1 Notes to JF: “Poincare method” section of new Chapter

What exists so far, if I haven’t forgotten anything, is

Chapter 4 section 4.3 (10/11/94 version)
Use in ’low-temperature Metropolis” (Chap 12 sec 6.1) (12/22/94 version)
Use in ”subperiodic trees” (saw.tex section 1.1)

The last two were intended as examples to be studied later in the book, in detail by various methods; but it’s OK with me if you prefer to put them in the new chapter.

I suggest that in writing the new chapter section you start with your own thoughts, rather than by editing the existing Chapter 4 sec 4.3. But here are two thoughts on section 4.3 that occurred to me while teaching.

1. Example 35 shows that Corollary 34 does not hold for vertex-transitive graphs. But a small modification of the proof of Cor 34 (bound flow thru edge by flow thru vertex) shows than on a vertex-transitive graph

$$\tau_2 \leq r ED^2; \quad r = \text{degree}.$$ 

2. Heuristically one expects that any “reasonable” graph has $\tau_2 = O(\Delta^2)$, for $\Delta =$ diameter. The argument for Cor 34 seems to imply one can’t hope to do better than this using the (naive, i.e. without choosing weights in Cauchy-S) Poincare method. The method is perhaps most relevant (xxx check with examples!!!!) where one believes that in fact $\tau_2 = \Theta(\Delta^2)$ and one seeks to prove a bound as close to this as one can. The (new) example below illustrates this point.

3. We should fix a name for this method. Persi (and you?) call it Poincare; I’ve been calling it distinguished paths, and Alistair Sinclair calls it multicommodity flow. I don’t really object to Poincare, except for preferring descriptive names in principle, so I would be happiest calling it the (adjective) flows method if we could find a suitable adjective: “locally bounded” or “diffuse” make sense but are a bit bland.
1.1 A chain on cladograms

xxx JF: I just made this up. Look complicated, but actually worked quite well in class.

An \( n \)-leaf cladogram is a tree with \( n \) leaves labeled \( \{1, 2, \ldots, n\} \), an unlabeled root of degree 1 and internal branchpoints of degree 3, where we do not distinguish between left and right branches. See figure 1. We define a Markov chain on the set \( I_n \) of such trees as follows.

Pick a uniform random leaf \( i \) and remove leaf \( i \) (in more detail: remove the edge from \( i \) to its branchpoint \( b \), and remove \( b \) to collapse two edges into one). Then pick a uniform random edge \( e \) of the remaining tree, create a new branchpoint \( b' \) in the interior of \( e \), and reattach leaf \( i \) via a new edge to \( b' \).

Figure 1 illustrates a typical transition: from the first tree, leaf 3 is removed and reattached to the edge above the branchpoint of \( \{11, 8\} \).

This chain has symmetric transition matrix, so is reversible with uniform stationary distribution \( \pi \). It is known (see Remarks later) that \( \tau_2 = \Omega(n^2) \) and there is reason to conjecture that in fact \( \tau_2 = \Theta(n^2) \). Since the diameter of the transition graph is \( O(n) \) (this can be deduced from our construction below), Corollary 34 (yyy 10/11/94 version of Chapter 4) would imply \( \tau_2 = O(n^2) \) if the chain were edge-transitive. In fact the chain is not even vertex-transitive (essentially, because different trees have different “shapes”), but (xxx tie up with comment 2 above: this is the type of example where we expect Poincare to do well) we shall use the distinguished paths method to prove

\[
\tau_2 = O(n^{7/2}). \tag{1}
\]

Our argument has “slack” at two places (which we will point out), and it would be interesting to seek to improve the analysis.

We first need some elementary observations concerning \( I_n \). Each tree \( x \in I_n \) has exactly \( 2n - 1 \) edges. A new tree in \( I_n \) can be obtained from an old tree in \( I_{n-1} \) by attaching leaf \( n \) to any edge of the old tree, and different choices of (old tree, edge) lead to different new trees. So \( |I_n| = |I_{n-1}| \times (2n - 3) \) and inductively

\[
|I_n| = (2n - 3)(2n - 5)(2n - 7) \cdots 3 \cdot 1 = c_n \text{ say}.
\]

This argument is tantamount to the observation that a uniform random tree in \( I_n \) can be constructed in the natural sequential way, as follows.
Lemma 1 Start with the unique tree in $I_2$, and for $k = 2, 3, \ldots, n-1$ attach leaf $k+1$ to the middle of a uniform random edge of the previous tree. The final random cladogram is distributed uniformly on $I_n$. This remains true if we add leaves in some arbitrary order $\pi(1), \ldots, \pi(n)$.

We now specify the distinguished paths. Fix an initial tree $x^0 \in I_n$. Create a uniform random permutation $\pi(1), \pi(2), \ldots, \pi(n)$ of leaves. Remove leaf $\pi(1)$ and reattach to a random edge of the remaining tree. Then remove $\pi(2)$ and reattach to the edge incident to $\pi(1)$. This creates a subtree $S_2$ which is a cladogram on the two leaves $\{\pi(1), \pi(2)\}$. Inductively, for $k = 2, 3, \ldots, n-1$ remove leaf $\pi(k+1)$ and reattach to a uniform random edge of $S_k$ to create the subtree $S_{k+1}$ on leaves $\pi(1), \ldots, \pi(k+1)$. We end with a random tree $S_n$.

Note that throughout the construction we want each $S_k$ to be a cladogram, so $S_k$ is the spanning subtree on leaves $\pi(1), \ldots, \pi(k)$ of the current tree, together with the edge upwards from the top branchpoint of that subtree. Write $x^0, x^1, x^2, \ldots, x^n = S_n$ for the sequence of $n$-leaf cladograms in this construction.

It follows from the lemma that $S_n$ is uniform on $I_n$. Thus by taking the initial tree $x^0$ to be uniform random, we have defined a flow from $\pi$ to $\pi$. Write $f(e)$ for the flow through a typical edge $e$ of the transition graph in this scheme. Since the stationary flow through $e$ equals $\frac{1}{c_n} \frac{1}{n} \frac{1}{2n-3}$ and each path has length $n$, by (xxx the fundamental inequality: Theorem 32)

$$\tau_2 \leq n \sup_e n(2n-3)c_n f(e).$$

To bound $f(e)$ we first write

$$f(e) = \sum_{k=0}^{n-1} f_k(e)$$

where $f_k(e)$ is the contribution to flow from cases where traversal of edge $e$ is caused by moving of leaf $\pi(k+1)$. Fix $e$; we illustrate with the edge from the first tree to the second tree in figure 1. First observe that $f_k(e)$ is non-zero only for certain values of $k$. In figure 1, $e$ could be traversed at the first step ($k = 0$), or at the third step ($k = 2$) if the subtree $S_2$ were the subtree on $\{11, 8\}$. But this $e$ cannot be traversed with $k = 1$, because then 3 must be reattached adjacent to some leaf $\pi(1)$. This $e$ could also be traversed with $k = 4$ or 5 but for no further values of $k$. Fix a value of $k$ for which the traversal (from some unspecified initial $x^0$) is possible. At the end of the argument we will sum over all $k$ without seeking to exploit
the “possibility” constraint – this is the first point where there is slack in the argument. We illustrate by considering the edge $e = (x^k, x^{k+1}$ in figure 1 and taking $k = 4$. So $S_k$ is the subtree shown on the right of figure 2. The initial tree $x^0$ must have the leaves (excluding $\{6, 11, 8\}$ ) in the same relative positions as in $x^k$. That is, $x^0$ must be like the tree on the left of figure 2 with leaves $\{6, 1, 11, 8\}$ added in arbitrary positions. The chance that a uniform random tree in $I_n$ is of this form equals $1/c_{n-k}$; this is the first term in inequality (3) below which summarizes the argument. Given $x^0$ is of this form, it is next necessary (in order that $x^k$ be as illustrated) that $\{\pi(1), \pi(2), \pi(3), \pi(4)\}$ be the (unordered) set $\{6, 1, 11, 8\}$, and this has chance $1/\binom{n}{k}$. Next, when $\pi(1)$ is reattached to form $x^1$ it must be reattached to a “permissible” edge, i.e. an edge which can lead eventually to $x^k$. At first sight it might appear that there is only one such edge, but figure 3 illustrates a “bad” initial configuration in which there are four possible such edges. We shall just bound the probability of reattachment to a permissible edge by 1; this is the second point of slack in the analysis. Next, in building the subtree $S_k$ we must build the correct subtree (illustrated on the right of figure 2), and this have chance $1/c_k$. Multiplying the terms so far gives an upper bound on the chance that a particular tree $x^k$ arises after step $k$.

In order than the next step traverses the edge $e = (x^k, x^{k+1})$ it is necessary that $\pi(k+1)$ is a particular leaf (leaf 3, in figure 1) and that it be reattached to the correct edge of $S_k$; these chances are $1/(n-k)$ and $1/(2k-1)$. In the case $k = 0$ the second chance is $1/(2n-3)$; we leave this variation implicit in the argument below.

Collecting these estimates

$$f_k(e) \leq \frac{1}{c_{n-k}} \quad (\text{possible initial } x^0)$$
$$\times \frac{1}{\binom{n}{k}} \quad (\text{choose } \{\pi(1), \ldots, \pi(k)\})$$
$$\times 1 \quad (\pi(1) \text{ reattached to feasible edge})$$
$$\times \frac{1}{c_k} \quad (\pi(1), \ldots, \pi(k) \text{ build correct subtree to create } x^k)$$
$$\times \frac{1}{n-k} \quad (\pi(k+1) \text{ is correct leaf})$$
$$\times \frac{1}{2k-1} \quad (\pi(k+1) \text{ reattached to correct edge}). \quad (3)$$

Rearranging,

$$n(2n-3)c_n f(e) \leq \frac{n(2n-3)}{(n-k)(2k-1)} \frac{c_n}{c_{n-k}c_k \binom{n}{k}}.$$

We can rewrite $c_n$ as $\frac{(2n)!}{(2n-1)!2^{n-1}n!}$, and then a routine argument from Stirling’s
formula shows the right side is asymptotic to
\[ 2\pi^{1/2}(k + 1)^{1/2}(n - k)^{1/2}n^{1/2} \quad \text{as } k \to \infty, \ n - k \to \infty \]
and has the same order of magnitude bound if \( n \to \infty \) with \( k \) or \( n - k \) bounded. So
\[ \sup_e n(3n - 1)c_n f_k(e) = O(n^{3/2}) \text{ uniformly in } k = 0, 1, \ldots, n - 1. \]

Since \( f(e) = \sum_{k=0}^{m-1} f_k(e) \), summing over \( k \) and applying (2) gives the desired bound (1).

Remarks. (a) For a typical edge \( e \) (rather than the worst-case edge) one can remove the slack in the argument above to show that the right side of (2) is \( O(n^2) \). So it is plausible that more elaborate analysis might be able to establish \( \tau_2 = O(n^2) \) using different bounds for the exceptional edges.

(b) Using coupling, Aldous [?] shows \( \tau_1 = O(n^3) \). The coupling construction uses similar ideas but its analysis is more complicated. By using a suitable test function in the extremal characterization, it is not hard to show [?] \( \tau_2 = \Omega(n^2) \). The conjecture \( \tau_2 = \Theta(n^2) \) parallels a conjecture that we can apply weak convergence methodology here (xxx point to discussion to be written in Chapter 13).
Figure 1. An edge $e = (x^k, x^{k+1})$ in the transition graph, for $n = 11$. 
Figure 2. In order that the transition at step $k = 5$ be the transition in figure 1, the subtree $S_4$ must be the right tree and the initial tree $x^0$ must be compatible with the left tree.

Figure 3. A bad possible initial tree $x^0$. 