition rate α_{ij} in eq#2 may be written as a matrix A, called transition rate matrix:

$$A = \begin{bmatrix} -\alpha_{00} & \alpha_{10} & \alpha_{20} & \cdots & \alpha_{r0} \\ \alpha_{01} & -\alpha_{11} & \alpha_{21} & \cdots & \alpha_{r1} \\ \alpha_{02} & \alpha_{12} & -\alpha_{22} & \cdots & \alpha_{r2} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ \alpha_{0r} & \alpha_{1r} & \alpha_{2r} & & -\alpha_{rr} \end{bmatrix}$$

For diagonal elements:

$$\alpha_{jj} = \sum_{\substack{k=0 \\ k\neq j}}^{r} \alpha_{jk}$$

Eq#2 now can be rewritten as in matrix form:

$$\dot{p}(t) = A\cdot p(t)$$

$$\begin{bmatrix} -\alpha_{00} & \alpha_{10} & \alpha_{20} & \cdots & \alpha_{r0} \\ \alpha_{01} & -\alpha_{11} & \alpha_{21} & \cdots & \alpha_{r1} \\ \alpha_{02} & \alpha_{12} & -\alpha_{22} & \cdots & \alpha_{r2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \alpha_{0r} & \alpha_{1r} & \alpha_{2r} & & -\alpha_{rr} \end{bmatrix} \begin{bmatrix} p_0(t) \\ p_1(t) \\ p_2(t) \\ \vdots \\ p_r(t) \end{bmatrix} = \begin{bmatrix} \dot{p}_0(t) \\ \dot{p}_1(t) \\ \dot{p}_2(t) \\ \vdots \\ \dot{p}_r(t) \end{bmatrix}$$