xxx Chap4-9.tex

## 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  $\{1, 2, ..., n\}$ , 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  $\mathbf{x} \in I_n$  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

$$|I_n| = (2n-3)(2n-5)(2n-7) \cdot 3 \cdot 1 := c_n$$
 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, ..., 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  $\pi(1), ..., \pi(n)$ .

We now specify the distinguished paths. Fix an initial tree  $\mathbf{x}^0 \in I_n$ . 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  $\mathbf{x}^0, \mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^n = S_n$  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  $\mathbf{x}^0$  to be uniform random, we have defined a flow from  $\pi$  to  $\pi$ . Write  $f(\mathbf{e})$  for the flow through a typical edge  $\mathbf{e}$  of the transition graph in this scheme. Since the stationary flow through  $\mathbf{e}$  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)

$$\tau_2 \le n \sup_{\mathbf{e}} n(2n-3)c_n f(\mathbf{e}).$$
<sup>(2)</sup>

To bound  $f(\mathbf{e})$  we first write

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

where  $f_k(\mathbf{e})$  is the contribution to flow from cases where traversal of edge  $\mathbf{e}$  is caused by moving of leaf  $\pi(k+1)$ . Fix  $\mathbf{e}$ ; we illustrate with the edge from the first tree to the second tree in figure 1. First observe that  $f_k(\mathbf{e})$  is non-zero only for certain values of k. In figure 1,  $\mathbf{e}$  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  $\mathbf{e}$  cannot be traversed with k = 1, because then 3 must be reattached adjacent to some leaf  $\pi(1)$ . This  $\mathbf{e}$  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  $\mathbf{x}^0$ ) 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  $\mathbf{e} = (\mathbf{x}^k, \mathbf{x}^{k+1})$  in figure 1 and taking k = 4. So  $S_k$  is the subtree shown on the right of figure 2. The initial tree  $\mathbf{x}^0$  must have the leaves (excluding  $\{6, 1, 11, 8\}$ ) in the same relative positions as in  $\mathbf{x}^k$ . That is,  $\mathbf{x}^0$  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  $\mathbf{x}^0$  is of this form, it is next necessary (in order that  $\mathbf{x}^k$  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  $\mathbf{x}^1$  it must be reattached to a "permissible" edge, i.e. an edge which can lead eventually to  $\mathbf{x}^k$ . 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  $\mathbf{x}^k$  arises after step k. In order than the next step traverses the edge  $\mathbf{e} = (\mathbf{x}^k, \mathbf{x}^{k+1})$  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

$$f_{k}(\mathbf{e}) \leq 1/c_{n-k} \quad \text{(possible initial } \mathbf{x}^{0}\text{)}$$

$$\times 1/\binom{n}{k} \quad (\text{ choose } \{\pi(1), \dots, \pi(k)\})$$

$$\times 1 \quad (\pi(1) \text{ reattached to feasible edge})$$

$$\times 1/c_{k} \quad (\pi(1), \dots, \pi(k) \text{ build correct subtree to create } \mathbf{x}^{k}\text{)}$$

$$\times 1/(n-k) \quad (\pi(k+1) \text{ is correct leaf})$$

$$\times 1/(2k-1) \quad (\pi(k+1) \text{ reattached to correct edge}). \quad (3)$$

Rearranging,

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

We can rewrite  $c_n$  as  $\frac{(2n)!}{(2n-1)2^n n!}$ , and then a routine argument from Stirling's

formula shows the right side is asymptotic to

$$2\pi^{1/2}(k+1)^{1/2}(n-k)^{1/2}n^{1/2}$$
 as  $k \to \infty, \ n-k \to \infty$ 

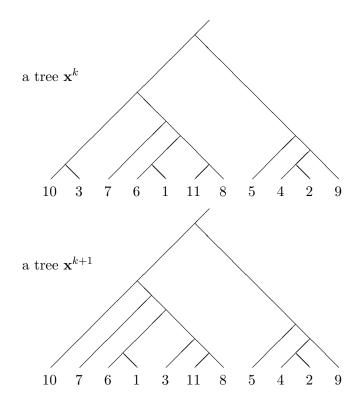
and has the same order of magnitude bound if  $n \to \infty$  with k or n-k bounded. So

$$\sup_{\mathbf{e}} n(3n-1)c_n f_k(\mathbf{e}) = O(n^{3/2}) \text{ uniformly in } k = 0, 1, \dots, n-1.$$

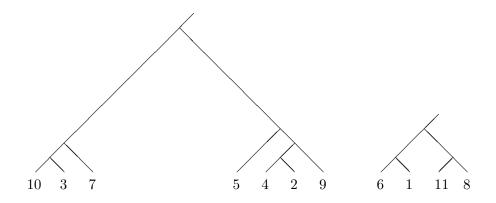
Since  $f(\mathbf{e}) = \sum_{k=0}^{m-1} f_k(\mathbf{e})$ , summing over k and applying (2) gives the desired bound (1).

*Remarks.* (a) For a typical edge **e** (rather that 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  $\mathbf{e} = (\mathbf{x}^k, \mathbf{x}^{k+1})$  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  $\mathbf{x}^0$  must be compatible with the left tree.

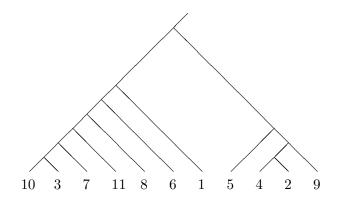


Figure 3. A bad possible initial tree  $\mathbf{x}^0$ .