COST OF SEQUENTIAL CONNECTION FOR POINTS IN SPACE

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A bound is given for the cost of the spanning tree produced by the sequential minimal insertion procedure as applied to n points in the unit d-cube. The technique developed is reasonably general and can be applied to several other problems of computational geometry, including the nearest neighbor heuristic for the traveling salesman problem. Attention is also given to bounding the sum of the powers of the edge lengths of sequentially constructed trees and paths. Examples illustrate that the bounds obtained are of best possible order as a function of the number of points.

spanning tree * minimal spanning tree * nearest neighbor heuristic * sequential insertion * traveling salesman problem

1. Introduction

This article develops a technique to provide sequentially constrained analogues to some classical inequalities of combinatorial optimization in Euclidean space. In particular, the technique provides sequential analogues to the following:

(1) If $S = \{x_1, x_2, ..., x_n\} \subset [0, 1]^d$ and $|x_i - x_j|$, denotes the Euclidean distance between x_i and x_j , then TSP(S), the minimum cost of a path through the points of S, satisfies

$$TSP(S) \le \alpha_d n^{(d-1)/d}, \tag{1.1}$$

where α_d is a constant that depends only on the dimension d.

(2) If MST(S) denotes the cost of the minimal Euclidean length spanning tree of $S = \{x_1, x_2, ..., x_n\} \subset [0, 1]^d$, then

$$MST(S) \le \alpha'_d n^{(d-1)/d}, \tag{1.2}$$

where the (smaller) constant α'_d again depends only on the dimension d.

Inequalities (1.1) and (1.2) have been the focus of many investigations and considerable ingenuity

has been expended to determine good values of the constants α_d and α_d' . For example, Verblunsky (1951) showed $\alpha_2 \leq (2.8)^{1/2}$, and Few (1955) improved this to $\alpha_2 \leq 2^{1/2}$. The first bounds on α_d for general d are given by Few (1955), and these have been improved by Moran (1984), Goldstein and Reingold (1988), and Goddyn (1988). If one does not press for the best values of α_d and α_d' , bounds (1.1) and (1.2) are both easy consequences of the pigeon-hole bound;

There is a constant $\beta_d > 0$ such that for any m-element set

$$S = \{x_1, x_2, \dots, x_m\} \subset [0, 1]^d,$$

the function defined by

$$g_m(x_1, x_2, ..., x_m) = \min_{1 \le j < k \le m} |x_j - x_k|$$

satisfies

$$g_m(x_1, x_2, ..., x_m) \le \beta_d m^{-1/d}.$$
 (1.3)

The problem that motivates this article is the derivation of an analogue to (1.2) for the heuristic construction of a spanning tree of $S = \{x_1, x_2, ..., x_n\}$ that is based on minimal sequential insertions. It turns out that one has the precise analogue of (1.2), and, moreover, an a priori inequality analogous to (1.3) is valid in an average sense. Before developing that a priori inequality

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(which is somewhat technical in appearance), we examine some of its consequences.

Given a fixed sequence $S = \{x_1, x_2, ..., x_n\}$ of points in \mathbb{R}^d , then we can build a spanning tree for S by sequentially joining x_i to the tree formed by $\{x_1, x_2, ..., x_{i-1}\}$ for $2 \le i \le n$. If $r_i = r(x_i; x_1, x_2, ..., x_{i-1})$ denotes the shortest distance between x_i and a point of $\{x_1, x_2, ..., x_{i-1}\}$, i.e.

$$r_i = r(x_i; x_1, x_2, \dots, x_{i-1}) = \min_{j:1 \le j < i} |x_i - x_j|,$$
(1.4)

then r_i is the minimal cost of joining x_i to a vertex of a spanning tree of $\{x_1, x_2, ..., x_{i-1}\}$. Naturally, $r(x_i; x_1, x_2, ..., x_{i-1})$ is at least as large as $g_i(x_1, x_2, ..., x_i)$ for each $1 \le i < n$, and by easy examples one can show r can be much greater than g. The cost of the minimal insertion tree constructed by sequentially connecting x_i to the tree already constructed on $\{x_1, x_2, ..., x_{i-1}\}$ is given by the sum of the r_i , $1 < i \le n$, and will be denoted by MIT(S). Despite the fact that the r_i are all at least as large as g it turns out that a bound is available for the sum of the r_i that is not substantially larger than the bound available for MST(S). Specifically, there is a constant, γ_d , depending only on the dimension d such that for all $n \ge 1$, we have

$$MIT(S) = \sum_{1 < i \le n} r(x_i; x_1, x_2, ..., x_{i-1})$$

$$\leq \gamma_d n^{(d-1)/d}.$$
(1.5)

Each of the inequalities (1.1), (1.2), and (1.5) says that the *average* cost of each edge is of order $n^{-1/d}$. The twist in (1.5) is that one maintains the same order of magnitude of average cost even when one is required to insert the x_i into the tree in a specified order.

The next section develops a general method for obtaining bounds in sequential problems, and, in particular, a proof is given of (1.5). The third section modifies the basic method to provide bounds for the nearest neighbor heuristic for the traveling salesman problem. In Section 4, the sum of the d-th powers of the edges of the minimal insertion tree are contrasted with those of the minimal spanning tree and some surprising differences emerge. The fifth section draws out the connections and distinctions between the present technique and a related method of Bentley and

Saxe (1980). The final section points out some open problems.

2. Sequential insertion trees

The following lemma provides the basis for many inequalities involving r_i . The key point is that the right-hand side of (2.1) does not depend on n and the left-hand side is almost the distribution function of the r_i . While the bounding constant is given explicitly, more attention has been given to obtaining a simple bound than to obtaining the sharpest possible constant. Although, the constant is irrelevant for most applications, it would be of interest to know if the right-hand side of (2.1) could be replaced by c^d for some c not depending on d.

Lemma 1. If
$$\{x_1, x_2, ..., x_n\} \subset [0,1]^d$$
 and $r_i = \min_{j:1 \le j < i} |x_j - x_i|$ for $1 < i \le n$,

then for any $0 < x < \infty$ we have

$$\sum_{x \le r_i < 2x} r_i^d \le 8^d d^{d/2}. \tag{2.1}$$

Proof. Let $C = \{i: x \le r_i < 2x\}$ and for each $i \in C$ let B_i be a ball of radius $\frac{1}{4}r_i$ with center x_i . We will argue by contradiction that $B_i \cap B_j = \emptyset$ for all i < j. If $B_i \cap B_j \neq \emptyset$, then the bounds $r_i \le 2x$ and $r_i \le 2x$ gives us

$$|x_i - x_j| \le \frac{1}{4}(r_i + r_j) < x.$$
 (2.2)

But, by definition of r_j we have $|x_i - x_j| \ge r_j$ for all i < j; and, by the lower bound on the summands in (2.1) we have $x \le r_j$, so we also see $|x_i - x_j| \ge x$. Since $|x_i - x_j| \ge x$ contradicts (2.2), we have $B_i \cap B_i = \emptyset$.

Now, since all of the balls B_i are contained in a sphere with radius $2d^{1/2}$, the fact that they are disjoint tells us the sum of their volumes is bounded by the volume of the sphere of radius $2d^{1/2}$. Thus, if ω_d denotes the volume of the unit ball in \mathbb{R}^d , we have the bound

$$\sum_{i \in S} \omega_d r_i^d 4^{-d} \le \omega_d 2^d d^{d/2}$$

from which (2.1) follows. \square

Information is easily extracted from (2.1) if one is guided by the theory of linear programming where duality tells us that essentially all inequalities that can be inferred from (2.2) are obtained by taking linear combinations of (2.2) with positive coefficients. This principle is made explicit by inequality (2.3) and its applications to the proof of (2.5) and (1.5).

The restriction in Lemma 2 to non-increasing functions is convenient, but inessential. Similar inequalities can be derived for Ψ that satisfy less taxing regularity assumptions.

Lemma 2. *I* is a positive and non-increasing function on the interval $(0, d^{1/2}]$, then for any $0 < \alpha < \beta \le d^{1/2}$

$$\sum_{\alpha \leqslant r_i \leqslant \beta} r_i^{d+1} \Psi(r_i) \leqslant 2 \cdot 8^d d^{d/2} \int_{\alpha/2}^{\beta} \Psi(x) \, \mathrm{d}x.$$
(2.3)

Proof. By (2.1) we have

$$\sum_{\alpha \leqslant r_i \leqslant \beta} r_i^d I(x \leqslant r_i < 2x) \leqslant 8^d d^{d/2},$$

where $I(x \le r_i < 2x) = I(\frac{1}{2}r_i \le x < r_i)$ is the indicator function. If we multiply by $\Psi(x)$ and integrate over $[\frac{1}{2}\alpha \beta]$, we find

$$\sum_{\alpha \leqslant r_i \leqslant \beta} r_i^d \int_{r_i/2}^{r_i} \Psi(x) \, \mathrm{d}x \leqslant 8^d d^{d/2} \int_{\alpha/2}^{\beta} \Psi(x) \, \mathrm{d}x. \tag{2.4}$$

Since Ψ is non-increasing, the integrand on the lefthand side of (2.4) is bounded from below by $\Psi(r_i)$, so

$$\Psi(r_i)r_i/2 \leqslant \int_{r_i/2}^{r_i} \Psi(x) \, \mathrm{d}x,$$

and (2.3) follows from (2.4). \Box

Our first application of (2.3) is to bound the sum of the d-th powers of the r_i . In Section 3 it will be proved that this bound cannot be essentially sharpened, even though we show that the minimal spanning tree satisfies an essentially stronger bound.

Lemma 3. There is a constant c_d depending only on d such that for all $n \ge 2$,

$$\sum_{i=1}^{n} r_i^d < c_d \log n. {(2.5)}$$

Proof. Setting $\Psi(x) = 1/x$ and $[\alpha, \beta] = [n^{-1/d}, d^{1/2}]$ in (2.3) gives us

$$\sum_{n^{-1/d} \leqslant r_i} r_i^d < 2 \cdot 8^d d^{d/2} \left\{ \log(d^{1/2}) - \log(\frac{1}{2}n^{-1/d}) \right\},$$
(2.6)

and the small values of r_i^d are trivial to bound

$$\sum_{r \le n^{-1/d}} r_i^d \le 1,\tag{2.7}$$

so (2.5) follows from (2.6). \Box

Inequality (2.5) can be used with Hölder's inequality to provide a bound on the basic sum of (1.5), Σr_i , but in this instance the bound one obtains is not the best possible. Specifically, applying Hölder's inequality with p = d and q = d/(d-1) to $\sum_{i=1}^{n} r_i \cdot 1$, we find

$$\sum_{i=1}^{n} r_i \leqslant c_d^{1/d} n^{(d-1)/d} (\log n)^{1/d}. \tag{2.8}$$

This bound falls short of the desired inequality (1.5) by a factor of $(\log n)^{1/d}$; so to prove (1.5), we use (2.3) directly. Letting $\Psi(x) = 1/x^d$ and $(\alpha, \beta) = [n^{-1/d}, d^{1/2}]$ in (2.3), we bound the sum of the larger r_i ,

$$\sum_{r_i \ge n^{-1/d}} r_i \le 2 \cdot 8^d d^{d/2} (d-1)^{-1} \cdot \left\{ 2^{d-1} n^{(d-1)/d} - d^{(d-1)/2} \right\}. \tag{2.9}$$

To handle the smaller r_i we again rely on the trivial bound

$$\sum_{r_i \leqslant n^{-1/d}} r_i \leqslant n \cdot n^{-1/d} = n^{(d-1)/d}, \tag{2.10}$$

and from (2.9) and (2.10) we conclude that (1.5) is proved with $\gamma_d = 1 + 2^{4d} d^{d/2} / (d-1)$.

3. Sharpness of bounds for MIT's and MST's

The presence of the logarithmic factor in (2.5) and the fact that it could be removed from (2.8) might lead one to question if (2.5) is sharp. Suspicions may be further raised by noting that Gilbert and Pollak (1968) showed for d = 2 that $\sum |e|^2$ is uniformly bounded for any minimal spanning tree of $\{x_1, x_2, \ldots, x_n\} \subset [0,1]^2$. It will be proved shortly that (2.5) is nevertheless sharp, but first it is instructive to look more deeply at the inequali-

ties that hold for sum of powers of edge lengths of minimal spanning trees.

The result of Gilbert and Pollak can be extended to arbitrary dimensions by using some recent results from the theory of spacefilling curves. In fact, the proof one obtains for general $d \ge 2$ is substantially simpler than the bare-handed proof given by Gilbert and Pollak in d = 2.

We will make use of a theorem of Milne (1980) that says there is a function f from [0,1] onto $[0,1]^d$ which is Lipschitzian of order 1/d, i.e.

$$|f(x) - f(y)| \le c |x - y|^{1/d}$$
 (3.1)

for a constant c > 0. To apply this to the bounding of edge weights of a minimal spanning tree, we suppose $V_n = \{x_1, x_2, ..., x_n\} \subset [0,1]^d$ and let T be a minimal spanning tree of V_n . Since f is surjective we can choose $\{y_1, y_2, ..., y_n\}$ in [0,1] such that $f(y_i) = x_i$. Next, we order the y_i to given $y_{(1)} \leq y_{(2)} \leq \cdots \leq y_{(n)}$ and define a new suboptimal spanning tree T_0 on V_n by choosing the n-1 edges $(f(y_{(i)}), f(y_{(i+1)})), 1 \leq i < n$. By the optimality of T and the Lipschitz property of f, we find

$$\sum_{e \in T} |e|^d \leq \sum_{e \in T_o} |e|^d$$

$$= \sum_{i=1}^{n-1} |f(y_{(i)}) - f(y_{(i+1)})|^d$$

$$\leq c^d \sum_{i=1}^{n-1} |y_{(i)} - y_{(i+1)}| \leq c^d.$$
(3.2)

In comparison with the complexity of the proof of Gilbert and Pollak (1968) in d = 2, this proof of the uniform boundedness of $\sum |e|^d$ is almost effortless. All of the geometry of $[0,1]^d$ has been compressed into the existence of the Lipschitz spacefilling curve. The use of spacefilling curves to provide heuristics for a variety of optimization problems is surveyed in Bartholdi and Platzman (1988).

Before leaving the problem of bounding $\sum |e|^d$ for minimal spanning trees we should note a fact that makes it possible to give an easy, new proof of the Gilbert and Pollak result in d=2 that does not require the relatively sophisticated machinery of spacefilling curves. The key observation is given in the following.

Pythagorean Lemma. Given n points in a right triangle, there is a path through the points such that the sum of the squares of the edges on the path is bounded by the square of the hypotenuse.

This lemma can be viewed as an adjunct to the Pythagorean theorem, and, when n = 3 and the points are the vertices of the triangle, the lemma even reduces to that result. For the details of the proof of the lemma, one can consult Newman (1982, p.8); but, if we gloss over some small points, it is easy to sketch the idea. The first trick is to consider a more specific induction hypothesis: any set of n points including the end points of the hypotenuse can be joined by a path with the required bound. Next, drop a perpendicular from the right-angled vertex to the hypotenuse, and add the point that was at the right angle to each of the sets of points in the two smaller triangles created by the bisection. One then applies the induction hypothesis and the Pythagorean theorem to complete the proof.

The fact inequality (2.5) of Lemma 3 cannot be essentially improved is a consequence of the following lemma that also shows that (1.3) is essentially sharp. As before, ω_d denotes the volume of the ball of unit radius in \mathbb{R}^d .

Lemma 4. For each $d \ge 1$, the constant $\delta_d = \frac{1}{2}\omega_d^{-1/d}$ has the property that for any $\{x_1, x_2, ..., x_n\} \subset [0,1]^d$ there is an $x_{n+1} \in [0,1]^d$ such that $|x_i - x_{n+1}| \ge \delta_d n^{-1/d}$ for all $1 \le i \le n$.

Proof. If B_i is a ball of radius $\delta_d n^{-1/d}$ and center x_i , then by setting $A = \bigcup_{i=1}^n B_i$ we find the complementary set A^c has measure at least $\frac{1}{2}$. We can thus take x_{n+1} to be any point in A^c . \square

Returning to (2.5) we can use Lemma 4 sequentially to construct $\{x_i, 1 \le i < \infty\}$ so that for all $i \ge 2$,

$$r_i \geqslant \delta_d (i-1)^{-1/d}. \tag{3.3}$$

From (3.3) we see that the order of the bounds (1.5), (2.1), and (2.5) cannot be improved.

4. Nearest neighbor traveling salesman path

Consider the path through $\{x_1, x_2, ..., x_n\} \subset [0,1]^d$ that is obtained by starting at x_1 and subse-

quently going to the nearest unvisited point. If we let $x_{j_1}, x_{j_2}, \ldots, x_{j_n}$ denote the ordering of the points on the path, then the n-1 values defined by

$$\tilde{r}_{i} = \min\{ |x_{j_{i}} - x_{k}| : x_{k} \notin \{x_{j_{1}}, x_{j_{2}}, \dots, x_{j_{i}}\} \},
1 \le i < n,$$
(4.1)

are the lengths of the edges in the path. Naturally, we also have

$$\tilde{r}_i = |x_{i,-} - x_{i,+1}|, \quad 1 \le i < n.$$
 (4.2)

Although the \tilde{r}_i are computationally and conceptually more difficult than the r_i of Section 2, we shall find inequalities analogous to (1.5), (2.1), (2.3), (2.5) and (2.7). Since each of these inequalities are consequences of (2.1), we only need to prove the analogue of that one bound. Even in this step, one sees close parallels to the proof of Lemma 1.

Lemma 5. If $S = \{x_1, x_2, ..., x_n\} \subset [0,1]^d$ and $\tilde{r}_i, 1 \leq i < n$, are the edge lengths of the nearest neighbor path, then for any $0 < x < \infty$ we have

$$\sum_{x \leqslant r_i < 2x} \tilde{r}_i^d \leqslant 8^d d^{d/2}. \tag{4.3}$$

Proof. Let $C = \{i: x \le \tilde{r}_i < 2x\}$ and for each $i \in C$ let B_i be a ball of radius $\frac{1}{4}\tilde{r}_i$ with center x_{j_i} where the j_i are defined as in (4.1). As before, we claim that $B_s \cap B_t = \emptyset$ for all s < t and we argue by contradiction. If $B_s \cap B_t \neq \emptyset$, then

$$|x_{i_s} - x_{i_t}| \le \frac{1}{4} (\tilde{r}_s + \tilde{r}_t) < x.$$
 (4.4)

Since s < t, we see $j_t \notin \{j_1, j_2, ..., j_s\}$, so (4.4) and (4.1) imply $\tilde{r}_s < x$. But $\tilde{r}_s < x$ contradicts the assumption that $s \in C$, so we conclude $B_s \cap B_t = \emptyset$ for all s, t contained in C. The remainder of the proof is exactly as in Lemma 1. \square

It remains only to summarize some consequences of (4.3).

Corollary. For all $n \ge 1$,

$$\sum_{i=1}^{n} \tilde{r}_i^d < c_d \log n, \tag{4.5}$$

and

$$\sum_{i=1}^{n} \tilde{r}_{i} < \gamma_{d} n^{(d-1)/d}. \tag{4.6}$$

The constants in (4.5) and (4.6) are exactly the same as those in (2.5) and (2.11).

5. Bentley-Saxe method

The method developed in the preceding section has a close relation to a method developed earlier in Bentley and Saxe (1980). Two immediate (but inessential) distinctions between the Bentley-Saxe method and that developed here are: (1) the Bentley-Saxe method was developed only in d=2; and (2) the Bentley-Saxe method focused on the overall cost of heuristic tours and paths rather than the cost of sequential connection.

A more important distinction is that Bentley and Saxe base their bounds is the notion of a compatible k-circling. If C_1, C_2, \ldots, C_m are m disks in \mathbb{R}^2 , $k \ge 2$, and cent(C) denotes the center of the disk C, then we say $\{C_i: 1 \le i \le m\}$ is a compatible k-circling provided

$$\operatorname{cent}(C_i) \in [0,1]^2, \tag{5.1a}$$

$$\partial C_i \cap [0,1]^2 \neq \emptyset, \tag{5.1b}$$

and

for any $1 \le i_1 < i_2 < \cdots < i_k \le m$, there is a j such that the relationship

$$\operatorname{cent}(C_{i_{i}}) \in \bigcap_{s=1}^{k} C_{i_{s}} \text{ fails.}$$
 (5.1c)

The main lemma of Bentley and Saxe says that for any $k \ge 2$ and any k-compatible circling $\{C_1, C_2, \ldots, C_m\}$ satisfying radius $(C_i) \ge \alpha$, for all $1 \le i \le m$, one has

$$\sum_{i=1}^{m} \text{radius}(C_i) \le 4(k-1)(1+\alpha^2)/(\pi\alpha^2). \quad (5.2)$$

Bentley and Saxe further show that if one places a circle \tilde{C}_i of radius \tilde{r}_i about x_{j_i} where $x_{j_i}, x_{j_2}, \ldots, x_{j_n}$ is the nearest neighbor tour of $\{x_1, x_2, \ldots, x_n\} \subset [0,1]^2$ described in Section 4, then $S = \{\tilde{C}_i : 1 \le i < n\}$ is a 3-compatible circling. Since a subset of a compatible circling is compatible, Bentley and Saxe apply (5.2) to appropriately chosen subsets of S to obtain

$$\sum_{1 \le i \le n} \tilde{r}_i \le 2\sqrt{2n/\pi} + O(\log n)$$
 (5.3)

and

$$\sum_{1 \le i \le n} \tilde{r}_i^2 \le 8 \log n + \mathcal{O}(1), \tag{5.4}$$

where the implied constants of the O-terms of (5.3) and (5.4) can be made explicit.

6. Concluding remarks and open problems

We know by (2.5) and (4.6) that if E is the set of edges for the minimal insertion tree or the nearest neighbor tour we have that

$$\sum_{e \in E} |e|^d < c \log n. \tag{6.1}$$

Moreover, by Lemma 4 one cannot essentially improve (6.1) despite the fact that by the argument of (3.1)–(3.2) we have the stronger bound

$$\sum_{e \in E} |e|^d < c \tag{6.2}$$

for the minimal spanning tree.

One intriguing question that is left open is whether one has the analogue of (6.2) for the minimal traveling salesman problem. To see the subtlety of this problem one first has to note that the argument in (3.1)–(3.2) does not apply. The crucial feature of the MST is that the trees one obtains are the same for the weight function $|e|^d$ as for the original weights |e|. This feature no longer holds for the traveling salesman problem so a new approach is required. One source of help might be in Rosenkrantz, Stearns and Lewis (1977), where one finds several results that complement the inequalities of this article.

To motivate the second problem, first define the sequence $\mu(n)$ by

$$\mu(n) = \max \{ MIT(S) \colon S = \{ x_1, x_2, ..., x_n \}$$

$$\subset [0,1]^d \}. \quad (6.3)$$

We have seen that $\mu(n)n^{-(d-1)/d}$ is bounded. Is it true that $\mu(n)n^{-(d-1)/d}$ converges as $n \to \infty$? The analogous question for minimal spanning trees and traveling salesman tours has been answered in the affirmative by Steele and Snyder (1988), but the fact that $\mu(n)$ is not determined by an optimality property makes the behavior of $\mu(n)$ more subtle.

The inequalities addressed in this article all concerned deterministic point sets, but they are closely related in spirit (and analytical content) to a number of probabilistic topics especially the

theory of subadditive Euclidean functionals. For a survey that addresses both probabilistic and deterministic issues, one can consult Steele (1988) where other open problems are also given.

Note added in proof

The Pythagorean Lemma of Section 3 is an unpublished result of R. Gomory established in 1966. It is cited by R. Adler in his comments on a paper of S. Kakutani (see *Collected Works of S. Kakutani, Vol. II*, R.R. Kallman (ed.), Birkhauser, Boston, 1986, p. 444).

Also the argument in (3.2) is cited by Adler in d = 2 as due to Kakutani (1966, unpublished).

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