Modeling Exopeptidase Activity from LC-MS Data

Proof of Proposition 1

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Recall that $(X(t))$ is a homogeneous Markov process with the following intensity of transitions $(x \neq x')$:

$$Q(x, x') = \begin{cases} a_{\star i} & \text{if } x'_{-i} = x_{-i}, x'_i = x_i + 1 \text{ for some } i, \\ a_{r(i,j)} x_i & \text{if } x'_{-i-j} = x_{-i-j}, x'_i = x_i - 1, x'_j = x_j + 1 \\ & \qquad \text{for some } i \to j, \\ a_{i\dagger} x_i & \text{if } x'_{-i} = x_{-i}, x'_i = x_i - 1 \text{ for some } i. \end{cases} \tag{1}$$

Proposition (Equilibrium distribution)**.** *The process $(X(t))$ has the equilibrium (stationary) distribution π given by*

$$\pi(x) = \prod_{i \in \mathcal{V}} \mathrm{e}^{-\lambda_i} \frac{\lambda_i^{x_i}}{x_i!},$$

where the configuration of intensities $(\lambda_i)_{i \in \mathcal{V}}$ is the unique solution to the

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following system of "balance" equations:

$$\sum_{k\to i} \lambda_k a_{r(k,i)} + a_{\star i} = \lambda_i \left(\sum_{i\to j} a_{r(i,j)} + a_{i\dagger} \right) \qquad \textit{for every } i \in \mathcal{V}.$$

Proof. We are to show that for every configuration x,

$$\sum_{x'\neq x} \pi(x)Q(x,x') = \sum_{x'\neq x} \pi(x')Q(x',x). \tag{2}$$

Using the formulas for $Q(x,x')$ it is easy to see that the LHS of (2) is

$$\begin{aligned}&\sum_{i\to j} \pi(x_{-i-j}) \mathrm{e}^{-\lambda_i} \frac{\lambda_i^{x_i}}{x_i!} \mathrm{e}^{-\lambda_j} \frac{\lambda_j^{x_j}}{x_j!} a_{r(i,j)} x_i \\ &\quad + \sum_i \pi(x_{-i}) \mathrm{e}^{-\lambda_i} \frac{\lambda_i^{x_i}}{x_i!} a_{i\dagger} x_i \\ &\qquad + \sum_k \pi(x_{-k}) \mathrm{e}^{-\lambda_k} \frac{\lambda_k^{x_k}}{x_k!} a_{\star k}.\end{aligned}$$

Putting the first and second term together we arrive at

$$\begin{aligned}\mathrm{LHS} = \sum_i \pi(x_{-i}) \mathrm{e}^{-\lambda_i} \frac{\lambda_i^{x_i - 1}}{(x_i-1)!} \left(\sum_{j\,:\, i\to j} a_{r(i,j)} + a_{i\dagger} \right) \lambda_i \\ + \pi(x) \sum_k a_{\star k}.\end{aligned}$$

Similarly, the RHS of (2) is

$$\sum_{k\to i}\pi(x_{-k-i})\mathrm{e}^{-\lambda_k}\frac{\lambda_k^{x_k+1}}{(x_k+1)!}\mathrm{e}^{-\lambda_i}\frac{\lambda_i^{x_i-1}}{(x_i-1)!}a_{r(k,i)}(x_k+1)$$
$$+\sum_{i}\pi(x_{-i})\mathrm{e}^{-\lambda_i}\frac{\lambda_i^{x_i-1}}{(x_i-1)!}a_{\star i}$$
$$+\sum_{j}\pi(x_{-j})\mathrm{e}^{-\lambda_j}\frac{\lambda_j^{x_j+1}}{(x_j+1)!}a_{j\dagger}(x_j+1).$$

Notice that the first term corresponds to transitions from x' to x with $x'_k = x_k+1$ and $x'_i = x_i-1$. In the second term we have transitions with $x'_i = x_i-1$ and in the third – those with $x'_j = x_j+1$. Analogously as when computing the LHS we obtain

$$\mathrm{RHS} = \sum_{i}\pi(x_{-i})\mathrm{e}^{-\lambda_i}\frac{\lambda_i^{x_i-1}}{(x_i-1)!}\left(\sum_{k:\,k\to i}a_{r(k,i)}\lambda_k + a_{\star i}\right)$$
$$+\pi(x)\sum_{j}\lambda_j a_{j\dagger}.$$

The balance equations imply that LHS=RHS and the proof is complete. □