Asymptotic theory of greedy approximations to minimal K-point random graphs

Alfred O. Hero and Olivier Michel

COMMUNICATIONS & SIGNAL PROCESSING LABORATORY
Department of Electrical Engineering and Computer Science
The University of Michigan
Ann Arbor, MI 48109-2122

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Abstract— **Let $\mathcal{X}_n = \{x_1, \ldots, x_n\}$, be an i.i.d. sample having multivariate distribution P on $[0,1]^d$. We derive a.s. limits for the power weighted edge weight function of greedy approximations to a class of minimal graphs spanning k of the n samples. The class includes all minimal k-point graphs constructed by the potential function partitioning method of Ravi, Sundaram, Marathe, Rosenkrantz and Ravi [1] where the edge weight function satisfies the quasi-additive property of Redmond and Yukich [2]. This includes greedy approximations to the k-point minimal spanning tree (k-MST), Steiner tree (k-ST), and the traveling salesman problem (k-TSP). An expression for the influence curve (IC) of the minimal weight function is given which characterizes sensitivity of the greedy algorithm to small perturbations in the underlying distribution. The form of the IC indicates that the weight function has robustness properties in $\mathbb{R}^d$ which are analogous to those of rank order statistics in one dimension. We also show that the log of the minimum weight function is a robust estimator of the Rényi entropy of order ν, where $\nu \in (0,1)$ is a function of the sample space dimension and the edge weight power exponent.**

I. Introduction

Assume that we are given a set $\mathcal{X}_n = \{x_1, \ldots, x_n\}$ of n points in $\mathbb{R}^d$. Fix k and denote by $\mathcal{X}_{n,k}$ a k-point subset of $\mathcal{X}_n$, $0 < k \leq n$. The elements of the subset $\mathcal{X}_{n,k}$ are distinct and there are $\binom{n}{k}$ possible k-point subsets of $\mathcal{X}_n$. The minimal k-point Euclidean graph problem is to find the subset of points $\mathcal{X}_{n,k}$ and the set of edges connecting these points such that the resultant graph has minimum total weight $L(\mathcal{X}_{n,k})$. This problem arises in competitive bidding for network routing contracts when some nodes may be left out of the connected network, the traveling salesman problem for visiting at least k out of n cities, and other combinatorial optimization problems.

For example, the Euclidean *minimal k-point spanning tree* (k-MST) is the minimum weight tree spanning any k of the points. As pointed out in Eppstein [3] the planar k-MST problem was shown to be NP-complete by Zelikovsky and Lozevanu [4] and Ravi, Sundaram, Marathe, Rosenkrantz and Ravi [1]. Ravi etal proposed a polynomial time approximation algorithm for the planar k-MST with approximation ratio $O(k^{1/4})$ which has been successively improved to $O(\log(k))$ by Garg and Hochbaum [5], $O(\log(k)/\log\log(n)$ by Eppstein [3], $O(1)$ by Blum, Chalasani and Vempala [6], $2\sqrt{2}$ by Mitchell [7], 3 by Garg [8], and $1+\epsilon$ by Arora [9]. Arora has recently obtained a linear time $1+\epsilon$ algorithm for multi-dimensional k-point TSP, MST and Steiner problems [10].

In this paper we derive a.s. limits for the power weighted edge weight function of greedy approximations to a class of minimal graphs spanning k of the n samples. The class includes all minimal k-point graphs constructed by the potential function partitioning method of Ravi, Sundaram, Marathe, Rosenkrantz and Ravi [1] where the edge weight function satisfies the quasi-additive property of Redmond and Yukich [2].

A direct result of the asymptotics of the minimal k-point weight function is that the log of the minimum weight function is a strongly consistent and robust estimator of the Rényi entropy of order ν of P, where $\nu \in (0,1)$ is a function of the sample space dimension and the edge weight power exponent. Entropy estimation has been of interest for pattern analysis, process complexity assessment, model identification, tests of distributions, and other applications where invariance to scale, translation and other invertible transformations is desired in the discriminant [11], [12], [13]. Another application is in vector quantization where Rényi entropy is related to asymptotic quantizer distortion via the Panter-Dite factor and Bennett's integral [14], [15]. Possible applications of our results include: estimation of Lyapounov exponents in non-linear models [16], [17], multi-modality image registration using mutual information matching criteria [18], stopping criteria for regression and classification trees [19], and other general entropy estimation problems [20], [11]

The principal results presented here are as follows:

1. A polynomial time greedy algorithm for constructing an approximation to the minimal k-point graph and its edge weight function is presented which is a direct generalization of the algorithm of Ravi, Sundaram, Marathe, Rosenkrantz and Ravi [1] developed therein for minimal k-point minimum spanning tree approximation on the plane.
2. A tight a.s. asymptotic bound on the entropy estimation error is given which can be used to determine the required partition resolution to obtain a prescribed estimator error when a bound on the total variation of the density function is known.
3. Zero asymptotic error is achieved when the density function is piecewise constant over the resolution $1/m$ partition cells of the greedy algorithm.
4. We give a condition, called a tightly coverable graph property, which holds when $k+o(k)$ of the vertices of the k-point graph can be covered by a resolution $1/m$ partition set (a.s.) as $k \to \infty$. This condition is satisfied for the greedy approximation by its construction. If the exact minimal k-point graph satisfies this condition then the weight of the mini-

[1]Alfred Hero is with the University of Michigan at Ann Arbor, MI 48109-2122 (hero@eecs.umich.edu), and Olivier Michel is with the Ecole Normale Superieure, Lyon cedex 07, France (omichel@ens-lyon.fr). This research was supported in part by AFOSR grant F49620-97-0028.

mal k-point graph converges to the same asymptotic limit as the greedy approximation, i.e. the greedy approximation is asymptotically optimal.
5. A robust Rényi entropy estimator is proposed based on the log of the weight of the minimal k-point graph with edge weight exponent γ. This estimator is shown to converge a.s. to a conditional Rényi entropy of order $\nu = (d-\gamma)/d \in (0,1)$, where $d > \gamma$ is the sample space dimension. Inspired by the convergence rates established in [21], for $\nu \leq 1/d$ we predict that the rate of convergence of the Rényi entropy estimator is equal to $1/\sqrt{n}$. This would make our estimator competitive with standard histogram estimation techniques of entropy estimation.
6. Influence curves studies are presented which quantitatively establish that the greedy minimal k-point graph construction generates a robust estimator of distribution entropy.
7. The influence curve study provides a threshold rule on the graph's edge weight function which can be applied to select an optimal threshold proportional number of points $(n-k)/n = 1-\alpha$. This threshold specifies the number of points which should be rejected from the sample to achieve maximum outlier rejection rate while preserving inliers.
8. The asymptotic results presented hold for a very general class of graphs constructed by minimizing an edge weight function which is a quasi-additive functional. This class includes the optimal Euclidean traveling salesman tour, the minimal spanning tree, the Steiner tree, and the two population minimal matching graph.

The outline of the paper is as follows. In Section II-A we review Euclidean minimal spanning graphs, including those arising from the solution of the traveling salesman problem, the minimal spanning tree, and the Steiner tree. In Section II-B we review the theory of quasi-additive functionals which were used by Redmond and Yukich to prove a general asymptotic theorem on the edge weight function of minimal spanning graphs. A minimal k-point graph is defined in Section III and in Section III-A we give a lemma giving a partition approximation for such graphs which satisfy a tightly coverable property. Then in Section IV we treat the asymptotic theory of greedy approximations with a series of lemmas and convergence results. This is followed in Section VII by a study of quantitative robustness of the greedy approximation via the influence function.

II. Background

Assume that $\mathcal{X}_n = \{x_1, \ldots, x_n\}$ is a realization of n i.i.d. random vectors where each x_k takes values in $\mathbb{R}^d$ and has distribution P with Lebesgue density f. Additional smoothness assumptions on f will be required and will be given in the sequel. To simplify certain mathematical technicalities we will assume that the distribution is supported on the unit cube $[0,1]^d$. Any finitely supported distribution can be mapped to this domain by invertible linear transformation. Although we do not prove it, the restriction to finite support can undoubtedly be relaxed for densities satisfying the tail decay bounds of [22].

A. Minimal Euclidean Graphs

An n-point (Euclidean) undirected graph G is defined by a set of vertices $\mathcal{X} = \{x_1, \ldots, x_n\}$ and a set of edges $\mathcal{E} = \{e_{ij}\}$, where each edge $e_{ij} = (x_i, x_j)$ connects a pair of vertices x_i, x_j. If for two vertices x and y a graph G has a sequence of edges $(x, x_{j_1}), (x_{j_1}, x_{j_2}), \ldots, (x_{j_p}, y)$ then G is said to contain a path from x to y. A graph is said to be connected if there exists a path between any pair of its vertices. If there exists a sequence of distinct edges which provide a path from any vertex back to itself the graph is said to contain a cycle. A graph which contains no cycles is an acyclic graph called a tree. By the span of a graph we mean the set of vertices which are connected by edges. The degree of a graph is the maximum number of edges which can be incident on any single vertex. The complete graph over $\mathcal{X}_n = \{x_1, \ldots, x_n\}$ is a graph for which each pair of vertices are connected by an edge; such a graph has $\binom{n}{2}$ edges, is connected, has cycles, and is of degree n.

Different graphs can be compared based on their weights which are defined as follows. If $x = [[x]_1, \ldots, [x]_d]^T$ and $y = [[y]_1, \ldots, [y]_d]^T$ are two vertices connected by an edge e we denote by $|e|$ the Euclidean length $\|x-y\| = \sqrt{\sum_{k=1}^d ([x]_k - [y]_k)^2}$ of the edge. Let ψ be an edge weight function which satisfies $\psi(|e|) \geq 0$. The total weight $L(\mathcal{X})$ of of a graph G with edges $\{e\}$ and vertices $\mathcal{X}$ is defined as the sum of the edge weights

$$L_G(\mathcal{X}) = \sum_{e \in G} \psi(|e|). \tag{1}$$

While as in [23] the results of this paper might be extended to general weight functions which satisfy $\psi(|e|) \sim O(|e|^\gamma)$ as $|e|$ approaches 0, we will restrict our attention to the case of "power weighted edges" of exponential order γ

$$\psi(|e|) = |e|^\gamma, \qquad 0 < \gamma < d. \tag{2}$$

A.1 Euclidean Traveling Salesman Problem

In the Euclidean traveling salesman (TSP) problem the objective is to find a graph of minimum weight among those that visit each point in $\mathcal{X}_n = \{x_1, \ldots, x_n\}$ exactly once. The resultant graph is called the *minimal TSP tour*. This problem is NP-hard and arises in many different areas of operations research [24]. Let $\mathcal{T}(\mathcal{X}_n)$ denote the possible sets of edges in the class graphs of degree 2 which span $\mathcal{X}_n$. The weight of the minimal TSP tour is specified by

$$L_{\text{TSP}}(\mathcal{X}_n) = \min_{\mathcal{T}(\mathcal{X}_n)} \sum_{e \in \mathcal{T}(\mathcal{X}_n)} |e|^\gamma.$$

A.2 Euclidean Minimal Spanning Tree Problem

In the Euclidean minimal spanning tree (MST) problem the objective is to find a graph of minimum weight which spans nodes $\mathcal{X}_n = \{x_1, \ldots, x_n\}$. This problem admits exact solutions which run in polynomial time and arises for $d=2$ in VLSI circuit layout and network provisioning [25], [26], two sample matching [27],pattern recognition [28], clustering [29], nonparametric regression [30] and testing for randomness [31]. Let $\mathcal{M}(\mathcal{X}_n)$ denote the possible sets of edges in the class of acyclic graphs which span $\mathcal{X}_n$. The weight of the MST is specified by

$$L_{\text{MST}}(\mathcal{X}_n) = \min_{\mathcal{M}(\mathcal{X}_n)} \sum_{e \in \mathcal{M}(\mathcal{X}_n)} |e|^\gamma.$$

A.3 Euclidean Steiner Tree Problem

In the Euclidean Steiner tree (ST) problem a set of additional nodes $\mathcal{Y}$, called Steiner nodes, can be inserted into the MST problem to reduce the weight required to span the nodes

$\mathcal{X}_n = \{x_1, \dots, x_n\}$. The first formulation of this problem seems to be attributed to Gauss in the context of connecting 3 towns with a network of roads of minimum overall length [9]. Steiner tree problems are NP-hard but have been of interest for minimum area routing problems, e.g. in VLSI layout [32]. Let $\mathcal{S}(\mathcal{X}_n \cup \mathcal{Y})$ denote the possible sets of edges in the class of acyclic graphs which span $\mathcal{X}_n \cup \mathcal{Y}$, where the finite set $\mathcal{Y}$ is free. The weight of the minimal ST is specified by

$$L_{\mathrm{ST}}(\mathcal{X}_n) = \min_{\mathcal{Y}, \mathcal{S}(\mathcal{X}_n \cup \mathcal{Y})} \sum_{e \in \mathcal{S}(\mathcal{X}_n \cup \mathcal{Y})} |e|^\gamma.$$

The asymptotic behavior of each of the weight functions $L_{\mathrm{TSP}}, L_{\mathrm{MST}}$ and L_{ST} can be studied using the more general concept of quasi-additive euclidean functionals introduced by Redmond and Yukich [2] and extended to the case of power weighted edges in [21] and [33].

B. Quasiadditive Euclidean Functionals

Let F be a finite subset of $[0,1]^d$, i.e. a set of points. Define the following conditions on a real valued set function L [2], [21]:

Null Condition: $L(\phi) = 0$, where ϕ is the null set.

Subadditivity: There exists a constant C_1 with the following property: If $\mathcal{Q}^m = \{Q_i\}_{i=1}^{m^d}$ is a uniform partition of $[0,1]^d$ into m^d cubes Q_i each of edge length m^{-1} and volume m^{-d} and if $\{q_i\}_{i \le m^d}$ is the set of points in $[0,1]^d$ which translate each Q_i back to the origin such that $Q_i - q_i = m^{-1}[0,1]^d$, then

$$L(F) \le m^{-1} \sum_{i=1}^{m^d} L(m[(F \cap Q_i) - q_i]) + C_1 m^{d-\gamma}$$

Superadditivity: There exists a constant C_2 with the following property:

$$L(F) \ge m^{-1} \sum_{i=1}^{m^d} L(m[(F \cap Q_i) - q_i]) - C_2 m^{d-\gamma}$$

Continuity: There exists a constant C_3 such that for all finite subsets F and G of $[0,1]^d$

$$|L(F \cup G) - L(F)| \le C_3 \,(\mathrm{card}(G))^{(d-\gamma)/d}$$

L is said to be a *continuous subadditive functional* if it satisfies the null condition, subadditivity and continuity. L is said to be a *continuous superadditive functional* if it satisfies the null condition, superadditivity and continuity.

Definition 1: A continuous subadditive functional L is said to be a *quasi-additive functional* when there exists a continuous superadditive functional L^* which satisfies $L(F) + 1 \ge L^*(F)$ and the approximation property

$$|E[L(U_1, \dots, U_n)] - E[L^*(U_1, \dots, U_n)]| \le C_4 n^{(d-\gamma-1)/d} \qquad (3)$$

where $U_1, \dots, U_n$ are i.i.d. uniform random vectors in $[0,1]^d$.

When such a functional L^* exists it is called the dual of L. As shown in Redmond and Yukich [2, Thm. 1.3] and [21, Thm 2.3] duals can frequently be constructed by identifying a related boundary rooted graph over $\mathcal{X}_n$. In [21, Thm 2.3] it is shown that L is quasi-additive for the following minimal graph problems: the minimal TSP tour, the MST, and the two population minimal matching problem. The following theorem is proven[2] in [21].

Theorem 1: Let L be a quasi-additive Euclidean functional with power-exponent γ, and let $\mathcal{X}_n = \{x_1, \dots, x_n\}$ be an i.i.d. sample drawn from a distribution on $[0,1]^d$ with an absolutely continuous component having (Lebesgue) density $f(x)$. Then

$$\lim_{n \to \infty} L(\mathcal{X}_n)/n^{(d-\gamma)/d} = \beta_{L,\gamma} \int f(x)^{(d-\gamma)/d} dx, \quad (a.s.) \qquad (4)$$

In Theorem 1 $\beta_{L,\gamma}$ is a constant which only depends on γ and the definition of the functional L, i.e. the graph optimality criterion (TSP, MST, or Steiner tree). In particular, $\beta_{L,\gamma}$ is independent of the distribution of the x_i's. Theorem 1 is a generalization of Steele's work [23] which itself is a generalization of the well known Beardwood, Halton and Hammersley Theorem [34].

III. Minimal k-point Euclidean Graphs

We denote by $\mathcal{X}_{n,k}$ a k-point subset of $\mathcal{X}_n$, $0 < k \le n$. The minimal k-point Euclidean graph problem is to find the subset of points $\mathcal{X}_{n,k} = \mathcal{X}^*_{n,k}$ and the set of edges connecting these points such that the resultant graph has minimum total weight $L(\mathcal{X}^*_{n,k})$

$$L(\mathcal{X}^*_{n,k}) \quad = \quad \min_{\mathcal{X}_{n,k}} L(\mathcal{X}_{n,k}).$$

Define $k = \lfloor \alpha n \rfloor$ as the integer part of αn. For the purposes of asymptotic analysis we will fix $\alpha \in (0,1)$ and study the behavior of $L(\mathcal{X}_{n,\lfloor \alpha n \rfloor})$ as $n \to \infty$. More generally define the weight functional $L_\alpha(F)$ as the k-minimal graph which spans $k = \lfloor \alpha \mathrm{card}(F) \rfloor$ of the points in the finite set F. Then $L(\mathcal{X}^*_{n,k}) = L_\alpha(\mathcal{X}_n)$. It is not difficult to see that $L_\alpha(F)$ neither satisfies the subadditivity property nor the continuity property. Hence, the elegant methods of Steele [23], Redmond and Yukich [2], and Rhee [35] cannot be directly applied.

A. A Tight Cover Property

Let $\mathcal{Q}^m$ be a uniform partition of $[0,1]^d$ into m^d cubes Q_i of edge length $1/m$. The quantity $1/m$ is called the resolution of the partition. The following definition of a tightly coverable graph specifies a class of k-point graph algorithms for which the vertices of the minimal graph can be covered by a small number of partition cells Q_i.

Definition 2 (**Tightly Coverable Graphs**) Let $\mathcal{Q}^m$, $m = 1, 2, \dots$, be a sequence of uniform partitions of $[0,1]^d$ of resolution $1/m$ and let $\sigma(\mathcal{Q}^m)$ denote the sigma-algebra generated by the partition cells in $\mathcal{Q}^m$. Let G_n be the complete graph spanning $\mathcal{X}_n$. For $\alpha \in [0,1]$ let $\mathcal{G}$ be an algorithm which constructs a subgraph of G_n with $k = \lfloor \alpha n \rfloor$ vertices $\mathcal{X}_{n,k} \subset \mathcal{X}_n$. Define $D^m_k = \cap_{\{C \in \sigma(\mathcal{Q}^m): \mathcal{X}_{n,k} \in C\}} D$ the minimum volume partition set which covers $\mathcal{X}_{n,k}$. The algorithm $\mathcal{G}$ is said to generate tightly coverable subgraphs if for any $\epsilon > 0$ there exists an M such that for all $m > M$

$$\limsup_{n \to \infty} \left| \frac{\mathrm{card}(\mathcal{X}_n \cap D^m_{\lfloor \alpha n \rfloor}) - \lfloor \alpha n \rfloor}{n} \right| \le \epsilon, \qquad (a.s.)$$

[2] In [21] Redmond and Yukich actually prove even stronger convergence (complete convergence) of the functional $L_n = L(\mathcal{X}_n)$ and give asymptotic convergence rate.

Tightly coverable subgraphs have the property that the vertices $\mathcal{X}_{n,k}$ can be dissected from the rest of the points in $\mathcal{X}_n$ using a scalpel of resolution $1/m$. For an arbitrary distribution of vertices $\mathcal{X}_n$, this property would allow us to index $\mathcal{X}_{n,k}$ over the $\binom{n}{k}$ possible combinations of k-point sets of $\mathcal{X}_n$ by indexing the sets of vertices $D \cap \mathcal{X}_n$ over the partition-generated subsets $D \in \sigma(\mathcal{Q}^m)$ of $[0,1]^d$.

B. A Covering Lemma

Consider the class (sigma algebra) $\sigma(\mathcal{Q}^m)$ of sets of resolution $1/m$. Out of this class we define C_α^m to be a set of probability at least α for which $L(C \cap \mathcal{X}_n)$ is minimized

$$C_\alpha^m = \mathrm{argmin}_{C \in \sigma(\mathcal{Q}^m): P(C) \geq \alpha} L(C \cap \mathcal{X}_n).$$

where $P(C) = P(x_i \in C)$. As in the tight cover definition, define D_k^m as the minimum volume set in $\sigma(\mathcal{Q}^m)$ containing $\mathcal{X}_{n,k}^*$

$$D_k^m = \cap_{C \in \sigma(\mathcal{Q}^m): C \supset \mathcal{X}_{n,k}^*} C.$$

Note that $\mathcal{X}_{n,k}^*$ is contained in set D_k^m but may not be contained in C_α^m.

With these definitions we have:

Lemma 1: Let L be a quasi-additive functional with power exponent γ as in Theorem 1. If $\mathrm{card}(\mathcal{X}_n \cap C_\alpha^m) \geq k$

$$\begin{aligned} &\left|L(\mathcal{X}_{n,k}^*) - L(\mathcal{X}_n \cap C_\alpha^m)\right| / n^{(d-\gamma)/d} \leq \\ C_3 &\left[\left(\frac{\mathrm{card}(\mathcal{X}_n \cap C_\alpha^m) - k}{n}\right)^{(d-\gamma)/d} + 2\left(\frac{\mathrm{card}(\mathcal{X}_n \cap D_k^m) - k}{n}\right)^{(d-\gamma)/d}\right]. \end{aligned} \tag{5}$$

Proof of Lemma 1

Let $\mathcal{X}_{n,k}^{C_\alpha^m}$ be any k-points in $\mathcal{X}_n \cap C_\alpha^m$. Due to continuity of L we have

$$\left|L(\mathcal{X}_n \cap C_\alpha^m) - L(\mathcal{X}_{n,k}^{C_\alpha^m})\right| \leq C_3 \left(\mathrm{card}(\mathcal{X}_n \cap C_\alpha^m) - k\right)^{(d-\gamma)/d}.$$

Hence, since $\mathcal{X}_{n,k}^*$ are the vertices of the minimal k-point graph

$$\begin{aligned} L(\mathcal{X}_n \cap C_\alpha^m) &\geq L(\mathcal{X}_{n,k}^{C_\alpha^m}) - C_3 \left(\mathrm{card}(\mathcal{X}_n \cap C_\alpha^m) - k\right)^{(d-\gamma)/d} \\ &\geq L(\mathcal{X}_{n,k}^*) - C_3 \left(\mathrm{card}(\mathcal{X}_n \cap C_\alpha^m) - k\right)^{(d-\gamma)/d}. \end{aligned} \tag{6}$$

Furthermore, again by continuity,

$$\left|L(\mathcal{X}_n \cap D_k^m) - L(\mathcal{X}_{n,k}^*)\right| \leq C_3 \left(\mathrm{card}(\mathcal{X}_n \cap D_k^m) - k\right)^{(d-\gamma)/d}, \tag{7}$$

so that

$$L(\mathcal{X}_n \cap D_k^m) \leq L(\mathcal{X}_{n,k}^*) + C_3 \left(\mathrm{card}(\mathcal{X}_n \cap D_k^m) - k\right)^{(d-\gamma)/d}. \tag{8}$$

Hence, combining (6) and (8)

$$\begin{aligned} &L(\mathcal{X}_n \cap D_k^m) - L(\mathcal{X}_n \cap C_\alpha^m) \\ &\leq C_3 \left[\left(\mathrm{card}(\mathcal{X}_n \cap D_k^m) - k\right)^{(d-\gamma)/d} + \left(\mathrm{card}(\mathcal{X}_n \cap C_\alpha^m) - k\right)^{(d-\gamma)/d}\right] \end{aligned} \tag{9}$$

On the other hand, by definition of C_α^m the left side of inequality (9) is greater than zero so that

$$\begin{aligned} &|L(\mathcal{X}_n \cap D_k^m) - L(\mathcal{X}_n \cap C_\alpha^m)| \\ &\leq C_3 \left[\left(\mathrm{card}(\mathcal{X}_n \cap D_k^m) - k\right)^{(d-\gamma)/d} + \left(\mathrm{card}(\mathcal{X}_n \cap C_\alpha^m) - k\right)^{(d-\gamma)/d}\right] \end{aligned}$$

which when combined with (7) gives

$$\begin{aligned} &\left|L(\mathcal{X}_{n,k}^*) - L(\mathcal{X}_n \cap C_\alpha^m)\right| \\ &\leq |L(\mathcal{X}_n \cap D_k^m) - L(\mathcal{X}_n \cap C_\alpha^m)| + \left|L(\mathcal{X}_{n,k}^*) - L(\mathcal{X}_n \cap D_k^m)\right| \\ &\leq C_3 \left[\left(\mathrm{card}(\mathcal{X}_n \cap C_\alpha^m) - k\right)^{(d-\gamma)/d} + 2\left(\mathrm{card}(\mathcal{X}_n \cap D_k^m) - k\right)^{(d-\gamma)/d}\right]. \end{aligned}$$

Dividing both sides by $n^{(d-\gamma)/d}$ establishes the lemma. □

When $k = \lfloor \alpha n \rfloor$ the first additive term on the right side of the inequality of Lemma 1 can be shown to converge a.s. to a term of order $O(m^{\gamma-d})$ using Lemma 6 and arguments similar to those used to prove Lemma 7. Thus if the minimal k-point graph can be shown to be tightly coverable, for any $\epsilon > 0$ there exists an M such that: $\limsup_{n\to\infty} |L(\mathcal{X}_{n,k}^*) - L(X_n \cap C_\alpha^m)|/n^{(d-\gamma)/d} \leq \epsilon$ (a.s.) for all $m > M$. It would then be possible to show that $L(\mathcal{X}_{n,k}^*)/n^{(d-\gamma)/d}$ would converge to the same a.s. limit as that of the greedy minimal k-point approximation given in the next section. Conversely, if the greedy approximation given below is not asymptotically equivalent to the exact minimal k-point graph then the latter graph does not satisfy the tightly coverable condition. The question whether the tightly coverable condition holds or not for the minimal k-point graph is still an open problem.

IV. Limit Theorem for k-point Greedy Approximation

Since the computation of the exact minimal k-point graph $\mathcal{X}_{n,k}^*$ has complexity which is exponential in the number of points n, the asymptotics of polynomial-time approximations are also of interest. Here we obtain asymptotic results for a greedy algorithm originally introduced by Ravi, Sundaram, Marathe, Rosenkrantz and Ravi [1] for constructing approximations to the k-MST on the plane. Their algorithm produces graphs which by construction satisfy the tightly coverable property introduceed in the last section. Here we define a generalized version of their algorithm which constructs graphs in d dimensions, $d > 1$, using arbitrary quasi-additive edge weight functions.

The algorithm is implemented in three steps: 1) the user specifies a uniform partition $\mathcal{Q}^m$ of $[0,1]^d$ having m^d cells Q_i of resolution $1/m$; 2) the algorithm finds the smallest subset $B_k^m = \cup_i Q_i$ of partition elements containing at least k points; 3) out of this smallest subset the algorithm selects the k points $\mathcal{X}_{n,k}$ which minimize $L(\mathcal{X}_{n,k})$. Stage 3 requires finding a k-point minimal graph on a much reduced set of points, which is typically only slightly larger than k if m is suitably chosen, which can be performed in polynomial time.

The smallest subset mentioned in Stage 2 of the algorithm is not unique. Figures 1 and 2 show an example with $m = 5$, $k = 17$ for which there are two possible smallest subsets, in this case both contain 18 points.

Similarly to [36], [1] we specify a small subset by the following greedy algorithm: i) find a reindexing $\{Q_{(i)}\}_{i=1}^{m^d}$ of the cells in $[0,1]^d$ ranked in decreasing order of the number of contained points, $\mathrm{card}(\mathcal{X}_n \cap Q_{(1)}) \geq \ldots \geq \mathrm{card}(\mathcal{X}_n \cap Q_{(m^d)})$ (if there are equalities arrange these in lexicographical order); ii) select the subset specified in Stage 2 by the recursion:

Greedy Subset Selection Algorithm

Intialize: $B = \phi$, $j = 1$
Do until $\mathrm{card}\{\mathcal{X}_n \cap B\} \geq k$
$B = B \cup Q_{(j)}$
End $j = j + 1$

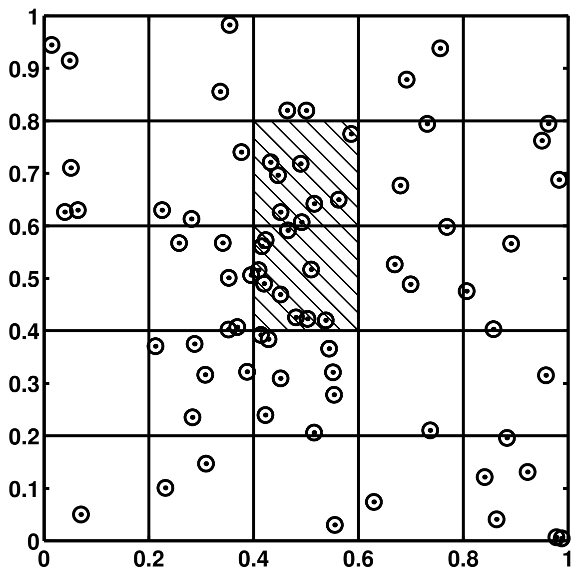

Fig. 1. *A sample of 75 points from the mixture density $f(x) = 0.25 f_1(x) + 0.75 f_o(x)$ where f_o is a uniform density over $[0,1]^2$ and f_1 is a bivariate Gaussian density with mean $(1/2, 1/2)$ and diagonal covariance* $\mathrm{diag}(0.01)$. *A smallest subset B_k^m is the union of the two cross hatched cells shown for the case of $m = 5$ and $k = 17$.*

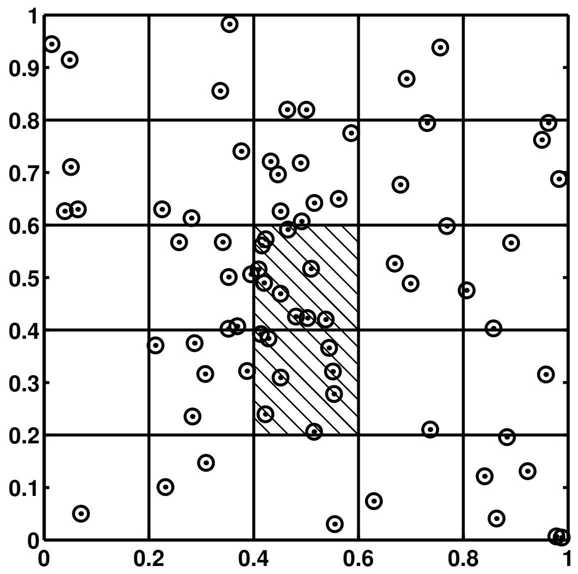

Fig. 2. *Another smallest subset B_k^m containing at least $k = 17$ points for the mixture sample shown in Fig 1.*

At termination of the algorithm $j = \tilde{q} \leq m^d$ and we have a minimal subset $B^m_{\lfloor \alpha n \rfloor} \stackrel{\text{def}}{=} B = \cup_{i=1}^{\tilde{q}} Q_{(i)}$ containing at least k points. Let $\mathcal{X}_{n,k}^{G_m}$ be the k vertices of the graph found by the greedy algorithm.

It should not be surprising that as $n \to \infty$ the greedy subset selection algorithm should produce the smallest resolution-$1/m$ set A of probability close to $\alpha = k/n$. Indeed, this is the basis for the asymptotic theorems stated below. Therefore we next specify a class of minimal subsets in the sigma-algebra $\sigma(\mathcal{Q}^m)$ which have coverage probability of at least α.

Define the cell probabilities $\varphi_i = \int_{Q_i} f(x)dx$, $i = 1, \ldots, m^d$. If for any $C \in \sigma(\mathcal{Q}^m)$ satisfying $P(C) \geq \alpha$ the set $A \in \sigma(\mathcal{Q}^m)$ satisfies

$$P(C) \geq P(A) \geq \alpha,$$

then A is called a *mininal resolution-$1/m$ set of probability at least α*. The class of all such sets is denoted $\mathcal{A}_\alpha^m$ and, as shown in the following construction, all sets in $\mathcal{A}_\alpha^m$ have identical coverage probabilities $p_{\mathcal{A}_\alpha^m} \geq \alpha$.

The class $\mathcal{A}_\alpha^m$ can be generated by the following greedy algorithm: i) find a reindexing $\{Q_{(i)}\}_{i=1}^{m^d}$ of the cells in $\mathcal{Q}^m$ ranked in decreasing order of cell probabilities, $\varphi_{(1)} \geq \ldots \geq \varphi_{(m^d)}$; ii) select a subset A using the Greedy Subset Selection Algorithm applied to the modified cell ordering prescribed in i). Assume the greedy algorithm terminates at iteration $j = q$. If $\varphi_{(q)} > \varphi_{(q+1)}$ then A is the only set in the class $\mathcal{A}_\alpha^m$. Otherwise, let there be $K - I$ identical values of φ_i satisfying $\varphi_{(I-1)} > \varphi_{(I)} = \ldots = \varphi_{(q)} = \ldots = \varphi_{(K)} > \varphi_{(K+1)}$ where $I \leq q$ and $K > q$. Then $\mathcal{A}_\alpha^m$ contains $S = \binom{K-I}{q-I+1}$ sets $\{A_i\}$ constructed by taking the last $q - I + 1$ cells that the greedy algorithm added to A and exchanging them with any of the $q - I + 1$ possible combinations of cells in the set $\{Q_{(I)}, \ldots, Q_{(K)}\}$. Each of these sets A_i is composed of an identical number q of dissecting cells $\{Q_j^{A_i}\}_{j=1}^q$ in $\mathcal{Q}^m$ having identical sets of coverage probabilities $\{P(Q_j^{A_i})\}_{j=1}^q = \{\varphi_{(j)}\}_{j=1}^q$, and satisfying $P(A_i) = p_{\mathcal{A}_\alpha^m} \geq \alpha$, $i = 1, \ldots, S$.

Before developing the main result of this section we define some notation.

We will be interested in two special subsets generated by $\mathcal{A}_\alpha^m$. The interior $\overline{\mathcal{A}_\alpha^m}$ defined as the intersection of all S sets in $\mathcal{A}_\alpha^m$

$$\overline{\mathcal{A}_\alpha^m} = \cap_{A_i \in \mathcal{A}_\alpha^m} A_i \tag{10}$$

and the associated residual set

$$\begin{aligned} \partial \mathcal{A}_\alpha^m &= \cup_{A_i \in \mathcal{A}_\alpha^m} A_i - \cap_{A_i \in \mathcal{A}_\alpha^m} A_i \\ &= \cup_{A_i, A_j \in \mathcal{A}_\alpha^m} A_i A_j^c. \end{aligned} \tag{11}$$

$\overline{\mathcal{A}_\alpha^m}$ is the "core" of the set $\mathcal{A}_\alpha^m$ and $\partial \mathcal{A}_\alpha^m$ is the "crust" of the set.

The total variation $v(Q)$ over a rectangle $Q \subset [0,1]^d$ of a function g on $\mathbb{R}^d$ is defined as [37]

$$v(Q) = \limsup_{\{z_i\} \in Q} \sum_i |g(z_i) - g(z_{i-1})| = v(Q), \tag{12}$$

where the limsup is taken over all countable subsets $\{z_1, z_2, \ldots,\}$ of points in Q. The function g is said to have bounded variation over Q if $v(Q) < \infty$. By convention, $v(\phi) = 0$ for ϕ the empty set.

To simplify the presentation we assume throughout that the distribution P of each of the i.i.d. points in $\mathcal{X}_n = \{x_1, \ldots, x_n\}$ is absolutely continuous with respect to Lebesgue measure and has a density $f(x)$. The results of [23] and [2] assert that the addition of singular components, e.g. delta functions, to the density does not change the asymptotics of $L(\mathcal{X}_n)$. Here it does change the asymptotics since the points of support of singular components entail zero edge weights and are therefore more attractive to include in the minimum k-point graph. However, the effect of singular components will only be to change the value of a threshold η on $f(x)$ (see remark below). The main result of this section is the following asymptotic theorem.

Theorem 2: Let $\mathcal{X}_n$ be an i.i.d. sample from a distribution having Lebesgue density $f(x)$. Fix $\alpha \in [0,1]$, $\gamma \in (0, d)$. Let

$f^{(d-\gamma)/d}$ be of bounded variation over $[0,1]^d$ and denote by $v(A)$ its total variation over a subset $A \subset [0,1]^d$. Then, the total edge weight $L(\mathcal{X}_{n,k}^{G_m})$ of a k-point graph constructed by the resolution-$1/m$ greedy algorithm satisfies

$$\limsup_{n\to\infty} \left| L(\mathcal{X}_{n,\lfloor \alpha n\rfloor}^{G_m})/n^{(d-\gamma)/d} - \beta_{L,\gamma}\int_{A_\alpha^m} f^{(d-\gamma)/d}(x)dx \right| < \delta, \qquad (a.s.), \qquad (13)$$

where $A_\alpha^m \in \mathcal{A}_\alpha^m$ is any minimal resolution-$1/m$ set of probability at least α,

$$\begin{aligned} \delta &= 2m^{-d}\beta_{L,\gamma}\sum_{i=1}^{m^d} v(Q_i \cap \partial\mathcal{A}_\alpha^m) + C_3(p_{\mathcal{A}_\alpha^m}-\alpha)^{(d-\gamma)/d} \\ &= O(m^{\gamma-d}), \end{aligned} \qquad (14)$$

and $p_{\mathcal{A}_\alpha^m}$ is the coverage probability of sets in $\mathcal{A}_\alpha^m$. Furthermore, the bound (13) holds pointwise when $L(\mathcal{X}_{n,\lfloor\alpha n\rfloor}^{G_m})$ is replaced by $E[L(\mathcal{X}_{n,\lfloor\alpha n\rfloor}^{G_m})]$.

We prove Theorem 2 in Section V. It is of interest here to relate the integral in (13) to the Rényi entropy of the density $f(x)$. The key to this relation is the following lemma which relates the integral over a set A in $\mathcal{A}_\alpha^m$ in (13) to a constrained minimum over $A \in \sigma(\mathcal{Q}^m)$.

Lemma 2: Under the assumptions of Theorem 2

$$\int_{A_\alpha^m} f^{(d-\gamma)/d}(x)dx = \min_{A\in\sigma(\mathcal{Q}^m):P(A)\geq\alpha}\int_A f^{(d-\gamma)/d}(x)dx + O(m^{-d}). \qquad (15)$$

Proof of Lemma 2

First recall that by construction of $\mathcal{A}_\alpha^m$ the coverage probability of any set in $\mathcal{A}_\alpha^m$ satisfies for some q: $\sum_{i=1}^{q-1}\varphi_{(i)} < \alpha$, $\sum_{i=1}^{q}\varphi_{(i)} = p_{\mathcal{A}_\alpha^m} \geq \alpha$, and $0 \leq p_{\mathcal{A}_\alpha^m} - \alpha < \varphi_{(q)}$, where $\varphi_{(1)} \geq \ldots \geq \varphi_{(m^d)}$, are the rank ordered cell probabilities.

In view of Lemma 4 it is sufficient to show that (15) holds for blocked densities of the form $f(x) = \tilde{f}(x) = \sum_{i=1}^{m^d}\theta_i I_{Q_i}(x)$. Observe that for any $A_\alpha^m \in \mathcal{A}_\alpha^m$ and for any η satisfying $m^d\varphi_{(q-1)} < \eta \leq m^d\varphi_{(q)}$: if $x \in A_\alpha^m$ then $\tilde{f}(x) \geq \eta$. Equivalently, $\tilde{f}^{(d-\gamma)/d}(x) - \lambda\tilde{f}(x) \leq 0$ where $\lambda = \eta^{-\gamma/d}$. With $I_{A_\alpha^m}(x)$ the indicator function of A_α^m this implies that for any $A \in \sigma(\mathcal{Q}^m)$

$$I_{A_\alpha^m}(x)(\tilde{f}^{(d-\gamma)/d}(x) - \lambda\tilde{f}(x)) \leq I_A(x)(\tilde{f}^{(d-\gamma)/d}(x) - \lambda\tilde{f}(x)),$$

for all x. Therefore, integrating this inequality over $x \in [0,1]^d$

$$\int_{A_\alpha^m}\left(\tilde{f}^{(d-\gamma)/d}(x) - \lambda\tilde{f}(x)\right)dx \leq \int_A \left(\tilde{f}^{(d-\gamma)/d}(x) - \lambda\tilde{f}(x)\right)dx,$$

or

$$\int_{A_\alpha^m}\tilde{f}^{(d-\gamma)/d}(x)dx - \int_A \tilde{f}^{(d-\gamma)/d}(x)dx \leq \lambda\left(\int_{A_\alpha^m}\tilde{f}(x)dx - \int_A\tilde{f}(x)dx\right). \qquad (16)$$

Now, as $P(A_\alpha^m) = p_{\mathcal{A}_\alpha^m}$, if $P(A) \geq \alpha$ then the right side of this inequality is upper bounded by $\lambda(p_{\mathcal{A}_\alpha^m} - \alpha) \leq \varphi_{(q)} = m^{-d}\theta_{(q)}$. Hence, minimizing both sides of the inequality (16) over A we obtain

$$\int_{A_\alpha^m}\tilde{f}^{(d-\gamma)/d}(x)dx \leq \min_{\{A\in\sigma(\mathcal{Q}^m):P(A)\geq\alpha\}}\int_A \tilde{f}^{(d-\gamma)/d}(x)dx + O(m^{-d}).$$

Since, obviously,

$$\int_{A_\alpha^m}\tilde{f}^{(d-\gamma)/d}(x)dx \geq \min_{\{A\in\sigma(\mathcal{Q}^m):P(A)\geq\alpha\}}\int_A (\tilde{f}^{(d-\gamma)/d}(x)dx$$

the lemma is established. □

We can now show how Theorem 2 can be related to estimation of Rényi entropy. Using Lemma 2 and the fact that $\sigma(\mathcal{A}^m)$ converges to the class of Borel subsets $\mathcal{B}$ of $[0,1]^d$, it is an easy exercise to show that

$$\begin{aligned} \lim_{m\to\infty}\int_{A_\alpha^m} f^{(d-\gamma)/d}(x)dx &= \inf_{A\in\mathcal{B}:P(A)\geq\alpha}\int_A f^{(d-\gamma)/d}(x)dx \\ &= \inf_{A\in\mathcal{B}:P(A)=\alpha}\int_A f^{(d-\gamma)/d}(x)dx \end{aligned} \qquad (17)$$

Now for any Borel set A in $[0,1]^d$ having $P(A) > 0$ define the conditional density $f(x|A) = f(x)/P(A)I_A(x)$ where $I_A(x)$ is the indicator function of A. The Rényi entropy of $f(x|A)$ of order $\nu \in (0,1)$ is defined as

$$R_\nu(f|A) = \frac{1}{1-\nu}\log\int f^\nu(x|A)dx. \qquad (18)$$

This is also called the conditional Rényi entropy given A. As $1-\nu > 0$ minimization of $R_\nu(f|A)$ over A is equivalent to minimization of the integral in (18). Let A_o be the probability-at-least-α Borel subset of $[0,1]^d$ which minimizes $R_\nu(f|A)$

$$R_\nu(f|A_o) = \inf_{\{A\in\mathcal{B}:P(A)\geq\alpha\}} R_\nu(f|A). \qquad (19)$$

For $\nu = (d-\gamma)/d$ define the following function of $L(\mathcal{X}_{n,\lfloor\alpha n\rfloor}^{G_m})$

$$\hat{R}_\nu \stackrel{\text{def}}{=} \frac{1}{1-\nu}\left(\log L(\mathcal{X}_{n,\lfloor\alpha n\rfloor}^{G_m})/(\lfloor\alpha n\rfloor)^\nu - \log\beta_{L,\gamma}\right) \qquad (20)$$

An immediate consequence of Theorem 2 is the following.

Theorem 3: Under the assumptions of Theorem 2 $\hat{R}_\nu$ is a strongly consistent estimator of the minimum conditional Rényi entropy $R_\nu(f|A_o)$ of order $\nu \in (0,1)$ as $m, n \to \infty$.

Before developing the proof of Theorem 2 in the next section, we make the following remarks.

1. The bound δ in Theorem 2 is tight since it reduces to zero for the case $\alpha = 1$, yielding the classical a.s. BHH limit theorem, Theorem 1, for minimal graphs spanning all n points $\mathcal{X}_n$. Indeed, in this case, for arbitrary $m > 0$ the class $\mathcal{A}_\alpha^m$ of resolution-$1/m$ probability-at-least-α sets contains only one set $A_1 = [0,1]^d$. Therefore, $p_{\mathcal{A}_\alpha^m} - \alpha = 0$, $\partial\mathcal{A}_\alpha^m = \phi$, the empty set, and $v(Q_i \cap \partial\mathcal{A}_\alpha^m) = 0$ as required.
2. Theorems 2 and 3 are easily extended to the case where the density of P contains singular components, e.g. delta functions. Specifically, let P have the mixed density $f(x)dx + \mu_s$ where dx is Lebesgue measure, $f(x)$ is the absolutely continuous component and μ_s is the singular component of P

relative to Lebesgue measure. Let the support of the singular measure be A_s and let $\alpha_s = \mu_s([0,1]^d) = P(A_s) < \alpha$. Then, we know from Lemma 6 that $\lim_{n\to} L(\mathcal{X}_n \cap A_s) = 0$ and hence points falling in the singular part A_s of $[0,1]^d$ contribute negligible weight. Thus, by the strong law of large numbers, $\alpha_s n$ of the n points can be included in the graph at negligible cost leaving only $(\alpha-\alpha_s)n$ points in $[0,1]^d - A_s$ whose edge weights are asymptotically significant. Therefore, in the case of a singular component with $\alpha_s < \alpha$, Theorem 2 holds with the class $\mathcal{A}_\alpha^m$ replaced by the class $\mathcal{A}_{\alpha-\alpha_s}^m$ of resolution $1/m$ subsets with coverage probability at least $\alpha - \alpha_s$. If $\alpha_s \geq \alpha$ then $\mathcal{A}_\alpha^m$ is replaced by the empty set and $L(\mathcal{X}_{\lfloor\alpha n\rfloor}^{G_m})$ converges to zero a.s. as $m,n \to \infty$. Likewise, it can be shown that when there is a singular component Lemma 2 holds with the minimization over the class $\{A \in \sigma(\mathcal{Q}^m) : P(A) \geq \alpha\}$ replaced by a minimization over the smaller class

$$\left\{A \in \sigma(\mathcal{Q}^m) : \int_A f(x)dx \geq \max\{\alpha-\alpha_s, 0\}\right\}.$$

3. As can be seen from Lemma 7, Theorem 2 holds for any method of selection of $k = \lfloor\alpha n\rfloor$ points from the minimal subset B_k^m of $\sigma(\mathcal{Q}^m)$ covering at least k points. It does not depend on the precise way that a few points are eliminated from the set B_k^m to form $\mathcal{X}_{n,k}^{G_m}$. This implies that for large n all methods of elimination are equivalent, including simply randomly rejecting points from B_k^m until exactly k points remain.
4. In smooth estimation problems the normalization factor required to ensure convergence of a parameter estimator to a finite non-zero constant is typically $1/n$. In contrast Theorem 2 says that the stabilization factor for $L(\mathcal{X}_{n,\lfloor\alpha n\rfloor}^{G_m})$ is the larger quantity $1/n^{(d-\gamma)/d}$, i.e., $L(\mathcal{X}_{n,\lfloor\alpha n\rfloor}^{G_m})$ is less explosive as a function of n. On the other hand, inspired by [21, Thm. 2.5] which gives the tight convergence rate $|E[L_{MST}(\mathcal{X}_n)] - \beta_{L_{MST},\gamma} n^{(d-\gamma)/d}| = O\left(\max(1, n^{(d-\gamma-1)/d})\right)$ for the MST under the uniform distribution, we conjecture that the rate of convergence in the limsup of Theorem 2 is only $O(1/n^{1/d})$ for $\gamma < d-1$ while it is the standard $O(1/\sqrt{n})$ for $\gamma \geq d-1$. For $d=2$ these rates are identical but for $d \gg 2$ the estimator (20) of Renyi entropy is best implemented for orders ν in the range $0 \leq \nu \leq 1/d$.
5. The bound δ of Theorem 2 decays to zero as a function of resolution $1/m$ at overall rate $O(m^{\gamma-d})$. The first term $2m^{-d}\beta_{L,\gamma}\sum_{i=1}^{m^d} v(Q_i \cap \partial A_\alpha^m) \leq 2\beta_{L,\gamma}m^{-d}v([0,1])$ decays as m^{-d} and and is due to non-uniqueness of the resolution-$1/m$ subsets $A_\alpha^m \in \mathcal{A}_\alpha^m$ all of which have identical coverage probability but over which f may have different variation. When f is, in the terminology of [23], a "blocked distribution," $f(x) = m^{-d} \cdot \sum_{i=1}^{m^d} \varphi_i I_{Q_i}(x)$, over the resolution-$1/m$ cells this term is equal to zero. The second additive term $C_3(p_{\mathcal{A}_\alpha^m} - \alpha)^{(d-\gamma)/d}$ is due to the overshoot of coverage probability by the subsets $A_\alpha^m \in \mathcal{A}_\alpha^m$. This term is zero when it so happens that the α chosen in the greedy algorithm is exactly attainable by a $1/m$ resolution subset. However, this term decays to zero only as $m^{\gamma-d}$ and dominates the resolution convergence rate. Note that this implies that the rate of convergence in m of the bound δ in Theorem 2 is fastest for small γ. For $d > 2$ this trend is opposite with respect to the rate of convergence in n (see previous remark) and is reminiscent of the fundamental tradeoff between bias or resolution (due to insufficient m) and variance (due to insufficient n) which characterizes most estimation problems.
6. Since $\sup_{x\in Q_{(q)}} f^{(d-\gamma)/d}(x) \leq v([0,1]^d)$ and $\sum_{i=1}^{m^d} v(Q_i \cap \partial\mathcal{A}_\alpha^m) \leq v([0,1]^d)$ we can weaken the a.s. bound in Theorem 2 by using the result (37), which was shown in the proof of Theorem 2. This results in the following
$$\delta \leq \left[2\beta_{L,\gamma}m^{-d} + C_3 m^{\gamma-d}\right] v([0,1]^d). \tag{21}$$
This a.s. bound holds uniformly over the class of all density functions such that $f^{(d-\gamma)/d}$ has total variation less than or equal to $v([0,1]^d)$. Thus if an upper bound $\overline{v}$ on the total variation of an unknown density is available and a consistent estimate of conditional Rényi entropy $R_\nu = R_\nu(f|A_o)$ is desired such that
$$|L(\mathcal{X}_{n,\lfloor\alpha n\rfloor}^{G_m})/(\lfloor\alpha n\rfloor)^\nu - \beta_{L,\gamma}\exp\{-(1-\nu)R_\nu)| < \epsilon$$
the weakened bound (21) can be used to give a selection rule for the required partition resolution $1/m$
$$1/m \leq \frac{\epsilon}{(2+C_3)\overline{v}}.$$
7. The Borel set A_o of probability-at-least-α defined in (19) which minimizes Rényi entropy of order ν is independent of ν and can be constructed by a simple water pouring procedure. To see this define the Lagrangian
$$\rho(A,\lambda) \quad \stackrel{\text{def}}{=} \quad \int_A f^{(d-\gamma)/d}(x)dx - \lambda\left(\int_A f(x)dx - \alpha\right)$$
for $\lambda > 0$. Consider an arbitrary Borel subset $\Delta A \subset [0,1]^d$ outside of A_o, $A_o \cap \Delta A = \phi$. By Kuhn-Tucker, A_o must satisfy $\rho(A_o + \Delta A, \lambda) - \rho(A_o, \lambda) \leq 0$ for A_o to minimize $\rho(A,\lambda)$ and hence minimize entropy. Here
$$\rho(A_o + \Delta A, \lambda) - \rho(A_o,\lambda) = \int_{\Delta A}\left(1 - \lambda f^{\gamma/d}\right) f^{(d-\gamma)/d},$$
which is negative when A_o is defined by
$$A_o = \{x : f(x) \geq \eta\}. \tag{22}$$
where, if possible, $\eta = \lambda^{-d/\gamma} \geq 0$ is selected to satisfy $P(A_o) = \alpha$. Hence, in this case, the conditional density $f(x|A_o)$ in (20) is obtained by truncating $f(x)$ wherever it falls below η and renormalizing to obtain a valid probability density integrating to 1 over $[0,1]^d$. See Fig. 3 for illustration.
When for any $a > 0$ the set $\{x : f(x) = a\}$ has (Lebesgue) measure zero $f(x)$ has no flat spots and it is always possible to select η in (22) to satisfy $P(A_o) = \alpha$. Otherwise, we need to slightly modify the definition (22) of A_o. Let η be such that the set $\{x : f(x) < \eta\}$ has probability α_-, the set $\{x : f(x) = \eta\}$ has probability $\alpha_+ - \alpha_- > 0$ and assume that $\alpha \in (\alpha_-, \alpha_+)$. Then defining
$$A_o = \{x : f(x) \geq \eta\} \cup C, \tag{23}$$
where C is an arbitrary Borel subset of $\{x : f(x) = \eta\}$ having $P(C) = \alpha - \alpha_-$, is an entropy minimizing subset of probability α.
8. The minimum entropy set A_o in (19) is not unique. For example any arbitrary probability zero set can be added to A_o without affecting the entropy. A more interesting example occurs when f is a uniform density for which case any set A of area α minimizes entropy. In this case the asssertion of Theorem 2 may come as a surprise since the largest distance

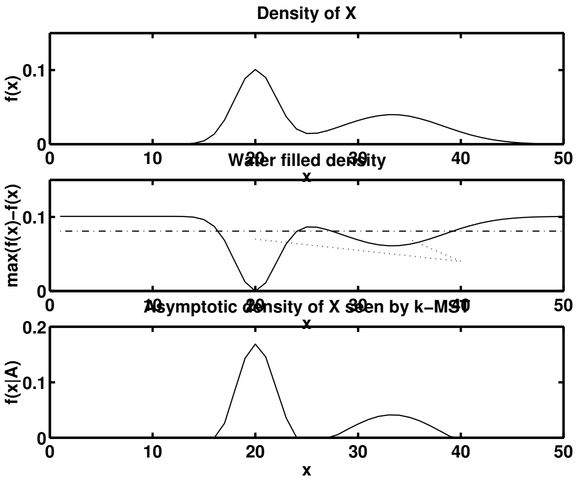

Fig. 3. *Water pouring construction of* $f(x|A_o)$

between points in A should be smallest for connected sets of small diameter, e.g., a sphere. However, let $A = \cup_{i=1}^{\infty} A_i$ be a countable union of disjoint sets A_i and having $\mathrm{vol}(A) = \alpha$. Note that only a single edge is needed between A_i and A_j to form a connected graph over any two sets. Thus in the limit of large n the total edge weight of the graph is dominated by connections between points within each A_i and not connections between different A_i. This is because the total edge weight depends more on the average edge weight than the maximum edge weight.

9. In the Rényi entropy estimator (20) the constant $\beta_{L,\gamma}$ is a bias offset which can in principle be computed offline as it does not depend on f. However, while upper and lower bounds are available, see e.g.[38] for MST bounds, analytic expressions for $\beta_{L,\gamma}$ are not available. Alternatively, for some estimation or classification problems only relative entropy may be needed, e.g. testing for different entropy rates between two populations via the ratio of k-point graph weight functionals, for which the bias offset need not be known.
10. Consider the case that $f = (1-\epsilon)f_1 + \epsilon f_o$ is a mixture of a nominal density f_1 of interest and a contaminating density f_0 and ϵ is small. Then, since f_1 increasingly dominates f_o as ϵ decreases, for small ϵ a suitable threshold η (α) exists for which: $f(x|A_o) \approx f_1(x)$. Thus (20) can be viewed as a robust estimator of the Rényi entropy of the nominal density f_1.

V. Proof of Theorem 2

Here we present a set of lemmas that are needed to prove Theorem 2. First we establish by Lemma 3 that any set B_n^m obtained by the greedy algorithm belongs to class $\mathcal{A}_\alpha^m$ with probability close to one. Then it is shown in Lemma 4 that replacing $f(x)$ by its piecewise constant approximation leads to an approximation error to the integral in (13) that goes like $O(m^{-d})$. This allows us to establish in Lemma 5 that the length of a MST spanning all points in B_n^m provides an estimate of $\int f^\nu(x)dx$. This result is then refined in Lemma 7 where it is shown that asymptotically the length of this MST increases at the same rate as the length of the k-MST spanning only $k = \lfloor \alpha n \rfloor$ of these points. It is then a simple matter to put Lemmas 5 and 7 together to prove Theorem 2.

Lemma 3: For given $\alpha \in [0,1]$ and a set of n i.i.d. points $\mathcal{X}_n = [x_1, \ldots, x_n]^T$ let B_n^m be the minimal cover of $\lfloor \alpha n \rfloor$ points with resolution-$1/m$ produced by the greedy subset selection algorithm. Then

$$P\left(\liminf_{n\to\infty} \{\mathcal{X}_n : B_n^m \in \mathcal{A}_\alpha^m\}\right) = 1.$$

Proof of Lemma 3

Define the m^d independent random variables $N_i = \mathrm{card}(\mathcal{X}_n \cap Q_i)$ of points in cell Q_i, $i = 1, \ldots, m^d$. By definition, the greedy algorithm gives a minimal cover $B_{\lfloor \alpha n \rfloor}^m$ containing at least αn points which satisfies the two conditions:

$$n^{-1} \sum_{i=1}^{\tilde{q}-1} N_{(i)} \quad < \quad \alpha \tag{24}$$

$$n^{-1} \sum_{i=1}^{\tilde{q}} N_{(i)} \quad \geq \quad \alpha. \tag{25}$$

Define $(i)_\varphi$ the index function which establishes a correspondance between rank ordered probabilities $\varphi_{(1)} \geq, \ldots, \geq \varphi_{(m^d)}$ and the cells Q_i which support each of these these probabilities: i.e. with this notation $P(x_i \in Q_{(i)_\varphi}) = \varphi_{(i)}$. For arbitrary $\epsilon > 0$ define the events $E_n(\epsilon)$ and F_n

$$E_n(\epsilon) \quad = \quad \left\{\mathcal{X}_n : n^{-1} \sum_{i=1}^{q-1} N_{(i)_\varphi} \leq \alpha - \epsilon\right\} \tag{26}$$

$$F_n \quad = \quad \left\{\mathcal{X}_n : n^{-1} \sum_{i=1}^{q} N_{(i)_\varphi} \geq \alpha\right\}. \tag{27}$$

Comparing these equations to (24) and (25) it will suffice to show $P(\liminf E_n \cap F_n) = 1$. Equivalently, since $P(\limsup E_n^c \cup F_n^c) \leq P(\limsup E_n^c) + P(\limsup F_n^c)$ we show that the latter two quantities are zero.

Define i.i.d. Bernouilli sequences $Y_n = \{y_1, \ldots, y_n\}$ and $Z_n = \{z_1, \ldots, z_n\}$ as

$$\begin{aligned} y_j &= I_{A_\alpha^m}(x_j) - I_{Q_{(q)_\varphi}}(x_j), \quad j = 1, \ldots, n \\ z_j &= I_{A_\alpha^m}(x_j), \quad j = 1, \ldots, n. \end{aligned}$$

and $p_y \stackrel{\mathrm{def}}{=} P(y_j = 1) = P(x_i \in A_\alpha^m) - P(x_i \in Q_{(q)_\varphi}) = \sum_{i=1}^{q-1} \varphi_{(i)}$ and $p_z \stackrel{\mathrm{def}}{=} P(z_j = 1) = P(x_i \in A_\alpha^m) = \sum_{i=1}^{q} \varphi_{(i)}$. Then we have the equivalent form for (26) and (27)

$$E_n(\epsilon) \quad = \quad \left\{Y_n : n^{-1} \sum_{j=1}^{n} y_j \leq \alpha - \epsilon\right\} \tag{28}$$

$$F_n \quad = \quad \left\{Z_n : n^{-1} \sum_{j=1}^{n} z_j \geq \alpha\right\}. \tag{29}$$

Let δ be defined as the smallest non-zero value of φ_i, $i = 1, \ldots, m^d$. Then by definition of A_α^m we have

$$p_y < \alpha \ \text{ and } \ p_z \geq \alpha + \delta. \tag{30}$$

From Sanov's theorem [39], [40]

$$\begin{aligned} P(E_n^c(\epsilon)) &\leq (n+1)^2 \exp\{-nK(\alpha - \epsilon, p_y)\} \\ P(F_n^c) &\leq (n+1)^2 \exp\{-nK(\alpha, p_z)\} \end{aligned}$$

where $K(p_1,p_2) = p_2 \ln p_1/p_2 + (1-p_2)\ln(1-p_2)/(1-p_1) \geq 0$ is the Kullback-Liebler distance between two Bernoulli probability distributions $\{p_1, 1-p_1\}$ and $\{p_2, 1-p_2\}$, $p_1, p_2 \in [0,1]$. Furthermore, from (30) and the fact that $K(p_1,p_2)$ is increasing in $|p_1-p_2|$, we have for $\epsilon < (\alpha - p_y)/2$

$$\begin{aligned} P(E_n^c(\epsilon)) &\leq (n+1)^2 \exp\{-nK(\alpha-\epsilon,\alpha)\} \\ P(F_n^c) &\leq (n+1)^2 \exp\{-nK(\alpha,\alpha+\delta)\}. \end{aligned}$$

It is easily verified that for any $\rho > 0$

$$\sum_{n=1}^{\infty}(n+1)^2 e^{-n\rho} \leq \int_0^{\infty}(u+2)^2 e^{-u\rho}du = C_\rho,$$

where $C_\rho = 2(2\rho^2+\rho+1)/\rho^3$. Hence,

$$\begin{aligned} \sum_{n=1}^{\infty} P(E_n^c(\epsilon)) &\leq C_{K(\alpha-\epsilon,\alpha)} < \infty \\ \sum_{n=1}^{\infty} P(F_n^c) &\leq C_{K(\alpha,\alpha+\delta)} < \infty, \end{aligned}$$

and by Borel-Cantelli we have $P(\limsup E_n^c(\epsilon)) = 0$, $P(\limsup F_n^c) = 0$ and the lemma follows. □

While $B^m_{\lfloor \alpha n \rfloor}$ does not necessarily converge to any fixed set as $n \to \infty$, the preceeding lemma establishes that it converges to the equivalence class of sets defined by $\mathcal{A}_\alpha^m$.

The next result relates the error of a blocked distribution approximation of $\int f^{(d-\gamma)/d}(x)dx$ to the total variation of f.

Lemma 4: For $\nu \in [0,1]$ let f^ν be of bounded variation over $[0,1]^d$ and denote by $v(A)$ its total variation over any subset $A \in [0,1]^d$. Define the resolution $1/m$ block density approximation $\tilde{f}(x) = \sum_{i=1}^{m^d} \theta_i I_{Q_i}(x)$ where $\theta_i = m^d \int_{Q_i} f(x)dx$. Then for any $A \in \sigma(\mathcal{Q}^m)$

$$0 \leq \int_A [\tilde{f}^\nu(x) - f^\nu(x)]dx \leq m^{-d}\sum_{i=1}^{m^d} v(Q_i \cap A).$$

Proof of Lemma 4

First note that as t^ν is a convex cap function, by Jensen's inequality $|C|^{-1}\int_C f^\nu(x)dx \leq \left(|C|^{-1}\int_C f(x)dx\right)^\nu$ for any Borel set C of positive volume $|C|$. The left side inequality of Lemma 4 now follows from the relation

$$\begin{aligned} &\int_A [\tilde{f}^\nu(x) - f^\nu(x)]dx \qquad (31) \\ &= m^{-d}\sum_{i:Q_i\cap A\neq\phi}^{m^d}\left[\left(m^d\int_{Q_i} f(x)dx\right)^\nu - m^d\int_{Q_i} f^\nu(x)dx\right]. \end{aligned}$$

We next deal with the right side of the inequality in Lemma 4. As functions of bounded variation are continuous except at possibly a countable number of points [37], by the mean value theorem for each Q_i there exist points $\xi_i \in Q_i$ and $\psi_i \in Q_i$ such that $\int_{Q_i} f(x)dx = f(\xi_i)m^{-d}$ and $\int_{Q_i} f^\nu(x)dx = f^\nu(\psi_i)m^{-d}$. Hence, using (31) and the definition (12) of v

$$\begin{aligned} &\left|\int_A [\tilde{f}^\nu(x) - f^\nu(x)]dx\right| \\ &= m^{-d}\left|\sum_{i:Q_i\cap A\neq\phi}(f^\nu(\xi_i) - f^\nu(\psi_i))\right| \\ &\leq m^{-d}\sum_{i:Q_i\cap A\neq\phi}|f^\nu(\xi_i) - f^\nu(\psi_i)| \\ &\leq m^{-d}\sum_{i:Q_i\cap A\neq\phi} v(Q_i) = m^{-d}\sum_{i=1}^{m^d} v(Q_i\cap A). \end{aligned}$$

This establishes the Lemma. □

Lemma 5: Assume f is of bounded total variation $v(Q_i)$ in each partition cell $Q_i \in \mathcal{Q}^m$. Let A be any set in the class $\mathcal{A}_\alpha^m$. Then for any quasi-additive functional $L_n(B^m_{\lfloor\alpha n\rfloor}) \stackrel{\text{def}}{=} L(\mathcal{X}_n \cap B^m_{\lfloor\alpha n\rfloor})$

$$\begin{aligned} &\limsup_{n\to\infty}\left|L_n(B^m_{\lfloor\alpha n\rfloor})/n^{(d-\gamma)/d} - \beta_{L,\gamma}\int_A f^{(d-\gamma)/d}(x)dx\right| \\ &< 2m^{-d}\beta_{L,\gamma}\sum_{i=1}^{m^d} v(Q_i\cap\partial\mathcal{A}_\alpha^m), \quad (a.s). \end{aligned}$$

Furthermore, this same bound holds when $L_n(B^m_{\lfloor\alpha n\rfloor})$ is replaced by $E[L_n(B^m_{\lfloor\alpha n\rfloor})]$.

The following follows directly from Theorem 1

Lemma 6: Assume the conditions of Theorem 1 and let A be an arbitrary Borel subset of $[0,1]^d$. Then for any quasi-additive functional $L_n(A) = L(\mathcal{X}_n \cap A)$

$$\lim_{n\to\infty} L_n(A)/n^{(d-\gamma)/d} = \beta_{L,\gamma}\int_A f^{(d-\gamma)/d}(x)dx, \quad (a.s.)$$

Furthermore, the above (a.s.) limit is the pointwise limit of $E[L_n(A)]/n^{(d-\gamma)/d}$ as $n \to \infty$.

Proof of Lemma 5

Let $\tilde{f}(x) = \sum_{i=1}^{m^d}\theta_i I_{Q_i}(x)$ be the blocked distribution approximation to $f(x)$ of Lemma 4. Now for any sets $A, A' \in \mathcal{A}_\alpha^m$ and $\nu = (d-\gamma)/d$, we have by the definitions (10), (11) of $\mathcal{A}_\alpha^m$, $\partial\mathcal{A}_\alpha^m$, and the triangle inequality

$$\begin{aligned} \left|\int_A f^\nu - \int_{A'} f^\nu\right| &= \left|\int_{A\cap\partial\mathcal{A}_\alpha^m} f^\nu - \int_{A'\cap\partial\mathcal{A}_\alpha^m} f^\nu\right| \\ &\leq \left|\int_{A\cap\partial\mathcal{A}_\alpha^m} f^\nu - \int_{A\cap\partial\mathcal{A}_\alpha^m} \tilde{f}^\nu\right| \\ &+ \left|\int_{A'\cap\partial\mathcal{A}_\alpha^m} f^\nu - \int_{A'\cap\partial\mathcal{A}_\alpha^m} \tilde{f}^\nu\right| \\ &+ \left|\int_{A\cap\partial\mathcal{A}_\alpha^m} \tilde{f}^\nu - \int_{A'\cap\partial\mathcal{A}_\alpha^m} \tilde{f}^\nu\right| \end{aligned}$$

By construction of $\mathcal{A}_\alpha^m$, the cell probabilities $\{\varphi_i\}_{i:Q_i\in A}$ and $\{\varphi_i\}_{i:Q_i\in A'}$ are identical so that the last term on the right side of the inequality is equal to zero. We therefore obtain by application of Lemma 4

$$\begin{aligned} \left|\int_A f^\nu - \int_{A'} f^\nu\right| &\leq 2\max_{A\in\mathcal{A}_\alpha^m} m^{-d}\sum_{i=1}^{m^d} v(Q_i\cap A\cap\partial\mathcal{A}_\alpha^m) \\ &\leq 2m^{-d}\sum_{i=1}^{m^d} v(Q_i\cap\partial\mathcal{A}_\alpha^m). \qquad (32) \end{aligned}$$

Next by Lemma 6 for any of the finite number of sets $A \in \mathcal{A}_\alpha^m$ and any $\epsilon > 0$ there exists an integer $n_0 = n_0(A)$ such that for all $n > n_0$

$$\left| L_n(A)/n^{(d-\gamma)/d} - \beta_{L,\gamma} \int_A f^{(d-\gamma)/d}(x)dx \right| \leq \epsilon, \quad (a.s.) \tag{33}$$

Let n_1 be defined as the largest of the $\{n_0(A)\}_{A \in \mathcal{A}_\alpha^m}$. By Lemma 3 there exists an integer n_2 such that for all $n > n_2$

$$\min_{A \in \mathcal{A}_\alpha^m} L_n(A) \leq L_n(B_{\lfloor \alpha n \rfloor}^m) \leq \max_{A \in \mathcal{A}_\alpha^m} L_n(A), \quad (a.s). \tag{34}$$

Now choosing $n_3 = \max(n_2, n_1)$ it follows from (33) and (34) that for all $n > n_3$

$$\begin{aligned} &\beta_{L,\gamma} \min_{A \in \mathcal{A}_\alpha^m} \int_A f^{(d-\gamma)/d}(x)dx - \epsilon \\ &\leq L_n(B_{\lfloor \alpha n \rfloor}^m)/n^{(d-\gamma)/d} \\ &\leq \beta_{L,\gamma} \max_{A \in \mathcal{A}_\alpha^m} \int_A f^{(d-\gamma)/d}(x)dx + \epsilon, \quad (a.s.). \end{aligned}$$

Applying the bound (32) we have for arbitrary $A \in \mathcal{A}_\alpha^m$ and all $n > n_3$

$$\begin{aligned} &\left| L_n(B_{\lfloor \alpha n \rfloor}^m)/n^{(d-\gamma)} d - \beta_{L,\gamma} \int_A f^{(d-\gamma)/d}(x)dx \right| \\ &\leq 2m^{-d} \beta_{L,\gamma} \sum_{i=1}^{m^d} v(Q_i \cap \partial \mathcal{A}_\alpha^m) + \epsilon, \quad (a.s.). \end{aligned}$$

Since ϵ is arbitrary the a.s. limit of Lemma 5 follows.

It remains to show that the same bound also holds for the limit $E[L_n(B_{\lfloor \alpha n \rfloor}^m)]/n^{(d-\gamma)/d}$. It follows from Lemmas 3 and 6 that for any $\epsilon > 0$ there exists n_o such that for $n > n_o$, $P(B_{\lfloor \alpha n \rfloor}^m \in \mathcal{A}_\alpha^m) \geq \epsilon$ and

$$\left| E[L_n(A)]/n^{(d-\gamma)/d} - \beta_{L,\gamma} \int_A f^{(d-\gamma)/d}(x)dx \right| \leq \epsilon$$

for any $A \in \mathcal{A}_\alpha^m$. Furthermore, as L_n is continuous it is bounded:

$$L_n(A) \leq C_3 \left(\text{card}(\mathcal{X}_n \cap A)\right)^{(d-\gamma)/d} \leq C_3 n^{(d-\gamma)/d}$$

and therefore for $n > n_o$

$$\begin{aligned} &\min_{A \in \mathcal{A}_\alpha^m} E[L_n(A)] - C_3 n^{(d-\gamma)/d} \epsilon \leq E[L_n(B_{\lfloor \alpha n \rfloor}^m)] \\ &\leq \max_{A \in \mathcal{A}_\alpha^m} E[L_n(A)] + C_3 n^{(d-\gamma)/d} \epsilon, \quad (a.s). \end{aligned}$$

Combining the above and again applying (32) yields for $n > n_o$

$$\begin{aligned} &\left| E[L_n(B_{\lfloor \alpha n \rfloor}^m)]/n^{(d-\gamma)/d} - \beta_{L,\gamma} \int_A f^{(d-\gamma)/d}(x)dx \right| \\ &< (1 + C_3)\epsilon + 2m^{-d} \beta_{L,\gamma} \sum_{i=1}^{m^d} v(Q_i \cap \partial \mathcal{A}_\alpha^m). \end{aligned}$$

Since ϵ is arbitrary we obtain the desired bound. □

We next extend Lemma 5 to a minimal graph constructed over any k points $\mathcal{X}_{n,k}$, e.g. $\mathcal{X}_{n,k}^{G_m}$, drawn from $B_{\lfloor \alpha n \rfloor}^m$.

Lemma 7: Let $\mathcal{X}_{n,\lfloor \alpha n \rfloor}$ be any $\lfloor \alpha n \rfloor$ points selected from $B_{\lfloor \alpha n \rfloor}^m$. Then, for any quasi-additive functional $L_n(B_{\lfloor \alpha n \rfloor}^m) \stackrel{\text{def}}{=} L_n(\mathcal{X}_n \cap B_{\lfloor \alpha n \rfloor}^m)$

$$\begin{aligned} &\limsup_{n \to \infty} \left| L_n(B_{\lfloor \alpha n \rfloor}^m) - L(\mathcal{X}_{n,\lfloor \alpha n \rfloor}) \right| / n^{(d-\gamma)/d} \\ &< C_3 (p_{\mathcal{A}_\alpha^m} - \alpha)^{(d-\gamma)/d}, \quad (a.s.) \end{aligned}$$

and

$$\begin{aligned} &\limsup_{n \to \infty} \left| E[L_n(B_{\lfloor \alpha n \rfloor}^m) - E[L(\mathcal{X}_{n,\lfloor \alpha n \rfloor})] \right| / n^{(d-\gamma)/d} \\ &< C_3 (p_{\mathcal{A}_\alpha^m} - \alpha)^{(d-\gamma)/d}, \end{aligned}$$

where $p_{\mathcal{A}_\alpha^m} = P(A_\alpha^m)$ is the coverage probability of sets A_α^m in $\mathcal{A}_\alpha^m$.

Proof of Lemma 7

Firstly, note that from continuity of L and the fact that $\alpha n - 1 \leq \lfloor \alpha n \rfloor \leq \alpha n$

$$\begin{aligned} &\left| L_n(B_{\lfloor \alpha n \rfloor}^m) - L(\mathcal{X}_{n,\lfloor \alpha n \rfloor}) \right| / n^{(d-\gamma)/d} \\ &\leq C_3 \left[\frac{\text{card}\left(B_{\lfloor \alpha n \rfloor}^m\right) - \lfloor \alpha n \rfloor}{n} \right]^{(d-\gamma)/d} \\ &\leq C_3 \left[n^{-1} \text{card}\left(B_{\lfloor \alpha n \rfloor}^m\right) - \alpha \right]^{(d-\gamma)/d} + C_3 n^{-(d-\gamma)/d}. \end{aligned} \tag{35}$$

Next we establish an a.s. limit for the first additive term on the right side. Lemma 3 guarantees that there exists an n_0 such that $B_{\lfloor \alpha n \rfloor}^m \in \mathcal{A}_\alpha^m$ with probability arbitrarily close to one. Therefore, for $n > n_o$ and for any $\epsilon > 0$, by Sanov's theorem we have

$$\begin{aligned} &P\left(n^{-1} \text{card}(\mathcal{X}_n \cap B_{\lfloor \alpha n \rfloor}^m) - \alpha \geq \epsilon\right) \\ &= P\left(n^{-1} \sum_{i=1}^n z_i \geq \epsilon + \alpha\right) \\ &\leq (n+1)^2 \exp\left\{-nK(\epsilon + \alpha, p_{\mathcal{A}_\alpha^m})\right\} \end{aligned}$$

where z_j's are i.i.d. Bernoulli random variables with $P(z_j = 1) = p_{\mathcal{A}_\alpha^m} = \sum_{i=1}^q \varphi_{(i)}$, as defined in the proof of Lemma 3. Now $\rho \stackrel{\text{def}}{=} K(\epsilon + \alpha, p_{\mathcal{A}_\alpha^m}) > 0$ for any $\epsilon > p_{\mathcal{A}_\alpha^m} - \alpha$ and therefore, since $\sum_{n > n_o} (n+1)^2 \exp^{-n\rho} \leq 2(2\rho^2 + \rho + 1)/\rho^3 < \infty$, by Borel-Cantelli we have

$$P\left(\limsup \left\{\mathcal{X}_n : n^{-1} \text{card}(\mathcal{X}_n \cap B_{\lfloor \alpha n \rfloor}^m) - \alpha \geq p_{\mathcal{A}_\alpha^m} - \alpha\right\}\right) = 0. \tag{36}$$

Since $C_3 n^{-(d-\gamma)/d}$ converges pointwise to zero as $n \to \infty$, the a.s. limit in the Lemma follows directly from (36) and (35).

Finally, as in the proof of 5, it can be shown that since $L(\mathcal{X}_n \cap B_{\lfloor \alpha n \rfloor}^m) - L(\mathcal{X}_{n,\lfloor \alpha n \rfloor})$ is bounded, $EL(\mathcal{X}_n \cap B_{\lfloor \alpha n \rfloor}^m) - EL(\mathcal{X}_{n,\lfloor \alpha n \rfloor}]$ satisfies the same asymptotic properties. □

We now have all the ingredients for the proof of Theorem 2.

Proof of Theorem 2

Combining Lemmas 5 and 7 and applying the triangle inequality we see that there exists an integer n_o such that for all $n > n_o$

$$\begin{aligned} &\left| L(\mathcal{X}_{n,\lfloor \alpha n \rfloor})/n^{(d-\gamma)/d} - \beta_{L,\gamma} \int_{A_\alpha^m} \tilde{f}^{(d-\gamma)/d}(x)dx \right| \\ &< 2m^{-d} \beta_{L,\gamma} \sum_{i=1}^{m^d} v(Q_i \cap \partial \mathcal{A}_\alpha^m) + C_3 (p_{\mathcal{A}_\alpha^m} - \alpha)^{(d-\gamma)/d}, \quad (a.s.) \end{aligned}$$

where A_α^m is any set in the class $\mathcal{A}_\alpha^m$.

It remains to show that $\delta = O(m^{\gamma-d})$. For this we recall as in the proof of Lemma 3 that the coverage probability of any set $A \in \mathcal{A}_\alpha^m$ is a sum of the rank ordered cell probabilities $P(Q_{(i)}) = \varphi_{(i)}$, $i = 1, \ldots, q$, where $\sum_{i=1}^{q-1} \varphi_{(i)} < \alpha$ and $\sum_{i=1}^{q} \varphi_{(i)} \geq \alpha$, and therefore

$$0 \leq P(A_\alpha^m) - \alpha \quad = \quad \sum_{i=1}^{q} \varphi_{(i)} - \alpha \leq \varphi_{(q)} = \int_{Q_{(q)}} f(x)dx = m^{-d} f(\xi)$$

where, by the mean value theorem, ξ is a point in $Q_{(q)}$. This gives the order $m^{\gamma-d}$ bound on the second additive term in δ of Theorem 2

$$0 \leq C_3(p_{\mathcal{A}_\alpha^m} - \alpha)^{(d-\gamma)/d} \leq C_3 m^{\gamma-d} \sup_{x \in Q_i} f^{(d-\gamma)/d}(x). \tag{37}$$

Since $\sup_{x\in Q_i} f^{(d-\gamma)/d}(x) \leq v([0,1]^d)$ and $\sum_{i=1}^{m^d} v(Q_i \cap \partial\mathcal{A}_\alpha^m) \leq v([0,1]^d)$ and $v([0,1]^d) < \infty$, Theorem 2 is established. □

□

VI. Examples

We first assume that f is a uniform density over the d-dimensional unit sphere $S(0,1)^d$. It is obvious that for $\alpha \in [0,1]$ a Borel subset A_o which minimizes Rényi entropy is

$$A_o = \left\{ x : \|x\| \leq \left(\frac{\alpha}{|S(0,1)^d|} \right)^{\frac{1}{d}} \right\}$$

and the associated minimum entropy conditional density is

$$f(x|A_o) = \left\{ \begin{array}{ll} \frac{1}{\alpha}, & x \in A_o \\ 0, & o.w. \end{array} \right.$$

By Theorem 2 $L(\mathcal{X}_{n.\lfloor\alpha n\rfloor}^{G_m})/n^{(d-\gamma)/d}$ converges a.s. to a linear function of α

$$\beta_{L,\gamma} \int f^{(d-\gamma)/d}(x|A_o)dx = \alpha \cdot \beta_{L,\gamma}.$$

Next assume that f is a multivariate Gaussian density with mean μ and covariance $\sigma^2 I$ on $\mathbb{R}^d$. Note that, unlike the previous example, the support of f is $\mathbb{R}^d$ which is not compact and cannot be mapped into $[0,1]^d$. However, in practice the range is finite and we can approximate by a truncated Gaussian density with compact support. The minimum entropy set for this case is

$$A_o = \left\{ x : \|x\| \leq \sigma \sqrt{Q_{\chi^2}^{-1}(\alpha; d)} \right\}$$

where $Q_{\chi^2}^{-1}(\cdot; d)$ is the quantile function of a Chi-squared density with d degrees of freedom. The associated conditional density is

$$f(x|A_o) = \left\{ \begin{array}{cc} \frac{1}{\alpha(2\pi\sigma)^{d/2}} e^{-\frac{\|x\|^2}{2\sigma^2}}, & x \in A_o \\ 0, & o.w. \end{array} \right. .$$

and $L(\mathcal{X}_n^{G_m})/n^{(d-\gamma)/d}$ converges a.s. to the non-linear function of α

$$\beta_{L,\gamma} \int f^{(d-\gamma)/d}(x|A_0)dx = Q_{\chi^2}(\nu Q_{\chi^2}^{-1}(\alpha; d)) \cdot (2\pi\sigma)^{\frac{\gamma}{2d}} \beta_{L,\gamma}$$

where $\nu = (d-\gamma)/d$.

These two examples suggest that the greedy k-point graph can be effectively used to discriminate between uniform and non-uniform densities based on plots of $L(\mathcal{X}_n^{G_m})/n^{(d-\gamma)/d}$ as a function of α.

VII. Influence Functions

Influence functions have been used to study quantitative robustness of estimators to outliers and other contaminating densities for over thirty years [41]. These functions provide a quantitative measure of outlier sensitivity of an estimator. An unbounded influence curve implies that the effect of an outlier on the estimator can be very severe. Robust estimators, such as the trimmed mean estimator which rejects observations which exceed a given sample quantile, have bounded influence curves (see Figure 4).

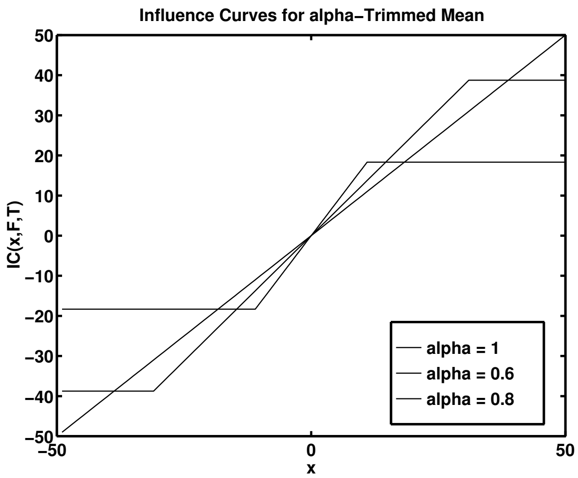

Fig. 4. *2in*

Trimmed mean influence curves for one dimesnsional observations and various trimming proportions $1-\alpha$. The trimmed mean estimator is a rank order statistic which robsutifies the sample mean estimate by rejecting all samples whose values exceed either of the sample quantiles $1-\alpha/2$ and $\alpha/2$.

Here we give the influence function for the normalized greedy minimal k-point graph weight $L(\mathcal{X}_{n,k}^{G_m})/(\lfloor\alpha n\rfloor)^{(d-\gamma)/d}$ described in Section IV. The influence function motivates the use of the weight function as a robust estimator of the entropy of a nominal density f_1 in the mixture model $f = (1-\epsilon) + f_1\epsilon$. It also establishes a kind of outlier robustness which is similar to that of rank order statistics for one dimensional observations. Finally, it gives an asymptotic approximation to the variance of $L(\mathcal{X}_{n,\lfloor\alpha n\rfloor}^{G_m})/(\lfloor\alpha n\rfloor)^{(d-\gamma)/d}$ which can be used to construct confidence intervals on finite sample accuracy.

Let P_n be the empirical distribution function of the n samples $\mathcal{X}_n = \{x_1, \ldots, x_n\}$

$$P_n(A) \stackrel{\text{def}}{=} \frac{1}{n} \int_A I_{x_i}(x)dx$$

for arbitrary Borel set A. For any statistic $T_n = T(P_n)$ converging a.s. to $T = T(P)$ the influence function (called an influence curve for one dimensional samples x_i) is defined as [42]

$$\text{IC}(x_o) = \lim_{s\to 0} \frac{T(\,(1-s)P + s\delta_{x_o}) - T(P)}{s}. \tag{38}$$

where δ_{x_o} is a concentrated distribution centered at $x_o \in \mathbb{R}^d$ and $s \in [0,1]$. For small s, $(1-s)P + s\delta_{x_o}$ is interpreted as a perturbed distribution resulting from exchanging sn of the n samples x_i from distribution P with sn samples from the concentrated distribution δ_{x_o}. Thus $\mathrm{IC}(x_o)$ can be used to probe the asymptotic sensitivity of the estimator T_n to localized perturbations of P.

The influence function can also be used to approximate asymptotic estimator variance [42] via the formula

$$n\mathrm{var}(T_n) \;\to\; \int \mathrm{IC}^2(x) f(x)dx$$

Now identifying $T_n = L^{G_m}_{n,\lfloor\alpha n\rfloor}/(\lfloor\alpha n\rfloor)^{(d-\gamma)/d}$ we have by Theorem 3 that T_n converges a.s. to the integral (17) which we thus identify as $T(P)$.

In the Appendix (Lemma 8) we show that $\mathrm{IC}(x_o)$ has the following form for densities f having no flat spots (cf Remark 2 of Section IV)

$$\mathrm{IC} = \beta_{L,\gamma} \left\{ \begin{array}{ll} \frac{\alpha-1}{\alpha^\nu}\zeta(\alpha) - \nu\int f^\nu(x|A_o)dx + \frac{\nu}{\alpha} f^{\nu-1}(x_o|A_o), & x_o \in A_o \\ \frac{\alpha}{\alpha^\nu}\zeta(\alpha) - \nu\int f^\nu(x|A_o)dx, & x_o \notin A_o \end{array} \right. \tag{39}$$

where ζ is a non-negative function and $A_o = \{x : f(x) \geq \eta\}$ is the entropy minimizing set of probability α.

Note that the influence function (39) may take on positive or negative values for x_o inside of A_o while it takes on positive values outside of A_o (observe that $f^{1-\nu} = f^{-|\nu-1|}$ increases without bound if the tails of f decreases to zero). This can be explained as follows. By the theory developed in the Section IV we know that asymptotically the minimal k-point graph spans all points within A_o and none of the points outside of A_o. Therefore exchanging a small number of vertices of the k-point graph within A_o with a small number of points outside of A_o necessarily increases the overall weight of the graph. On the other hand, the value of IC on the interior of A_o corresponds to the effect on the weight due to perturbing the locations of a small number of vertices. Thus, depending on the direction of these perturbations the weight of the graph can either increase or decrease.

We illustrate these phenomena in Figure 5 where IC is plotted as a function of $x_o \in \mathbb{R}^2$ for the case of the bivariate Gaussian distribution considered in the previous subsection. Two cases are shown, the figure on the left is the influence function for $\alpha = 1$, i.e., for the minimal graph spanning all points (labeled MST), and the figure on the right is for $\alpha = 0.8$, i.e. for the minimal k-point graph (labeled k-MST) spanning only 80% of the n points. Note that, as expected, the influence function is bounded for the k-point graph but unbounded for the graph spanning all n points. This suggests that the greedy k-point minimal graph is a natural multi-dimensional extension of rank order statistical methods such as the trimmed mean. This complements the comments of Friedman and Rafsky [27] in which they proposed the MST as a natural generalization of one dimensional rank order statistical tests of Smirnov and Wald Wolfowitz.

VIII. Conclusion

We have given strong asymptotic convergence results for greedy approximations to minimal k-point graphs. These convergence results indicate that the weight function of minimal k-point graphs provide natural extensions of one dimensional rank order statistics to multiple dimensions. Our results also provide an interesting alternative to kernel or histogram methods of entropy estimation. In addition to this and other applications mentioned in the introduction of this paper, our results can also be applied to robustification of minimal graph methods proposed for pattern recognition [28], exploratory non-linear regression [43], clustering [29], and testing for randomness [31].

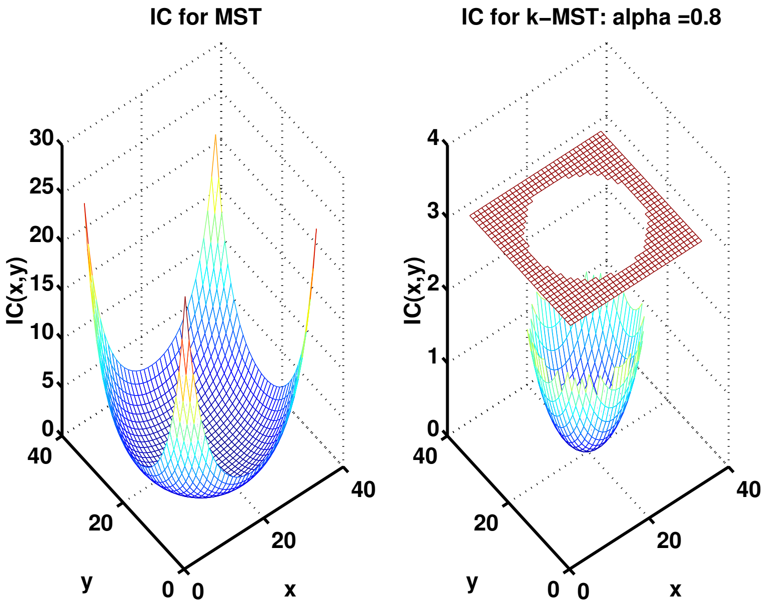

Fig. 5. *MST and k-MST influence curves for bivariate Gaussian density on the plane.*

IX. Appendix

For $\nu \in (0,1]$ define the function

$$g_\nu(\eta) = \int_{\{x: f(x)\geq\eta\}} f^\nu(x)dx. \tag{40}$$

Note that when A_o is the minimum entropy subset of probability α defined in (22) then $g_\nu(\eta) = \int_{A_o} f^\nu(x)dx$ and $g_1(\eta) = P(A_o) = \alpha$.

Lemma 8: Let f be a Lebesgue density over $\mathbb{R}^d$ and assume that for any $a > 0$ the set $\{x : f(x) = a\}$ has measure zero. Assume α, η have the relation $\alpha = g_1(\eta)$. Let δ_{x_o} be a uniform distribution over a hypercube with center x_o and volume Δ^d, where Δ is smaller than the modulus of continuity of f. Then the influence function (38) of $T_n = L(\mathcal{X}^{G_m}_{n,\lfloor\alpha n\rfloor})/(\lfloor\alpha n\rfloor)^{(d-\gamma)/d}$ has the form

$$\mathrm{IC}(x_o) = \tag{41}$$
$$\beta_{L,\gamma} \left\{ \begin{array}{ll} \frac{\alpha-1}{\alpha^\nu}\zeta(\alpha) - \nu\int f^\nu(x|A_o) + \frac{\nu}{\alpha} f^{\nu-1}(x_o|A_o), & x_o \in A_o \\ \frac{\alpha}{\alpha^\nu}\zeta(\alpha) - \nu\int f^\nu(x|A_o)dx, & x_o \notin A_o \end{array} \right.$$

where $\nu = (d-\gamma)/d$,

$$\zeta(\alpha) = \frac{g'_\nu\left(g_1^{-1}(\alpha)\right)}{g'_1\left(g_1^{-1}(\alpha)\right)}$$

is non-negative and $A_o = \{x : f(x) \geq \eta\}$ is the entropy minimizing set of probability α.

Proof of Lemma 8

First we define an entropy minimizing set A_s of probability α analogously to definition (22) of A_o

$$A_s = \{x : f_s \geq \eta\}$$

where η satisfies

$$\int_{A_s} f_s = \alpha. \tag{42}$$

Using $f_s = (1-s)f + s\delta_{x_o}$ this latter relation implies

$$\begin{aligned} \alpha &= (1-s)\int_{A_s} f + s\int_{A_s} \\ &= \begin{cases} (1-s)\int_{A_s} f + s, & (1-s)f(x_o) + s\Delta^{-d} \geq \eta \\ (1-s)\int_{A_s} f, & o.w. \end{cases} . \end{aligned}$$

Therefore

$$\int_{A_s} f = \begin{cases} \frac{\alpha-s}{1-s}, & (1-s)f(x_o) + s\Delta^{-d} \geq \eta \\ \frac{\alpha}{1-s}, & o.w. \end{cases} . \tag{43}$$

On the other hand, using the definition $g_1(a) = \int_{\{x: f(x)\geq a\}} f$ and the assumption that Δ is less than the modulus of continuity of f, which implies that over the support of δ_{x_o} the density $f(x) \approx f(x_o)$, it is seen that

$$\int_{A_s} f = \tag{44}$$

$$\begin{cases} g_1(\eta/(1-s)) + \Delta^d f(x_o), & 0 < \eta - (1-s)f(x_o) \leq s\Delta^{-d} \\ g_1(\eta/(1-s)), & o.w. \end{cases} .$$

Hence, combining (43) and (44) we have an equation for the threshold $\eta = \eta(s)$ which guarantees (42)

$$\eta = \tag{45}$$

$$\begin{cases} (1-s)g_1^{-1}\left(\frac{\alpha-s}{1-s} - \Delta^d f(x_o)\right), & 0 < \eta - (1-s)f(x_o) \leq s\Delta^{-d} \\ (1-s)g_1^{-1}\left(\frac{\alpha-s}{1-s}\right), & (1-s)f(x_o) \geq \eta \\ (1-s)g_1^{-1}\left(\frac{\alpha}{1-s}\right), & o.w. \end{cases} .$$

where we have used the obvious fact that, as $\{x : f(x) = a\}$, $a > 0$, has measure zero, $g_1(a)$ is strictly monotone decreasing and thus has an inverse $g_1^{-1}(b)$.

Next we express $\int_{A_s} f_s^\nu$ to order $o(s)$

$$\int_{A_s} f_s^\nu = \int_{A_s} f^\nu + s\nu \int_{A_s} (\delta_{x_o} - f) f^{\nu-1} + o(s),$$

and note the following identities

$$\int_{A_s} f^\nu$$

$$= \begin{cases} g_\nu\left(\eta/(1-s)\right) + \Delta^{-d\nu} f^\nu(x_o), & 0 < \eta - (1-s)f(x_o) \leq s\Delta^{-d} \\ g_\nu\left(\eta/(1-s)\right), & o.w. \end{cases} .$$

$$\int_{A_s} \delta_{x_o} f^{\nu-1} = \begin{cases} f^{\nu-1}(x_o), & (1-s)f(x_o) + s\Delta^{-d} \geq \eta \\ 0, & o.w. \end{cases} . \tag{46}$$

To simplify the notation we define the partition E_0, E_1, E_2 of $\mathbb{R}^d$

$$\begin{aligned} E_0(s) &= \{x : 0 < \eta - (1-s)f(x) \leq s\Delta^{-d}\} \\ E_1(s) &= \{x : (1-s)f(x) \geq \eta\} \\ E_2(s) &= \{x : (1-s)f(x) + s\Delta^{-d} < \eta\}. \end{aligned}$$

Putting (46) and (46) together and using (45) we obtain

$$\begin{aligned} \int_{A_s} f_s^\nu = (1-s\nu)g_\nu &\left(g_1^{-1}\left(\frac{\alpha-s}{1-s} - \Delta^{-d} f(x_o) I_{E_0}(x_o)\right.\right. \\ &+ \left.\left.\frac{s}{1-s} I_{E_2}(x_0)\right)\right) + s\nu f^{\nu-1}(x_o) I_{E_0 \cup E_1}(x_o) \\ &+ \Delta^{-d\nu} f^\nu(x_o) I_{E_0}(x_o) + o(s) \end{aligned} \tag{47}$$

To compute $\mathrm{IC}(x_o)$ it remains to evaluate the limit

$$\begin{aligned} \mathrm{IC}(x_o)/\beta_{L,\gamma} &= \lim_{s\downarrow 0} \frac{1}{s}\left[\int f_s^\nu(x|A_s)dx - \int f^\nu(x|A_o)dx\right] \\ &= \frac{1}{\alpha^\nu} \cdot \lim_{s\downarrow 0} \frac{1}{s}\left[\int_{A_s} f_s^\nu(x)dx - \int_{A_o} f^\nu(x)dx\right] \end{aligned} \tag{48}$$

First observe that $E_0 = E_0(s)$ converges to the empty set as $s \to 0$. Hence, in what follows we can safely neglect terms in (47) which are multiplied by I_{E_0}. Next observe that, as $\{x : f(x) = a\}$ has measure zero g_v, g_1 and g_1^{-1} are differentiable a.e. Furthermore, applying the chain rule to the identity $g_1(g_1^{-1}(q(s))) = q(s)$, for any differentiable function $q(s)$

$$\frac{d}{ds} g_1^{-1}(q(s)) = q'(s)/g_1'(g_1^{-1}(q(s))).$$

Identifying $q(s) = (\alpha-s)/(1-s)$ over $E_1(s)$ and $q(s) = \alpha/(1-s)$ over $E_2(s)$, observing that $E_1(0) = A_o$ and $E_2(0) = A_o^c$, and $o(s)/s \to 0$, it can be verified after some algebra that the limit (48) takes the form

$$\begin{aligned} \mathrm{IC}(x_o)/\beta_{L,\gamma} = \frac{1}{\alpha^\nu} &\frac{g_\nu'\left(g_1^{-1}(\alpha)\right)}{g_1'\left(g_1^{-1}(\alpha)\right)} \cdot \left[(\alpha-1)I_{A_o}(x_o) + \alpha I_{A_o^c}(x_o)\right] \\ &- \frac{\nu}{\alpha^\nu} g_\nu\left(g^{-1}(\alpha)\right) + \frac{\nu}{\alpha^\nu} f^{\nu-1}(x_o) I_{A_o}(x_o) \end{aligned}$$

Finally, using $g_\nu\left(g^{-1}(\alpha)\right) = \int_{A_o} f^\nu$ and the definition of the conditional density $f(x|A_o)$ we obtain the assertion of Lemma 8.

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