Appendix C

Pathway Sums for Chain Graphs, $\mathcal{S}_{\alpha,\beta}^{C_N}$

To obtain the total probability of leaving the chain C_N via node α if started from node β, i.e. $\mathcal{E}_{\alpha}^{C_N}\mathcal{S}_{\alpha,\beta}^{C_N}$, we must calculate the pathway sum $\mathcal{S}_{\alpha,\beta}^{C_N}$. We start with the case $\alpha = \beta$ and obtain $\mathcal{S}_{\beta,\beta}^{C_N}$. Consider any path that has reached node $N-1$. The probability factor due to all possible $N-1$ to N recrossings is simply $R_{N-1} = 1/(1 - P_{N-1,N}P_{N,N-1})$. We need to include this factor every time we reach node $N-1$ during recrossings of $N-2$ to $N-1$. The corresponding sum becomes

$$R_{N-2} = \sum_{m=0}^{\infty} (P_{N-2,N-1}P_{N-1,N-2}R_{N-1})^m = \frac{1}{1 - P_{N-2,N-1}P_{N-1,N-2}R_{N-1}}. \quad \text{(C.1)}$$

Similarly, we can continue summing contributions in this way until we have recrossings of β to $\beta+1$, for which the result of the nested summations is $R_\beta = 1/(1 - P_{\beta,\beta+1}P_{\beta+1,\beta}R_{\beta+1})$. Hence, R_β is the total transition probability for pathways that return to node β and are confined to nodes with index greater than β without escape from C_N.

We can similarly calculate the total probability for pathways returning to β and confined to nodes with indices smaller than β. The total probability factor for recrossings between nodes 1 and 2 is $L_2 = 1/(1 - P_{1,2}P_{2,1})$. Hence, the required probability for recrossings between nodes 2 and 3 including arbitrary recrossings between 1 and 2 is $L_3 = 1/(1 - P_{2,3}P_{3,2}L_2)$. Continuing up to recrossings between nodes $\beta - 1$ and β we obtain the total return probability for pathways restricted to this side of β as

$L_\beta = 1/(1 - P_{\beta-1,\beta}P_{\beta,\beta-1}L_{\beta-1})$. The general recursive definitions of L_j and R_j are:

$$\begin{aligned} L_j &= \begin{cases} 1, & j = 1, \\ 1/(1 - P_{j-1,j}P_{j,j-1}L_{j-1}), & j > 1, \end{cases} \\ \text{and} \quad R_j &= \begin{cases} 1, & j = N, \\ 1/(1 - P_{j,j+1}P_{j+1,j}R_{j+1}), & j < N. \end{cases} \end{aligned} \tag{C.2}$$

We can now calculate $\mathcal{S}^{C_N}_{\beta,\beta}$ as

$$\begin{aligned} \mathcal{S}^{C_N}_{\beta,\beta} &= \sum_{m=0}^{\infty}\sum_{n=0}^{m} \frac{n!}{m!(n-m)!} \left(P_{\beta-1,\beta}P_{\beta,\beta-1}L_{\beta-1}\right)^n \left(P_{\beta,\beta+1}P_{\beta+1,\beta}R_{\beta+1}\right)^{m-n} \\ &= \sum_{m=0}^{\infty} (P_{\beta-1,\beta}P_{\beta,\beta-1}L_{\beta-1} + P_{\beta,\beta+1}P_{\beta+1,\beta}R_{\beta+1})^m \\ &= (1 - P_{\beta-1,\beta}P_{\beta,\beta-1}L_{\beta-1} - P_{\beta,\beta+1}P_{\beta+1,\beta}R_{\beta+1})^{-1} \\ &= \left(1 - \frac{L_\beta - 1}{L_\beta} - \frac{R_\beta - 1}{R_\beta}\right)^{-1} \\ &= \frac{L_\beta R_\beta}{L_\beta - L_\beta R_\beta + R_\beta}, \end{aligned} \tag{C.3}$$

where we have used Equation C.2 and the multinomial theorem [242].

We can now derive $\mathcal{S}^{C_N}_{\alpha,\beta}$ as follows. If $\alpha > \beta$ we can write

$$\mathcal{S}^{C_N}_{\alpha,\beta} = \mathcal{S}^{C_N}_{\alpha-1,\beta} P_{\alpha,\alpha-1} R_\alpha. \tag{C.4}$$

$\mathcal{S}^{C_N}_{\alpha-1,\beta}$ gives the total transition probability from β to $\alpha - 1$, so the corresponding probability for node α is $\mathcal{S}^{C_N}_{\alpha-1,\beta}$ times the branching probability from $\alpha - 1$ to α, i.e. $P_{\alpha,\alpha-1}$, times R_α, which accounts for the weight accumulated from all possible paths that leave and return to node α and are restricted to nodes with indexes greater than α. We can now replace $\mathcal{S}^{C_N}_{\alpha-1,\beta}$ by $\mathcal{S}^{C_N}_{\alpha-2,\beta}P_{\alpha-1,\alpha-2}R_{\alpha-1}$ and so on, until $\mathcal{S}^{C_N}_{\alpha,\beta}$ is expressed in terms of $\mathcal{S}^{C_N}_{\beta,\beta}$. Similarly, if $\alpha < \beta$ we have

$$\mathcal{S}^{C_N}_{\alpha,\beta} = \mathcal{S}^{C_N}_{\alpha+1,\beta} P_{\alpha,\alpha+1} L_\alpha, \tag{C.5}$$

and hence

$$\mathcal{S}^{C_N}_{\alpha,\beta} = \begin{cases} \mathcal{S}^{C_N}_{\beta,\beta} \displaystyle\prod_{i=\alpha}^{\beta-1} P_{i,i+1}L_i, & \alpha < \beta, \\ \mathcal{S}^{C_N}_{\beta,\beta} \displaystyle\prod_{i=\beta+1}^{\alpha} P_{i,i-1}R_i, & \alpha > \beta. \end{cases} \tag{C.6}$$