A new upper bound for the Euclidean TSP constant

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Abstract

Let $X_1, X_2, \ldots, X_n$ be n independent and uniformly distributed random points in a compact region $R \subset \mathbb{R}^2$ of area 1. Let $\mathsf{TSP}(X_1, \ldots, X_n)$ denote the length of the optimal Euclidean travelling salesman tour that traverses all these points. The classical Beardwood-Halton-Hammersley theorem proves the existence of a universal constant β_2 such $\mathsf{TSP}(X_1, \ldots, X_n)/\sqrt{n} \to \beta_2$ almost surely, which satisfies $0.625 \leq \beta_2 \leq 0.92117$. This paper presents a computer-aided proof using numerical quadrature and decision trees that $\beta_2 < 0.90304$. Although our improvement is still somewhat small, our approach has the advantage that it is primarily limited by computer hardware, and is thus amenable to further improvements over time.

1 Introduction

The Beardwood-Halton-Hammersley (BHH) theorem is a seminal result in the probabilistic analysis of combinatorial optimization that characterizes the length of a Euclidean travelling salesman tour [5]. It is stated as follows:

Theorem 1 (BHH theorem). *Let $\{X_i\}$ be a sequence of independent random variables uniformly distributed in the unit square, and let $\mathsf{TSP}(X_1, \ldots, X_n)$ denote the length of the optimal Euclidean travelling salesman tour of $X_1, \ldots, X_n$. There exists a universal constant β_2 satisfying $0.625 \leq \beta_2 \leq 0.92117$, such that*

$$\lim_{n\to\infty} \frac{\mathsf{TSP}(X_1, \ldots, X_n)}{\sqrt{n}} \to \beta_2$$

almost surely. Moreover, when the elements of $\{X_i\}$ are independently sampled from a distribution μ with compact support $\mathcal{R} \subset \mathbb{R}^2$, we have

$$\lim_{n\to\infty} \frac{\mathsf{TSP}(X_1, \ldots, X_n)}{\sqrt{n}} \to \beta_2 \int_{\mathcal{R}} \sqrt{f(x)}\, dx\,,$$

almost surely, where $f(x)$ is the density of the absolutely continuous part of the distribution μ.

Even more generally, [5] also proved the existence of absolute constants β_d for every integer $d \geq 2$. The value of β_2 is presently unknown, though prior work has given numerical Monte Carlo estimates for β_2 [9, 17, 19, 20, 21, 22, 26, 30], β_3, and β_4 [19, 22]. These approximations were mainly built upon the Held-Karp linear programming relaxation [15, 16]. The most recent estimates obtained in [2, 3] come from simulating very large instances, and show with a high degree of confidence that $\beta_2 \approx 0.71$. However, the original bounds $0.625 \leq \beta_2 \leq 0.92117$ of [5] were not improved until over 50 years later, in the papers [13, 27].

The purpose of this paper is to improve the upper bound $\beta_2 \leq 0.92117$; we prove the following:

Theorem 2. $\beta_2 < 0.90304$.

The approach we describe consists of a computer-aided proof that combines computer algebra tools, numerical quadrature, and decision trees. Although our improvement is still somewhat small, our approach has the advantage that it is primarily limited by computer hardware, and is thus amenable to further improvements over time.

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1.1 Related work

This paper is devoted to bounding β_2 from [5], although the fact that $\mathsf{TSP}(X_1, \ldots, X_n) \in \mathcal{O}(\sqrt{n})$ was observed earlier in [8, 29, 32], together with explicit upper bounds. Theorem 1 has been discussed extensively in the contexts of both combinatorial optimization and probability theory [2, 6, 10, 14, 25, 31, 35], and it is further known that similar limiting behaviors are seen in a wide variety of related problems, such as the minimum spanning tree, Steiner tree, and minimum weight matching problems [23, 24, 35].

The problem of determining bounds for proportionality constants is common in *continuous approximation analysis* of logistics systems [1, 7, 11]. Certain problems are structured so that their proportionality constants have exact expressions, such as the minimum spanning tree [4] and variations of the location-routing problem [33]. The paper [12] takes a different perspective, and proves that β_2 is *strictly* greater than constants for e.g. the minimum spanning tree or the Held-Karp relaxation [15, 16].

2 Background

The purpose of this section is to provide a short overview of the progress on bounding β_2 from above thus far. The original argument that $\beta_2 \leq 0.92117$, as put forth in [5] (and concisely summarized in Section 2 of [27]), is as follows: to begin, we will make our analysis simpler by observing that for independent and uniformly distributed $X_1, \ldots, X_n$ in the unit square, we have

$$\frac{\mathbb{E}[\mathsf{TSP}(X_1, \ldots, X_n)]}{\sqrt{n}} \to \beta_2 \,.$$

This is helpful to us because we are now free to study the tour length in expectation only, as opposed to the almost sure sense as in Theorem 1; the heavy lifting has already been done for us.

The original upper bound [5] produces a "reasonably good" tour by dividing the square into horizontal strips of height $h/\sqrt{n}$, for some constant h of our choosing, and then connecting the points in each strip horizontally to form a family of paths, as shown in Figure 1a. It is routine to show that we can merge these paths together to form a single tour by adding a total length that is almost surely $o(\sqrt{n})$, as shown in Figure 1b. Thus, it suffices to determine the expected total length of these paths.

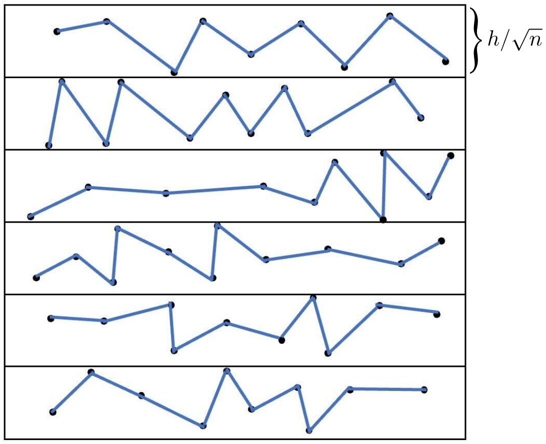
Consider a path $(X_1, Y_1), \ldots, (X_k, Y_k)$, where by construction we have $X_1 \leq \cdots \leq X_k$. It is easy to see that $Y_i = \frac{h}{\sqrt{n}} U$, where U is uniform on the interval $[0, 1]$. Furthermore, [5] also shows that the difference between consecutive x-coordinates, $X_{i+1} - X_i$, follows a scaled exponential distribution as $n \to \infty$, i.e. that

$$h\sqrt{n}(X_{i+1} - X_i) \sim Z \,,$$

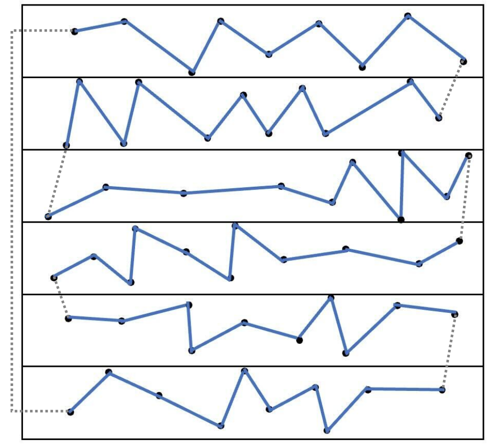
where Z is exponentially distributed with mean 1. Therefore, the expected distance between each consecutive pair (X_i, Y_i) and (X_{i+1}, Y_{i+1}) is

$$\mathbb{E}\left\| \begin{pmatrix} X_i - X_{i+1} \\ Y_i - Y_{i+1} \end{pmatrix} \right\| = \frac{1}{h\sqrt{n}} \mathbb{E} \left\| \begin{pmatrix} Z \\ h^2(U_0 - U_1) \end{pmatrix} \right\|$$

where U_1 and U_0 are uniform on the interval $[0, 1]$, and we obtain an upper bound for the length of the total tour



(a)



(b)

Figure 1: In 1a we divide the square into 6 horizontal strips and traverse them horizontally. The additional length needed to aggregate these paths into one is shown in 1b with dashed lines, and it is routine to show that their total contribution is $o(\sqrt{n})$ almost surely.

by multiplying the right hand side of the above by n. We therefore have the following, for all h:

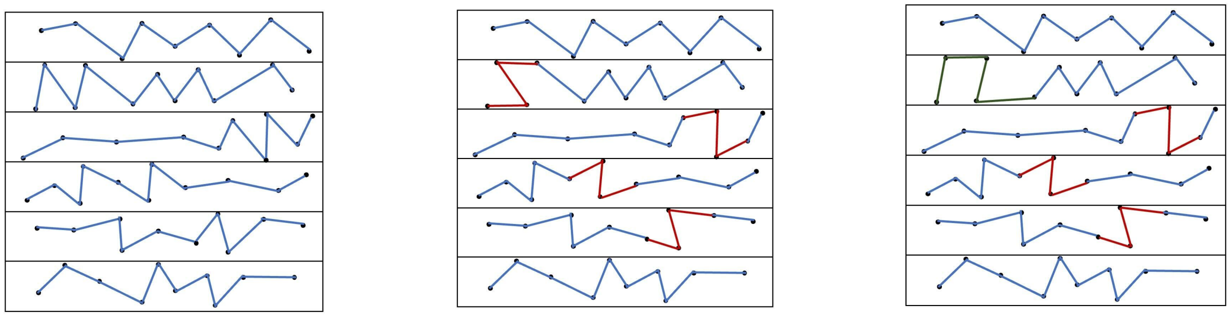
$$\begin{aligned}\beta_2 &\leq \frac{1}{h}\mathbb{E}\left\|\begin{pmatrix} Z \\ h^2(U_0 - U_1) \end{pmatrix}\right\| \qquad (1)\\ &= \frac{1}{h}\int_0^\infty \int_0^1 \int_0^1 e^{-z}\sqrt{z^2 + h^4(u_0-u_1)^2}\,du_0\,du_1\,dz \\ &= \frac{1}{3h^5}\int_0^\infty e^{-z}\left(3h^2z^2\log(h^2/z + \sqrt{h^4/z^2+1}) + 2z^3 + (h^4 - 2z^2)\sqrt{h^4+z^2}\right)dz\,.\end{aligned}$$

It turns out that the above expression is minimized at $h = \sqrt{3}$, at which point the integral evaluates numerically to 0.92116. In fact, [5] makes a numerical error using Simpson's rule to obtain the incorrect estimate 0.92037, a fact not observed (and corrected) until 56 years later in [27].

The paper [27] improves the upper bound by $\frac{9}{16}10^{-6}$ by observing that, unsurprisingly, the left-to-right ordering is not always optimal, and identifies a specific configuration (which they call a *zigzag structure*) for which an alternate ordering is preferable. The numerical improvement is obtained by bounding from below the probability of this configuration occurring, as well as the amount of improvement that is realized. The author notes that the improvement is small, but emphasizes that the underlying idea is of greater interest than the actual numerical improvement.

3 An improved upper bound

The central idea to our improved upper bound, which is also alluded to in Section 2.5 of [27], is to replace the horizontal traversal strategy from Section 2 with a more general sequence. Specifically, we consider the same set of strips of height $h/\sqrt{n}$, but we now select ordered $(k+1)$-tuples $(X_i, Y_i), \ldots, (X_{i+k}, Y_{i+k})$ for fixed (small) k, and select the permutation that minimizes the total tour length of those $k+1$ points, as shown in Figure 2. Note that it is necessary to restrict ourselves to those permutations that begin with the leftmost endpoint (X_i, Y_i) and end



(a) $k = 1, 2$ (b) $k = 3$ (c) $k = 4$

Figure 2: A collection of strips as in the original argument (2a), as well as optimal permutations for $(k+1)$-tuples in (2b) and (2c).

with the rightmost endpoint (X_{i+k}, Y_{i+k}), because we have to stitch all of the paths together to form a single path. The original bound of [5] simply corresponds to the case where $k = 1$ (or $k = 2$, since the endpoints are fixed). For example, whereas the original bound (1) is

$$\beta_2 \leq \frac{1}{h}\mathbb{E}\left\| \begin{pmatrix} Z \\ h^2(U_0 - U_1) \end{pmatrix} \right\|,$$

we can take $k = 3$ to obtain a tighter bound

$$\beta_2 \leq \frac{1}{3h}\mathbb{E}\min\left\{ \begin{array}{c} \left\|\begin{pmatrix} Z_1 \\ h^2(U_0 - U_1) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_2 \\ h^2(U_1 - U_2) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_3 \\ h^2(U_2 - U_3) \end{pmatrix}\right\| \\ \left\|\begin{pmatrix} Z_1 + Z_2 \\ h^2(U_0 - U_2) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_2 \\ h^2(U_2 - U_1) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_3 \\ h^2(U_1 - U_3) \end{pmatrix}\right\| \end{array} \right\},$$

where (as before) all Z_i's are exponential with mean 1 and all U_i's are uniform on the unit interval. Here the top expression simply consists of moving from left to right (i.e. the original upper bound), and the bottom expression consists of swapping the two middle points. Purely for the sake of exposition, for $k = 4$ the bound is

$$\beta_2 \leq \frac{1}{4h}\mathbb{E}\min\left\{ \begin{array}{c} \left\|\begin{pmatrix} Z_1 \\ h^2(U_0 - U_1) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_2 \\ h^2(U_1 - U_2) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_3 \\ h^2(U_2 - U_3) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_4 \\ h^2(U_3 - U_4) \end{pmatrix}\right\| \\ \left\|\begin{pmatrix} Z_1 \\ h^2(U_0 - U_1) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_2 + Z_3 \\ h^2(U_1 - U_3) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_3 \\ h^2(U_3 - U_2) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_3 + Z_4 \\ h^2(U_2 - U_4) \end{pmatrix}\right\| \\ \left\|\begin{pmatrix} Z_1 + Z_2 \\ h^2(U_0 - U_2) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_2 \\ h^2(U_2 - U_1) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_2 + Z_3 \\ h^2(U_1 - U_3) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_4 \\ h^2(U_3 - U_4) \end{pmatrix}\right\| \\ \left\|\begin{pmatrix} Z_1 + Z_2 \\ h^2(U_0 - U_2) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_3 \\ h^2(U_2 - U_3) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_2 + Z_3 \\ h^2(U_3 - U_1) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_2 + Z_3 + Z_4 \\ h^2(U_1 - U_4) \end{pmatrix}\right\| \\ \left\|\begin{pmatrix} Z_1 + Z_2 + Z_3 \\ h^2(U_0 - U_3) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_2 + Z_3 \\ h^2(U_3 - U_1) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_2 \\ h^2(U_1 - U_2) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_3 + Z_4 \\ h^2(U_2 - U_4) \end{pmatrix}\right\| \\ \left\|\begin{pmatrix} Z_1 + Z_2 + Z_3 \\ h^2(U_0 - U_3) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_3 \\ h^2(U_3 - U_2) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_2 \\ h^2(U_2 - U_1) \end{pmatrix}\right\| + \left\|\begin{pmatrix} Z_2 + Z_3 + Z_4 \\ h^2(U_1 - U_4) \end{pmatrix}\right\| \end{array} \right\}; \tag{2}$$

Figure 3 shows an example of a 5-tuple for which the fourth entry of the above expression is the optimal permutation. The remainder of this paper is devoted to bounding integrals such as (2) from above in a rigorous fashion; the main problems are that such integrals are high-dimensional, as a $(k+1)$-tuple ends up requiring $2k+1$ variables, and do

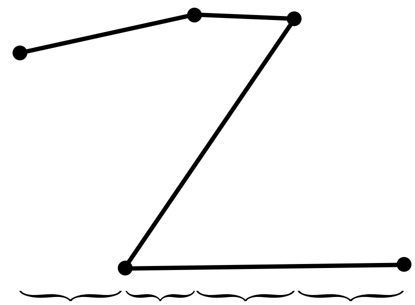


Figure 3: A 5-tuple (5 points and 4 intervals Z_i) for which the fourth entry in (2) is the minimum-cost permutation.

not have closed form expressions. We will describe how to simplify them in the next section.

3.1 Analysis of the high-dimensional integral

The next step in our analysis is to change variables back to the original entries X_i, i.e. by defining $X_i = \sum_{j=1}^{i} Z_i$ for $i \in \{1, \ldots, k\}$, and setting $X_0 = 0$ for notational convenience. The bounds from the previous section are now easily expressed for any $(k+1)$-tuple by writing

$$\beta_2 \leq \frac{1}{kh} \mathbb{E} \min_{\pi \in \Pi_k} \sum_{i=1}^{k} \left\| \begin{pmatrix} X_{\pi(i)} - X_{\pi(i-1)} \\ h^2(U_{\pi(i)} - U_{\pi(i-1)}) \end{pmatrix} \right\| \tag{3}$$

where Π_k consists of all permutations π of $\{0, \ldots, k\}$ such that $\pi(0) = 0$ and $\pi(k) = k$. To evaluate the expectation, we need to transform it into an integral, which means we require the joint pdf on $(X_1, \ldots, X_k)$. Fortunately, this turns out to be straightforward:

Lemma 3. *The joint density function of $(X_1, \ldots, X_k)$ is $f(x_1, \ldots, x_k) = e^{-x_k}$ for $0 \leq x_1 \leq \cdots \leq x_k$.*

Proof. This is a standard textbook-level exercise when introducing exponential random variables and their properties, but we include an inductive proof here for completeness. Assume that the statement holds for $(X_1, \ldots, X_{k-1})$. The joint distribution on $(X_1, \ldots, X_{k-1}, X_k)$ is

$$f(x_1, \ldots, x_{k-1}) g(x_k | X_{k-1} = x_{k-1})$$

where g is the conditional pdf on x_k. Since $X_k = X_{k-1} + Z_k$, we have

$$g(x_k | X_{k-1} = x_{k-1}) = e^{-(x_k - x_{k-1})} \text{ for } x_k \geq x_{k-1}$$

from which the result follows. $\square$

We can now write (3) as the integral

$$\beta_2 \leq \frac{1}{kh} \int_{\mathcal{D}} e^{-x_k} \min_{\pi \in \Pi_k} \sum_{i=1}^{k} \left\| \begin{pmatrix} x_{\pi(i)} - x_{\pi(i-1)} \\ h^2(u_{\pi(i)} - u_{\pi(i-1)}) \end{pmatrix} \right\| dV \,, \tag{4}$$

where

$$\mathcal{D} = \{(x_1, \ldots, x_k), (u_0, \ldots, u_k) : 0 \leq x_1 \leq \cdots \leq x_k \,,\, 0 \leq u_i \leq 1\} \,,$$

and the remainder of this paper consists of bounding the integral (4) rigorously from above. For notational convenience, we define the integrand $g_\pi = g_\pi(x_1, \dots, x_k, u_0, \dots, u_1)$ as

$$g_\pi = \frac{e^{-x_k}}{kh} \sum_{i=1}^{k} \left\| \begin{pmatrix} x_{\pi(i)} - x_{\pi(i-1)} \\ h^2(u_{\pi(i)} - u_{\pi(i-1)}) \end{pmatrix} \right\| ,$$

so that (4) is equivalent to writing

$$\beta_2 \le \int_{\mathcal{D}} \min_{\pi \in \Pi_k} g_\pi \, dV$$

(note that the term e^{-x_k} can appear either inside or outside the $\min_{\pi \in \Pi_k}$ expression because we have assumed that $\pi(k) = k$).

To realize an improvement over the original bound from Section 2, suppose we have a box $B \subset \mathcal{D}$ for which some permutation π^* other than the identity is preferable (note that π^* need not be the optimal permutation *everywhere* in B, merely on average). We can use this box to realize a (very small) improvement over the original bound by writing

$$\begin{aligned} \beta_2 &\le \int_{\mathcal{D}} \min_{\pi \in \Pi_k} g_\pi \, dV \\ &= \int_{\mathcal{D} \setminus B} \min_{\pi \in \Pi_k} g_\pi \, dV + \int_B \min_{\pi \in \Pi_k} g_\pi \, dV \\ &\le \int_{\mathcal{D} \setminus B} g_{\mathrm{Id}} \, dV + \int_B g_{\pi^*} \, dV , \end{aligned}$$

where Id denotes the identity permutation. In other words, we use the identity permutation (i.e. left-to-right traversal) everywhere outside B, and we use π^* inside B. The domain $\mathcal{D} \setminus B$ is cumbersome, but we can obviously simplify things in the usual way by expressing the integral as the difference of an integral over $\mathcal{D}$ and the same integral over B:

$$\int_{\mathcal{D} \setminus B} g_{\mathrm{Id}} \, dV = \underbrace{\int_{\mathcal{D}} g_{\mathrm{Id}} \, dV}_{(*)} - \int_B g_{\mathrm{Id}} \, dV .$$

Finally, since the original bound from [5] already used the identity permutation in its analysis, we see that the integral over $\mathcal{D}$ marked $(*)$ above is already a known quantity, because

$$\begin{aligned} \int_{\mathcal{D}} g_{\mathrm{Id}} \, dV &= \frac{1}{kh} \int_{\mathcal{D}} e^{-x_k} \sum_{i=1}^{k} \left\| \begin{pmatrix} x_i - x_{i-1} \\ h^2(u_i - u_{i-1}) \end{pmatrix} \right\| dV \\ &= \frac{1}{kh} \int_{z_k=0}^{\infty} \cdots \int_{z_1=0}^{\infty} \int_{u_k=0}^{1} \cdots \int_{u_0=0}^{1} \sum_{i=1}^{k} \left\| \begin{pmatrix} z_i \\ h^2(u_i - u_{i-1}) \end{pmatrix} \right\| du_0 \cdots du_k \, dz_1 \cdots dz_k \\ &= \frac{1}{3h^5} \int_0^{\infty} e^{-z} \left(3h^2 z^2 \log(h^2/z + \sqrt{h^4/z^2 + 1}) + 2z^3 + (h^4 - 2z^2)\sqrt{h^4 + z^2} \right) dz \end{aligned}$$

from (1). If we use $h = \sqrt{3}$ as in the original bound from [5], then the above procedure is guaranteed to yield a small improvement by our original assumption that π^* is preferable (on average) in B.

3.2 Separating the integral

We have now established that we can improve the original bound from Section 2 anytime we have a box B for which the identity permutation is (on average) inferior to some other permutation π^*. Not surprisingly, the net improvement in the upper bound that we give in this paper comes from aggregating a large disjoint collection of such boxes and repeatedly performing the steps in the preceding section. In order to achieve guaranteed bounds, we must next show that integration over B is tractable.

Suppose as before that π^* is the non-identity permutation that minimizes $\int_B g_\pi \, dV$. Expanding terms, and using linearity of integration, we can write

$$\begin{aligned}\int_B g_\pi \, dV &= \frac{1}{kh}\int_B e^{-x_k}\sum_{i=1}^{k}\left\|\begin{pmatrix} x_{\pi(i)} - x_{\pi(i-1)} \\ h^2(u_{\pi(i)} - u_{\pi(i-1)})\end{pmatrix}\right\| \\ &= \frac{1}{kh}\sum_{i=1}^{k}\int_B e^{-x_k}\left\|\begin{pmatrix} x_{\pi(i)} - x_{\pi(i-1)} \\ h^2(u_{\pi(i)} - u_{\pi(i-1)})\end{pmatrix}\right\|,\end{aligned} \tag{5}$$

so that the integral over B separates into a sum of integrals, each of which involves no more than 5 variables, namely x_k, $x_{\pi(i)}$, $x_{\pi(i-1)}$, $u_{\pi(i)}$, and $u_{\pi(i-1)}$; when we consider the last summand with $i = k$, there are only 4 variables since $\pi(k) = k$. The first $k-1$ summands, which do not contain x_k in the $\|\cdot\|$ expression, can be reduced to the form

$$\begin{aligned}& C\int_{t_0}^{t_1}\int_{c_2}^{d_2}\int_{c_1}^{d_1}\int_{a_2}^{b_2}\int_{a_1}^{b_1} e^{-s}\left\|\begin{pmatrix} x_2 - x_1 \\ h^2(y_2 - y_1)\end{pmatrix}\right\| dx_1\, dy_1\, dx_2\, dy_2\, ds \\ =& C'\int_{c_2'}^{d_2}\int_{a_2}^{b_2}\int_{c_1'}^{d_1}\int_{a_1}^{b_1}\sqrt{(x_2-x_1)^2+(y_2-y_1)^2}\, dx_1\, dy_1\, dx_2\, dy_2\end{aligned}$$

where C is a constant obtained by integrating out the variables that do not appear in the integrand, C' is further obtained by integrating out the e^{-s} term and eliminating h by a change of variables in y_1 and y_2, and $c_i' = h^2 c_i$. Fortunately, it turns out that this integral has a closed form:

Lemma 4. *We have*

$$\int_{c_2}^{d_2}\int_{a_2}^{b_2}\int_{c_1}^{d_1}\int_{a_1}^{b_1}\sqrt{(x_2-x_1)^2+(y_2-y_1)^2}\, dx_1\, dy_1\, dx_2\, dy_2 = \quad F(x_1,y_1,x_2,y_2)\Big|_{y_2=c_2}^{d_2}\Big|_{x_2=a_2}^{b_2}\Big|_{y_1=c_1}^{d_1}\Big|_{x_1=a_1}^{b_1}$$

where

$$\begin{aligned}F(x,y,u,v) =& \int\int\int\int\sqrt{(x-u)^2+(y-v)^2}\, dx\, dy\, du\, dv \\ =& \frac{-1}{288}(3u^4 + 4u^2v^2 + 3uv^3 - 12u^3x - 8uv^2x - 3v^3x + 18u^2x^2 - 12ux^3 - 12u^3y \\ & -28uv^2y + 12v^2xy + 42uvy^2 - 18vxy^2 - 28uy^3 + 12xy^3) \\ & -\frac{1}{24}(v^2 - 2vy + 2y^2)u(v-2y)v\log 2 \\ & +\frac{1}{24}[(x-u)^2 + (y-v)^2 + uv - vx - uy + xy](u - x + y - v)(u-x)(v-y)\log(\sqrt{(x-u)^2+(y-v)^2} - y + v) \\ & +\frac{1}{12}(u-x)(v-y)^4\log\left|\sqrt{(x-u)^2+(y-v)^2} - x - y + u + v\right| \\ & -\frac{1}{60}[(x-u)^2 - (y-v)^2 + uv - vx - uy + xy][(x-u)^2 - (y-v)^2 - uv + vx + uy - xy]\sqrt{(x-u)^2+(y-v)^2}\end{aligned}$$

Proof. This can be verified by differentiating the antiderivative function F with a computer algebra system. We used FriCAS [28] to compute F directly. □

The other possibility for the integrals in (5) is when $i = k$, which does not have a closed-form antiderivative because of the exponential term. However, we can still reduce it to a univariate integral by integrating the other three variables, and the following result is sufficient to this end:

Lemma 5. *We have*

$$
\begin{aligned}
&\int_{a_2}^{b_2}\int_{c_2}^{d_2}\int_{c_1}^{d_1}\int_{a_1}^{b_1} e^{-x_2}\sqrt{(x_2-x_1)^2+(y_2-y_1)^2}\,dx_1\,dy_1\,dy_2\,dx_2 \\
&=\int_{a_2}^{b_2} e^{-x_2}\left(\int_{c_2}^{d_2}\int_{c_1}^{d_1}\int_{a_1}^{b_1}\sqrt{(x_2-x_1)^2+(y_2-y_1)^2}\,dx_1\,dy_1\,dy_2\right)dx_2 \\
&=\int_{a_2}^{b_2} e^{-x_2}G(x_2)\,dx_2\,, \qquad (6)
\end{aligned}
$$

where

$$
G(x_2) = \left. \left. F(x_1,y_1,x_2,y_2)\right|_{y_2=c_2}^{d_2}\right|_{y_1=c_1}^{d_1}\Bigg|_{x_1=a_1}^{b_1}
$$

and

$$
\begin{aligned}
F(x,y,u,v) &= \int\int\int \sqrt{(x-u)^2+(y-v)^2}\,dx\,dy\,dv \\
&= \frac{1}{6}(u-x)^3 y\log\left(\sqrt{(x-u)^2+(y-v)^2}+y-v\right) \\
&+ \frac{1}{6}(7u^2-2ux+x^2)(u-x)v\log\left(\sqrt{(x-u)^2+(y-v)^2}-y+v\right) \\
&+ \frac{1}{24}(12u^2+v^2)v^2\log\left|\sqrt{(x-u)^2+(y-v)^2}-x+u-y+v\right| \\
&- \frac{1}{24}(12u^2+v^2)v^2\log\left|\sqrt{(x-u)^2+(y-v)^2}+x-u-y+v\right| \\
&+ \frac{1}{12}(2v^2-3vy+2y^2)vy\log\left(\frac{\sqrt{(u-x)^2+(y-v)^2}-u+x}{|y-v|}\right) \\
&- \frac{1}{24}\left(12u^2-y^2\right)y^2\log\left|\sqrt{(x-u)^2+(y-v)^2}-x+u+y-v\right| \\
&+ \frac{1}{24}\left(12u^2-y^2\right)y^2\log\left|\sqrt{(x-u)^2+(y-v)^2}+x-u+y-v\right| \\
&- \frac{1}{24}(14u^2-3v^2-4ux+2x^2+6vy-3y^2)(u-x)\sqrt{(x-u)^2+(y-v)^2}
\end{aligned}
$$

Proof. Again, we used FriCAS [28] to compute the antiderivative F. $\square$

The fact that the preceding integral does not have a closed form means that numerical methods are required, which have the potential to introduce approximation error, which would thus render our analysis unreliable. Fortunately, there is structure that we can exploit to maintain true rigorous upper and lower bounds:

Remark 6. The function $G(x_2)$ is convex, as it is obtained by integrating $\sqrt{(x_2-x_1)^2+(y_2-y_1)^2}$, which is itself convex. Thus, the integrand $e^{-x_2}G(x_2)$ in (6) is the product of two convex functions. We can bound $\int_{a_2}^{b_2} e^{-x_2}G(x_2)\,dx_2$ from above by bounding the functions e^{-x_2} and $G(x_2)$ from above individually with piecewise linear functions, namely the trapezoidal rule, and then taking their product, which is merely a piecewise quadratic function.

Remark 7. When evaluating a box B, we are interested in determining if a given permutation π is preferable to the identity permutation π_{Id}. To this end, distinct from Remark 6, it is also helpful to determine a *lower bound* of $\int_{a_2}^{b_2} e^{-x_2}G(x_2)\,dx_2$ where we use the identity permutation. That is, if an upper bounding integral obtained from π is superior to a lower bounding integral obtained from π_{Id}, then we are guaranteed that π is indeed the superior permutation. We can also bound $\int_{a_2}^{b_2} e^{-x_2}G(x_2)\,dx_2$ from below by bounding the functions e^{-x_2} and $G(x_2)$ from below individually with piecewise linear functions, namely tangent lines, and then taking their product, which is merely a piecewise quadratic function.

We now conclude this section, as we have all the machinery required to improve the upper bound of β_2 via repeated integration over a large collection of disjoint boxes B. The following section addresses how to determine these boxes and to address any remaining numerical error.

4 Numerical experiments

Recall that the entirety of our analysis consists of bounding the right-hand side of (4). Section 3 describes how to bound the integral over $\mathcal{D}$, by accumulating improvements over a large collection of disjoint boxes B. We furthermore must specify h and k, which for this paper we chose to set $h = \sqrt{3}$ as in the original paper [5] and $k = 4$, as we found that higher values of k required too much additional computing power. Per Remarks 6 and 7, when numerical integration was required (albeit in one dimension only!), we chose (somewhat arbitrarily) to use approximations consisting of 100 piecewise linear components.

4.1 Constructing B with a decision tree

A natural technique for finding many boxes B as in Section 3 is to use a decision tree applied to a Monte Carlo simulation. More specifically, we draw a large number N of samples from the set

$$\mathcal{D} = \{(x_1, \ldots, x_k), (u_0, \ldots, u_k) : 0 \leq x_1 \leq \cdots \leq x_k \, , \, 0 \leq u_i \leq 1\}$$

with independent uniform distributions on the u_i's and the distribution from Lemma 3 for the x_i's. Then, we determine which of the $(k-1)!$ permutations is optimal for each sample, and label that sample with that permutation as an outcome. Thus, at the end of the process, we have N points in $\mathcal{D}$, each of which is labelled with one of $(k-1)!$ categorical outcomes.

Given these N samples, together with their categorical outcomes, we train a decision tree to predict the outcome as a function of the $2k + 1$ coordinates of the N samples. Recall that the leaves of a decision tree are precisely a disjoint collection of boxes, and are in fact a partition of the search space, and are thus suitable for use as a collection of boxes for our bounds. After training our decision tree (using cross entropy to determine splitting thresholds), we obtain a partition of $\mathbb{R}^{2k+1}$ induced by the leaves of the tree.

The last step in this process is to note that the leaves of the tree do indeed induce a partition of $\mathbb{R}^{2k+1}$ into boxes, but those boxes that intersect the boundary of $\mathcal{D}$ are not usable by our procedure since $\mathcal{D}$ is not rectangular. For any box B such that $B \cap \mathcal{D}$ and $B \setminus \mathcal{D}$ are non-empty, we can find the largest-volume box B' such that $B' \subset B \cap \mathcal{D}$ via convex optimization (specifically, a logarithmic transform on the product term used to compute the volume of a box).

4.2 Results

Setting $k = 4$ and $h = \sqrt{3}$, we ran 20 instances each for $N \in \{10^3, 10^4, 10^5, 10^6, 10^7\}$, and a single instance for $N \in \{3 \cdot 10^7, 5 \cdot 10^7, 7.5 \cdot 10^7\}$. Our experiments for the larger instances were conducted on an Intel Xeon E5-2640 v3, 2.60 GHz CPUs with 59 GB memory per node, supported by USC Center for Advanced Research Computing (CARC). The rest of our experiments were done on a personal computer with Apple M1 chip, 8 cores and 8GB memory. In order to avoid any possibility of floating point error, we used the Python package mpmath [18], which uses variable-precision interval arithmetic. Table 1 shows how we achieve better upper bounds of β_2 as the sample size N increases, thus proving Theorem 2. For reproducibility, our source code is available at [34].

As an aside, Figure 4 illustrates how the selection of different h would affect β_{UB}^{new}. Fixing $k = 4$ and $N = 10^7$, we ran 10 instances each for $h^2 = 2, 2.25, 2.5, 2.75, 3, 3.25, 3.5, 3.75, 4, 4.25, 4.5$. Computational results show that the

N	Upper bound of β_2
10^3	0.921042
10^4	0.91995
10^5	0.9169
10^6	0.91172
10^7	0.90577
$3 \cdot 10^7$	0.90387
$5 \cdot 10^7$	0.90317
$\mathbf{7.5 \cdot 10^7}$	**0.90304**

Table 1: The best upper bounds of β_2 obtained by our method, for increasing values of N. The best upper bound $\beta < 0.90304$ is highlighted.

original selection $h = \sqrt{3}$ still gives us the best upper bound under our current scheme of selecting boxes B, which we find surprising, though it does not eliminate the potential of choosing alternative h.

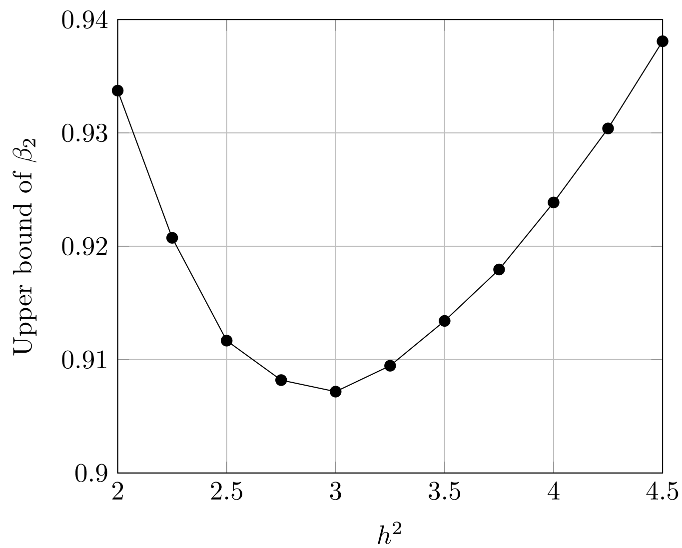


Figure 4: New upper bounds as h changes, for $k = 4$ and $N = 10^7$.

5 Conclusions and future work

We have proven that $\beta_2 < 0.90304$, although it is clear that the bound can be improved by additional computing power. Our approach also suggests extensions to improve estimates for the corresponding constants β_d for TSPs having higher dimension $d > 2$, although these constants appear less frequently in the literature. Our approach is also applicable (with much simpler antiderivative expressions) to bound constants for, say, the Manhattan metric, though these also do not appear to be the subject of much interest.

As a final future direction, we note that [13] improved the lower bound of β_2 partially based on the arguments put forth in [27]. We also suggest an alternative direction for improving the lower bound, although it appears computationally intractable at present.

We first let L_k be a random variable representing the length of a TSP tour of k points uniformly distributed in the unit square, but with the additional feature that all distance traversed along the boundary is free (thus, L_k is a lower bound of the true TSP tour). We can write

$$\ell_k := \mathbb{E}L_k = \int_0^1 \cdots \int_0^1 \min_{\pi \in \Pi_k} \sum_{i=1}^{k} d(x_{\pi(i)}, x_{\pi(j)})\, dV\,,$$

where $d(x_i, x_j)$ denotes the shortest distance between x_i and x_j, possibly utilizing the boundary. The integral is the minimum of convex functions, and can therefore be bounded below by taking a (very large) collection of tangent planes. One could also apply the same techniques as in our paper and find boxes in which certain permutations are known to be optimal everywhere, and then apply Lemma 4.

To see how this helps us, now assume that n points $\mathscr{X} = \{X_1, \ldots, X_n\}$ are independently and uniformly sampled in the unit square, and divide the square into n/k square cells C_i. A lower bound of the TSP tour length of all n points is the *rooted dual* [25], also known as the *boundary functional* [35], which consists of modifying the distance matrix between points X_i so that there is no cost incurred when travelling along the boundary of any of the square cells (as opposed to the boundary of the unit square as we just did). We write this as TSP_0, so that we have

$$\mathsf{TSP}(\mathscr{X}) \geq \sum_{i=1}^{n/k} \mathsf{TSP}_0(\mathscr{X} \cap C_i)\,.$$

However, we note that if we have $|\mathscr{X} \cap C_i| = k$, then the entries $\mathsf{TSP}_0(\mathscr{X} \cap C_i)$ follow the same distribution as the L_k's, scaled by a factor of $\sqrt{k/n}$. Furthermore, for large n, the number of points in each cell C_i follows a Poisson distribution with mean k, and hence

$$\beta_2 \geq \frac{1}{\sqrt{n}} \mathbb{E} \sum_{i=1}^{n/k} \mathsf{TSP}_0(\mathscr{X} \cap C_i) = \frac{1}{\sqrt{n}} \cdot \frac{n}{k} \sum_{i=1}^{\infty} \sqrt{\frac{k}{n}} \Pr(Z = i) \ell_i = \frac{e^{-k}}{\sqrt{k}} \sum_{i=1}^{\infty} \frac{k^i}{i!} \ell_i\,,$$

where Z is a Poisson random variable with mean k. We can therefore improve estimates of β_2 by lower bounding as many terms ℓ_i as computing power permits, and using simpler analytic lower bounds such as nearest-neighbor distances for $i \to \infty$.

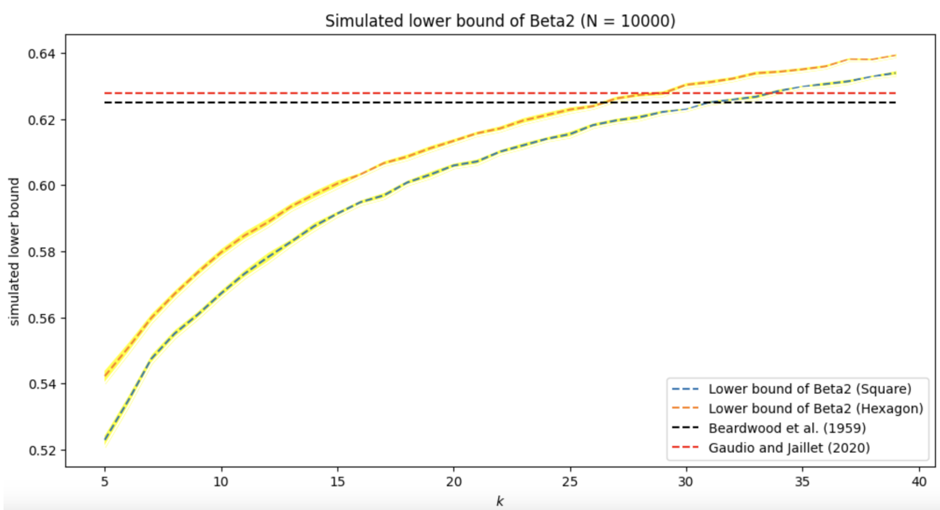


Figure 5: Simulated lower bound of β_2

Figure 5 demonstrates how different Poisson means k would affect the expected lower bound of β_2, which we denote as β_{LB}^{sim} (these are not true lower bounds, merely Monte Carlo estimates). We ran 10000 instances each for $5 \leq k \leq 39$ and computed sample averages to estimate the ℓ_i's. Computational results show that when k increases,

β_{LB}^{sim} also increases as would be expected. The yellow region represents the 95% confidence interval of the average lower bound of β_2, which shows that it takes around $k = 29$ to surpass the best known lower bound from [13]. This is likely beyond the reach of current computing limits, but we include it for posterity.

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