1 A special aggregation-fragmentation process

Consider the state space $S_n = \{\mathbf{m} = (m_j) : m_j \geq 0, \sum_j j m_j = n\}$. Picture a state as a partition of n items into clusters, with m_j clusters of size j, $1 \leq j \leq n$. Picture each cluster as a linear polymer, with j items linked by $j-1$ edges. Fix a parameter $0 < \beta < \infty$, and define a continuous-time chain $(\mathbf{M}(t))$ on S_n as follows. Let each edge disappear at rate β, splitting a size-j (say) item into two items of sizes i and $j-i$, for some $1 \leq i \leq j/2$. And for each distinct pair of clusters, of sizes i and $j-i$ say, let them merge into one cluster of size j (by creation of a linking edge) at rate $2/n$. So the transition rates are as follows. Write δ^j for the unit vector $\delta^j_i = 1_{(i=j)}$.

$$
\begin{array}{rcl}
\mathbf{m} \to & \mathbf{m} - \delta^j + \delta^i + \delta^{j-i} & : \text{ rate } 2\beta m_j, \quad 1 \leq i < j/2 \\
 & \text{(fragmentation)} & : \text{ rate } \beta m_j, \quad i = j/2
\end{array}
$$

$$
\begin{array}{rcl}
\mathbf{m} \to & \mathbf{m} + \delta^j - \delta^i - \delta^{j-i} & : \text{ rate } 2 m_i m_{j-i}/n, \quad 1 \leq i < j/2 \\
 & \text{(aggregation)} & : \text{ rate } m_i(m_i - 1)/n, \quad i = j/2.
\end{array}
$$

Writing $c(\mathbf{m}) = \sum_j m_j$ for the number of clusters in configuration $\mathbf{m}$, it is easy to check that the chain is reversible with stationary distribution

$$\pi(\mathbf{m}) \propto (\beta n)^{c(\mathbf{m})} \prod_j \tfrac{1}{m_j!}.$$

In fact this model is a particular case of general reversible models of aggregation and fragmentation: see Kelly [**?**] Chapter 8. We will use special structure of this particular case to prove a bound on the relaxation time.

Proposition 1 *For the aggregation-fragmentation chain* $(\mathbf{M}(t))$ *specified above,*

$$(1 - o(1))(\beta^2 + 4\beta)^{-1/2} \leq \tau_2 \leq \beta^{-1} \text{ as } n \to \infty.$$

Proof. Consider the following interacting particle process $\mathbf{B}(t) = (B_i(t), 1 \leq i \leq n)$ on the edges of the n-cycle. Each edge can be in state 0 or state 1, so the states are $\mathbf{b} = (b_1, \ldots, b_n) \in C_n := \{0,1\}^n$. The transition rates at each edge are:

$$
\begin{array}{ll}
0 \to 1 & \text{rate } \beta \\
1 \to 0 & \text{rate } \frac{s(\mathbf{b})-1}{n}, \text{ where } s(\mathbf{b}) := \sum_i b_i.
\end{array}
$$

This chain is reversible with stationary distribution

$$\pi(\mathbf{b}) \propto (\beta n)^{s(\mathbf{b})}/(s(\mathbf{b})-1)!.$$

Now we can specify a function $f : C_n \to S_n$ as follows. In a configuration $\mathbf{b}$, cut each edge in state 1. Let m_j be the resulting number of connected components with exactly j vertices, and let $f(\mathbf{b}) = (m_j)$. We claim that the chain on S_n induced by f (recall Chapter 4 section 6.1) from the interacting particle process $\mathbf{B}(t)$ on C_n is precisely the aggregation-fragmentation chain $(\mathbf{M}(t))$. The key fact is that the process $(B_i(t))$ is exchangeable in the edge-labels i. So conditional on $f(\mathbf{B}(t)) = \mathbf{m}$, for fixed t and $\mathbf{m}$, the blocks comprising $\mathbf{m}$ are in uniform random order. Thus if a particular edge changes state from 1 to 0 at time t, the chance that it causes some size-i block and some size-$(j-i)$ block to join together equals $\frac{2m_i m_{j-1}}{s(\mathbf{b})(s(\mathbf{b})-1)}$, where $\mathbf{b} = \mathbf{B}(t)$. Since there are $s(\mathbf{b})$ edges in state 1 and each makes a transition at rate $(s(\mathbf{b})-1)/n$, the total rate of aggregation of size-i and size-$(j-i)$ blocks equals $2m_i m_{j-i}/n$, as required. Verifying the other transition rates is similar.

So the contraction principle (Chapter 4 section 6.1) says $\tau_2 \le \tilde{\tau}_2$, where $\tilde{\tau}_2$ is the relaxation time of the process $\mathbf{B}(t)$. We shall bound $\tilde{\tau}_2$ by coupling. Let $D = \{(\mathbf{b},\mathbf{b}) : \mathbf{b} \in C_n\}$ be the diagonal in $C_n \times C_n$ and let

$$\begin{aligned} D_1 &= \{(\mathbf{b},\mathbf{b}') : \mathbf{b}' - \mathbf{b} = \delta^e \text{ for some edge } e\} \\ D_2 &= \{(\mathbf{b},\mathbf{b}') : \mathbf{b}' - \mathbf{b} = \delta^e - \delta^{e'} \text{ for some edges } e, e'\}. \end{aligned}$$

We now specify a coupling $(\mathbf{B}(t), \mathbf{B}'(t))$ such that, from any initial states $(\mathbf{b},\mathbf{b}') \in D_1$, the coupled process stays in D_1 until entering $D \cup D_2$. Specify the transition rates for the coupled process at each edge to be

$$\begin{array}{lcl} (0,0) \to (1,1) & ; & \text{rate } \beta \\ (0,1) \to (1,1) & : & \text{rate } \beta \\ (1,1) \to (0,0) & : & \text{rate } (s(\mathbf{b})-1)/n \\ (1,1) \to (1,0) & : & \text{rate } 1/n. \end{array}$$

Note that the coupled process exits D_1 at rate $\beta + (s(\mathbf{b})-1)/n \ge \beta$, We next specify a coupling $(\mathbf{B}(t), \mathbf{B}'(t))$ such that, from any initial states $(\mathbf{b},\mathbf{b}') \in D_2$, the coupled process stays in D_2 until entering D. In this coupling, if e, e' are the initially unmatched edges, then the other edges remain matched and we specify that when one of the unmatched edges in $\mathbf{B}(t)$ makes a transition then the other unmatched edge in $\mathbf{B}'(t)$ makes the same transition. So the process becomes coupled at rate $2\beta + 2(s(\mathbf{B}(t)) - 1)/n \geq 2\beta$.

Combining the two couplings, it is easy to deduce from the coupling inequality that for any $(\mathbf{b}, \mathbf{b}') \in D_1 \cup D_2$

$$||P_{\mathbf{b}}(\mathbf{B}(t) \in \cdot) - P_{\mathbf{b}'}(\mathbf{B}(t) \in \cdot)|| = O(e^{-(\beta-\varepsilon)t}) \text{ as } t \to \infty$$

for any $\varepsilon > 0$. Using the triangle inequality this extends to any $(\mathbf{b}, \mathbf{b}') \in C_n \times C_n$ and so

$$||P_{\mathbf{b}}(\mathbf{B}(t) \in \cdot) - \pi(\cdot)|| = O(e^{-(\beta-\varepsilon)t}).$$

So by the characterization of relaxation time as asymptotic rate of convergence to stationarity, (Chapter 4 Lemma yyy; currently sitting as Lemma 16 of Chapter 13), we have $\tilde{\tau}_2 \leq 1/(\beta + \varepsilon)$ and the upper bound in Proposition 1 follows.

The process $s(\mathbf{B}(t))$ is clearly the continuous-time birth-and-death chain (Q_t, say) on states $\{1, 2, \ldots, n\}$ with transition rates

$$i \to i+1: \text{ rate } \beta(n-i); \quad i \to i-1: \text{ rate } i(i-1)/n.$$

One can check that in the aggregation-fragmentation process $\mathbf{M}(t)$ the number $c(\mathbf{M}(t))$ of clusters also evolves as this birth-and-death chain Q_t. Appealing again to the contraction principle, the relaxation time τ_2^* for Q_t is a lower bound for the relaxation time τ_2 for $\mathbf{M}(t)$. So to prove the lower bound in Proposition 1 it is enough to prove

$$\tau_2^* \geq (1 - o(1))(\beta^2 + 4\beta)^{-1/2} \text{ as } n \to \infty.$$

From the explicit formula for the stationary distribution π^Q of Q_t it is straightforward to show that π^Q is asymptotically Normal$(n\mu, n\sigma^2)$ as $n \to \infty$, where

$$\mu = \sqrt{\beta^2/4 \ + \beta} - \beta/2, \quad \sigma^2 := \mu(1-\mu)/(2-\mu)$$

and μ is the positive solution of $\mu^2 = \beta(1-\mu)$. We apply the extremal characterization with test function $f(i) := i$ and find

$$\begin{aligned} \mathrm{var}_\pi f &\sim n\sigma^2 \\ \mathcal{E}(f,f) &= \sum_i \pi^Q(i) q(i, i+1) \sim q_{i^*, i^*+1} \sim \beta(1-\mu)n \text{ where } i^* := \lfloor \mu n \rfloor. \end{aligned}$$

The extremal characterization now implies

$$\tau_2^* \geq (1 - o(1)) \frac{\sigma^2}{\beta(1-\mu)}.$$

Finally,

$$\begin{aligned}
\frac{\sigma^2}{\beta(1-\mu)} &= \frac{\mu}{\beta(2-\mu)} \text{ (definition of } \sigma) \\
&= \frac{1}{\beta + 2\mu} \text{ (use quadratic satisfied by } \mu \text{ to check } \mu(\beta+2\mu) = \beta(2-\mu)) \\
&= (\beta^2 + 4\beta)^{-1/2} \text{ (definition of } \mu).
\end{aligned}$$

■

Remarks. From the stationary distribution of $\mathbf{B}(t)$ we see that the size of a typical cluster has geometric(μ) distribution, asymptotically.

Our arguments continue to apply in the setting where $\beta = \beta_n \sim b/n$, say, though here the upper and lower bounds on τ_2 have orders n and $n^{1/2}$. Here the size of a typical cluster is geometric($\mu = \beta_n^{1/2}$) and it gets split at rate $\beta_n/\mu =$ order $n^{-1/2}$, suggesting that the relaxation time should indeed be order $n^{1/2}$. The coupling analysis we gave is very crude in this setting and can perhaps to improved. In particular, since the exit rate from D_1 is typically about $\beta + \mu$ one might hope to get $1/(\beta + \mu)$ as an upper bound for τ_2, and this would be the same order of magnitude as the lower bound.

2 Example: horizontally convex polyominoes

Here we give an elementary, but non-obvious, example of a reversible chain arising in the study of the uniform distribution on a combinatorial set.

Consider *horizontally convex polyominoes*, which we'll abbreviate to *polyominoes.* A size-n polyomino is obtained by breaking unit cells $\{1, 2, \ldots, n\}$ into consecutive blocks, and placing each block on top of the previous block, where "on top" means that some component of the current block is immediately above some component of the previous block. The figure shows a polyomino with $n = 17$.