1. INTRODUCTION

1.1. Chief Goals

This monograph concerns the study of the lengths of graphs on random vertex sets in Euclidean space $\mathbb{R}^d$, $d \geq 2$. We are interested primarily in the lengths of those graphs representing the solutions to problems in Euclidean combinatorial optimization.

This work was originally motivated by a desire to understand the asymptotics of the solutions of the classic problems of Euclidean combinatorial optimization, including the well-known traveling salesman problem. Later, as the tools and methods were refined and generalized, it was realized that the approach was general enough to describe the behavior of a variety of Euclidean graphs, including random tessellations, triangulations, and geometric location problems. We will limit our discussion to the lengths of some of the better known Euclidean graphs, particularly those occurring naturally in combinatorial optimization, computational geometry, and operations research. We expect that the methods and approach here can be used to treat other Euclidean graphs.

Within combinatorial optimization, there are several graphs which are of central importance. Many problems in combinatorial optimization involve the construction of the shortest possible network of some kind; we will be interested in the total edge length of these networks. Typical problems include the following ones, which, for the sake of brevity, are stated here in only an informal manner. Here V is a *random* vertex set in Euclidean space.

(i) Traveling Salesman Problem (TSP). Find the length of the shortest closed path traversing each vertex in V exactly once.

(ii) Minimum Spanning Tree (MST). Find the minimal total edge length of a spanning tree through V.

(iii) Minimal Euclidean Matching. Find the minimal total edge length of a Euclidean matching of points in V.

These three archetypical problems are central to combinatorial optimization and operations research. Precise statements of these problems appear at the end of the chapter.

Within computational geometry, we are motivated by the following problems.

(i) Find the total edge length of the Voronoi and Delaunay tessellations of V.

(ii) Find the length of the k nearest neighbors graph on V.

The graphs defined by these problems are not only useful in the theory of Euclidean optimization (Preparata and Shamos, 1985), but they are also of widespread interest in the natural and social sciences (Okabe et al., 1992).

Within the theory of minimal surfaces, optimization problems involve lengths of graphs and, more generally, areas of surfaces. In two dimensions one such problem involves minimizing the sum of the lengths of the edges in a triangulation of V; in three dimensions the analogous problem involves minimizing the sum of the areas of the faces of a tetrahedralization of V.

Our central goal is to develop a general unifying approach which describes the stochastic behavior of the total edge length of a variety of graphs, including the above mentioned ones. This is the main focus of the monograph. Considerable effort has gone into understanding the total edge length behavior of Euclidean graphs; however, up until now different problems have relied upon different approaches. We formulate a single approach which is simple and yet general enough to treat a variety of graphs arising in diverse areas. The approach contains known results as special cases and also opens up the way to proving new results.

We have two secondary goals. The first is to provide an overview of recent progress and to review related work. We will not present a complete history of the subject but will emphasize that work which is most relevant. We also indicate to the researcher some of the main unsettled problems in the field.

The second goal is to provide a set of tools which should be useful for future endeavors. Chief among these tools is the combined use of geometric subadditivity and superadditivity. Although subadditive methods have been used since the seminal work of Beardwood, Halton, and Hammersley (1959), superadditivity has not been explicitly used before. What is new here and what is not well recognized, is that most graphs having a subadditive structure admit canonical modifications, called boundary graphs, which possess an intrinsic superadditive structure. This insight can be put to good use and serves as the starting point towards deepening our understanding of total edge lengths of Euclidean graphs. Boundary graphs provide the key conceptual and technical tool of this monograph. They allow us to systematically and simultaneously exploit the inherent subadditivity and superadditivity of many Euclidean graphs. The combined use of subadditivity and superadditivity yields *two-sided additivity* and this forms the core of our approach.

Although the main new tool is the use of boundary graphs, there are other tools as well. One such tool is isoperimetry, developed by Talagrand (1995, 1996a, 1996b) and Rhee (1993b). Isoperimetry has already been recognized for its mathematical depth and breadth and it comes as no surprise that it finds applications in our subject. Indeed, Talagrand (1995) and Steele (1997) have showed that isoperimetric methods are germane to several problems of geometric probability.

1.2. A Brief History

We now consider the background of our subject, sketch its historical development, and review recent progress. Much of the probability theory of combinatorial optimization has been heavily influenced by the work of Steele.

Beardwood, Halton, and Hammersley (1959) proved the following celebrated result, which serves as a starting point for Steele's work as well as for this monograph:

Theorem 1.1. *Let $X_i,\ i \geq 1,$ be independent and identically distributed random variables with values in the unit cube $[0,1]^d,\ d \geq 2$. Let $T(X_1,...,X_n)$ denote the length of the shortest tour through $X_1,...,X_n$. Then with probability one*

$$\lim_{n\to\infty} T(X_1,...,X_n)/n^{(d-1)/d} = \alpha(d)\int_{[0,1]^d} f(x)^{(d-1)/d}, \tag{1.1}$$

where f is the density of the absolutely continuous part of the law of X_1 and $\alpha(d)$ is a positive constant which depends only on d.

Beardwood, Halton, and Hammersley (1959) recognized that the methods used to prove Theorem 1.1 had the potential to treat various problems. They indicated that Theorem 1.1 holds for the minimal spanning tree and Steiner minimal spanning tree problems, but did not explicitly develop the limit theory. They also conjectured that their approach could be useful in the probabilistic versions of Plateau's problem, Douglas's problem, and other problems in minimal surfaces. *A central goal of this monograph is to show through simple and general methods that an unexpectedly large number of problems in Euclidean combinatorial optimization and computational geometry have solutions satisfying the limit law (1.1).*

The elegant limit law (1.1) has several implications. Jensen's inequality shows that the right side of (1.1) is largest when f is the density of the uniform distribution. Hence non-uniformity in the distribution of X will tend to decrease the total tour length $T(X_1,...,X_n)$. Also, since every probability distribution is the sum of a singular and a continuous component, the singular component of a probability distribution contributes nothing to the limit in (1.1). As pointed out by Beardwood, Halton, and Hammersley (1959), it represents the extreme case of non-uniformity.

Simple scaling arguments show that Theorem 1.1 holds if the unit cube is replaced by an arbitrary compact subset K of $\mathbb{R}^d$. In particular if $X_i,\ i \geq 1,$ are independent and identically distributed (i.i.d.) random variables with the uniform distribution on a set K of Lebesgue measure one, then the limit in (1.1) exists and equals $\alpha(d)$ almost surely (a.s.). In other words, we find the rather surprising result that the limit is independent of the shape of the compact set K. In the sequel we will review the numerical estimates for the constant $\alpha(d)$.

The landmark work of Beardwood, Halton, and Hammersley (1959) stood virtually by itself for over fifteen years. In an unrelated effort, Miles (1970) showed that the mean total edge lengths of planar tessellations, including the Voronoi and Delaunay tessellations, satisfy the limit law (1.1). Moreover, he explicitly computed values for the limiting constants. However, his results are limited to the homogeneous planar Poisson point process and do not approach (1.1) in generality.

Several years later Karp recognized that the a.s. asymptotics (1.1) could be used to deepen our understanding of the approximate algorithmic solutions to the TSP. In his seminal work, Karp (1976,1977) introduced for all $\epsilon > 0$ a partitioning heuristic for the TSP which runs in polynomial time and with probability one yields a tour whose length is within a factor of $1 + \epsilon$ of the minimal tour length. In this way he was the first to show that the stochastic version of an NP-complete problem a.s. has a polynomial time algorithm yielding a nearly optimal solution.

Soon after Karp's deep results, Papadimitriou (1978a) recognized that the proof of Theorem 1.1 could be modified to show a similar result for the minimal matching problem, at least in dimension $d = 2$. More generally, he showed that if a functional L satisfies four key combinatorial conditions then it also satisfies the asymptotics (1.1). Two of these conditions, subadditivity and superadditivity, foreshadow the approach taken here.

Steele (1981a) also approached the subject from a general point of view. He abstracted the properties used in the proof of Theorem 1.1 and laid out a set of sufficient conditions guaranteeing that a large class of functionals, termed Euclidean functionals, satisfy the asymptotics (1.1). Steele's conditions involve geometric subadditivity, scaling, monotonicity, and translation invariance and he recognized that they form the key ingredients to the proof of Theorem 1.1. Using these abstract properties, Steele (1981a) proved a general result and deduced Theorem 1.1 as a corollary. He also showed via this general result that the length of the Steiner minimal spanning tree satisfies (1.1).

Steele's (1981a) classic paper opened the way for further research and soon it was shown that several other problems in combinatorial optimization enjoyed asymptotics similar to (1.1). Most of the effort however was confined to the study of problems on uniform samples, which, while certainly the most interesting case, does not tell the whole story. In the uniform setting Steele (1982) showed that a version of the minimal triangulation problem satisfies (1.1). Later, Steele (1988) explicitly showed that the length of the minimal spanning tree satisfies (1.1); Steele's work covers the case of power-weighted edges as well.

Steele's work was followed by several similar results. Avis, Davis, and Steele (1988) showed that the greedy matching heuristic satisfies the asymptotics (1.1). Talagrand (1991) showed that in the case of uniform random variables, (1.1) holds for the directed TSP, a modification of the usual TSP where edges are assigned directions according to an independent coin-tossing scheme. Goemans and Bertsimas (1991) employed Steele's general approach to show that (1.1) holds for the Held-Karp relaxation of the TSP. Later, Steele (1992) showed that the limit (1.1) holds for the semi-matching problem.

Several related results followed. Jaillet (1992), guided by the general abstract properties put forth by Steele, found suboptimal rates of convergence in (1.1). Rhee (1993) showed that the limit (1.1) could be strengthened to complete convergence for many optimization problems, including the minimal matching problem. Alexander (1994) discovered an approach which yields rates of convergence for the archetypical problems of combinatorial optimization. His rates are optimal in some cases.

These research efforts collectively suggest that (1.1) is a special case of a general "umbrella theorem" which includes the above results as special cases. As already indicated, our main goal is to show that this is indeed so. Our umbrella result opens the door for proving limit theorems for a variety of graphs. The methods used to prove this general "umbrella theorem" provide asymptotics for the lengths of graphs on arbitrary sequences of i.i.d. random variables. The methods also give rates of convergence.

1.3. Methods

Optimization problems and related problems involving lengths of graphs have been customarily viewed as functionals defined on point sets in Euclidean space. This approach is traditional and not unnatural. However, it is also useful to view these problems as functionals defined on *pairs* (F, R), where F is a point set in $\mathbb{R}^d$ and R is a d-dimensional rectangle in $\mathbb{R}^d$. Thus it will be useful to write, for example, $T(F, R)$ for the functional denoting the shortest tour through the set $F \cap R$.

This viewpoint helps identify the intrinsic similarities of optimization problems, especially geometric subadditivity, geometric superadditivity, ergodicity, translation invariance, and scaling. When considered as functionals on pairs (F, R), many optimization problems become superadditive functionals over the collection of d-dimensional rectangles. We use superadditivity to capture ergodicity. This is done by drawing upon a multiparameter version of Kingman's famous subadditive ergodic theorem.

One of our central ideas is that many problems in combinatorial optimization and computational geometry are not only subadditive, but admit simple and natural modifications having a superadditive structure. These modifications are found by examining the "boundary problem" or "boundary functional", an idea articulated in Redmond's (1993) thesis. It is easily seen and well-known that many optimization problems and problems in graph theory suffer from boundary effects. This peculiarity is an annoying irritant at best. At worst, it can lead to nearly insurmountable technical and conceptual difficulties. It is somewhat of an irony that it is precisely the peculiar boundary behavior which produces the coveted superadditive structure.

Roughly speaking, if the functional $L(F, R)$ denotes the length of a graph on a vertex set $F \subset R$, then the boundary functional $L_B(F, R)$ will denote the canonical functional associated with $L(F, R)$ which treats the boundary of R as a single point. Edges in the graph given by $L_B(F, R)$ which lie on the boundary of R are assigned zero length. In the case of the TSP functional, this means that travel along the boundary is "free". This simple idea leads to the valuable superadditive relation

$$L_B(F \cap (R_1 \cup R_2), R_1 \cup R_2) \geq L_B(F \cap R_1, R_1) + L_B(F \cap R_2, R_2)$$

which holds for all disjoint rectangles R_1 and R_2 whose union is a rectangle. Superadditive relations for L_B, coupled with subadditive relations for L, lead to two-sided additivity estimates for L. This monograph will explore the multiple benefits of two-sided additivity.

Boundary functionals L_B have a second crucial property which lies at the heart of our approach: the boundary functional L_B is "close" to the standard functional L. "Close" essentially means that the a.s. stochastic behavior of L is governed by that of L_B. Thus, to determine the stochastic behavior of L on point sets of large cardinality, it is usually easier to understand the stochastic behavior of the canonical boundary functional L_B and then use the closeness of L and L_B to capture the stochastic behavior of L.

Boundary problems and boundary functionals are essential tools, but they are not the only ones. Other tools involve isoperimetric methods, which are often more powerful than martingale methods. In particular, the Rhee and Talagrand isoperimetric inequalities have considerably furthered our understanding of the lengths of graphs. Their work, described in Chapter 6, essentially shows that the a.s. behavior of optimization functionals is governed by the behavior of the mean of the functional. Thus, to prove a.s. limit theorems for optimization functionals, it will be enough to prove limit results for the *mean* of the functionals. This observation dramatically simplifies the proofs.

There are several contributions provided by the general approach taken here:

(i) We provide a set of theorems which unifies probabilistic limit results for solutions to problems in optimization and computational geometry. The approach contains the classic asymptotic results and it also furnishes asymptotics for related problems in geometric probability, thereby generalizing and extending (1.1).

(ii) The level of generality of our main results includes the case of graphs with power-weighted edges. It also treats the case of vertex sets with unbounded support.

(iii) We use the intrinsic superadditivity of boundary functionals to find rates of convergence in (1.1) in a simple and natural way.

(iv) Limit results hold in the sense of complete convergence, which is stronger than a.s. convergence and which is necessary for some problems of model generation.

(v) We use boundary functionals to formulate large deviation results for the total edge lengths of graphs.

There are other benefits to the approach taken here. We recall that Karp (1976, 1977) introduced a partitioning heuristic for the TSP which runs in polynomial time and which a.s. yields a tour whose length is within a factor of $1 + \epsilon$ of the minimal tour length. We will generalize and extend Karp's result in the following way: given an optimization functional L, we will show that boundary functionals help analyze the performance of partitioning heuristics L_H which are analogous to Karp's partitioning heuristic and which approximate L to within a factor of $1 + \epsilon$.

There is a final benefit to our approach. Our motivation for considering boundary functionals came from a desire to better understand the stochastic behavior of the classic Euclidean optimization problems. It is a pleasant surprise that boundary functionals are useful in the *deterministic* setting as well. More precisely, boundary functionals are a natural tool in the study of the *worst case* values of problems in combinatorial optimization and operations research. The worst case value of L, denoted by $L(n)$, is the largest value of $L(V)$, where V ranges over all subsets of $[0, 1]^d$ of size n. Worst case versions of L are purely deterministic objects and it is somewhat surprising that they may be successfully analyzed using the approach developed for the stochastic analysis. We will see in Chapter 11 that the asymptotic behavior of the worst case versions parallels that of the stochastic versions.

1.4. Definitions

We recall the formal definitions of some of the classic problems of combinatorial optimization. The first several chapters use these concrete problems to illustrate the general theory. We emphasize that the general theory applies to a large variety of problems in geometric probability, including those motivated by problems in operations research and computational geometry. Some of these applications are explored in Chapters 8, 9, 10, and 11.

Our three-part definition begins with the problem of finding the shortest tour through a vertex set. This is perhaps the most famous problem of combinatorial optimization. Throughout $V := \{x_1, ..., x_n\} \subset \mathbb{R}^d,\ d \geq 2$.

Definition 1.2.

(a) (Traveling salesman problem; TSP) A closed tour or closed Hamiltonian tour is a closed path traversing each vertex in V exactly once. For all $p > 0$, let $T^p(V)$ be the length of the shortest closed tour T on V with pth power weighted edges. Thus

$$T^p(V) := \min_T \sum_{e \in T} |e|^p,$$

where the minimum is over all tours T and where $|e|$ denotes the Euclidean edge length of the edge e. Thus,

$$T^p(V) := \min_\sigma \left\{ \|x_{\sigma(n)} - x_{\sigma(1)}\|^p + \sum_{i=1}^{n-1} \|x_{\sigma(i)} - x_{\sigma(i+1)}\|^p \right\},$$

where the minimum is taken over all permutations σ of the integers $1, 2, ..., n$. $T^1(V)$ is the length of the classic traveling salesman tour on V.

(b) (Minimum spanning tree; MST) For all $p > 0$, let $M^p(V)$ be the length of the shortest spanning tree on V with pth power weighted edges, namely

$$M^p(V) := \min_T \sum_{e \in T} |e|^p,$$

where the minimum is over all spanning trees T of the vertex set V.

(c) (Minimal matching) For all $p > 0$, the minimal matching on V with pth power weighted edges has length given by

$$S^p(V) := \min_\sigma \sum_{i=1}^{n/2} \|x_{\sigma(2i-1)} - x_{\sigma(2i)}\|^p,$$

where the minimum is over all permutations of the integers $1, 2, ..., n$. If n has odd parity, then the minimal matching on V is the minimum of the minimal matchings on the n distinct subsets of V of size $n - 1$.

The above definition tells us that T^p, M^p, and S^p represent the canonical length functionals associated with the graphs given by the TSP, MST, and minimal matching problems, respectively. Definition 1.2 considers problems of combinatorial optimization which are more general than the classic ones which restrict attention to the case $p = 1$. The case of power-weighted edges ($p > 1$) is not studied as much as the linear case $p = 1$. The approach taken here treats the general case with no additional work and so we have deliberately chosen to work with these general definitions.

Terminology, Notes, and References

(i) When $p = 1$ we will abbreviate notation and write $T(V)$ for $T^1(V)$ with similar meanings for $M(V)$ and $S(V)$.

(ii) $\mathcal{F} := \mathcal{F}(d)$ denotes the finite subsets of $\mathbb{R}^d$ and $\mathcal{R} := \mathcal{R}(d)$ denotes the d-dimensional rectangles of $\mathbb{R}^d$. These are sets of the form $[x_1, y_1] \times [x_2, y_2] \times ... \times [x_n, y_n]$, where $x_i, y_i \in [-\infty, \infty]$.

(iii) Throughout we use the symbol C to denote a constant which may depend on d and p and whose value may vary at each occurrence.

(iv) The Euclidean TSP problem is NP-complete (see e.g. Garey and Johnson (1979)) and there is no known algorithm for solving the TSP in a time which grows polynomially with the size of the vertex set. On the other hand, to solve the MST problem $M^p(V)$, a greedy algorithm (join the nearest two points with an edge, then the next pair of nearest points, and so on, being sure not to form a circuit) will work in polynomial time. We refer to Kruskal (1956), Prim (1957), and Borůvka (1926).

Among the many methods for finding the length $S^1(V)$ of a Euclidean minimal matching, Edmond's (1965) algorithm is probably the best known. Its running time, while not optimal, is of the order of $(\text{card}(V))^3$. Tarjan (1983) has a fine exposition of algorithms for optimization problems.

(v) It is well-known that combinatorial optimization problems can be formulated as problems in statistical mechanics. See e.g. Mézard, Parisi, and Virasoro (1987). Minimal matchings occur naturally in statistical mechanics. Finding the ground state energy of Ising models is equivalent to finding a spin configuration which minimizes the Hamiltonian of the system. This amounts to finding a minimum matching between the so-called frustrated plaquettes (the weights may not be Euclidean and therefore may not satisfy the triangle inequality). See Bieche et al. (1980) and Barahona et al. (1982).