EXPECTED NUMBER OF INVERSIONS AFTER A SEQUENCE OF RANDOM ADJACENT TRANSPOSITIONS

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Abstract. In the evolution of a genome, the gene sequence is sometimes rearranged, for example by transposition of two adjacent gene blocks. In biocombinatorics, one tries to reconstruct these rearrangement incidents from the resulting permutation. It seems that the algorithms used are too effective and find a shorter path than the real one. For the simplified case of adjacent transpositions, we give expressions for the expected number of inversions after $t$ random moves. This average can be much smaller than $t$, a fact that has largely been neglected so far.

1. Background

The genome rearrangement problem is a combinatorial problem arising in the area of molecular evolution. Basically, it can be stated as a problem about permutations of gene sequences. Given a permutation $\pi$ as a word in the symbols $\{1, \ldots, n\}$ (corresponding to genes), find the “best” path to the identity permutation when the feasible steps are block moves (removing a contiguous segment and inserting it somewhere else) and block reversals (reversing the order of a segment). The shortest path between the two permutations is the parsimonious solution, and finding algorithms for computing the shortest (or at least a short) path has been given a good deal of attention in [3], [2] etc. Although no particular solution is more probable than the parsimonious one, the shortest distance is not necessarily the most probable length of a path. The number of shortest paths from the identity to $\pi$ is much less than the number of paths using just a few extra steps. If a probabilistic model of the process is formulated, a maximum-likelihood
distance could be defined. We have not seen this problem considered in the literature.

One approach is to try to determine the expected distance to the identity permutation after a random walk of given length. This seems to be a difficult problem. Of course, one can obtain intuition from computer simulation, but a mathematical treatment would be preferable.

In the present paper, we simplify the model so that the only steps allowed are adjacent transpositions. Observe that the set of adjacent transpositions is the intersection of the set of block moves and the set of block reversals. For this simpler problem, we are able to obtain good lower and upper bounds by modelling the random walks in terms of a discrete heat equation.

2. Introduction

We are studying random walks of fixed length $t$ on the Cayley graph of the Coxeter group $A_n$, which is isomorphic to the symmetric group $S_{n+1}$. The Cayley graph has an edge between two permutations if one is obtained from the other by an adjacent transposition. (See [1] for similar problems on $S_{n+1}$ and other groups.)

The walk starts at the identity permutation 1234... and consists of $t$ random steps, chosen with uniform probability among the $n$ possible adjacent transpositions. Let $\pi$ be the permutation where this random walk stops and let $\text{inv}(\pi)$ denote the number of inversions. The shortest possible walk from the identity to $\pi$ has length $\text{inv}(\pi)$, so this number is less than or equal to $t$. Clearly, for $t = 1$, all permutations have $\text{inv}(\pi) = 1$, but for $t \geq 2$, a later move may cancel an inversion created by an earlier move. We would like to determine the expected number of inversions $E(\text{inv}(\pi))$, and we will denote it by $E_{nt}$ to make the dependence on the parameters $n$ and $t$ explicit.

The set of adjacent transpositions is denoted by $S = \{s_1, \ldots, s_n\}$ where $s_i$ is the transposition of the positions $i$ and $i + 1$. Let $P_{nt}$ be the set of all walks of length $t$, that is of all words in $S$ of length $t$:

$$P_{nt} = \{s_{i_1}s_{i_2}\ldots s_{i_t} : 1 \leq i_1, \ldots, i_t \leq n\}.$$  

Obviously $P_{nt}$ has cardinality $n^t$. As the same notation is used for a word and its product $\pi = s_{i_1}s_{i_2}\ldots s_{i_t}$, the notation $P_{nt}$ will be used also for the multiset of permutations. By counting all inversions in $P_{nt}$ we can find the average number.

$$n^t E_{nt} = \sum_{\pi \in P_{nt}} \text{inv}(\pi).$$
Using a computer, we have calculated the integers \(n^t E_{nt}\) for \(n, t \leq 10\). These data suggested a formula of unexpected simplicity. Let \(C_i\) denote the Catalan number \(\frac{1}{i+1} \binom{2i}{i}\).

**Theorem 2.1.** For a fixed \(t\) and for all \(n \geq t\), the expected number of inversions after \(t\) random adjacent transpositions is

\[
E_{nt} = t - \frac{2}{n} \binom{t}{2} + \sum_{r=2}^{t} \frac{(-1)^r}{n^r} \left[ 2^r C_r \left( \frac{t}{r+1} \right) + 4d_r \left( \frac{t}{r} \right) \right],
\]

where \(d_2, d_3, d_4, \ldots\) is a certain integer sequence starting by \(0, 1, 9, 69, 510\). No expression for \(d_r\) is known, but the following inequalities hold.

\[
t - \frac{2}{n} \binom{t}{2} + \sum_{r=2}^{t} \frac{(-1)^r}{n^r} \left[ 2^r C_r \left( \frac{t}{r+1} \right) - 2^{r-1} C_{r-1} \left( \frac{t}{r} \right) \right] \leq E_{nt} \leq t - \frac{2}{n} \binom{t}{2} + \sum_{r=2}^{t} \frac{(-1)^r}{n^r} 2^r C_r \left( \frac{t}{r+1} \right)
\]

A direct proof of the theorem seems difficult, so our approach has been a reformulation of the problem to a discrete heat flow model.

### 3. The Heat Flow Analogy

Instead of directly counting all inversions in \(P_{nt}\), we introduce the following fine-grading. Fixing \(n\) and \(t\), let

\[
p_{ij} := \text{Prob}(\pi_i < \pi_j)
\]

for a random permutation \(\pi \in P_{nt}\). Equivalently,

\[
n^t p_{ij} = \#\{\pi \in P_{nt} : \pi_i < \pi_j\}.
\]

Since every inversion is counted by one such class, we have

\[
E_{nt} = \sum_{i>j} p_{ij}.
\]

The matrices \((p_{ij})\) can be computed recursively. For \(t = 0\), the set \(P_{nt}\) consists of the identity permutation only, so \((p_{ij})\) has ones above the main diagonal and zeroes below, as in the leftmost matrix of Figure 1. The transformation to \(t = 1, t = 2\) and so on turns out to be a heat flow process. The total heat is invariant, for \(p_{ij} + p_{ji} = 1\) by the law of the Excluded Middle. The main diagonal in the matrix may be left blank, as in the figure, or we may set all its entries to \(1/2\) so that the rule \(p_{ij} + p_{ji} = 1\) is satisfied.

For any graph with real numbers (signifying temperature or heat) on the vertices, a heat flow process with thermal conductivity \(x\) means the

\[
E_{nt} = \sum_{i>j} p_{ij}.
\]
Proposition 3.1. The sequence of \((p_{ij})\)-matrices for \(t = 0, 1, 2, \ldots\) describes a heat flow process with conductivity \(x = \frac{1}{n}\) on the graph depicted in Fig. 1. The expected number of inversions, \(E_{nt}\), equals the total heat below the diagonal.

Proof. Consider the \((p_{ij})\)-matrix after \(t\) steps and let \(\pi\) be one of the permutations contributing to \(p_{ij}\), that is, \(\pi\) satisfies \(\pi_i < \pi_j\). Each neighbour of \(p_{ij}\) corresponds to a move that affects either \(\pi_i\) or \(\pi_j\). For example, the neighbour to the right, \(p_{i,j+1}\), corresponds to the transposition \((\pi_j, \pi_{j+1})\). When \(i\) and \(j\) are adjacent, the transposition \((\pi_i, \pi_j)\) is possible, which explains the graph edges across the main diagonal.

Except for these moves (at most four), the new \(p'_{ij}\) would be the same as the old \(p_{ij}\), but now the following is true:

\[
p'_{ij} = p_{ij} + \frac{1}{n} \sum (p\text{neighbour} - p_{ij}),
\]

where the sum is taken over all graph neighbours of \(p_{ij}\). For after, say, the transposition \((\pi_j, \pi_{j+1})\), the \(p'_{ij}\)-condition \(\pi'_i < \pi'_j\) means that we must have had \(\pi_i < \pi_{j+1}\), which is the \(p_{i,j+1}\)-condition.

From now on our analysis concerns the more general heat flow process where \(x\) is not necessarily \(\frac{1}{n}\). For the matrix entries we write \(p_{ij}(x)\) and for the total heat below the diagonal we use the notation \(E_{nt}(x)\). For example, Fig. 1 demonstrates that \(E_{41}(x) = 4x\) and \(E_{42}(x) = 8x - 8x^2\).

This analysis is complicated by the special edges across the diagonal. However, if we replace the graph of Fig. 1 by the simple grid graph of Fig. 2 and set all diagonal values to 1/2, then the heat flow process is
unchanged! For thanks to the symmetry property $p_{j,j+1} = 1 - p_{j+1,j}$ we have

$$p_{j,j+1} - p_{j+1,j} = 1 - 2p_{j+1,j} = 2(1/2 - p_{j+1,j}).$$

In other words, the loss of the neighbour across the diagonal is compensated for by the two new neighbours on the diagonal.

![Grid graph with initial values](image)

**Figure 2.** Grid graph with initial values

**Proposition 3.2.** The sequence of $p_{ij}(x)$-matrices for $t = 0, 1, 2, \ldots$ describes a heat flow process on the $(n+1) \times (n+1)$ grid graph depicted in Fig. 2.

3.1. **Hot boundary condition.** The above heat flow process on a grid with insulated boundary can be reformulated as a heat flow process on the lower triangle with the hot boundary condition $p_{ii} = 1/2$ on the diagonal. This should be obvious from the fact that the only connection between the lower and upper triangle of the grid graph is the diagonal, and the property of the original process that the diagonal has constant temperature $p_{ii} = 1/2$.

Note that the subdiagonal element $p_{j+1,j}(x)$ receives $2x/2$ from its diagonal neighbours and sends back $2x p_{j+1,j}(x)$. The net heat transfer to the lower triangle is $\sum_j (x - 2x p_{j+1,j}(x))$, so we have the following result.

**Proposition 3.3.**

$$E_{n+1}(x) = E_n(x) + nx - 2x \sum_j p_{j+1,j}$$

For example, in Fig. 1 we see that $8x - 8x^2 = 4x + 4x - 2x(4x).$
3.2. **Symmetric model and semi-infinite model.** The insulated left and lower boundaries can be gotten rid of in two different ways, by symmetric extension or by just neglecting their effect.

The reflection trick in Fig. 3 demonstrates that the diamond graph with hot boundaries all around is equivalent to the triangle. This model is what we will use for our exact solution later in this paper.

Neglecting the effect of the left and lower boundaries is equivalent to moving them to infinity. Then we are left with the whole half-plane below an infinite hot diagonal. As we will see, this problem is not so difficult and we can use its solution as a lower bound.

It is clear that the temperature at a given inner point in the diamond model must be at least as hot as a point at the same distance from the diagonal in the semi-infinite model, since the former point has heat flowing to it from three additional sides. Hence, solving the semi-infinite model gives a lower bound for the actual finite case.

![Figure 3. Triangle with hot diagonal and symmetric extension of the same problem](image)

### 4. Heat flow combinatorics

Our goal in this section is to find combinatorial expressions for the $p_{ij}(x)$-matrices describing heat flow on a triangular grid graph. As explained above, the triangular graph can be considered as embedded either in a finite diamond graph or in a semi-infinite grid graph.

At day $t = 0$ the diagonal entries are $p_{ii} = \frac{1}{2}$ with zeroes below the diagonal. Referring to Fig. 1 and the recursion ($p'$ means next day)

$$p'_{ij}(x) = p_{ij}(x) + x \sum (p_{\text{neighbour}}(x) - p_{ij}(x)),$$

(3)

it is obvious that the entries $p_{ij}(x)$ in step $t$ will be polynomials in $x$ of degree $t$ (or less). We can give each coefficient in these polynomials a combinatorial significance. Vaguely expressed, they count journeys for $t$ days from the hot boundary to the location of $p_{ij}(x)$. The recursion states that such a journey ending in a certain location on a certain day $[p'_{ij}(x)]$ may have been either at the same location yesterday $[p_{ij}(x)]$ and
had a resting day or at a neighbouring location $[p_{\text{neighbour}}(x)]$ and had a travel day (the $x$-factor means travel day) or at the same location $[p_{ij}(x)]$ and travelled half-way to the neighbour and then back (the $-x$-factor means round trip).

![Grid graph with mid-vertices](image)

**Figure 4.** Grid graph with mid-vertices

In order to make our statements precise, we will modify the grid graph as in Fig. 4. Each of the original edges is split in two by a new *mid-vertex*. Mid-vertices are introduced for counting purposes only, they do not carry heat.

Each day, the vertices on the hot boundary send out heat packets with the value $\frac{x}{2}$ to their neighbours. These packets are sent on and on, back and forth, always multiplied by $x$ or $-x$. Consider one such heat packet at a certain location in the morning of a certain day. What can happen to it during the day?

1. It stays on its vertex unchanged.
2. It travels a half-edge, gets multiplied by $x$, and travels the other half-edge to the next vertex.
3. It travels a half-edge, gets multiplied by $-x$, and returns the same half-edge to the same vertex.

If the start value is $\frac{1}{2}$ and the journey has $r$ travel days (type 2 or 3), the final value is $\pm \frac{1}{2}x^r$. The sign depends on the number of days of type 3, and is easily seen to be $(-1)^{r+i-j}$ if the journey ends at $(i, j)$. Hence we have the following result.

**Lemma 4.1.** The coefficient of the $x^r$-term in $p_{ij}(x)$ is $(-1)^{r+i-j}$ times the number of journeys from the hot boundary to $(i, j)$ in $t$ days, $r$ of which are travel days.

4.1. **The semi-infinite model.** Our next step is counting the journeys specified in the lemma. This is easy in the semi-infinite case where all points on the $k$-subdiagonal are equivalent. We define the *sublevel* of $(i, j)$ as $k = i - j$. The journey from sublevel $k$ to sublevel 0 can be specified by three items:

- Out of the $t$ days, $r$ travel days must be chosen. This can be done in $\binom{t}{r}$ ways.
For each of the $r$ travel days, horizontal or vertical travel must be chosen. This can be done in $2^r$ ways.

A Catalan walk in $2r$ half-steps from sublevel $k$ to sublevel 0 must be specified. By Catalan walk we mean that sublevel 0 must not be reached until the last half-step. It is well-known that the number of such walks is
\[
\binom{2r-1}{r-k} - \binom{2r-1}{r-k-1}.
\]

For $k = 1$ this is the Catalan number $C_r$.

Combining this journey count with Lemma 4.1, we get the expressions for $p_{i,j}(x)$ and eventually the total heat in the triangle.

**Proposition 4.2.** After $t$ time steps in the semi-infinite model,
\[
p_{i,j}(x) = \frac{1}{2} \sum_{r=k}^{t} (-1)^{r+k} \binom{t}{r} 2^r \left[ \binom{2r-1}{r-k} - \binom{2r-1}{r-k-1} \right] x^r,
\]
where $k = i - j$. The total heat under the diagonal is
\[
E_{nt}(x) = ntx - \frac{n+1}{2} \sum_{r=2}^{t} (-1)^r \binom{t}{r} 2^r C_{r-1} x^r
\]

**Proof.** As there are $n+1-k$ locations on sublevel $k$, we must do the following sum.

\[
E_{nt}(x) = \sum_{k=1}^{n} (n+1-k) \frac{1}{2} \sum_{r=k}^{t} (-1)^{r+k} \binom{t}{r} 2^r \left[ \binom{2r-1}{r-k} - \binom{2r-1}{r-k-1} \right] x^r.
\]

\[
= \sum_{r=1}^{t} (-1)^r \binom{t}{r} 2^r x^r \sum_{k=1}^{r} \frac{n+1-k}{2} \binom{2r-1}{r-k} - \binom{2r-1}{r-k-1},
\]
and the last sum simplifies to give the desired result. \qed

As we observed in Sec. 4.1, the total heat in the semi-infinite model gives a lower bound for the total heat in the finite case. In particular, we can plug in $x = \frac{1}{n}$ to obtain a lower bound for the expected number of inversions.

**Corollary 4.3.** The lower bound for $E_{nt}$ in Theorem 2.1 holds true.

**Proof.** Substitute $x = \frac{1}{n}$ and collect like powers of $\frac{1}{n}$. \qed

Remarkably, the semi-infinite model also provides an upper bound for the total heat in the finite case. By iterating the recursion 3.3 for the $E_{nt}$ in the finite case, we obtain the following formula.
Lemma 4.4. Let $e_t(x)$ denote the sum of the subdiagonal entries of the $p_{ij}(x)$-matrix for time step $t$ in the finite case. Then

$$E_{nt} = ntx - 2x[e_{t-1}(x) + e_{t-2}(x) + \cdots + e_1(x)].$$

We know that all $p_{ij}(x)$ in the semi-infinite model are less than or equal to the $p_{ij}(x)$ in the finite case. In particular, the subdiagonal sums must be less, so if we use them for $e_t(x)$ in the lemma above, we obtain an upper bound for $E_{nt}$.

Corollary 4.5. The upper bound for $E_{nt}$ in Theorem 2.1 holds true.

Proof. Use the lemma together with Eq. 4, then substitute $x = \frac{1}{n}$ and simplify. □

4.2. The finite case. Lemma 4.1 tells us that $p_{ij}(x)$ is an alternating polynomial and that its coefficients counts journeys from the hot boundary to $(i,j)$. In the finite case, counting journeys is difficult when $n < t$, for there are four boundaries and wherever you start it is possible to reach more than one of them in $t$ days. But when $n \geq t$, the situation is better.

The expression for the number of journeys with $r$ travel days starting at $(i,j)$ and ending at a hot boundary used to be

$$\binom{t}{r}2^r\left[\binom{2r-1}{r-k} - \binom{2r-1}{r-k-1}\right]$$

but for some $(i,j)$ that are close to two boundaries, this number will now increase. For the extra journeys, horizontal and vertical steps cannot be chosen freely, so the factor $2^r$ does not apply. For example, from $(2,1)$ it is possible to reach the left boundary in two steps, at least one of which must be horizontal. Therefore, the contribution of the extra journeys to $E_{nt}(x)$ will be of the form

$$\sum_{r=2}^{t}(-1)^r\binom{t}{r}2g_r x^r.$$  \hspace{1cm} (6)

The factor 2 comes from symmetry. More important than the exact value of the $g_r$-numbers is the fact that they do not depend on $n$. Therefore, these correction terms become less and less important as $n$ increases. For the expected number of inversions, $E_{nt}$, the correction terms may be written as in Theorem 2.1.

5. Open problems

(1) Is there a nice expression for the $d_r$-numbers of Theorem 2.1?
(2) Is there a nice expression for the $g_r$-numbers of Eq. 6?
(3) Can the analysis be extended to adjacent block tranpositions?
(4) Can the analysis be extended to block reversals?
(5) If the result of some random moves is a permutation with a
    certain number of inversions, what number of moves is the most
    probable?

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