

# A phase transition in the random transposition random walk

Nathanael Berestycki, Rick Durrett

#### ▶ To cite this version:

Nathanael Berestycki, Rick Durrett. A phase transition in the random transposition random walk. 2004. hal-00001309v1

## HAL Id: hal-00001309 https://hal.science/hal-00001309v1

Preprint submitted on 16 Mar 2004 (v1), last revised 12 Aug 2015 (v3)

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

## A phase transition in the random transposition random walk

Nathanaël Berestycki<sup>1,2</sup> and Rick Durrett<sup>2</sup>

March 16, 2004

#### Abstract

Our work is motivated by Bourque and Pevzner's (2002) simulation study of the effectiveness of the parsimony method in studying genome rearrangement, and leads to a surprising result about the random transposition walk on the group of permutations on n elements. Consider this walk in continuous time starting at the identity and let  $D_t$  be the minimum number of transpositions needed to go back to the identity from the location at time t.  $D_t$  undergoes a phase transition: the distance  $D_{cn/2} \sim u(c)n$ , where u is an explicit function satisfying u(c) = c/2 for  $c \le 1$  and u(c) < c/2 for c > 1. In addition, we describe the fluctuations of  $D_{cn/2}$  about its mean in each of the three regimes (subcritical, critical and supercritical). The techniques used involve viewing the cycles in the random permutation as a coagulation-fragmentation process and relating the behavior to the Erdős-Renyi random graph model.

**Keywords** random transposition, random graphs, phase transition, coagulation-fragmentation, genome rearrangement, parsimony method

- 1. Ecole Normale Supérieure, Département de Mathématiques et Applications, 45, rue d'Ulm F-75005 Paris, France
- 2. Department of Mathematics, Malott Hall, Cornell University, Ithaca, NY 14853, U.S.A. Both authors are partially supported by a joint NSF-NIGMS grant DMS-0201037, and would like to thank David Aldous for taking the time to answer a number of questions as this paper was being written.

#### 1 General motivation

The relationship between the orders of genes in two species can be described by a signed permutation. For example the relationship between the human and mouse X chromosomes may be encoded as (see Pevzner and Tesler (2003))

$$1 \quad -7 \quad 6 \quad -10 \quad 9 \quad -8 \quad 2 \quad -11 \quad -3 \quad 5 \quad 4$$

In words the two X chromosomes can be partitioned into 11 segments. The first segment of the mouse X chromosome is the same as that of humans, the second segment of mouse is the 7th human segment with its orientation reversed, etc. The parsimony approach to estimation of evolutionary changes of the X chromosome between human and mouse is to ask: what is the minimum number of reversals (i.e., moves that reverse the order of a segment and therefore change its sign) needed to transform the arrangement above back into  $1, \ldots, 11$ ? In other words, what is the (reversal) distance between the human and mouse X chromosomes?

Hannehalli and Pevzner (1995) developed a polynomial algorithm for answering this question. The first step in preparing to use the HP algorithm is to double the markers. When segment i is doubled we replace it by two consecutive numbers 2i - 1 and 2i, e.g., 6 becomes 11 and 12. A reversed segment -i is replaced by 2i and 2i - 1, for example, -7 is replaced by 14 and 13. The doubled markers use up the integers 1 to 22. To these numbers we add a 0 at the front and a 23 at the end. Using commas to separate the ends of the markers we can write the two genomes as follows:

The next step is to construct the breakpoint graph (see Figure 1) that results when the commas are replaced by edges that connect vertices with the corresponding numbers. In the picture we have written the vertices in their order in the mouse genome. Commas in the mouse order become thick lines (black edges), while those in the human genome are thin lines (gray edges).

Each vertex has one black and one gray edge, so the connected components of the graph are easy to find: start with a vertex and follow the connections in either direction until you come back to where you start. In this example there are five components:

$$0-1-0$$
  $2-14-15-3-2$   $4-22-23-8-9-5-4$   $19-17-16-18-19$   $13-11-10-7-6-21-20-12-13$ 

To compute a lower bound for the distance, we take the number of commas seen when we write out one genome. In this example that is 12. In general, it is 1 plus the number of markers. We then subtract the number of components in the breakpoint graph. In this example that is 5, so the result is 7. This is a lower bound on the distance, since any reversal can at most reduce this quantity by 1, and it is 0 when the two genomes are the same. We can verify that 7 is the minimum distance by constructing a sequence of 7 moves that transforms the mouse X chromosome into the human order. There are thousands of solutions, so we leave this as an exercise for the reader. Here are some hints: (i) To do this it suffices to at each step choose a reversal that increases the number of cycles by 1. (ii) This never occurs if the two chosen black edges are in different cycles. (iii) If

the two black edges are in the same cycle and are (a, b) and (c, d) as we read from left to right, this will occur unless in the cycle minus these two edges a is connected to d and b to c, in which case the number of cycles will not change. For example, in the graph in Figure 1 a reversal that breaks black edges 19-17 and 18-16 will increase the number of cycles but the one that breaks 2-14 and 15-3 will not.

In general the distance between genomes can be larger than the lower bound from the breakpoint graph. There can be obstructions called *hurdles* that can prevent us from decreasing the distance and hurdles can be intertwined in a *fortress of hurdles* that takes an extra move to break. See Hannehalli and Pevzner (1995). In symbols if  $\pi$  is the signed permutation that represents the relative order and orientation of segments in the two genomes

$$d(\pi) = n + 1 - c(\pi) + h(\pi) + f(\pi)$$

where  $d(\pi)$  is the distance from the identity, n is the number of markers,  $c(\pi)$  is the number of components in the breakpoint graph,  $h(\pi)$  is the number of hurdles, and  $f(\pi)$  is the indicator of the event  $\pi$  is a fortress of hurdles. See Section 5.2 of Durrett (2002) or Chapter 10 of Pevzner (2000) for more details.

Although  $d_0(\pi) = n + 1 - c(\pi)$  is only a lower bound on the distance, it is the right answer in most biological examples. Bafna and Pevzner (1995) consider 11 comparisons of mitochondrial and chloroplast genomes and found that this lower bound gave the right answer in all cases. This pattern has continued in more recent work, see York, Durrett, and Nielsen (2002), and Durrett, Nielsen, and York (2003). The simulations in Figure 2 will give more evidence that  $d_0(\pi)$  and  $d(\pi)$  are close in many cases.

To motivate our main question, we will introduce a second data set. Ranz, Casals, and Ruiz (2001) located 79 genes on chromosome 2 of *D. repleta* and on chromosome arm 3R of *D. melanogaster*. If we number the genes according to their order in *D. repleta* then their order in *D. melanogaster* is given in Table 1. This time we do not know the orientation of the segments, but that is not a serious problem. Using simulated annealing one can easily find an assignment of signs that minimizes the distance, which in this case is 54. Given the large number of rearrangements relative to the number of markers we should ask: when is the parsimony estimate reliable?

Bourque and Pevzner (2002) approached this question by taking 100 markers in order, performing k randomly chosen reversals to get a permutation  $\pi_k$ , computing the minimum number of reversals needed to return to the identity,  $d(\pi_k)$ , and then plotting the average value of  $d(\pi_k) - k \le 0$  for 100 simulations. They concluded, based on their simulations, that the parsimony distance for n markers was a good estimate as long as the number of reversals performed was at most 0.4n. In Figure 2 we have given -1 times their data. We have also repeated their experiment for the approximate distance  $d_0(\pi) = n + 1 - c(\pi)$  and plotted the average value of  $k - d_0(\pi_k) \ge 0$  for 10,000 replications. Our curve is less random, but close to data of Bourque and Pevzner (2000). The smooth curve gives result of Theorem 3 for the limiting behavior of  $(tn - d_0(\pi_{tn}))/n$  (as a function of t).

The biological question concerns the random reversal walk. However, it is also interesting to consider the analogous problem for random transpositions. In that case the distance from the identity can be easily computed: it is the number of markers n minus the number of cycles in the permutation. For an example, consider the following permutation of 14 objects written in its cyclic decomposition:

which indicates that  $1 \to 7$ ,  $7 \to 4$ ,  $4 \to 1$ ,  $2 \to 2$ ,  $3 \to 12$ ,  $12 \to 3$ , etc. There are 5 cycles so the distance from the identity is 9. If we perform a transposition that includes markers from two different cycles (e.g., 7 and 9) the two cycles merge into 1, while if we pick two in the same cycle (e.g., 13 and 11) it splits into two.

The situation is similar but slightly more complicated for reversals. There a reversal that involves edges in two different components merges them into 1, but a reversal that involves two edges of the same cycle may or may not increase the number of cycles. One can attempt to couple the components of the breakpoint graph for random reversals on n-1 markers and the cycles of random transposition of n markers as follows: number the edges between markers in the reversal chain (including the ends 0 and n); when markers i and j are transposed, do the inversion of edges numbered i and j. The result of the coupled simulation is given in Figure 2. As expected time minus distance is smaller for reversals but the qualitative behavior is similar. Thus, we will begin by considering the biologically less relevant case of random transpositions, and ask a question that in terms of the rate 1 continuous time random walk on the symmetric group is: how far from the identity are we at time cn/2? We will see later that parts of the answer can be extended to the reversal random walk.

## 2 The coagulation-fragmentation process and the random graph process

Let  $(\sigma_t, t \geq 0)$  be the continuous-time random walk on the group of permutations, starting at the identity, in which, at times of a rate one Poisson process, we perform a transposition of two elements chosen uniformly at random, with replacement, from  $\{1, \ldots, n\}$ . Choosing with replacement causes the chain to do nothing with probability 1/n, but makes some of the calculations a little nicer. If we think of the permutation  $\sigma$  as being represented by numbered balls sitting on numbered locations with ball  $\sigma(k)$  sitting at k, then transposition of i and j,  $\rho_{i,j}$ , can be implemented in two ways. We can exchange the balls at i and j or the balls numbered i and j. Algebraically these correspond to  $\rho_{i,j}\sigma$  and  $\sigma\rho_{i,j}$ . Since  $(\sigma\rho_{i,j})^{-1} = \rho_{i,j}\sigma^{-1}$  and the partition of  $\{1,\ldots,n\}$  induced by the cycle decompositions of  $\sigma$  and  $\sigma^{-1}$  are equal, the results are the same for either random walk.

Define the distance to the identity  $D_t$  to be the minimum number of transpositions you need to perform on  $\sigma_t$  to go back to the identity element. A different way of looking at  $D_t$  is the following.  $(\sigma_t, t \geq 0)$  can be viewed as a random walk on a graph G, where G is the Cayley graph of the symmetric group for the set of generators given by the set of all transpositions. Using this language, we see that  $D_t$  is nothing but the graph distance from  $\sigma_t$  to the origin, the identity element.

It is clear that if  $N_t$  is the number of transpositions distinct from the identity performed up to time t (a Poisson random variable with mean t[1-2/(n-1)]), then  $D_t \leq N_t$ . As mentioned earlier  $D_t$  is given by  $D_t = n - |\sigma_t|$ , where  $|\sigma_t|$  is the number of cycles in the cycle decomposition of  $\sigma_t$ . This formula allows us to turn any question about  $D_t$  into a question about  $|\sigma_t|$ . The key to studying  $|\sigma_t|$  is that the cycles evolve according to the dynamics of a coagulation-fragmentation process. When a transposition  $\rho_{i,j}$  occurs, if i and j belong to two different cycles then the cycles merge. On the contrary, if they belong to the same cycle, this cycle is split into two cycles. From the definition it can be seen that the ranked sizes of the cycles form a coagulation-fragmentation process (see Aldous (1999) and Pitman (2002),(2003)) in which components of size x and y merge at rate  $K_n(x,y) = 2xy/n^2$  and components of size x split at rate  $F_n(x) = x(x-1)/n^2$  and are

broken at a uniformly chosen random point. Diaconis, Mayer-Wolf, Zeitouni, and Zerner (2003) have recently considered the corresponding Markov chain on partitions of the unit interval and shown that the Poisson-Dirichlet distribution is the unique invariant measure.

To study the evolution of the cycles in the random permutation, we construct a random graph process. Start with the initial graph on vertices  $\{1, \ldots, n\}$  with no edge between the vertices. When a transposition of i and j occurs in the random walk, draw an edge between the vertices i and j. To avoid multiple edges, we will not draw a second edge if one is already present. It is easy to see that in our continuous time process, at time t this graph is a realization of the Erdős-Renyi random graph G(n, p), in which edges are independently present with probability  $p = 1 - \exp(-2t/n^2)$ , see Bollobás (1985) or Janson, Luczak, and Ruczinski (2000). It is also easy to see that in order for two integers to be in the same cycle in the permutation it is necessary that they are in the same component of the random graph.

To estimate the difference between cycles and components, let  $F_t$  denote the event that a fragmentation occurs at time t. It is clear that

$$D_t = N_t - 2\sum_{s \le t} \mathbf{1}_{\{F_s\}} \tag{1}$$

A fragmentation occurs in the random permutation when a transposition occurs between two integers in the same cycle, so tree components in the random graph correspond to unfragmented cycles in the random walk. Unicyclic components (with an equal number of vertices and edges) correspond to cycles in the permutation that have experienced exactly one fragmentation, but we need to know the order in which the edges were added to determine the resulting cycles. For more complex components, the relationship between the random graph and the permutation is less clear. Fortunately, these can be ignored in the proofs of our results.

#### 3 Limit Theorems

We will now describe our results and sketch their proofs. Rigorous proofs of the results stated in this section can be found in sections 4, 5 and 6.

#### 3.1 The subcritical regime

**Theorem 1.** Let 0 < c < 1. The number of fragmentations

$$Z_c := \sum_{s < cn/2} \mathbf{1}_{\{F_s\}} \Rightarrow \text{Poisson}(\kappa(c))$$
 (2)

where  $\kappa(c) = (-\log(1-c)-c)/2$ . In fact, the convergence holds for the process  $\{Z_c : 0 \le c < 1\}$  with the limit being a Poisson process with compensator  $\kappa(c)$ .

**Remark.** The result for fluctuations is formulated in terms of fragmentations rather than the distance since  $D_{cn/2} - cn/2 \approx N_{cn/2} - cn/2 = O(n^{1/2})$ . For the embedded discrete time chain, if  $k = \lfloor cn/2 \rfloor$ , then

$$(k - D_k)/2 \Rightarrow \text{Poisson}(\kappa(c)) \text{ as } n \to \infty$$
 (3)

We divide by 2 since a fragmentation reduces the distance by 1 instead of increasing it by 1. To deduce (3) from (2) we note that time k in the discrete walk corresponds to time  $N^{-1}(k) \approx cn/2$  in the continuous time walk.

Sketch of the proof. The process  $\{Z_c, 0 \leq c < 1\}$  is a càdlàg counting process. Therefore by arguments from Jacod and Shiryaev (1987), it is enough to show that its compensator  $\kappa^n$  converges to the deterministic limit  $\kappa(c)$ . If  $f_k(t)$  is the fraction of vertices that belong to cycles of size k, the rate at which fragmentations occur is just  $\sum_k f_k(t)(k-1)/n$ . Hence  $\kappa^n$  is just the integral w.r.t time of this rate. We first show that the variance converges to 0 and then, by Chebycheff's inequality, it only remains to show  $E\kappa^n(c) \to \kappa(c)$ . But by exchangeability  $E[f_k(t)] = P[|\mathcal{C}_1| = k]$  where  $|\mathcal{C}_1|$  is the size of the component that contains 1 at time t. It is not hard to see that this quantity at time bn/2 converges in distribution to the total progeny  $\tau$  of a Galton-Watson branching process with offspring distribution Poisson(b), or PGW(b). Summing the geometric series, we see that  $E\tau = 1/(1-b)$ . Integrating w.r.t. b we get the desired expected value,  $\kappa(c)$ .

To prepare for later developments, it is useful to take a second combinatorial approach to this result. We begin with Cayley's result that there are  $k^{k-2}$  trees with k labeled vertices. At time cn/2 each edge is present with probability  $1 - \exp(-c/n) \sim c/n$  so the expected number of trees of size k present is

$$\binom{n}{k}k^{k-2}\left(\frac{c}{n}\right)^{k-1}\left(1-\frac{c}{n}\right)^{k(n-k)+\binom{k}{2}-k+1}\tag{4}$$

since each of the k-1 edges need to be present and there can be no edges connecting the k point set to its complement or any other edges connecting the k points. For fixed k the above is asymptotic to

$$n\frac{k^{k-2}}{k!}c^{k-1}\left(1-\frac{c}{n}\right)^{kn}$$

The quantity in parentheses at the end converges to  $e^{-ck}$  so we have an asymptotic formula for the number of tree components at time cn/2. As a side result we get the following known result:

**Corollary 1.** The probability distribution of the total progeny T of a Poisson(c) branching process with c < 1 is given by  $P(T = k) = \frac{1}{c} \frac{k^{k-1}}{k!} (ce^{-c})^k$ 

See section 4.1 of Pitman (1998) for another proof of this result. It was first discovered by Borel (1942) and the distribution of T is called the Borel distribution. It is a particular case of the so-called Borel-Tanner distribution, see Devroye (1992) and Pitman (1997) for further references. In this context it appeared in the problem of the total number of units served in the first busy period of a queue with Poisson arrivals and constant service times. See also Tanner (1961). Of course, this becomes a branching process if we think of the customers that arrive during a person's service time as their children.

#### 3.2 The critical regime

It is well known in the theory of random graphs that the critical regime takes place at times  $(n/2)(1+\lambda n^{-1/3})$ ,  $\lambda \in (-\infty,\infty)$ . See Aldous (1997) for an interesting account that relates the growth of large clusters in the critical random graph to the multiplicative coalescent. At times  $(n/2)(1-n^{-r})$  with r < 1/3, we are still in the subcritical regime, so the arguments in the proof of Theorem 1, when done more carefully, are still valid. More precisely, we can show that if

 $c_n(r) = 1 - n^{-r/3}$  for  $0 \le r \le 1$ , then the expected number of fragmentations up to time  $c_n(r)n/2$  is again given by  $\kappa(c_n(r)) \sim (r/6) \log n$ . Hence define:

$$W_n(r) = \left(\frac{6}{\log n}\right)^{1/2} \left(\sum_{s \le c_n(r)n/2} \mathbf{1}_{\{F_s\}} - \frac{r}{6} \log n\right)$$
 (5)

**Theorem 2.** As  $n \to \infty$ ,  $W_n(\cdot)$  converge weakly, with respect to the Skorokhod topology on the space of càdlàg functions on [0,1], to  $\{W(r), 0 \le r \le 1\}$ , a standard Brownian Motion on [0,1]. Furthermore,

$$\left(\frac{6}{\log n}\right)^{1/2} \left(\sum_{s \le n/2} \mathbf{1}_{\{F_s\}} - \frac{1}{6} \log n\right) \Rightarrow W(1), \tag{6}$$

**Sketch of the proof.** Intuitively, the first result is an immediate consequence of the Poisson limit in Theorem 1 and the normal approximation to the Poisson. To prove it, we show that  $W_n(r)$  is a martingale, whose jumps are asymptotically zero, and whose quadratic variation process is r thanks to our time-change  $c_n(r) = 1 - n^{-r/3}$ . Therefore it converges to Brownian Motion.

At times  $(1 - n^{-1/3})n/2 \le t \le n/2$  we are in the critical range of the random graph. Results of Luczak, Pittel, and Wierman (1994) and computations with (4) imply that the number of fragmentations in this interval is bounded in expectation and hence can be ignored.

**Remark.** While Theorem 2 is a nice theoretical result, it does not have much to say about any biological example. If we think of the human genome and set n=3 billion nucleotides, Theorem 2 says that after n/2=1.5 billion transpositions there have been an average of  $(\log n)/6=3.63$  fragmentations, with a standard deviation of 1.91. These numbers are small so even for n=3 billion, we can't expect a very good approximation to the normal distribution. In the example that we simulated n=100 and  $(\log n)/6=0.767$  versus an observed average number of fragmentations =0.662 (which translates into a value of 1.224 in Figure 2). While our estimation of the mean is not very accurate, Figure 3 shows that the distribution of the number of fragmentations is almost Poisson.

#### 3.3 The supercritical regime

This is the most interesting case, and also the hardest one. We start by establishing a law of large numbers. For all c > 0 define

$$\beta_k(c) = \frac{1}{c} \frac{k^{k-1}}{k!} (ce^{-c})^k$$

so that for c < 1 it coincides with the Borel distribution of Corollary 1. When c > 1,

$$\lim_{n \to \infty} P(|\mathcal{C}_1| = k) = \beta_k(c)$$

still holds but the  $\beta_k(c)$ 's no longer sum up to 1 because there is a probability  $\beta_{\infty}(c) = 1 - \sum_{k\geq 1} \beta_k(c) > 0$  that  $\mathcal{C}_1$  is the giant component.

Let us denote by  $\Upsilon(c)$  a random variable that takes the value 1/k with probability  $\beta_k(c)$  when  $1 \le k < \infty$  and the value 0 with probability  $\beta_{\infty}(c)$ . The motivation for this definition is that  $1/|\mathcal{C}_k|$  has the same distribution as  $\Upsilon(c)$  and  $\sum_{k=1}^n 1/|\mathcal{C}_k|$  gives the number of components in the random graph.

**Theorem 3.** Let c > 0 be a fixed positive number. Then the number of cycles in the random permutation at time cn/2,  $|\sigma_{cn/2}| = g(c)n + \omega(\sqrt{n})$ , where

$$g(c) := E\Upsilon(c) = \sum_{k=1}^{\infty} \frac{1}{c} \frac{k^{k-2}}{k!} (ce^{-c})^k$$
(7)

and the error term  $\omega(n)/a_n\sqrt{n}\to 0$  in probability if  $a_n\to\infty$ .

Note that the theorem is valid for all regimes and implies that the distance is given by  $D_{cn/2} = u(c)n + \omega(\sqrt{n})$  where u(c) = 1 - g(c). Although it is not obvious from the formula, u(c) = c/2 for c < 1 and u(c) < c/2 when c > 1. Using Stirling's formula,  $k! \sim k^k e^{-k} \sqrt{2\pi k}$ , it is easy to check that g' exists for all c and is continuous, but g''(1) does not exist. In words, there is phase transition in the behavior of the distance of the random walk to the identity at time n/2 from linear to sublinear.

*Proof.* In the supercritical regime the dynamics of the large components is quite complicated, but there can never be more than  $\sqrt{n}$  components of size  $\sqrt{n}$  or larger. The expected number of fragmentations that produce clusters of size  $\leq \sqrt{n}$  by time cn/2 is at most  $n^{-1/2} \cdot cn/2$ . From this and Chebyshev's inequality we see that up to a term  $\omega(n^{1/2})$ ,  $|\sigma_{cn/2}|$  is the number of components of the random graph, and the result follows Theorem 12 in Chapter V of Bollobás (1985).

**Theorem 4.** Let c > 1. As  $n \to \infty$ ,

$$\frac{D_{cn/2} - u(c)n}{n^{1/2}} \Rightarrow \mathcal{N}(0, \sigma^2)$$
(8)

where  $\sigma = \rho[1 + \rho(c/2 - 1)]$ , and  $\rho = 1 - \theta(c)$  is the extinction probability of a supercritical PGW(c).

**Remark.** Note that the constant  $\sigma$  is different from the one given in Berestycki and Durrett (2003). We were correct in claiming that the central limit theorem in Theorem 4 is the same as the one for the number of components of the random graph, but we naively thought that the terms in  $\sum_{k=1}^{n} 1/|\mathcal{C}_k|$  were sufficiently independent so that  $\sigma^2 = \text{var}(\Upsilon(c))$ .

Sketch of Proof. By Pittel's (1990) central limit theorem for the number of components of a random graph, see his Corollary 1 and note that  $T/c = \rho$ , it suffices to prove that the number of extra components due to fragmentation at time cn/2 is  $o(\sqrt{n})$ . Our first step is to increase the cutoff for large cycles to  $n^a$  where a > 1/2, so that the number of large cycles is  $\leq n^{1-a} = o(n^{1/2})$ . The number of fragmentations that produce "small" cycles is now  $n^{-(1-a)} \cdot cn/2 = O(n^a)$  and cannot be ignored, so we need to use the fact that fragmented cycles are reabsorbed by the large components. If the fraction of mass in large cycles ("upstairs") at time tn is  $\lambda_t$  then new fragments of size k are produced at rate  $\leq 2\lambda_t$  and each fragment of size k is reabsorbed at rate  $2k\lambda_t$ . After time change this is bounded by an  $M/M/\infty$  queue in which the expected number of customers in equilibrium is 1/k. Using this, we can show that with high probability the number of small fragments at any time is  $\leq (\log n)^2$ . Of course, the coagulation fragmentation process is not exactly the queuing system. Customers can split into two, coalesce with other customers, gain weight (and increase their fragmentation rate) by eating small components, etc. However,  $(\log n)^2$  is much smaller than  $n^{1/2}$  so crude but robust estimates and patience eventually lead to a proof.

#### 3.4 Results for Reversals.

Theorems 3 and 4 extend easily to the approximate distance for reversal chain. Recall that the main difference lies in the fact that, a reversal involving edges from different components in the breakpoint graph always yields a coagulation, but one involving two edges in the same component may or may not cause a fragmentation. The proofs of the results for transpositions are based on showing that fragmentations can be ignored, so this difference is unimportant and the result extends to reversals. As Figure 2 shows, this is not true for the more precise results in Theorems 1 and 2. For example, the underlying data shows that up to c=1, an average of 23% of the reversals have caused no change in the distance. Since inversions that affect an edge are much more frequent than those that involve it, it seems reasonable to guess that in the limit as  $n \to \infty$  the relative orientations of the black edges in a component of the breakpoint graph are independent. This would imply that the Poisson process of fragmentations in the reversal case is a 1/2-thinning of the one for transpositions, and Theorem 2 would hold with 6 replaced by 12.

#### 3.5 Emergence of a giant cycle?

Since cycles in the random permutation are smaller than components of the random graph, it follows that if c < 1 then the largest cycle at time cn/2 is of size  $\leq \alpha_c \log n$  where  $\alpha_c = 1/(c-1 - \log c)$ . (See Theorem 10 in Chapter V of Bollobás (1985) or Lemma 3 below.)

For c > 1, the largest component of the random graph is, as is well known, "giant", meaning that it is of order n. In fact it is asymptotic to  $\theta(c)n$  where  $\theta(c)$  is the survival probability of a supercritical Poisson Galton-Watson with mean c. It is a natural question to ask whether the largest cycle of the random permutation is also giant in the supercritical regime.

Conjecture. Let  $L_1(t)$  be the size of the largest cycle at time t. If c > 1 then

$$\frac{L_1(cn/2)}{\theta(c)n} \Rightarrow V$$

where V is an a.s. positive random variable on [0,1].

A partial result in this direction is given by Theorem 5, where it is proved that the amount of mass in cycles of size larger than  $n^a$  for a = .55 at time cn/2 is asymptotic to  $\theta(c)n$ . As we were finishing this paper, we learned that Oded Schramm (private communication) has proved this conjecture. His proof is simple but does not provide very precise information about the sizes of the large cycles.

David Aldous (private communication) conjectures that the relative sizes of the pieces of the giant cycle are in equilibrium at all times in the supercritical regime, i.e., have the Poisson-Dirichlet PD(0,1) distribution, which gives the limiting behavior of the ordered sizes of cycles in a uniform random permutation. According to this conjecture, V would be distributed as the first coordinate of a PD(0,1) random variable. One way to approach this conjecture would be to generalize Aldous (1997) to show that the large cycles in the critical regime converge to a coagulation-fragmentation process and to study the growth of clusters in that process.

Alternatively, one could look at the size of the cycle containing 1,  $K_1(t)$ , and try to show that

$$\frac{K_1(cn/2)}{\theta(c)n} \Rightarrow U$$

where U has a point mass of size  $1 - \theta(c)$  at 0 and is otherwise uniform on  $(0, \theta(c))$ . Figure 4 shows the average growth of  $K_1(cn/2)/n$  in 10,000 simulations of n = 100, n = 1000, and compares the results to  $EU = \theta(c)^2/2$ . Although this considers only one aspect of the distribution of large cycles, it agrees well with Aldous' conjecture.

Figure 5 shows a histogram of the result of 100,000 simulations of  $K_1(100)$  when n = 100. As the graph shows, the spike in the frequency of clusters of size 4 or smaller is what one would predict from the random graph cluster size distribution. The remainder of the distribution is roughly uniform except for rounding at the upper end. The latter is to be expected if Aldous' conjecture is correct, since the size of the giant component satisfies the central limit theorem.

**Remark.** The problem of the emergence of a giant cycle is closely related to Angel's (2003) work on the existence of infinite orbits for the random stirring process, which is the random transposition random walk on an infinite graph such as  $\mathbb{Z}^d$  or a tree, rather than the complete graph on  $\{1,\ldots,n\}$  considered in this work. To explain the connection, suppose that we construct our process using a Poisson process with rate  $2/n^2$  for each  $i \neq j$ , and at these times draw an edge between i and j to indicate that i and j are to be transposed. To compute the cycles in the permutation at time cn/2, we repeat the first [0, cn/2] units of time periodically and then observe the sites that a walker starting at i visits at times kcn/2, for  $k = 1, 2, \ldots$  Angel (2003) calls this construction the cyclic time random walk. Its relevance to his work is that the cyclic time random walk is transient if, and only if, the cycles are infinite.

#### 4 The subcritical regime

Let us introduce some notations for the different probability laws involved. For each n, we have the coagulation-fragmentation process, and the Erdős-Renyi random graph model. To emphasize when computations are being done for the random graph we will use  $Q_p$ , for the random graph with Bernoulli percolation parameter p, and Q for the law of the evolving random graph that at time s has  $p_s = 1 - \exp(-2s/n^2)$ . When s = cn/2 this probability is  $p(c, n) = 1 - \exp(-c/n) \le c/n$ . To simplify notation we will use QX to denote the expected value of X with respect to the probability Q.

Our first result provides a useful upper bound.

**Lemma 1.** The cluster size  $|\mathcal{C}_1|$  in  $Q_{c/n}$  is dominated by Z, the total progeny of a branching process in which each individual has a Binomial(n-1,c/n) number of children, i.e., we can construct these random variables on the same probability space so that  $|\mathcal{C}_1| \leq Z$  a.s. It follows from this that if c < 1 then  $Q_{c/n}|\mathcal{C}_1| \leq 1/(1-c)$ .

*Proof.* Intuitively, this holds since a vertex in generation k may have children among all of the n vertices of the graph except those of the first k generations. To begin to prove this formally, let  $\xi_{i,j}$ ,  $1 \le i,j \le n$  be independent random variables, taking values 1 with probability c/n and 0 with probability 1 - c/n. To start the random graph let  $Y_0 = \{1\}$  and let  $Y_1 = \{j \notin Y_0 : \xi_{1,j} = 1\}$ . To start the branching process let  $Z_0 = 1$ ,  $Z_1 = |Y_1|$ , and let  $\phi_1 : Y_1 \to \{1, 2, ..., Z_1\}$  be 1-1 and onto.

If the first k stages of the construction have been done and we have  $Y_k \neq \emptyset$  and a  $\phi_k : Y_k \rightarrow \{1, \ldots, Z_k\}$  that is 1-1 (but not onto in general), then let

$$Y_{k+1} = \bigcup_{i \in Y_k} \{ j \notin \bigcup_{\ell=0}^k Y_\ell : \xi_{i,j} = 1 \}$$

We let individual  $\phi_k(i)$  in the kth generation of the branching process have  $|\{j \neq i : \xi_{i,j} = 1\}|$  children. The individuals in the branching process that are not in  $\phi_k(Y_k)$  have a number of children given by independent binomials. It should be clear from the construction that can again define  $\phi_{k+1}: Y_{k+1} \to \{1, \dots Z_{k+1}\}$  to be 1-1, and the comparison follows by induction. The inequality follows by computing EZ by summing a geometric series.

The next result shows that the bound in Lemma 1 is exact in the limit. Let  $\{Z_k\}_{k=0}^{\infty}$  be a Poisson Galton-Watson process with offspring mean c and let  $Z = \sum_{k=0}^{\infty} Z_k$  be its total progeny.

**Lemma 2.** Let  $C_1$  be the cluster that contains vertex 1. If  $0 \le c < 1$  then as  $n \to \infty$ 

$$Q_{p(c,n)}(|\mathcal{C}_1|=k) \to P(Z=k)$$

*Proof.* The number of children of vertex 1,  $Z_n^1 = |Y_1|$  has distribution Binomial(n-1, p(c, n)), which converges to a Poisson(c) limit. Let  $k \ge 1$  and let  $(n_1, ..., n_{k+1}) \in \mathbb{N}^{k+1}$ . If we let  $Z_j^n = |Y_j|$  then

$$Q_{p(c,n)}(Z_{k+1}^n = n_{k+1}|Z_1^n = n_1, ..., Z_k^n = n_k) = P\left(\sum_{i=1}^{n_k} B_i^n = n_{k+1}\right)$$

where  $B_i^n$  are i.i.d. Binomial(n-s, p(c, n)) random variables, and  $s = \sum_{i=0}^k n_k$  with  $n_0 = 1$ . From this it follows easily that the convergence of finite-dimensional distributions of  $\{Z_j^n\}_{j\geq 1}$  to those of PGW(c). Markov's inequality and the domination result in Lemma 1 imply that

$$Q_{p(c,n)}\left(\sum_{k=K}^{\infty} Z_k^n > 0\right) \le Q_{p(c,n)}\left(\sum_{k=K}^{\infty} Z_k^n\right) \le c^K/(1-c)$$

and the desired conclusion follows.

Our next ingredient is

**Lemma 3.**  $Q_{c/n}(|\mathcal{C}_1| \ge y) \le \frac{1}{c} \exp(-(c-1-\ln c)y).$ 

*Proof.* In view of Lemma 1, it suffices to prove the result for Z, rather than  $|C_1|$ . To do this, let

$$\phi_n(\theta) = e^{-\theta} \sum_{m=0}^{n-1} \binom{n-1}{m} \left(\frac{c}{n}\right)^m \left(1 - \frac{c}{n}\right)^{n-1-m} e^{\theta m}$$
$$= e^{-\theta} \left(1 - \frac{c}{n} + \frac{c}{n}e^{\theta}\right)^{n-1}$$

be the moment generating function of the distribution of the number offspring minus 1. Let  $S_m$  be a random walk that takes steps with this distribution and  $S_0 = 1$ , so that  $S_m$  explores the Galton-Watson tree. Then  $\tau = \inf\{m : S_m = 0\}$  has the same distribution as Z. Let  $R_m = \exp(\theta S_m)/\phi_n(\theta)^m$ .  $R_m$  is a nonnegative martingale. Stopping at time  $\tau$  we have  $e^{\theta} \geq E(\phi_n(\theta)^{-\tau})$ . If  $\phi_n(\theta) < 1$  it follows that

$$P(\tau \ge y)\phi_n(\theta)^{-y} \le E[\phi_n(\theta)^{-\tau}] \le e^{\theta}$$

Using  $\phi_n(\theta) \leq e^{-\theta} \exp(c(e^{\theta} - 1))$  now we have

$$P(\tau \geq y) \leq e^{\theta} \left( e^{-\theta} \exp(c(e^{\theta} - 1)) \right)^{y}$$

To optimize the bound we want to minimize  $c(e^{\theta}-1)-\theta$ . Differentiating this means that we want  $ce^{\theta}-1=0$  or  $\theta=-\log(c)$ . Plugging this and recalling that  $\tau$  and Z have the same distribution we have

$$P(Z \ge y) \le \frac{1}{c} \exp(-(c - 1 - \ln c)y)$$

It follows that

$$Q_{c/n}(|\mathcal{C}_1| \ge y) \le \frac{1}{c} \exp(-(c-1-\ln c)y)$$

which completes the proof of lemma 3.

Now recall that for c < 1,  $Z_c = \sum_{s \le cn/2} \mathbf{1}_{\{F_s\}}$  is the number of fragmentations up to time cn/2.

**Lemma 4.** Let  $f_k(s)$  be the empirical fraction of vertices in cycles of size k at time s. If  $0 \le c < 1$  then  $Ef_k(cn/2) \to P(Z=k)$  and  $EZ_c \to \kappa(c)$ , where  $\kappa(c)$  was defined in Theorem 1.

*Proof.* The cycle sizes at time s in the coagulation-fragmentation process are dominated by the cluster sizes in the random graph model with  $p_s = 1 - \exp(-2s/n^2) \le 2s/n^2$ . Therefore,

$$EZ_c \le \int_0^{cn/2} Qf_k(s) \frac{k-1}{n} ds \le \int_0^{cn/2} Q_{2s/n^2} |\mathcal{C}_1| - \frac{1}{n} ds$$

Using Lemma 1  $Q_{2s/n^2}|\mathcal{C}_1| \leq 1/(1-(2s/n))$ . Changing variables un/2 = s we have

$$EZ_c \le -\frac{1}{2}(\log(1-c) + c) = \kappa(c) \tag{9}$$

Since unfragmented cycles are the same as tree components in the random graph, the first convergence result follows from Lemma 2. The second one follows from Fatou's lemma and (9).

The final preparatory step is:

**Lemma 5.** If c < 1 the expected number of fragmentations that occur to cycles that have already been fragmented is  $\leq K_c(\log n)^2/n$ , and  $K_c = c\kappa(c)(3\alpha_c)^2$ . (Recall  $\alpha_c = (c-1-\log c)^{-1}$ ).

*Proof.* The expected number of such fragmentations is at most:

$$\leq E \int_0^{cn/2} \frac{\text{#vertices in fragments}}{n} \frac{L_1(bn/2)}{n} dt$$
$$\frac{n}{2} \int_0^c EZ_b \left(\frac{L_1(bn/2)}{n}\right)^2 db$$

where  $L_1(t)$  is the size of the largest component at time t. On the event that  $L_1(cn/2) \leq 3\alpha_c \log n$ , the above is at most

$$(n/2)(3\alpha_c \log n/n)^2 \int_0^c \kappa(b)db \le \frac{1}{2} K_c \frac{(\log n)^2}{n}$$

On the other hand by Lemma 3 the complement of this event has probability at most  $n^{-2}$ , and there can never be more than cn/2 such fragmentations, so Lemma 5 is proved.

We are now ready to prove Theorem 1. Let  $\bar{Z}_c^n = \sum_{s \leq cn/2} \mathbf{1}_{\{\bar{F}_s\}}$ ,  $0 \leq c < 1$  be the counting process of fragmentations that occur to cycles which (a) have not been fragmented previously and (b) have size  $\leq n^{0.7}$ . The second condition is irrelevant in this section, but imposing it now will help in the next one. Unfragmented cycles correspond to trees in the random graph so the compensator of  $\bar{Z}_c^n$  is

$$\bar{\kappa}^n(c) = \int_0^{cn/2} \bar{\psi}_s^n \, ds \tag{10}$$

where  $\bar{\psi}^n_s = \sum_{k=1}^{n^{0.7}} \bar{f}_k(s)(k-1)/n$  and  $\bar{f}_k(s)$  is the fraction of vertices that belong to tree components of size k. As noted in the sketch of the proof, it is enough to show that for each fixed c,  $\kappa^n(c)$  converges in probability to  $\kappa(c)$ , or, by Lemma 5, that  $\bar{\kappa}^n(c)$  converges to  $\kappa(c)$  in probability. Lemmas 3 and 4 imply that  $E[\int_0^{cn/2} \bar{\psi}^n_s ds] \to \kappa(c)$ . It remains to show that  $\operatorname{var} \int_0^{cn/2} \bar{\psi}^n_s ds \to 0$ .

**Lemma 6.** For all time  $s \le cn/2$ 

$$\operatorname{var}(\bar{\psi}_s^n) \le \frac{K}{n^3} Q_{p(c,n)}[|\mathcal{C}_1|^3]$$

where K is a constant that depends only on c.

*Proof.* In terms of cluster sizes

$$\bar{\psi}_s^n = \frac{1}{n^2} \sum_{i=1}^n (|\mathcal{C}_i| - 1) I_i$$

where  $I_i$  is the indicator of the event that  $C_i$  is a tree. Let  $d_i = (|C_i| - 1)I_i$ .

$$\operatorname{var} \frac{1}{n^2} (d_1 + \dots + d_n) = \frac{1}{n^4} \left( n \operatorname{var} (d_1) + n(n-1) \operatorname{cov} (d_1, d_2) \right)$$
(11)

Monotonicity and Lemma 3 imply,

$$\operatorname{var}(d_1) \le Q_{p(c,n)}[|\mathcal{C}_1|^2] \le K$$
 (12)

It remains to bound  $cov(d_1, d_2)$ . If we let

$$\pi_{n,i} = i^{i-2} (p_s)^{i-1} (1 - p_s)^{i(n-i) + \binom{i}{2} - (i-1)}$$

where  $p_s = 1 - \exp(-2s/n^2)$  then by the reasoning for (4) we have

$$Q_{p_s}[\mathcal{C}_1 \cap \mathcal{C}_2 = \emptyset, |\mathcal{C}_1| = j, |\mathcal{C}_2| = k, \ \mathcal{C}_1 \text{ and } \mathcal{C}_2 \text{ are trees}] = \binom{n-2}{j-1} \pi_{n,j} \binom{n-j-1}{k-1} \pi_{n-j,k}$$

$$Q_{p_s}[\mathcal{C}_1 = \mathcal{C}_2, |\mathcal{C}_1| = k, \ \mathcal{C}_1 \text{ is a tree}] = \binom{n-2}{k-2} \pi_{n,k}$$

From this it follows that  $cov(d_1, d_2)$ 

$$= \sum_{j,k} \left[ \binom{n-2}{j-1} \binom{n-j-1}{k-1} (1-p_s)^{-j} - \binom{n-1}{j-1} \binom{n-1}{k-1} \right] (j-1)(k-1)\pi_{n,j}\pi_{n,k}$$

$$+ \sum_{k} \binom{n-2}{k-2} (k-1)^2 \pi_{n,k}$$

The term in square brackets is

$$\leq \frac{(n-2)!e^c}{(j-1)!(k-1)!(n-j-k)!} - \frac{(n-1)!}{(j-1)!(n-j)!} \frac{(n-1)!}{(k-1)!(n-k)!} \leq 0$$

since  $(n-2)!e^c \le (n-1)!$  for large n and  $(n-j)!/(n-j-k)! \le (n-1)!/(n-1-k)!$ . The second term is

$$\leq \frac{1}{n-1} \sum_{k} k^{3} \binom{n-1}{k-1} \pi_{n,k} \leq \frac{1}{n-1} Q_{p(c,n)}[|\mathcal{C}_{1}|^{3}]$$

Combining this with (11) and (12) gives the result.

Hence by the Cauchy-Schwarz inequality we get:

$$\operatorname{var}\left(\int_{0}^{t} \bar{\psi}_{s}^{n} ds\right) = Q\left[\left(\int_{0}^{t} (\bar{\psi}_{s}^{n} - Q[\bar{\psi}_{s}^{n}]) ds\right)^{2}\right] \leq t \int_{0}^{t} \operatorname{var}\left(\bar{\psi}_{s}^{n}\right) ds$$

$$\leq \frac{cn}{2} \int_{0}^{cn/2} \frac{K}{n^{3}} ds = \frac{c^{2}K}{4n} \to 0$$

$$(13)$$

This completes the proof of Theorem 1.

#### 5 The critical regime

The first step in the proof of Theorem 2 is to argue that fragmentations of previously fragmented cycles can be ignored. The number of such fragmentations is smaller than the total number of cycles in multicyclic components (i.e., components with at least 2 cycles) in the random graph. Theorem 1 and Corollary 3 in Luczak, Pittel, and Weirman (1994) imply that the total number of cycles in multicyclic components in the critical regime is bounded in probability. In particular, divided by  $(\log n)^{1/2}$  it converges to 0 in probability. As a result, by the converging together lemma (see e.g., Durrett (1996), Chap.2, Ex. 2.10), it suffices to prove the central limit theorem for the number of fragmentations on tree components.

As in the previous section, we will in addition restrict our attention to fragmentations of tree components of size  $n^{0.7}$ , and continue to use the notation introduced there. Let  $\bar{W}_n(r) := (6/\log n)^{1/2}(\bar{Z}^n(r) - \bar{\kappa}^n(r))$ . By standard methodology in the theory of stochastic processes (see Jacod and Shiryaev (1987) or Revuz and Yor(1999) for instance), to prove convergence of  $\bar{W}_n(\cdot)$  to Brownian Motion, the two things we need to check are: (i)  $E[\sup_{0 \le r \le 1} |\bar{W}_n(r) - \bar{W}_n(r^-)|] \to 0$  and (ii) The quadratic variation of  $W_n$ , i.e. the increasing process associated with  $\bar{W}_n(\cdot)^2$ , must converge to r at time r. (i) is obvious because  $\bar{Z}^n$  is a counting process, and (ii) turns into  $E(6\bar{Z}^n(r)/\log n) \to r$  and  $\operatorname{var}(6\bar{Z}^n(r)/\log n) \to 0$ . These two steps are dealt with respectively in lemmas 7 and 9.

Lemma 7.

$$E\left[\frac{6}{\log n} \int_0^{c_n(r)n/2} \bar{\psi}_s^n \ ds\right] \to r$$

<sup>&</sup>lt;sup>1</sup>This result could also be derived from the Folk Theorem 1 in Aldous (1997) which gives the limit for the joint distribution of the component sizes and the number of cycles they contain. See the discussion page 850 of his paper.

*Proof.* The upper bound follows from (9) which holds for all c < 1. In the other direction, changing variables  $s = c_n(v)n/2$  where  $c_n(v) = 1 - n^{-v/3}$  and noting  $c'_n(v) = (1/3)(\log n)n^{-v/3}$  gives

$$E\left[\frac{6}{\log n}\bar{Z}^{n}(r)\right] = n \int_{0}^{r} Q[\bar{\psi}_{c_{n}(v)n/2}^{n}]n^{-v/3} dv$$

$$= \int_{0}^{r} \sum_{k=1}^{n^{0.7}} \frac{k-1}{n} Q_{p(c_{n}(v),n)}[kT_{k}]n^{-v/3} dv$$
(14)

where  $T_k$  is the number of tree components of size k, and  $p(c,n) = 1 - \exp(-c/n)$ .

To take the limit of the last expression we will use formula (4) which gives the expected number of trees of size k. For this and other similar calculations the following will be useful.

**Lemma 8.** If  $k \to \infty$  and  $k = o(n^{3/4})$  then

$$\gamma_{n,k}(c) \equiv \binom{n}{k} k^{k-2} \left(\frac{c}{n}\right)^{k-1} \left(1 - \frac{c}{n}\right)^{kn-k^2/2 - 3k/2 + 1}$$

$$\sim \frac{nk^{-5/2}}{c\sqrt{2\pi}} \exp\left(-\alpha(c)k + (c-1)\frac{k^2}{2n} - \frac{k^3}{3n^2}\right) \equiv \lambda_{n,k}(c)$$

where  $\alpha(c) = c - 1 - \log(c)$ . There is a constant K so that if  $1 \le k \le n^{0.7}$  and  $c \le 1$  then  $\gamma_{n,k}(c) \le K\lambda_{n,k}(c)$ .

*Proof.* Stirling's formula implies  $k! \sim k^k e^{-k} \sqrt{2\pi k}$ . Using this we have that

$$\gamma_{n,k}(c) \sim \frac{nk^{-5/2}}{c\sqrt{2\pi}} \left[ \prod_{j=1}^{k-1} \left( 1 - \frac{j}{n} \right) \right] e^k c^k \left( 1 - \frac{c}{n} \right)^{kn - k^2/2 - 3k/2 + 1}$$

Using the expansion  $\log(1-x) = -x - x^2/2 - x^3/3 - \dots$  we see that if k = o(n) then

$$\left(1 - \frac{c}{n}\right)^{kn - k^2/2 - 3k/2 + 1} \sim \exp(-ck + k^2/2n)$$

while if  $k = o(n^{3/4})$  we have

$$\prod_{j=1}^{k-1} \left( 1 - \frac{j}{n} \right) = \exp \left( -\frac{1}{n} \sum_{j=1}^{k-1} j - \frac{1}{n^2} \sum_{j=1}^{k-1} j + O\left(\frac{j^4}{n^3}\right) \right) \\
\sim \exp \left( -\frac{k(k-1)}{2n} - \frac{k(k-1)(2k-1)}{6n^2} \right) \sim \exp\left( -\frac{k^2}{2n} - \frac{k^3}{3n^2} \right)$$

Combining the last three formulas gives the asymptotic formula. To prove the bound we note that Stirling's formula implies  $k! \ge \delta k^k e^{-k} \sqrt{2\pi k}$  for some  $\delta > 0$ . Using the bounds  $\log(1-x) \le -x$  and  $\log(1-x) \le -x - x^2/2$  in the last two calculations gives the upper bound.

Setting c = 1 - b with  $b \to 0$  and using Taylor's theorem

$$-(c-1-\log(c))k - b\frac{k^2}{n} \approx -\frac{b^2}{2}k - b\frac{k^2}{n}$$

The first term becomes significantly negative when  $k \approx 1/b^2$ , the second when  $k \approx \sqrt{n/b}$ . If  $b = n^{-a}$  with a < 1/3 the first threshold is smaller and the second term can be ignored. Recalling that (4) implies  $ET_k = \gamma_{n,k}(c)$  and using Lemma 8 with the last observation we see that if v < 1

$$\sum_{k=1}^{n^{0.7}} \frac{k^2}{n} Q_{p(c_n(v),n)}[T_k] \sim \frac{1}{\sqrt{2\pi}} \sum_{k=1}^{n^{0.7}} k^{-1/2} \exp(-n^{-2v/3}k/2)$$
(15)

Here we have used the asymptotic formula for all k. However, the next computation will show that the sum grows like  $n^{v/3}$  so the contributions from small k can be ignored.

If we view the sum in (15) as a Riemann sum with spacing  $n^{-2v/3}$ , we can rewrite it as

$$n^{v/3} \sum_{k=1}^{n^{0.7}} n^{-2v/3} (n^{-2v/3}k)^{-1/2} \exp(-n^{-2v/3}k/2)$$

From this it follows that

$$n^{-v/3} \sum_{k=1}^{n^{0.7}} \frac{k(k-1)}{n} Q_{p(c_n(v),n)}[T_k] \to \int_0^\infty \frac{x^{-1/2}}{\sqrt{2\pi}} e^{-x/2} dx$$

Changing variables  $x = y^2$ , dx = 2y dy the integral becomes  $(2\pi)^{-1/2} \int_0^\infty 2e^{-y^2/2} dy = 1$ . Therefore, by Fatou's lemma:

$$\lim \inf_{n \to \infty} E\left[\frac{6}{\log n} \bar{Z}^n(r)\right] \ge \int_0^r n^{-v/3} \cdot n^{v/3} \ dv = r$$

We turn now to the analysis of the variance.

**Lemma 9.** var 
$$\left(\frac{6}{\log n}\bar{\kappa}_n(r)\right) \to 0$$

*Proof.* Changing variables as in (14) and using Cauchy-Schwarz inequality as in (13),

$$\operatorname{var}\left(\frac{6}{\log n} \int_{0}^{c_{n}(r)n/2} \bar{\psi}_{s}^{n} ds\right) = \operatorname{var}\left(n \int_{0}^{r} \bar{\psi}_{c_{n}(v)n/2}^{n} n^{-2v/3} dv\right)$$

$$\leq n^{2} \int_{0}^{r} n^{-2v/3} \operatorname{var}\left(\bar{\psi}_{c_{n}(v)n/2}^{n}\right) dv$$

$$\leq \frac{2}{n} \int_{0}^{r} n^{-2v/3} Q_{p(c_{n}(v),n)}[|\mathcal{C}_{1}|^{3} I_{1}] dv$$

Reasoning as in (15) but using the bound in Lemma 8

$$\sum_{k=1}^{n} k^{3} Q_{p(c_{n}(v),n)}[kT_{k}] \le K \sum_{k=1}^{n} k^{3/2} \exp(-n^{-2v/3}k/2)$$

To check the right-hand side note that the power of k has increased by 2, from the previous calculation. If we view the last sum as a Riemann sum with spacing  $n^{-2v/3}$ , we can rewrite it as

$$n^{5v/3} \sum_{k=1}^{n} n^{-2v/3} (n^{-2v/3}k)^{3/2} \exp(-n^{-2v/3}k/2)$$

Now  $x^{3/2}e^{-x/2}$  has derivative  $((3/2)x^{1/2} - (1/2)x^{3/2})e^{-x/2}$  so it is increasing on [0,3] and then decreasing on  $[3,\infty)$ . Thus if we discard the term with the largest k so that  $n^{-2v/3}k \leq 3$  we have a lower bound on the integral.

$$n^{-2v/3} \sum_{k=1}^{n} k^{3} Q_{p(c_{n}(v),n)}[kT_{k}] \leq n^{v} \frac{1}{\sqrt{2\pi}} \int_{0}^{\infty} x^{3/2} e^{-x/2} dx + n^{v/3} 3^{3/2} e^{-3/2}$$

Using this it follows that

$$\operatorname{var}\left(\frac{6}{\log n}\bar{\kappa}^n(r)\right) \leq \frac{K}{n} \int_0^r n^u \, du$$

Writing  $n^u = \exp(-u \log n)$  and integrating we have that the right-hand side is  $\leq K/(\log n) \to 0$ . This concludes the proof of the first result in theorem 2.

The final step is to estimate the number of fragmentations that occur to tree components of size  $\leq n^{0.7}$  at times between  $(1 - n^{-1/3})n/2$  and n/2:

$$\int_{(1-n^{-1/3})n/2}^{n/2} Q\bar{\psi}_s^n \, ds$$

For each s in the interval the integrand is smaller than  $\sum_{k=1}^{n^{0.7}} \frac{k^2}{n} Q_{1/n} T_k$ . Using Lemma 8, the last quantity is smaller than

$$\frac{K}{n} \sum_{k=1}^{\infty} k^{-1/2} \exp(-k^3/3n^2)$$

which we can rewrite as

$$\frac{K}{n}n^{1/3}\sum_{k=1}^{\infty}n^{-2/3}(kn^{-2/3})^{-1/2}\exp(-(kn^{-2/3})^3/2)$$

The above sum is a Riemann sum so it converges to  $\int_0^\infty x^{-1/2}e^{-x^3/2}dx$ . Therefore,  $Q\bar{\psi}_s^n \leq Kn^{-2/3}$ . Since the duration of the critical regime is  $n^{2/3}/2$ , the expected number of fragmentations is bounded and the proof of Theorem 2 is complete.

### 6 The supercritical regime

As indicated in the sketch of the proof of Theorem 4, it is enough to show that, with probability going to 1 as  $n \to \infty$ , at time cn/2 there are fewer than  $o(n^{1/2})$  extra components due to fragmentation. Let a=0.55. (In fact the results stated would also be valid for any 1/2 < a < 2/3 but making this choice makes some proofs slightly easier). We call cycles of size  $k \ge n^a$  large. These can be ignored since there cannot be more than  $n^{1-a} = o(n^{1/2})$  such components. We define the amount of mass "upstairs" by

$$N_t^{\uparrow} = \sum_{k > n^a} k X_k(t)$$

where  $X_k(t)$  is the number of cycles of size k at time t. If all of the mass was upstairs, then the expected number of cycles of size  $\leq n^a$  produced by fragmentation would be  $2n^{a-1}(cn/2) = O(n^a)$ .

It is overly pessimistic to think that all of the mass will be upstairs, but by analogy with the random graph, we expect that at times c > 1 a positive fraction of the mass will be there, so this estimate of the number of fragmentations is too large to ignore.

To improve this crude estimate, we take advantage of the fact that fragmented pieces are reabsorbed upstairs. Let  $X_k^{\downarrow}(t)$  be the number of cycles of size k produced by fragmentation of cycles upstairs. To increase  $X_k^{\downarrow}(t)$ , we need to pick for the transposition one of the  $N_t^{\uparrow}$  vertices upstairs and then one of the 2 points located k steps away when writing the corresponding cycle of the current permutation, giving a rate  $2N_t^{\uparrow}/n^2$ . As for the death rate, one way to get rid of a component of size k is by picking one of the k vertices of one of the  $X_k^{\downarrow}(t)$  components and one of the  $N_t^{\uparrow}$  vertices upstairs. This happens with rate  $2kX_k^{\downarrow}(t)N_t^{\uparrow}/n^2$ . For the moment we are ignoring the fact that cycles may experience coalescence or fragmentation while downstairs. We will deal with these complexities once we have an understanding of the basic birth and death process of fragments of large clusters.

#### 6.1 The cluster queuing system

It is fortunate that the unknown quantity  $N_t^{\uparrow} \leq n$  appears in both rates, so that as along as  $N_t^{\uparrow} > 0$  we can remove it by time change. Once this is done, we have a system of stochastic processes  $\xi_t^k$ , for  $1 \leq k \leq n^a$  that we call a *cluster queuing system*: let  $\xi_t^k$  be independent birth-and-death chains with birth rate 1 and death rate  $k\xi_t^k$ , that begin with  $\xi_0^k = 0$ .

**Lemma 10.** With probability  $\rightarrow 1$  as  $n \rightarrow \infty$  we have

$$\sum_{k=1}^{n^a} \xi_t^k \le (\log n)^2 \quad and \quad \sum_{k=1}^{n^a} k \xi_t^k \le n^a (\log n)^2$$

for all  $t \leq cn/2$ .

Proof. The second result is a trivial consequence of the first. The key idea to handle these processes is to consider strips  $2^j \leq k < 2^{j+1}$ . Because there are no simultaneous jumps, we can prove that the queues  $\xi_t^k$  at each level k are independent processes (see e.g. Revuz-Yor (1999), chap. XII, prop. (1.7), for a proof of this fact in the case of Poisson processes). Therefore, for each  $1 \leq j \leq \log_2 n^a$ , the number of cycles with sizes in  $[2^j, 2^{j+1}), \zeta_t^j$ , is dominated by a birth and death chain with birth and death rates respectively  $2^j$  and  $2^j \zeta_t^j$ . To analyze these processes, we consider the successive excursions away from 0. Their embedded discrete time processes  $Y_s$  jump from m to m-1 with probability m/(m+1) and from m to m+1 with probability 1/(m+1). Let us try to find a function  $\phi$  such that  $\phi(0) = 0$ ,  $\phi(1) = 1$  and  $\phi(Y_s)$  is a martingale. The latter implies

$$\frac{1}{m+1}[\phi(m+1) - \phi(m)] = \frac{m}{m+1}[\phi(m) - \phi(m-1)]$$

so  $\phi(x) = \sum_{k=1}^{x} (k-1)!$ . Since  $\phi(1) = 1$  and  $\phi(0) = 0$ , it follows by optional sampling that the maximum level reached during an excursion of  $\zeta^{j}$ , M, satisfies

$$P(M > x) = 1/\phi(x+1) < 1/x! \tag{16}$$

To bound the number of excursions for the process in the  $j^{\text{th}}$  strip before time cn/2,  $N_j(cn/2)$ , we note that jumps from 0 to 1 occur at rate  $2^j$  so ignoring the amount of time it takes to return

to 0 from 1, the number of excursions by time cn/2 is bounded by a Poisson random variable with mean  $2^{j}cn/2 \le cn^{a+1}$ . Markov's inequality implies that  $P(N_{j}(cn/2) > n^{2}) \le cn^{a-1}$  so

$$P\left(\max_{1 \le j \le a \log_2 n} N_j(cn/2) > n^2\right) \to 0 \tag{17}$$

To estimate the probability that the maximum of  $n^2$  excursions is  $> \log n$  we recall (16) and that Stirling's formula implies  $k! \ge \delta_0 k^k e^{-k} / \sqrt{2\pi k}$  for some  $\delta_0 > 0$ , so

$$(\log n)! \ge \delta_1 (\log n)^{\log n} n^{-1} (\log n)^{-1/2} = \delta_1 n^{\log \log n - 1} (\log n)^{-1/2}$$

The right-hand size goes to  $\infty$  faster than  $n^2 \log_2 n$  so using (17) we have

$$P\left(\max_{1 \le j \le a \log_2 n} \max_{0 \le t \le cn/2} \zeta_t^j > \log n\right) \to 0$$

When the last event does not occur we have

$$\sum_{k=1}^{n^{a}} \xi_{t}^{k} \le a(\log_{2} n) \log n = \frac{a}{\log 2} (\log n)^{2}$$

Since  $a < 2/3 < \log 2 \approx 0.69$ , this gives the desired result.

#### 6.2 The initial mass upstairs

Before going any further we must ensure that upstairs never becomes empty in this process: i.e. that  $N_t^{\downarrow} > 0$  for all t > 0 with high probability, so that we can indeed time-change the queues by  $(N_t^{\downarrow})^{-1}$ , and use all the analysis carried out in the previous section. This will be done by showing that initially there are already more vertices upstairs than will ever (with high probability) be taken away by fragmentation in the cluster queuing system.

Lemma 8 implies that when c = 1 the expected number of trees of size k

$$ET_k \sim \frac{nk^{-5/2}}{\sqrt{2\pi}} \exp(-k^3/3n^2)$$

If we let  $|\mathcal{C}_{\geq a}| = \sum_{k=n^a}^{\infty} T_k$  then it follows that

$$E|\mathcal{C}_{\geq a}| \sim \frac{n}{\sqrt{2\pi}} \sum_{k=n^a}^{\infty} k^{-5/2} \sim \frac{2}{3\sqrt{2\pi}} n^{1-3a/2}$$

Bollobás (1985) has calculated (see page 107) that the expected number of ordered pairs of trees of sizes j and k,

$$E(T_i, T_k) \leq ET_i ET_k$$

When  $j \neq k$  this implies  $\operatorname{cov}(T_j, T_k) \leq 0$  and for j = k that  $ET_k(T_k - 1) \leq (ET_k)^2$  or  $\operatorname{var}(T_k) \leq ET_k$ . Summing we have

$$\operatorname{var}(|\mathcal{C}_{\geq a}|) \leq E|\mathcal{C}_{\geq a}|$$

and it follows from Chebyshev's inequality that  $|\mathcal{C}_{\geq a}|/E|\mathcal{C}_{\geq a}| \to 1$  in probability. These trees have not experienced fragmentation so their size is always  $\geq n^a$  and the total mass in large components is at least  $Kn^{1-a/2}$ . When a < 2/3 and n is large, this is much larger than the  $n^a(\log n)^2$  upper bound on the missing mass due to fragmentations.

#### 6.3 Fragmentation in the cluster queuing system

We will now estimate the effect of fragmentation and coagulation of members of the cluster queuing system. The latter is good news because it reduces the number of components by 1, but is bad news because it makes a cluster with a fragmentation rate larger than the sum of the rates for the two merged clusters. If we imagine that the coagulation involves a red cluster and a yellow cluster then the additional fragmentations are those that involve a red site and a yellow site. Summing we see that while the total mass in the cluster queuing system is  $\leq n^a \log n$ , the expected number of fragmentations of original clusters and possible additional fragmentations of coagulated clusters is at most

 $\left(\frac{n^a \log n}{n}\right)^2 \frac{cn}{2} = Kn^{2a-1} (\log n)^2 = o(n^{1/2})$ 

#### 6.4 The effect of small random graph components

Up to this point we have concentrated on the effect of the fragmentation of the large cycles. To complete the proof we have to consider the influence of cycles that are contained in components of the random graph that are small, i.e., smaller than  $n^a$ . Two things can happen to these cycles that do not happen in the random graph. (i) They can merge with clusters in the queuing system. (ii) They can experience fragmentation.

(i) is good news because it reduces the number of components by 1, but is bad news because it generates a cluster with a fragmentation rate larger than the sum of the rates for the two merged clusters. However, when this happens, the death rate of the cluster can only increase, and it does not affect the number of clusters in the queuing system. Therefore, the number of clusters in this queuing system can not be more than  $(\log n)^2$  with probability  $\to 1$  as  $n \to \infty$  even when (i) is taken into account.

(ii) By a now familiar estimate, the expected number of fragmentations that produce clusters of size  $\leq n^p$  at times between n and n+t is at most  $2n^{p-1}t$ , so we can ignore fragmentations that (a) produce clusters of size  $\leq n^{0.45}$  before time cn/2 and (b) produce clusters of size  $\leq n^{0.55}$  at times between n and  $n+n^{0.9}$ .

If c > 1 the distribution of nongiant components in the random graph is given by progeny of a Poisson Galton Watson process with mean c on the event of its extinction. If we let  $\rho$  denote its extinction probability, then the offspring distribution conditional on extinction is given by

$$\frac{1}{\rho}e^{-c}\frac{(c\rho)^k}{k!} = e^{-c\rho}\frac{(c\rho)^k}{k!}$$

since  $\rho = e^{-c(1-\rho)}$ . In short, PGW(c) conditioned on extinction is  $PGW(c\rho)$ . The last observation implies that results for finite supercritical clusters can be derived from those for subcritical clusters. In particular, by Lemma 3 the largest nongiant components seen at times  $\geq n + n^{0.9}$  are smaller than  $n^{0.2}$ . Since fragmentations of such clusters necessarily produce pieces smaller than  $n^{0.2}$  these fragmentations can be ignored by (a).

#### 6.5 A sharper estimate for the mass upstairs

It follows from the fact that the cluster queuing system never has more than  $n^a(\log n)^2$ , that the total mass upstairs must be close to that of the giant component in the random graph. Indeed, the

pieces giant component must be located either upstairs or in the cluster queuing system, or in some other small component having experienced multiple fragmentation. But the mass in the latter is easily shown to be  $O(n^a(\log n)^2)$  and we have just proved that the cluster queuing system never weighs more than  $n^a(\log n)^2$ . Therefore, upstairs must contain  $\theta(c)n - O(n^a(\log n)^2)$  ( $\theta(c)n$  being the number of vertices in the giant component by time cn/2 with high probability, and  $\theta(c)$  is the survival probability of a supercritical PGW(c)).

To rephrase the above:

**Theorem 5.** For any c > 1, at time cn/2 there are at least  $\theta(c)n - o(n)$  vertices located on large cycles (i.e., of size greater than or equal to  $n^a$ ).

#### REFERENCES

Aldous, D. (1997) Brownian excursions, critical random graphs and the multiplicative coalescent. *Ann. Prob.* 25, 812–854

Aldous, D. (1999) Deterministic and stochastic models for coalescence (aggregation and coagulation): a review of the mean-field theory for probabilists. *Bernoulli.* 5, 3–48

Angel, O. (2003) Random infinite permutations and the cyclic time random walk. Pages 9–16 in Banderier and Krattenthaler (2003)

Arratia, R. and Barbour, A. and Tavaré, S. (2003) Logarithmic combinatorial structures: a probabilistic approach. European Math. Society Monographs, 1.

Bafna, V. and Pevzner, P. (1995) Sorting by reversals: Genome rearrangement in plant organelles and evolutionary history of X chromosome. *Mol. Biol. Evol.* 12, 239–246

Banderier, C., and Krattenthaler, C. (2003) Proceedings of the conference Discrete Random Walks. Discrete Math and Computer Science. dmtcs.loria.fr/proceedings/dmACind.html

Berestycki, N. and Durrett, R., (2003) A phase transition in the random transposition random walk. Pages 17-26 in Banderier and Krattenthaler (2003)

Bollobás, B. (1984) The evolution of random graphs. Trans. Amer. Math. Soc. 286, 257–274

Bollobás, B. (1985) Random Graphs, Cambridge University Press.

Borel, E. (1942) Sur l'emploi du théorème de Bernouilli pour faciliter le calcul d'une infinité de coefficients. Application au problème de l'attente à un guichet. *C.R. Acad. Sci. Paris.* 214, 452–456

Bourque, G. and Pevzner, P. A. (2002) Genome-scale evolution: reconstructing gene orders in the ancestral species. *Genome Research.* 12, 26–36

Devroye, L. (1992) The branching process method in the Lagrange random variate generation, cgm.cs.mcgill.ca/~luc/branchingpaper.ps

Diaconis, P., Mayer-Wolf, E., Zeitouni, O., and Zerner, M. (2003) Uniqueness of invariant distributions for split-merge transformations and the Poisson-Dirichlet law. *Ann. Prob.*, to appear

Durrett, R. (1996) Probability: Theory and Examples, Second Edition, Duxbury Press

Durrett, R. (2002) Probability Models for DNA Sequence Evolution. Springer-Verlag, New York

Durrett, R. (2003) Shuffling Chromosomes. J. Theor. Prob. 16, 725–750

Durrett, R., Nielsen, R., and York, T.L. (2003) Bayesian estimation of genomic distance. *Genetics*, to appear

Hannehalli, S. and Pevzner, P.A. (1995) Transforming cabbage into turnip (polynomial algorithm for sorting signed permutations by reversals). *Proceedings of the* 27<sup>th</sup> Annual Symposium on the Theory of Computing, 178–189. Full version in the Journal of the ACM. 46, 1–27

Jacod, J. and Shiryaev, A. (1987) Limit Theorems for Stochastic Processes, Springer New-York

Janson, S., Knuth, D. E., Luczak, T. and Pittel, B. (1993) The birth of the giant component. *Rand. Struct. Algor.* 4, 231–358

Janson, S., Luczak, T., and Ruczinski, A. (2000) Random Graphs, Wiley-Interscience, New York

Luczak, T., Pittel, B., and Wierman, J. C. (1994) The structure of a random graph near the point of the phase transition. *Trans. Amer. Math. Soc.* 341, 721–748

Mayer-Wolf, E. and Zeitouni, O. and Zerner, M. (2002) Asymptotics of certain coagulation-fragmentation processes and invariant Poisson-Dirichlet measures. *Electr. Journ. Prob.* 7, 1–25

Pevzner, P.A. (2000) Computational Molecular Biology: An Algorithmic Approach. MIT Press, Cambridge

Pevzner, P.A. and Tesler, G. (2003) Genome rearrangement in mammalian evolution: lessons from human and mouse genomes. *Genome Research.* 13, 37–45

Pitman, J. (1997) Enumerations of trees and forests related to branching processes and random walks, www.stat.berkeley.edu/~pitman

Pitman, J. (1998) Coalescent random forests, Preprint 457, Dept. of Statistics, U.C. Berkeley

Pitman, J. (2002) Poisson-Dirichlet and GEM invariant distributions for split-and-merge transformations of an interval partition. *Combin. Prob. Comput.* 11, 501–514

Pitman, J. (2003) Combinatorial stochastic processes. Lecture Notes for St. Flour Course, to appear www.stat.berkeley.edu/~pitman

Pittel, B. (1990) On tree census and the giant component in sparse random graphs, Rand. Struct. Algor., 1, 311–342

Ranz, J.M. and Casals, F. and Ruiz, A. (2001) How malleable is the eukaryotic genome? Extreme rate of chromosomal rearrangement in the genus *Drosophila*. Genome Research. 11, 230–239

Revuz, D. and Yor, M., (1999) Continuous martingales and Brownian Motion, Springer-Verlag, New York

Tanner, J.C. (1961) A derivation of the Borel distribution. Biometrika 48, 222–224

York, T.L., Durrett, R., and Nielsen, R. (2002) Bayesian estimation of inversions in the history of two chromosomes. *J. Comp. Bio.* 9,808–818

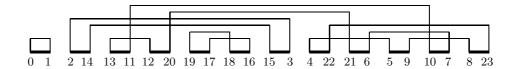


Figure 1: Breakpoint graph for human-mouse X chromosome comparison

```
36
    37
         17
             40
                  16
                       15
                           14
                                63
                                    10
                                          9
55
    28
         13
             51
                  22
                       79
                           39
                                70
                                    66
                                          5
     7
6
         35
             64
                  33
                       32
                           60
                                61
                                     18
                                         65
62
    12
                  23
                       20
                            4
                                52
                                    68
                                         29
         1
              11
48
     3
         21
             53
                  8
                       43
                           72
                                58
                                    57
                                         56
19
    49
                  30
                                          2
         34
             59
                       77
                           31
                                67
                                    44
27
    38
         50
              26
                  25
                       76
                           69
                                41
                                    24
                                         75
71
    78
         73
             47
                  54
                       45
                                42
                                    46
                           74
```

Table 1: Order of the genes in D. repleta compared to their order in D. melanogaster