

Lemma 1.

$$p_{\xi\xi}(t) = 1 - \binom{|\xi|}{2} (1 + O(N^{-1})) c_N(t).$$

Proof. We will show that the claimed expression is both a lower bound and an upper bound for $p_{\xi\xi}(t)$, beginning with the latter. By definition,

$$\begin{aligned} p_{\xi\xi}(t) &= \frac{1}{(N)^{|\xi|}} \sum_{\substack{i_1 \neq \dots \neq i_{|\xi|}=1 \\ \text{all distinct}}}^N \nu_t^{(i_1)} \dots \nu_t^{(i_{|\xi|})} \\ &= \frac{1}{(N)^{|\xi|}} \left[\left(\sum_{i=1}^N \nu_t^{(i)} \right)^{|\xi|} - \binom{|\xi|}{2} \sum_{i=1}^N (\nu_t^{(i)})^2 \left(\sum_{j=1}^N \nu_t^{(j)} \right)^{|\xi|-2} \right] \\ &= \frac{1}{(N)^{|\xi|}} \left[N^{|\xi|} - N^{|\xi|-2} \binom{|\xi|}{2} \sum_{i=1}^N (\nu_t^{(i)})^2 \right] \\ &= \frac{N^{|\xi|}}{(N)^{|\xi|}} \left[1 - \binom{|\xi|}{2} \frac{1}{N^2} \sum_{i=1}^N (\nu_t^{(i)})^2 \right]. \end{aligned}$$

Now

$$\frac{1}{N^2} \sum_{i=1}^N (\nu_t^{(i)})^2 = \frac{1}{N^2} \left(N + \sum_{i=1}^N (\nu_t^{(i)})_2 \right) = \frac{1}{N} + \frac{1 + O(N^{-1})}{\cancel{(N)}_2} c_N(t),$$

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so that

$$p_{\xi\xi}(t) = \frac{N^{|\xi|}}{(N)^{|\xi|}} \left[1 - \binom{|\xi|}{2} \frac{1}{N} - \binom{|\xi|}{2} (1 + O(N^{-1})) c_N(t) \right]. \quad (1)$$

Next,

$$\begin{aligned} \frac{N^{|\xi|}}{(N)^{|\xi|}} &= \left[\left(1 - \frac{1}{N} \right) \dots \left(1 - \frac{|\xi|-1}{N} \right) \right]^{-1} \\ &= \left[1 - \left(\sum_{i=1}^{|\xi|-1} i \right) \frac{1}{N} + \left(\sum_{i=1}^{|\xi|-1} \sum_{j \neq i}^{|\xi|-1} ij \right) \frac{1}{N^2} + O(N^{-3}) \right]^{-1}, \end{aligned}$$

and we have that

$$\begin{aligned} \sum_{i=1}^{|\xi|-1} i &= \binom{|\xi|}{2}, \\ \sum_{i=1}^{|\xi|-1} \sum_{j \neq i}^{|\xi|-1} ij &= \sum_{i=1}^{|\xi|-1} i \left[\binom{|\xi|}{2} - i \right] = \binom{|\xi|}{2}^2 - \sum_{i=1}^{|\xi|-1} i^2 = \binom{|\xi|}{2}^2 - \binom{|\xi|}{2} \frac{2|\xi|-1}{3}, \end{aligned}$$

Presumably a known result

so that

$$\frac{N^{|\xi|}}{(N)^{|\xi|}} = \left[1 - \binom{|\xi|}{2} \frac{1}{N} + \left\{ \binom{|\xi|}{2}^2 - \binom{|\xi|}{2} \frac{2|\xi|-1}{3} \right\} \frac{1}{N^2} + O(N^{-3}) \right]^{-1}.$$

A Taylor expansion gives

$$\frac{1}{1+x} = 1 - x + x^2 + O(x^3),$$

so that

$$\begin{aligned}\frac{N^{|\xi|}}{(N)_{|\xi|}} &= 1 + \binom{|\xi|}{2} \frac{1}{N} - \left\{ \binom{|\xi|}{2}^2 - \binom{|\xi|}{2} \frac{2|\xi| - 1}{3} \right\} \frac{1}{N^2} + \binom{|\xi|}{2}^2 \frac{1}{N^2} + O(N^{-3}) \\ &= 1 + \binom{|\xi|}{2} \frac{1}{N} + \binom{|\xi|}{2} \frac{2|\xi| - 1}{3} \frac{1}{N^2} + O(N^{-3}).\end{aligned}$$

Substituting back into (1), we obtain

$$\begin{aligned}p_{\xi\xi}(t) &= \left[1 + \binom{|\xi|}{2} \frac{1}{N} + \binom{|\xi|}{2} \frac{2|\xi| - 1}{3} \frac{1}{N^2} + O(N^{-3}) \right] \left[1 - \binom{|\xi|}{2} \frac{1}{N} - \binom{|\xi|}{2} (1 + O(N^{-1})) c_N(t) \right] \\ &= 1 - \left\{ \binom{|\xi|}{2}^2 - \binom{|\xi|}{2} \frac{2|\xi| - 1}{3} \right\} \frac{1}{N^2} + O(N^{-3}) - \binom{|\xi|}{2} (1 + O(N^{-1})) c_N(t) \\ &= 1 - \binom{|\xi|}{2} \frac{(3|\xi| - 1)(|\xi| - 2)}{6} \frac{1}{N^2} + O(N^{-3}) - \binom{|\xi|}{2} (1 + O(N^{-1})) c_N(t).\end{aligned}$$

It is clear the second order term is always non-positive, and so we have the asymptotic bound

$$p_{\xi\xi}(t) \leq 1 - \binom{|\xi|}{2} (1 + O(N^{-1})) c_N(t)$$

as soon as $|\xi| \geq 3$. For $|\xi| = 2$, we need to check the signs of higher order terms. We have

$$N^2 / (N)_2 = \frac{N^2}{N(N-1)} = \frac{1}{1 - 1/N} = 1 + \frac{1}{N} + \frac{1}{N^2} + \frac{1}{N^3} + \dots,$$

so that

$$\begin{aligned}p_{\xi\xi}(t) &= \left[1 + \frac{1}{N} + \frac{1}{N^2} + \frac{1}{N^3} + \dots \right] \left[1 - \frac{1}{N} - (1 + O(N^{-1})) c_N(t) \right] \\ &= 1 - (1 + O(N^{-1})) c_N(t).\end{aligned}$$

All the corrections cancel, and hence the upper bound holds for $|\xi| = 2$, and in fact is an asymptotic equality in that case.

For a lower bound, let $\kappa_i := \#\{j : b_j = i\}$ denote the multiplicity of mergers of size i , with the slight abuse of terminology in that κ_1 counts non-merger events. In particular, we have that $\kappa_1 + 2\kappa_2 + \dots |\xi| \kappa_{|\xi|} = |\xi|$. Now

$$p_{\xi\xi}(t) = 1 - \frac{1}{(N)_{|\xi|}} \sum_{k=1}^{|\xi|-1} \sum_{\substack{b_1 \geq \dots \geq b_k = 1 \\ b_1 + \dots + b_k = |\xi|}} \frac{|\xi|!}{\prod_{j=1}^{|\xi|} (j!)^{\kappa_j} \kappa_j!} \sum_{\substack{i_1 \neq \dots \neq i_k = 1 \\ \text{all distinct}}}^N (\nu_t^{(i_1)})_{b_1} \dots (\nu_t^{(i_k)})_{b_k},$$

because the right hand side subtracts the probabilities of all possible merger events. See [Fu, 2006, eq (11)] for the combinatorial factor. The omitted $k = |\xi|$ summand would correspond to the probability of an identity transition. The non-increasing ordering of (b_1, \dots, b_k) is arbitrary, but without loss of generality: choosing any ordering of the same set of merger sizes would give the same result.

Because $b_1 \geq 2$ and the summands are all non-negative, we can separate out one pair-merger, replace falling factorials with exponents, and write

$$\begin{aligned}p_{\xi\xi}(t) &\geq 1 \\ &- \frac{1}{(N)_{|\xi|}} \sum_{i=1}^N (\nu_t^{(i)})_2 \sum_{k=1}^{|\xi|-2} \sum_{\substack{b_1 \geq \dots \geq b_k = 1 \\ b_1 + \dots + b_k = |\xi|}} \frac{|\xi|!}{\prod_{j=1}^{|\xi|} (j!)^{\kappa_j} \kappa_j!} \sum_{\substack{i_2 \neq \dots \neq i_k \neq i \\ \text{all distinct}}}^N (\nu_t^{(i)})_{b_1-2} (\nu_t^{(i_2)})_{b_2} \dots (\nu_t^{(i_k)})_{b_k}.\end{aligned}$$

Now, for each $k \in \{1, \dots, |\xi| - 2\}$ we have

$$\frac{|\xi|!}{\prod_{j=1}^{|\xi|} (j!)^{\kappa_j} \kappa_j!} = \underbrace{\binom{|\xi|}{b_1, \dots, b_k}}_{\text{unfamiliar notation: multinomial coefficient}} \prod_{j=1}^{|\xi|} \frac{1}{\kappa_j!} = \binom{|\xi|}{2} \frac{\binom{|\xi|-2}{b_1-2, b_2, \dots, b_k}}{\binom{b_1}{2}} \prod_{j=1}^{|\xi|} \frac{1}{\kappa_j!} \leq \binom{|\xi|}{2} \binom{|\xi|-2}{b_1-2, b_2, \dots, b_k},$$

which gives

$$p_{\xi\xi}(t) \geq 1 - \frac{\binom{|\xi|}{2}}{(N)^{|\xi|}} \sum_{i=1}^N (\nu_t^{(i)})_2 \sum_{k=1}^{|\xi|-2} \sum_{\substack{b_1 \geq \dots \geq b_k = 1 \\ b_1 + \dots + b_k = |\xi|}}^{|\xi|-2} \binom{|\xi|-2}{b_1-2, b_2, \dots, b_k} \sum_{\substack{i_2 \neq \dots \neq i_k \neq i \\ \text{all distinct}}}^N (\nu_t^{(i)})^{b_1-2} (\nu_t^{(i_2)})^{b_2} \dots (\nu_t^{(i_k)})^{b_k}.$$

We also have the following identity, which is due to the fact that the left hand side is just an obtuse way to write a multinomial expansion of the right hand side:

$$\begin{aligned} & \sum_{k=1}^{|\xi|-2} \sum_{\substack{b_1 \geq \dots \geq b_k = 1 \\ b_1 + \dots + b_k = |\xi|}}^{|\xi|-2} \binom{|\xi|-2}{b_1-2, b_2, \dots, b_k} \sum_{\substack{i_2 \neq \dots \neq i_k \neq i \\ \text{all distinct}}}^N (\nu_t^{(i)})^{b_1-2} (\nu_t^{(i_2)})^{b_2} \dots (\nu_t^{(i_k)})^{b_k} \\ &= \left(\sum_{j \neq i}^N \nu_t^{(j)} \right)^{|\xi|-2} \leq N^{|\xi|-2}. \end{aligned}$$

Thus

$$p_{\xi\xi}(t) \geq 1 - \frac{\binom{|\xi|}{2}}{(N)^{|\xi|}} \sum_{i=1}^N (\nu_t^{(i)})_2 N^{|\xi|-2} = 1 - \binom{|\xi|}{2} \frac{1 + O(N^{-1})}{(N)_2} c_N(t),$$

as required. □

References

Yun-Xin Fu. Exact coalescent for the Wright-Fisher model. *Theor. Popln Biol.*, 69:385–394, 2006.