Problems in Extremal and Combinatorial Geometry

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Dedications

To Mom and Dad, for all their love, support, and patience over the years.

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Abstract

Problems in Extremal and Combinatorial Geometry

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This thesis deals with three families of optimization problems: (1) Euclidean optimization problems on random point sets; (2) independent sets in hypergraphs; and (3) packings in point lattices. First, we consider bounds on several monochromatic and bichromatic optimization problems including minimum matching, minimum spanning trees, and the travelling salesman problem. Many of these problems lend themselves to representations in terms of *hierarchically separated trees* — trees with uniform branching factor and depth, and having edge weights exponential in the depth of the edge in the tree. In the second part, we consider the independent set problem on uniform hypergraphs, in anticipation of applying it to the third part, packing problems on point lattices. In these problems we wish to select a subset of points from an $n \times n \times ... \times n$ grid avoiding particular patterns. We also study several generalizations of these problems that have not been handled previously.

1. Introduction

This thesis covers three fields in discrete and computational geometry: (1) the behavior of Euclidean optimization problems on random point sets; (2) graph and hypergraph theory; and (3) packing problems in point lattices. We review each of these fields in turn.

1.1 Optimization problems on Euclidean sets and hierarchically separated trees

Euclidean optimization problems are of interest to many real-world applications, such as routing and transportation. Although worst-case bounds are useful, for many problems the expected bound is a better indicator of the overall behavior of the algorithm[1] — even more so if we can show that the variance is small, so that the results are tightly concentrated around the mean. When such concentration holds, derandomization of these results can provide a fast deterministic algorithm that, although having a poor worst-case bound, provides good results with overwhelming probability.

Let us consider, as a first example, the travelling salesman problem (TSP) on the d-dimensional unit hypercube $[0,1]^d$: given a point set $\{x_1, \ldots, x_n\} \subseteq [0,1]^d$, the TSP asks for the route of shortest distance that starts at x_1, visits all the other points exactly once, and returns to x_1. Beardwood, Halton and Hammersley's landmark result [10] showed that for the TSP functional T on i.i.d. random variables $X_i \in [0,1]^d$,

$$\lim_{n\to\infty} \frac{T(X_1, X_2, \ldots, X_n)}{n^{(d-1)/d}} = \alpha(T,d) \cdot \int_{[0,1]^d} f(x)^{(d-1)/d}\, dx$$

[1] Hoare's quicksort is a good example: its expected running time is $\Theta(n \log n)$ but its worst case is $\Theta(n^2)$.

almost surely, where $\alpha(T, d)$ is a constant depending on d, and $f(x)$ is the c.d.f. of the continuous part of the distribution of the X_i's. The integral is maximized (and in fact evaluates to 1) when the X_i's obey a uniform distribution.[2] Rhee [38] later extended this result to apply to the minimum matching functional and shows complete convergence (instead of almost sure convergence) for minimum matchings and for the TSP; in [39] she showed how to extend the result to cover unbounded distributions over the entire space $\mathbb{R}^d$.

Yukich [58] uses the relationships between smooth subadditive Euclidean functionals and their corresponding superadditive *boundary functionals*, introduced by Redmond in his dissertation [37]. In the boundary version of the TSP, the boundary of the hypercube is treated as a "highway" on which travel costs nothing; it is clear that the optimal solution to the boundary TSP is less than the optimal solution of the ordinary TSP. Similar boundary versions can be defined for other Euclidean functionals as well. By relating a wide class of Euclidean functionals to their respective boundary versions, Yukich generalized these results into his "umbrella theorem":

Theorem 1.1 (Yukich) *If L^p is a subadditive Euclidean functional and is close in mean to a superadditive Euclidean functional L^p_B, both smooth of order p; if $1 \leq p < d$; and if $d \geq 2$; then*

$$\lim_{n\to\infty} \frac{L^p(X_1, X_2, \ldots, X_n)}{n^{(d-p)/d}} = \alpha(L^p, d) \cdot \int_{[0,1]^d} f(x)^{(d-p)/d}\, dx$$

with complete convergence.

Here $\alpha(L^p, d)$ is a constant depending on d, p, and the functional L; and L^p denotes the sum of the p-th powers of each edge. Yukich also strengthened this result to handle distributions on unbounded subsets of $\mathbb{R}^d$.

[2] Intuitively, this is to be expected; if the distribution is biased toward one region of the hypercube, we expect more of the points to fall there, shortening the length of the average optimal tour.

The problems whose functionals satisfy the hypothesis of the theorem include the TSP, the minimum spanning tree (MST) problem, and the minimum matching problem (MMP). We will have more to say about these problems later, but for now we give quick definitions of the latter two. Given a set of points $\{x_1, \ldots, x_n\}$, the MST is the minimum weight graph that connects the points, where the edge between two points is weighted by Euclidean distance. The minimum matching (when n is even) is a pairing of these points that minimizes the sum of the distances between each pair.

Yukich [58] provides an additional reason to care about the *expected* behavior of these optimization problems. Suppose that for a given n, we wish to find a set of n points in $[0, 1]^d$ that maximizes the cost of the solution to the TSP (or to another problem). In general this is hard to solve; but it turns out that for many problems, the cost is of the same order of magnitude as the expected cost for a randomly chosen point set. We thereby see that the expected behavior of these problems provides insight into their worst-case behavior.

In a different direction, Ajtai, Komlós, and Tusnády [3] considered the bichromatic matching problem, which is to minimize the expected matching cost between two randomly chosen point sets $R = \{r_1, \ldots, r_n\} \subseteq \mathbb{R}^d$ and $B = \{b_1, \ldots, b_n\} \subseteq \mathbb{R}^d$. Here each red point is matched to a unique blue point; the cost of the matching is the sum of the distance between each red point and its matched blue point.[3] Leighton and Shor [31] analyzed the problem of minimizing the *maximum* distance in the matching instead of the sum of the distances (similar to the distinction between the L_1 and L_∞ norms). Much later, Abrahamson, Csaba, and Shokoufandeh [1, 2] rederived some of the results of [3] using *hierarchically separated trees* (HSTs), trees with a regular

[3]This distance is sometimes called the *earth mover's distance* (EMD), where the points of R are analogized to mounds of earth (here of the same size) and the points of B represent holes that will hold them.

structure and regular edge weights. (The HST was introduced by Bartal [8].) For the bichromatic matching problem on $[0,1]^d$ for $d \neq 2$, they were able to derive upper bounds identical to those of [3].

In this thesis, we will extend their results to cover the expected costs of an optimal matching or Hamiltonian tour on HSTs; we will consider monochromatic and bichromatic versions of both these problems, as well as the monochromatic matching problem. We also offer concentration results for the monochromatic problems. We anticipate that these results will be useful to others in the future, since many optimization problems can be reduced to problems on HSTs. To demonstrate, we will apply these bounds to derive previously unknown bounds on the costs of the bichromatic minimum spanning tree problem and TSP in high-dimensional Euclidean hypercubes $[0,1]^d$.

1.2 Independent sets in graphs and hypergraphs

We now turn to graph theory, before returning later to geometry proper. There is a rich history of interplay between geometric problems and problems in graph theory; see Bárány [7] for a survey. It happens often that the constraints of a geometric problem can be encoded into a graph, onto which all the tools of graph theory can then be brought to bear. We will demonstrate the reduction of several lattice-point packing problems to the *independent set problem* on uniform hypergraphs. The reduction is fairly natural: many problems dealing with conflicts between elements of a set can be recast as independent set problems on suitably defined hypergraphs.

After carrying out the reduction, we must then determine the independence number of the graph, either by algorithmic means (constructing an independent set) or by bounding the independence number (finding an expression for it). The independent set problem is, like many (hyper)graph problems, NP-hard — assuming P $\neq$

NP, a polynomial-time algorithm can only provide a good solution that is not necessarily optimal. For completeness, we mention that the TSP is also NP-hard; several constant-factor approximation algorithms exist for the TSP, and we will examine two of these in Chapter 4.

For independent sets, the situation is different: the best-known general bound on the independence number is given by probabilistic methods. For some problems, it happens that a randomly chosen configuration often provides a good solution; if the expected value is sufficient, we can take advantage of the linearity of expectation to generate a solution that achieves this expected value. This strategy is called *E-M*, meaning *expectation maximization* in maximization problems and *expectation minimization* in minimization problems. We give an example of this process in Chapter 4, where we demonstrate the derandomization of a probabilistic result of Caro and Wei [13, 56] on the independence number of a graph.

Their result is related to Turán's famous theorem [55]. Let us define the (n, k) Turán graph $\mathcal{T}(n, k)$ to be the complete k-partite graph on n vertices where the division of the vertices into k classes is as equal as possible. Turán proved

Theorem 1.2 (Turán [55]) *Of all the graphs on n vertices not containing a subgraph isomorphic to K_{k+1}, the graph $\mathcal{T}(n, k)$ has the smallest independence number, namely $\lceil n/k \rceil$; and every such graph with the same independence number is isomorphic to $\mathcal{T}(n, k)$.*

Equivalently,

Theorem 1.3 (Turán [55]) *The independence number of a graph on n vertices with average degree δ is at least $n/(\delta + 1)$.*

Turán's paper actually proved Theorem 1.2, but many people also refer to Theorem 1.3 as Turán's theorem.

Extensions of Caro and Wei's theorem due to Caro and Tuza [14] and to Thiele [54] provide a generalization of the E-M algorithm to K-uniform hypergraphs; in Chapter 5, we will use their bounds to improve bounds on some high-dimensional lattice-point packing problems. We also have novel results to report, Theorems 4.13 and 4.17, that follow from the Caro-Tuza bound.

1.3 Lattice packing problems

Our final topic in this thesis is packing problems on lattice points. A *lattice* in d dimensions is a point set of the form $A \cdot \mathbb{Z}^d$ where A is a $d \times d$ nonsingular matrix. In this thesis we will normally be concerned with the *square lattice* $\mathbb{Z}^d$ and subsets thereof; this is what we will mean when we speak of "the" lattice. Another frequently encountered type of lattice is the triangular lattice, generated by setting $A = \begin{bmatrix} 1 & 1/2 \\ 0 & \sqrt{3}/2 \end{bmatrix}$ (or a multiple); this lattice resembles a tessellation of the plane by triangles. The *d-dimensional lattice of width n* is the set $\{1, \ldots, n\}^d$. The two-dimensional lattice turns up in many bounds involving planar point sets in $\mathbb{R}^d$ (that is, questions involving points with *real* coordinates, not just integer coordinates). We briefly describe some of these problems.

The Heilbronn triangle problem [42] asks how to place n points inside the unit square $[0, 1]^2$ in a way that maximizes the minimum area of the $\binom{n}{3}$ triangles so formed. Heilbronn believed the maximum to be c/n^2, which is obtainable with a simple modular construction on lattice points (see Section 5.2). To the contrary, Komlós, Pintz, and Szemerédi [29] proved a lower bound of $\Omega(\log n/n^2)$ using a probabilistic construction.

A question of Erdős asked for the maximum number of incidences between n points and m lines in the plane. The famous Szemerédi-Trotter theorem [50] bounds this number from above by $O(n^{2/3}m^{2/3} + n + m)$. This bound is in fact attained by taking a $\lfloor\sqrt{n}\rfloor \times \lfloor\sqrt{n}\rfloor$ lattice and drawing m lines in such a way that maximizes the point incidences on each line.

Another problem considered by Erdős [20] was that of finding the maximum number of pairs of n points that can lie a unit distance apart. A scaled version of the square lattice gives a lower bound of $ne^{c\log n/\log\log n}$, which is believed to be tight. The best known upper bound is $O(n^{4/3})$, first proved by Spencer, Szemerédi, and Trotter [46]. Also in [20], Erdős considered the problem of minimizing the number of distinct distances occurring among n points. The $\lfloor\sqrt{n}\rfloor \times \lfloor\sqrt{n}\rfloor$ lattice contains $O(n/\sqrt{\log n})$ distinct distances; again this is believed to be the tight bound, but the best known lower bound[4] is $\Omega(n^{C-\epsilon})$ where $C \approx 0.8641$.[5] Curiously, over a wide range of values of n, the minimum number of distinct distances among n points is realized by a section of the triangular lattice (in other words, it seems that we only have to consider subsets of the triangular lattice); Erdős and Fishburn [22] conjectured this to be true for all n greater than some n_0.

Lattices also come into play in questions about geometric packings and coverings in the plane. Let T be a convex set, and let $A_1, A_2, \ldots$ be a set of shape-preserving affine transformations (thus each is a composition of translations, rotations, and reflections). The A_i's and T induce an arrangement $\bigcup_i A_iT$. It is a *packing* if no point in the plane is contained in two of the copies of T (with the possible exception of the boundaries of T, if T is a closed set). The complementary notion of a *covering* is an arrangement in which every point in the plane is contained in at least one copy of T. Over a domain D, we can define the *efficiency* of a packing by the ratio of the area of the packing

[4]This is found in [12, Chapter 5] as the consequence of two results, one by Solymosi and Tóth [45] and the other by Katz and Tardos [28].

[5]Recently (in 2010), Guth and Katz [24] have demonstrated a lower bound of $\Omega(n/\log n)$ for this problem, which gives an almost-tight bound. As far as we can tell, this paper has not yet been published; it is available at `http://arxiv.org/abs/1011.4105`

to the area of D; packings have efficiency ≤ 1, coverings ≥ 1. If D is unbounded, we can take the limit of the efficiency on the bounded domains $D \cap \{(x, y) : x^2 + y^2 \leq r\}$ for $r = 1, 2, 3, \ldots$. Many results on the optimal efficiency of packings involve *lattice-centered packings*,[6] which are packings of the form $\bigcup_{c \in C}(T + c)$ for some $C \subseteq \mathbb{R}^2$. Here, rotations and reflections are not allowed. When T is centrally symmetric, it turns out that the lattice-centered packing often gives optimal results over all possible packings. Similar considerations are true for non-crossing coverings.[7] The most efficient non-crossing coverings tend to be lattice-centered. A good overview of geometric packing and covering can be found in the book by Pach and Agarwal [34, Chapters 3 and 4].

Lattices have received considerable attention from researchers even beyond their relations to the above problems. In Chapter 5 we will consider packing problems on the $n \times n$ lattice; these problems entail finding a maximum subset of the lattice that contains no instance of a forbidden subset. Solutions to problems of this type are of great use in computational geometry and in sampling theory.

The most famous open problem in this class is the *no-three-in-line* problem, which asks for a maximal subset of the $n \times n$ lattice containing no three collinear points. The upper bound is $2n$, and this bound is generally believed to be attainable. The best known lower bound is $(1.5 - o(1)) \cdot n$, given by a construction of Hall et al. [25]. Thiele [52, 53] considered the related problem of choosing points from the lattice while avoiding four co-circular points (considering four collinear points to lie on a circle of infinite radius). He demonstrated a lower bound of $(1/4 - o(1)) \cdot n$. Erdős and Guy [21] considered the problem of choosing a subset of k points such that the $\binom{k}{2}$ pairs of points all have distinct distances; they give a greedy algorithm that constructs a set

[6] These are generally called just "lattice packings," but we add "centered" to the term to distinguish this notion from the type of problems we consider later on.

[7] A covering is *non-crossing* if for any copies T_1 and T_2 of the tile, the differences $T_1 - T_2$ and $T_2 - T_1$ form connected sets. This condition is believed not to be essential to the theory, but exisiting proofs about coverings rely on it.

of $n^{2/3-o(1)}$ points. We review these constructions in Sections 5.2 and 5.5.

Higher-dimensional lattices present additional problems; these problems generally have not been explored as deeply as their two-dimensional equivalents. Riddell [40] considered the problem of choosing points from the lattice $\{1,\ldots,n\}^d$ such that no n points are collinear. Thiele [52] considered subsets of $\{1,\ldots,n\}^d$ that avoid **(1)** $d+1$ points on the $(d-1)$-dimensional hyperplanes, and **(2)** $d+2$ points on the d-dimensional hyperspheres (including $(d-1)$-dimensional hyperplanes as degenerate hyperspheres).

In a similar vein, we will consider generalizations of the no-K-in-line and no-four-on-circle problems to higher dimensions. Our results will be obtained with the aid of the results in Chapter 4 on the independence number of uniform hypergraphs. These packing problems have natural representations as hypergraphs — take the vertex set to be the points of the lattice, and form an edge from every forbidden subset (collinear K-tuple or co-circular 4-tuple) of points.

1.4 Plan of the thesis

The rest of this thesis is laid out as follows. In Chapter 2 we discuss monochromatic optimization problems on HSTs. In Chapter 3 we consider the bichromatic versions of these problems. Then, in Chapter 4, we turn to graph and hypergraph theory, looking into questions concerning the independence number of uniform hypergraphs. In Chapter 5, we apply these results to packing problems on lattice structures. We offer conclusions in Chapter 6.

A summary of the mathematical notation used in this thesis is found in Appendix A. Appendix B contains proofs of some theorems and lemmata used in the main text; we have placed them there so as not to disrupt the flow (such as it is) of the main text. Appendix C contains some material that we produced late in the writing of this thesis; the ideas are elegant but the proofs are lacking. Perhaps the reader will have some insights into the questions raised there.

2. Monochromatic HST problems

2.1 Introduction

The notion of the hierarchically (well-)separated tree (HST) was introduced by Bartal [8]. A λ-HST is a rooted weighted tree satisfying two properties: (1) for a given node v, the edges connecting v to its children have the same weight; and (2) for a given node v that is neither a root nor a leaf, the ratio of each of v's child edge weights to the weight of v's parent edge is λ. Therefore, along any path from the root to a leaf, the weights of the edges will be $c, c\lambda, c\lambda^2$, etc. In what follows, we only consider HSTs that are balanced (those for which the branching factor of all nodes other than the leaves is the same, denoted by b) and uniform (having every leaf at the same depth δ). We also require $0 < \lambda < 1$. We describe an HST with these parameters as a (b, δ, λ)-HST.

There is a little ambiguity here, in that we have not specified the weight of the edges incident on the root; most of the time, we will assume that this weight is λ, giving us a weight sequence of $\lambda, \lambda^2, \ldots, \lambda^d$. If the weight is different, it only affects our results by constant factors, and so we feel free to ignore them.

Bartal [9] showed that arbitrary metric spaces on n points can be $O(\log n \log\log n)$-probabilistically approximated by a collection of HSTs; the factor of the approximation (here $c \log n \log\log n$) indicates the maximum factor by which a randomly chosen tree from the collection will overestimate, in expectation, the distance between any pair of points. Fakcharoenphol, Rao and Talwar [23] improved the factor in Bartal's result from $O(\log n \log\log n)$ to $O(\log n)$.

General HSTs are well suited to approximating arbitrary Euclidean metric spaces. In this paper we consider only balanced uniform HSTs, but even these are useful in

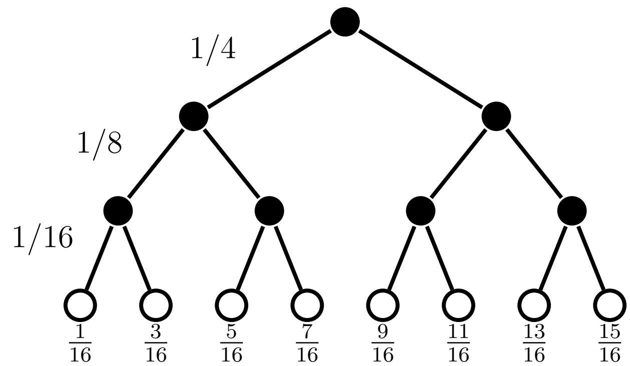


Figure 2.1: Eight equispaced points on $[0, 1]$ and their HST approximation. For every pair of points x, y, the distance between x and y in the tree exceeds or equals their Euclidean distance $|x - y|$.

approximating "well-behaved" spaces. To start, let us consider a set P_n of n equally spaced points on the interval $[0, 1]$. For simplicity, let us assume the points are placed at the midpoints of the subintervals $[0, 1/n], [1/n, 2/n], \ldots, [(n-1)/n, 1]$. For n a power of two, we can draw a full binary tree of height $\log_2 n$ whose leaves are collocated with P_n. Figure 2.1 shows the tree for $n = 8$. The edge weight ratio is set to $1/2$, and the edges incident on the root are given weights of $1/4$; the tree then has a diameter of $1 - 1/n$.

This tree defines a metric on the leaves of P_n: the distance between two leaves is the length of the path connecting them. It is clear that the distance between the two leaves p and q in the tree is greater than or equal to the Euclidean distance between the points p and q; thus it is said that the tree metric *dominates* the Euclidean metric on these points. While the tree metric is close to the Euclidean distance for many point pairs (consider the two extreme points), other point pairs are assigned an exaggerated distance. Consider the two middle points: their Euclidean distance is $1/n$, but their distance in the tree is nearly 1.

We obtain better results with a more complex technique. Let us embed P_n into

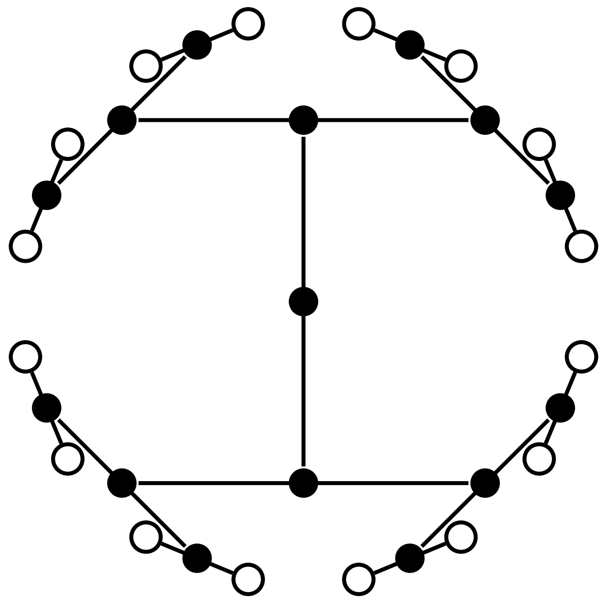


Figure 2.2: The sixteen white points represent sixteen equispaced points on the toric interval $[0,2]$. They are paired off, and the midpoint of each pair is drawn, with edges to the points of its pair. This process is repeated until only one point remains.

the interval $[0,2]$ equipped with a torus distance metric: the distance between two points x and y is defined as $\min(|x-y|, 2-|x-y|)$. Thus the interval wraps around — the points 0 and 2 are coincident — but for two points inside $[0,1]$, the torus metric agrees with the Euclidean metric. Define $P'_n = P_n \cup (1+P_n)$. We can repeat our construction from above: choose one of the points to be the "first" leaf, and build a binary tree whose leaves are collocated with P'_n. In this way we obtain a set of n trees; one such tree is shown in Figure 2.2. Now, for a fixed pair of points p and q from P_n, some trees will greatly overestimate the distance between p and q, but most of the trees will give a fairly close value to the Euclidean distance. Choosing a tree at random will provide an approximation that is accurate with high probability; one can show that the expected distance in the tree is no more than $O(\log_2 n)$ times the actual Euclidean distance.

Our construction easily generalizes to higher dimensions. Given n points equally spaced in $[0,1]^d$, we can embed them into a set of $n \cdot 2^d$ points in $[0,2]^d$ equipped with a torus metric. The resulting tree will now have a branching factor of 2^d. Furthermore, the restriction to equispaced points is, for many applications, not essential: points on $[0,1]^d$ can be discretized to an equispaced grid of points. The most convenient such grid is the one formed by cutting the hypercube into n parts along every dimension, forming n^d smaller hypercubes, and taking the midpoint of each cube. This setup introduces some error, which depends on the coarseness of the discretization; the optimal error is often negligible when compared to the cost of the problem. For more on the application of HSTs to problems on metric spaces, we refer the reader to the papers by Bartal [8, 9] and Fakcharoenphol et al. [23].

2.2 Definitions of problems

Given an HST H and a submultiset V' of its leaves, we let G be the complete graph with vertex set V. Here V contains the elements of V', and if there are multiple copies of a leaf in V', we distinguish them in V by indexing the different copies. For every $v, w \in V$, the weight of the path from v to w is denoted by $d_H(v, w)$. Note that we will have distinct vertices of G that are at a distance zero from each other, when these are copies of the same leaf of H.

In this chapter, we will demonstrate tight bounds on the expected costs of solutions to three problems on HSTs. These problems are the minimum matching problem, the travelling salesman problem (TSP), and the minimum spanning tree (MST) problem.

Minimum Matching Problem (MMP): The minimum matching on V has cost given by

$$M(V) = \min_{M \subseteq G} \sum_{e \in M} |e|,$$

where $|e|$ denotes the weight of the edge e and the minimum is taken over all possible perfect matchings of G. If n is odd, one of the vertices is excluded from the matching, and so the minimum matching on V is the minimum of the minimum matchings on the n subsets $V \backslash \{x_1\}, V \backslash \{x_2\}, \ldots, V \backslash \{x_n\}$.

Travelling Salesman Problem (TSP): A closed tour or Hamiltonian cycle is a simple cycle that visits each vertex of V exactly once. We denote by $T(V)$ the length of the shortest closed tour on V. Thus

$$T(V) = \min_{\tau \subseteq G} \sum_{e \in \tau} |e|,$$

where the minimum is taken over all tours τ.

Minimum Spanning Tree Problem (MST): We let $MST(V)$ be the cost of the minimum spanning tree on V, namely

$$MST(V) = \min_{F \subseteq G} \sum_{e \in F} |e|,$$

where the minimum is taken over all spanning trees F.

2.3 The minimum matching problem

Let H be an HST, and let W be a set of points assigned to the leaves of H. In this section, we will prove that the optimal matching cost is on the order of $\sum_{k=1}^{h} (b\lambda)^k$, where $h = \min(\delta, \log_b n)$. The proof proceeds in two broad stages. First, we determine, based on the leaves that form W, the number of matches τ_v occurring at each node v of the tree; the idea of a matching occurring at a node is formalized as a *transit*. Once this question is resolved, the value of $\mathbf{E}[M(W)]$ can be found as the expectation of a weighted sum of the τ_v's.

For each vertex $v \in V(H)$, we define $X(v)$ to be the number of points assigned to the descendants of v in H. We consider a node to be a descendant of itself, so that when v is a leaf, $X(v)$ is simply the number of points assigned to v. For a non-leaf vertex v with children $u_1, u_2, \ldots, u_k$, we have

$$X(v) = \sum_{i=1}^{k} X(u_i).$$

For a pair of matched points (x, y) in W belonging to distinct leaves u_x and u_y in H, we will say the pair (x, y) results in a *transit* at vertex v when v is the lowest common ancestor of u_x and u_y — that is, when the path between u_x and u_y passes through v. We denote by τ_v the total number of transits at vertex v in an optimal matching. Given an integer N, we define $Odd(N)$ to be the parity of N, i.e., 1 when N is odd and 0 when N is even.

Lemma 2.1 *Let H be an HST, and let W be a submultiset of the leaves of H. The number of transits at any non-leaf vertex v in a minimum matching $M(W)$ is*

$$\tau_v = \frac{1}{2}\left(\left(\sum_{i=1}^{k} Odd(X(u_i))\right) - Odd\left(X(v)\right)\right),$$

where $u_1, u_2, \ldots, u_k$ are the children of v.

Proof: First consider a vertex v at height 1 and its children $u_1, u_2, \ldots, u_k$. For each u_i, only $Odd(X(u_i))$ instances need to look for a match elsewhere in the tree, since an even number of the instances can be paired off in the leaf. The number of remaining unmatched points will therefore be $\sum_i Odd(X(u_i))$. These points can now be paired off at v; if this quantity is odd, there will be one point left over. The number of pairs that transit through v is thus

$$\frac{1}{2}\left(\sum_i Odd(X(u_i)) - Odd\left(\sum_i Odd(X(u_i))\right)\right)$$

$$= \frac{1}{2}\left(\sum_i Odd(X(u_i)) - Odd\left(\sum_i X(u_i)\right)\right).$$

We will now modify the HST in the following way. Each point resident at a leaf of the tree will be transferred to its parent, and the leaves will be removed. Thus each vertex v that was formerly at depth 1 will become a leaf, and every remaining vertex will retain its previous X-value. It is clear that the number of transits at every vertex w in this new tree remains the same, since any unmatched point at u_i would have had to search above v in any case, and these points will transit at the same vertex as they would have before. Successive applications of the argument in the preceding paragraph will reduce the tree to a single node, showing that $\tau_v = \frac{1}{2}\left(\sum_i Odd(X(u_i)) - Odd\left(\sum_i X(u_i)\right)\right)$ for every vertex v in the original tree. $\square$

The above argument also shows that $\tau_v \leq \frac{1}{2} deg_H(v)$: the number of transits at v is upper-bounded by the number of children of v, regardless of the number of descendants v has in the HST.

Lemma 2.2 *Let v be a non-root vertex in level ℓ of an HST H. Then*

$$\mathbf{Pr}[X(v) \text{ is odd}] \leq \frac{1}{2},$$

so that $\mathbf{E}[Odd(X(v))] \leq \frac{1}{2}$. If n, the number of points chosen, is at least b^ℓ, then

$$\mathbf{Pr}[X(v) \text{ is odd}] \geq \frac{1}{4},$$

so that $\mathbf{E}[Odd(X(v))] \geq \frac{1}{4}$.

Proof: Let r be the ratio of leaves of H that are descendants of v. We have $r = 1/b^\ell$. Let us start with an empty multiset of points and add points one by one. Some of these points will belong to leaves that are descendants of v, while others will not. For $i = 1, \ldots, n$, define m_i to be the number of the first i points that belong to descendants of v, and let $\chi_i = Odd(m_i)$. The variables χ_i form a Markov process where each transition changes state with probability r and remains at the current state with probability $1-r$; this gives us the transition matrix $\mathcal{P} = \begin{bmatrix} 1-r & r \\ r & 1-r \end{bmatrix}$. The initial state of the process is $\pi = [1,\ 0]$.

We can diagonalize $\mathcal{P}$ as $U^{-1}DU$, where $D = \begin{bmatrix} 1 & 0 \\ 0 & 1-2r \end{bmatrix}$ and $U = U^{-1} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$. After n points have been chosen, the state of the system will be

$$\begin{aligned} \pi\mathcal{P}^n &= \pi U^{-1} D^n U \\ &= \left[\frac{1}{2} + \frac{1}{2}(1-2r)^n,\ \frac{1}{2} - \frac{1}{2}(1-2r)^n\right], \end{aligned}$$

and we have $\mathbf{Pr}[X(v) \text{ is odd}] = \frac{1}{2} - \frac{1}{2}(1-2r)^n$.

Set $\Delta = (1-2r)^n$. Notice that Δ cannot be negative, since $b \geq 2$ and $r \leq 1/b$. This shows the first statement of the lemma. For the lower bound, we wish to show $\Delta \leq \frac{1}{2}$. When $n \geq b^\ell$, the worst case is clearly for $r = 1/b^\ell$ and $n = b^\ell$, which gives us

$$\Delta \leq (1 - 2/b^\ell)^{b^\ell} < \exp(-2) < \frac{1}{2},$$

and the second statement is proved. □

We now have

Corollary 2.3 *Let $H = H(b, \delta, \lambda)$ be a balanced HST, and let v be one of its non-leaf vertices in level $\ell > 0$. Then*

$$\mathbf{E}[\tau_v] \leq \frac{1}{4}(b-1),$$

and if $n \geq b^\ell$,

$$\mathbf{E}[\tau_v] \geq \frac{1}{8}(b-1).$$

Proof: Take the expectation of τ_v as given by Lemma 2.1. The values of

$\mathbf{E}[Odd(X(v))]$ and $\mathbf{E}[Odd(X(u_i))]$ are bounded by Lemma 2.2. $\square$

Theorem 2.4 *Let $H = H(b, \delta, \lambda)$ be a balanced HST, and let W be a randomly chosen n-element submultiset of its leaves. The value of $\mathbf{E}[M(W)]$, the expected weight of the optimal matching of W, obeys*

$$\mathbf{E}[M(W)] \leq B_{b,\lambda} \sum_{k=1}^{\delta} (b\lambda)^k$$

for some positive constant $B_{b,\lambda}$ depending only on b and λ. If $n \geq b^\delta$, then

$$\mathbf{E}[M(W)] \geq A_{b,\lambda} \sum_{k=1}^{\delta} (b\lambda)^k$$

for some positive constant $A_{b,\lambda}$ depending only on b and λ.

Proof: Consider the contribution of level k (where $k > 0$) to the value of $M(W)$. Level k contains b^k vertices, and the expected number of transits at each of these vertices is between $\frac{1}{8}(b-1)$ and $\frac{1}{4}(b-1)$, by Corollary 2.3. The weight of a match at level k is $2(\lambda^k + \lambda^{k+1} + \lambda^{k+2} + \ldots + \lambda^\delta)$; this is bounded from below by $2\lambda^k$ and from above by $2\sum_{i=k}^{\infty} \lambda^i = 2\lambda^k/(1-\lambda)$. The total contribution of levels $1, 2, \ldots, \delta$ can therefore be bounded from above by

$$\sum_{k=1}^{\delta} \left(b^k \cdot \frac{1}{4}(b-1) \cdot \frac{2\lambda^k}{1-\lambda} \right) = \frac{b-1}{2(1-\lambda)} \cdot \sum_{k=1}^{\delta} (b\lambda)^k.$$

and bounded from below, when $n \geq b^\delta$, by

$$\sum_{k=1}^{\delta} \left(b^k \cdot \frac{1}{8}(b-1) \cdot 2\lambda^k \right) = \frac{b-1}{4} \cdot \sum_{k=1}^{\delta} (b\lambda)^k.$$

Choose $A_{b,\lambda} < (b-1)/4$ and $B_{b,\lambda} > (b-1)/2(1-\lambda)$. We have not counted the contribution of the root, but it is negligible, at most the constant b. $\square$

Remark 2.5 *Let us perform a walk on the tree, starting at the root, and visiting each leaf in order from left to right. This walk will use each edge twice. At level ℓ there are b^ℓ edges, and their cost is λ^ℓ. Therefore the total cost will be*

$$2 \cdot \sum_{\ell=1}^{\delta} b^\ell \lambda^\ell.$$

Note the similarity to the bounds in Theorem 2.4.

Now we have

Theorem 2.6 *Let $H = H(b, \delta, \lambda)$ be a balanced HST, let W be a randomly chosen n-element submultiset of its leaves, and let $h = \min(\delta, \log_b n)$. Then*

$$\mathbf{E}[M(W)] \leq C_{b,\lambda} \sum_{k=1}^{h} (b\lambda)^k$$

for some positive constant $C_{b,\lambda}$ depending only on b and λ.

Note that the upper index of the summation has changed from δ to h.

Proof: If $\delta \leq \log_b n$ then there is nothing to prove. Hence, we may assume that $\delta > \log_b n$, and consider the case $h = \log_b n$ for n a power of b.

Each node at depth h will have an average of one element of W in its subtree. The worst case occurs when each node at depth h has *exactly* one element: otherwise, elements can be paired off in the subtrees without looking above level h. Thus the situation is the same as locating points at level h instead of at level δ. More generally, when n is not a power of b, the average number of elements of W in each subtree will still be $O(1)$, giving us the same result (with a different constant). The bound then comes from applying Theorem 2.4 to a tree of height h. $\square$

Relaxing the index of the second summation in Theorem 2.4 from δ to h, we conclude

Theorem 2.7 *Let $H = H(b, \delta, \lambda)$ be a balanced HST, let W be a randomly chosen n-element submultiset of its leaves, and let $h = \min(\delta, \log_b n)$. Then*

$$A'_{b,\lambda} \sum_{k=1}^{h} (b\lambda)^k \leq \mathbf{E}[M(W)] \leq B'_{b,\lambda} \sum_{k=1}^{h} (b\lambda)^k$$

for some positive constants $A'_{b,\lambda}, B'_{b,\lambda}$ depending only on b and λ.

(Above, and throughout the rest of this thesis, we implicitly assume that the value $\log_b n$ appearing in the index of the summation is an integer. The reader may substitute $\lfloor \log_b n \rfloor$ or $\lceil \log_b n \rceil$ if he wishes; the results are not affected.)

2.4 The TSP and the MST problem

Now we turn our attention to the MST problem and the TSP. Let us first consider the TSP. We construct a tour on the multiset W as follows: we build a tree T' that contains each edge $e = (p, c)$, where p is the parent vertex of c, if and only if some descendant of c is identified with a point of W. The tour $\mathcal{T}$ is formed by visiting the leaves of T' in order; it is clear that the weight of $\mathcal{T}$ is exactly twice the weight of T', since each edge of T' will be traversed exactly twice to form the tour $\mathcal{T}$. We can easily show that an optimal tour on W and the root of the HST can be formed in this way: Suppose we have a tour that does not have the form described above. There are two leaves u and v that are out of order in the tour. Switching the positions of u and v in the tour can only decrease the total cost.

Observe that even though the root is not always needed to create a tour on W, it will be needed with high probability. More precisely, the probability that it will *not* be needed is the same as the probability that all n chosen leaves of T have the same ancestor at level 1 of the tree; this probability is $1/b^{n-1}$, which is at most $1/2$ for $b, n \geq 2$. In the following, we presume that the root is needed; this only changes the true values of the expectations by a constant factor, which we can ignore. We will show that the expected cost of the optimal tour is on the order of $\sum_{\ell=1}^{h}(b\lambda)^{\ell}$, where $h = \min(\delta, \log_b n)$.

Let v be a non-root vertex in T, and let ℓ be its level in the tree (with the root being at level 0). The probability that a randomly chosen leaf of T is a descendant of v is $1/b^{\ell}$. Since n points will be chosen, the probability that the parent edge of v is needed in $\mathcal{T}$ is

$$1 - \left(1 - \frac{1}{b^{\ell}}\right)^{n}.$$

Since there are b^{ℓ} vertices in level ℓ and each of their parent edges has weight λ^{ℓ}, the total contribution of level ℓ to the weight of $\mathcal{T}$ is

$$2 \cdot (b\lambda)^{\ell} \cdot \left(1 - \left(1 - \frac{1}{b^{\ell}}\right)^{n}\right),$$

hence

Theorem 2.8 *Let $H = H(b, \delta, \lambda)$ be a balanced HST, and let W be a randomly chosen n-element submultiset of its leaves. Then the expected cost of a tour on W and the root of T is*

$$2 \cdot \sum_{\ell=1}^{\delta} \left[(b\lambda)^{\ell} \cdot \left(1 - \left(1 - \frac{1}{b^{\ell}}\right)^{n}\right)\right].$$

The result of Theorem 2.8 is exact, though unwieldy in this form. Our goal now is to massage this quantity into the expression of Theorem 2.12.

Since removing the root from the tour can only decrease its cost, we have

$$\mathbf{E}[TSP(W)] \leq 2 \cdot \sum_{\ell=1}^{\delta} \left[(b\lambda)^{\ell} \cdot \left(1 - \left(1 - \frac{1}{b^{\ell}}\right)^{n}\right)\right],$$

and

Corollary 2.9

$$\mathbf{E}[TSP(W)] \leq 2 \cdot \sum_{\ell=1}^{\delta} (b\lambda)^{\ell}.$$

By the inequality $1 + x \leq e^x$, when $n \geq b^\ell$ we have

$$\left(1 - \frac{1}{b^\ell}\right)^n \leq e^{-n/b^\ell} \leq \frac{1}{e},$$

hence

Lemma 2.10 *Given that the root is necessary in the tour,*

$$\mathbf{E}[TSP(W)] \geq 2 \cdot (1 - 1/e) \cdot \sum_{\ell=1}^{h} (b\lambda)^{\ell}$$

where $h = \min(\delta, \log_b n)$.

Since the root is necessary with probability at least 1/2,

Corollary 2.11

$$\mathbf{E}[TSP(W)] \geq (1 - 1/e) \cdot \sum_{\ell=1}^{h} (b\lambda)^{\ell}$$

where $h = \min(\delta, \log_b n)$.

All that remains is to reconcile these two corollaries.

Theorem 2.12

$$\mathbf{E}[TSP(W)] = \Theta\left(\sum_{\ell=1}^{h} (b\lambda)^{\ell}\right)$$

where $h = \min(\delta, \log_b n)$.

Proof: Assume $h = \log_b n$, since otherwise the theorem follows directly from Corollaries 2.9 and 2.11. We divide the tour into two parts in relation to the h-th level of the tree: the "upper" part consists of the edges above this level, while the "lower" part consists of the edges below this level. The theorem will be proved if we can show that the expected cost of the lower part is dominated by that of the upper part.

Let us change the lower part in the following way: instead of building the optimal tour within each subtree, we will just connect each leaf (that has a point) to its ancestor in the h-th level. This is a more direct or "lazier" tour, where we ignore the cheaper edges in these subtrees. Clearly this increases the cost; moreover, this new cost is easier to calculate. There are n points, and the cost of connecting each point to its ancestor in the h-th level is $2 \cdot (\lambda^{h+1} + \lambda^{h+2} + \ldots + \lambda^{\delta-1}) \leq 2 \cdot \lambda^{h+1}/(1-\lambda)$. This cost is therefore bounded from above by $2n \cdot \lambda^{h+1}/(1-\lambda)$.

We now consider the upper part of the tour — in fact, we need only consider those edges connecting nodes in the $(h-1)$-st and h-th levels. Let us mark every node in the h-th level that has a point in its subtree. The parent edge of every marked node must be included in the tour: how many of these n nodes do we expect to be marked? It is not hard to see that the probability of a node remaining unmarked is $(1-1/n)^n$; this is bounded from above by $1/e$. Thus the expected number of marked nodes exceeds $n \cdot (1-1/e)$, and the total expected cost of their parent edges is at least $2n \cdot (1-1/e) \cdot \lambda^h$. We conclude that the cost of the lower part of the tour is less than a constant factor (depending on b and λ) times the cost of the upper part of the tour. $\square$

Let us turn to the MST problem. It is well known that on a graph whose edge weights obey the triangle inequality, the optimal solutions to the MST problem and to the TSP are within constant factors of each other. An algorithm appearing in the work of Rosenkrantz et al. [41][1] uses this fact to find a 2-approximation for the TSP on metric graphs. Our goal in the remainder of this section is to show that the

[1] This reference is one of the earliest to the algorithm, but is not clear who first came up with it first.

optimal solutions to these two problems *on HSTs* are, in fact, approximately equal: we will have

$$MST(W) \leq T(W) \leq MST(W) + \Delta,$$

where Δ is the diameter of the tree. The minimum spanning tree is obtained by removing one edge from the optimal tour, and this edge will have weight less than or equal to the tree diameter.

As observed above, with probability at least 1/2, the root is needed to form the MST; in what follows, we assume that the root is part of the MST. Let F be a rooted tree with positive edge weights, and let r be its root. Assume further that every leaf lies in level k of the tree. Let us denote by $d(u, v)$ the total edge weight of the path connecting the leaves u and v. These distances clearly determine a metric space $\mathcal{M}_F$ on the leaf set of F. For any $x \in V(F)$, let $F(x)$ denote the subtree of F rooted at x.

Lemma 2.13 *Let W be a submultiset of the leaves of F. Denote by T the minimum spanning tree on W with distances determined by $\mathcal{M}_F$. Also, for an arbitrary non-root vertex $x \in V(F)$, let $T(x)$ be the forest spanned by the vertices of $V(T) \cap V(F(x))$. Then the forest $T(x)$ is either connected or empty.*

Proof: Assume on the contrary that some $T(x)$ is disconnected and non-empty. Let C_1 and C_2 be two of its components. We will change T in the following way: delete the edge that connects C_1 to $T - T(x)$, and connect C_1 to C_2 by an edge. This new tree has a smaller total edge weight, since we can connect C_1 and C_2 by keeping the edges of the $C_1 - (T - T(x))$ path from C_1 to x and deleting the other edges. $\square$

We can say more about the structure of the minimum spanning tree if we impose another condition on F:

Lemma 2.14 *Assume that all edges that connect a parent with its children have equal weight. Then one of the minimum spanning trees is a path.*

Proof: Let us first consider the case when F is a star tree. In this case, the distance between any two distinct leaves is the same, so there is an MST which is a path.

When F is not a star tree, we apply the lemma inductively to the subtrees rooted at the children of r; each subtree has an MST that is a path. Stitching together these MSTs creates an MST of F that is a path. To see its minimality, note that if it were not optimal, the suboptimal pieces could be replaced by optimal ones. We know that the MST can be formed piecewise in this way from Lemma 2.13. □

The next lemma follows easily.

Lemma 2.15 *For any HST F, it holds that* $0 < TSP(F) - MST(F) \leq diam(F)$.

Proof: By the preceding lemma, we may take the MST to be a path. The first inequality follows from the fact that removing an edge from a Hamiltonian tour yields a spanning tree. To see the second inequality, observe that the TSP solution and the MST differ only in that the former is a cycle and the latter is a chain; the TSP tour is obtained by adding one edge to the MST. This edge has weight at most $diam(F)$.
□

Notice that $diam(F) = 2\sum_{i=1}^{\delta} \lambda^i < 2\lambda/(1-\lambda)$, which we consider constant. The bounds (expectation and, later, concentration inequalities) obtained for the TSP will therefore apply to the MST problem as well.

Corollary 2.16

$$0 < \mathbf{E}[TSP(W)] - \mathbf{E}[MST(W)] \leq diam(F).$$

Thus Theorem 2.12 also applies to MSTs, viz.,

Theorem 2.17

$$\mathbf{E}[MST(W)] = \Theta\left(\sum_{\ell=1}^{h} (b\lambda)^{\ell}\right)$$

where $h = \min(\delta, \log_b n)$.

2.5 The lifting lemma [17]

Our results for the monochromatic problems give us a sense that there is something special about the $(\log_b n)$-th level of the tree; deeper levels of the tree seem to have negligible effect on the solutions' asymptotic costs. We formalize this notion as a process that we call "lifting," in which points in deep levels are moved up to the $(\log_b n)$-th level.

Given an HST $H(b, \delta, \lambda)$ and an n-point multiset W with $\delta \geq \log_b n$, we define the *lifting of* W, written $\mathcal{L}_H(W)$, to be the multiset formed from the level-$(\log_b n)$ ancestor of each point in W. Stated otherwise, if we define $A(v)$ to be the ancestor of the point v that lies in level $\log_b n$ of the tree, then

$$\mathcal{L}_H(W) = \bigcup_{v \in W} A(v),$$

where each point in level $\log_b n$ is included as many times as it has descendants in W. Notice that if the points of W are chosen i.i.d. uniformly from the leaves of H, then $\mathcal{L}_H(W)$ is an i.i.d. uniformly chosen multiset of tree nodes from the $(\log_b n)$-th level of H.

For convenience we again define $h = \log_b n$.

Claim 2.18 *Let v be a vertex of H that sits in level $\ell \geq h$. Then*

$$d_H(v, \mathcal{L}_H(v)) \leq \sum_{i=h+1}^{\infty} \lambda^i = \frac{\lambda^{h+1}}{1-\lambda},$$

where $d_H(x, y)$ denotes the distance of x and y in H.

The claim follows easily from the definition of the edge weights in an HST. From this claim follows

Lemma 2.19 (the lifting lemma) *Assume that a balanced HST $H(b, \delta, \lambda)$ has depth $\delta > h$. Let W be an n-element multiset of the leaves. Then*

$$d_H(W, \mathcal{L}_H(W)) = O((b\lambda)^h).$$

Proof: $d_H(W, \mathcal{L}_H(W)) \leq n \cdot \lambda^{h+1}/(1-\lambda) = (b\lambda)^h/(1-\lambda)$. $\square$

The lifting lemma enables us to use a three-part strategy on these problems when $\delta > h$:

1. Lift the points from the leaves to level h. This incurs a certain cost, say α.
2. Solve the problem with the points placed at level h. Let us say the cost is β.
3. If we can show $\alpha = O(\beta)$, the cost of the original problem is $\Theta(\beta)$.

We now present new proofs of the monochromatic matching and TSP theorems.

Theorem 2.20 *Let $H = H(b, \delta, \lambda)$ be a balanced HST, let W be a randomly chosen n-element submultiset of its leaves, and let $h = \min(\delta, \log_b n)$. Then*

$$\mathbf{E}[M(W)] \leq C_{b,\lambda} \sum_{k=1}^{h} (b\lambda)^k$$

for some positive constant $C_{b,\lambda}$ depending only on b and λ.

Proof: If $\delta \leq \log_b n$ then there is nothing to prove. Hence, we may assume that $\delta > \log_b n$, and consider the case $h = \log_b n$ for n a power of b. From Lemma 2.19, the cost of lifting every point to level h is $O((b\lambda)^h)$. The cost of the matching on the lifted points is $O\left(\sum_{k=1}^{h}(b\lambda)^k\right)$ by Theorem 2.4. Summing these two costs proves the theorem. $\square$

Theorem 2.21

$$\mathbf{E}[TSP(W)] = \Theta\left(\sum_{\ell=1}^{h}(b\lambda)^{\ell}\right)$$

where $h = \min(\delta, \log_b n)$.

Proof: Assume $h = \log_b n$, since otherwise the theorem follows directly from Corollaries 2.9 and 2.11. The lower bound is evident from Corollary 2.11. From Lemma 2.19, the cost of lifting the points residing at the leaves to level h is $O((b\lambda)^h)$. Since the points are now at level h of the HST, we will treat h as the new height: by Corollary 2.9, the cost of this tour on the lifted points is $\Theta\left(\sum_{\ell=1}^{h}(b\lambda)^{\ell}\right)$. The sum of these two costs is $\Theta\left(\sum_{\ell=1}^{h}(b\lambda)^{\ell}\right)$.

The tour so constructed is not in fact the optimal tour, but instead a "lazier" one: above level h the tour is unchanged, but below level h there are n direct circuits, one between each point and its ancestor in level h. The cost of the optimal tour is therefore $O\left(\sum_{\ell=1}^{h}(b\lambda)^{\ell}\right)$. Since, by Corollary 2.11, the cost above level h is $\Omega\left(\sum_{\ell=1}^{h}(b\lambda)^{\ell}\right)$, the theorem is proved. □

While the lifting lemma was not essential to our proofs in this chapter, it will be crucial when we consider the bichromatic problems in the next chapter.

2.6 Concentration inequalities

Many of the ideas in this section stem from those of Yukich [58, Chapter 6], who in turn used methods of Talagrand [51], Rhee [38] and Steele [48]. Given a hierarchically separated tree T with branching factor b and weight ratio λ satisfying $0 < \lambda < 1$ and $b\lambda \geq 1$, we investigate the probability that the matching length of a random point set X deviates widely from its expectation. We will consider both the monochromatic case and the bichromatic case. As it turns out, we have much better concentration results for the former than for the latter, since in the monochromatic case we can use an isoperimetric inequality which, unfortunately, cannot be applied to the bichromatic problems.

First we briefly discuss Azuma's inequality, which will be of use to us in both cases. Let $(\Omega, \mathcal{A}, P)$ be a finite probability space with the filtration (in this case a sequence of partitions of Ω)

$$(\emptyset, \Omega) = A_0 \subseteq \mathcal{A}_1 \subseteq \ldots \subseteq \mathcal{A}_t = \mathcal{A}.$$

Let X be a random variable. For each $1 \leq i \leq t$ we define the *martingale difference* $d_i = \mathbf{E}(X|\mathcal{A}_i) - \mathbf{E}(X|\mathcal{A}_{i-1})$, and assume that $\|d_i\|_\infty \leq \sigma_i$. We have the following well-known result:

Theorem 2.22 (Azuma's inequality) *For all $a > 0$,*

$$\mathbf{Pr}(|X - \mathbf{E}X| \geq a) \leq 2e^{-a^2/2\sigma^2},$$

where $\sigma^2 \equiv \sum_{i=1}^{t} \sigma_i^2$.

First we will consider the minimum matching problem.

Lemma 2.23 *Assume that k points are assigned to vertices of T, with k even. Then the minimum matching for this point set has total cost at most $2 \cdot Top(k)/(1-\lambda)$, where $Top(k)$ is the sum of the edge lengths of the first $\lceil \log_b k \rceil$ levels of T.*

Proof: Let y_1 and y_2 be two points below level $\ell = \lceil \log_b k \rceil$ that are matched in the minimum matching. Denote their ancestors at level ℓ by x_1 and x_2, respectively. Then $d_T(y_1, y_2) \leq d_T(x_1, x_2) + 2\lambda^\ell/(1-\lambda)$ by Lemma 2.19. If one of the points, say y_1, is at level ℓ, we still have the same inequality. It is easy to see that no edge of the tree is used more than once in a minimum matching. Hence, the minimum matching length is at most $Top(k) + k\lambda^\ell/(1-\lambda)$, since we have $k/2$ pairs to be matched.

It is easy to see that $Top(k) = b\lambda + \dots b^\ell \lambda^\ell \geq k\lambda^\ell$. This implies that the minimum matching length is at most $2 \cdot Top(k)/(1-\lambda)$. $\square$

We are now going to use isoperimetric methods in order to prove strong concentration inequalities. Toward this end, let $(\Omega, \mathcal{A}, \mu)$ be the finite probability space with the atoms of Ω corresponding to the leaves of T, with each atom having equal probability. We define Ω^n to be the n-fold product space on Ω, and we denote by μ^n its probability measure.

Given $X, Y \in \Omega$, the Hamming distance H between X and Y is the number of coordinates in which X and Y disagree:

$$H(X, Y) = |\{i : X_i \neq Y_i\}|.$$

With the following lemma, we show that if two n-tuples are close in Hamming distance, the corresponding minimum matching costs are close to each other. This property is called the *smoothness* of the minimum matching functional.

Lemma 2.24 *Let $X, Y \in \Omega^n$. If $H(X, Y) = k$ then*

$$M(X) \leq M(Y) + 2 \cdot Top(k)/(1-\lambda),$$

where Top is as defined in Lemma 2.23.

Proof: Assume that we have a minimum matching for Y, and then delete/add k points in order to make X. We construct a matching (not necessarily minimum) for X that will satisfy the inequality of the lemma.

There are three kinds of matched pairs in Y. First, there are those that are unaffected — that is, both points belong to X as well. We will keep them matched in the new matching. Second, there are matched pairs from which we deleted one point each. The remaining points of these pairs became unmatched, as well as the points of $X - Y$. Since $H(X,Y) = k$, we have k unmatched points (here k must be even). We find a minimum matching for these points; the cost is at most $2 \cdot Top(k)/(1-\lambda)$ by Lemma 2.23. In this way, we constructed a matching for X having total length at most $M(Y) + 2 \cdot Top(k)/(1-\lambda)$, and the lemma is proved. $\square$

Let us now consider the smoothness of the TSP functional on HSTs. Earlier we saw that the difference between the costs of the TSP and MST are bounded by a constant (the limit of the diameter of the tree as $\delta \to \infty$). Therefore, the concentration we show below for the TSP holds for the MST as well. First we need an analogue of Lemma 2.23.

Lemma 2.25 *Assume that k points are assigned to vertices of T, with k even. Then the travelling salesman tour for this point set has total cost at most $4 \cdot Top(k)/(1-\lambda)$, where $Top(k)$ is the sum of edge lengths of the first $\lceil \log_b k \rceil$ levels of T.*

Proof: The proof is very similar to the proof of Lemma 2.23, so we emphasize the differences only. First, the TSP tour that connects all the vertices in level k has total length $2 \cdot Top(k)$. We use the lifting lemma again to prove that for points below level k, we have to add at most an extra cost of $2\lambda/(1-\lambda)$. Since there are k points, we can have at most $2k\lambda/(1-\lambda)$ extra cost. This adds up to $2 \cdot Top(k) + 2k\lambda/(1-\lambda) \leq 4 \cdot Top(k)/(1-\lambda)$. $\square$

With this we are prepared to show the smoothness of the TSP.

Lemma 2.26 *Let $X, Y \in \Omega^n$. If $H(X,Y) = k$ then*

$$TSP(X) \leq TSP(Y) + 8 \cdot Top(k)/(1-\lambda).$$

Proof: Assume that we have an optimal tour $\mathcal{T}$ for Y, and then delete/add k points in order to make X. We construct a tour (not necessarily optimal) for X that will satisfy the inequality of the lemma.

Notice that even if we delete points from $\mathcal{T}$, the optimal cost of the tour $\mathcal{T}_1$ that skips the deleted points, going through only the remaining points in their original order, is at most as large as the cost of $\mathcal{T}$. This follows from the triangle inequality: say, u, v, w are in this order in the optimal tour, and then we delete v. Then $d(u, v) + d(v, w) \geq d(u, w)$.

Next, we construct an optimal tour $\mathcal{T}_2$ through the new points, with cost at most $4 \cdot Top(k)$ by Lemma 2.25. Then we delete one edge from $\mathcal{T}_1$ and one edge from $\mathcal{T}_2$. This way we get two paths. We will get a new tour by connecting the endpoints of the paths; this has cost at most twice the diameter, which is at most $4\lambda/(1 - \lambda)$. The total additional cost is therefore $4 \cdot Top(k) + 4\lambda/(1 - \lambda) \leq 8 \cdot Top(k)/(1 - \lambda)$. $\square$

It will be convenient to introduce a new notation L for a smooth functional. We will assume that $L(X) \leq L(Y) + K \cdot Top(k)/(1 - \lambda)$, if $H(X, Y) \leq k$, with $K > 0$ a constant. We further assume that $\mathbf{E}L = \Theta\left(\sum_{i=1}^{h} (b\lambda)^i\right)$. Notice that by Lemmata 2.24 and 2.26, we have the smoothness conditions for M, TSP and MST, albeit with different values for K. We showed in previous sections that for these functionals the expectation has the above form. As it turns out, smoothness and expectation value are the most important properties we need for showing strong concentration about the mean.

The isoperimetric inequality we need is standard, but for completeness we present the proof. For a subset $A \subseteq \Omega$, we define

$$H(A, X) = \min_{Y \in A} H(X, Y).$$

Let us fix a set A such that $\mu^n(A) \geq 1/2$. For a number t we define

$$A_t = \{X : H(X, A) \leq t\}.$$

We will show, with the aid of Azuma's inequality, that $\mu^n(\overline{A_t}) = 1 - \mu^n(A_t)$ tends to zero very fast as we increase t. Let

$$\alpha = \int H(A, X)\ d\mu^n;$$

this is the expected Hamming distance of a randomly chosen n-tuple of Ω^n from A. Then by Azuma's inequality,

$$\mu^n(\{X : |H(A, X) - \alpha| \geq t\}) \leq 2e^{-t^2/2n}.$$

(Here we have used the fact that changing one coordinate results in a change of at most 1 in the Hamming distance.)

Next we give a bound for α. Observe that when $Y \in A$, we have $H(A, Y) = 0$. Thus

$$A \subseteq \{X : |H(A, X) - C| \geq C\}$$

for all $C > 0$. Setting $t = \alpha$ in the above inequality, we have

$$1/2 \leq \mu^n(A) \leq \mu^n(\{X : |H(A, X) - \alpha| \geq \alpha\}) \leq 2e^{-\alpha^2/2n},$$

which implies $\alpha \leq \sqrt{2n \log 4}$. Hence

$$\mu^n(\{X : H(A, X) \geq t + \sqrt{2n \log 4}\}) \leq 2e^{-t^2/2n}.$$

Some consideration of the cases $t \geq 2\sqrt{2n \log 4}$ and $t < 2\sqrt{2n \log 4}$, after necessary modifications of the parameters, produces the following *isoperimetric inequality*, valid for all t independently of α.

Proposition 2.27 (isoperimetric inequality) *If $A \subseteq \Omega^n$ satisfies $\mu^n(A) \geq 1/2$, then*

$$\mu^n(\overline{A_t}) \leq 4e^{-t^2/8n}.$$

We are going to use the *median* of the L functional:

$$med(L) = \inf\{t \in \mathbb{R} : \mu^n(\{X \in \Omega^n : L(X) \leq t\}) \geq 1/2\}.$$

Let

$$A = \{X \in \Omega^n : L(X) \leq med(L)\};$$

then $\mu^n(A) \geq 1/2$. Applying Lemma 2.24, we obtain

$$\begin{aligned}
\mathbf{Pr}(L(X) \geq med(L) + t) &= \mu^n(\{X \in \Omega^n : L(X) \geq med(L) + t\}) \\
&\leq \mu^n(\{X \in \Omega^n : med(L) + K \cdot Top(k)/(1-\lambda) \geq med(L) + t\}) \\
&= \mu^n(\{X \in \Omega^n : K \cdot Top(k)/(1-\lambda) \geq t\}),
\end{aligned}$$

where $k = H(A, X)$. One can also prove a similar inequality using the set $B = \{X \in \Omega^n : L(X) \geq med(L)\}$, to bound the probability $\mathbf{Pr}(L(X) \leq med(L) - t)$. Putting the two together, we see

$$\mathbf{Pr}(|L(X) - med(L)| \geq t) \leq 2\mu^n(\{X \in \Omega^n : K \cdot Top(k)/(1-\lambda) \geq t\}).$$

In the cases that interest us most, we can find the inverse of $Top(k)$, and hence we can apply the isoperimetric inequality (Proposition 2.27) to prove strong concentration around the expected value.

First, we consider the case when $b\lambda = 1$. Then

$$Top(k) = \sum_{i=1}^{\lceil \log_b k \rceil} (b\lambda)^i = \lceil \log_b k \rceil.$$

In this case, using the isoperimetric inequality, we have

$$\mathbf{P}(|L(X) - med(L)| \geq t) \leq 2\mu^n(\{X \in \Omega^n : KC(\lambda)Top(k) \geq t\}) \leq$$

$$2\mu^n(\{X \in \Omega^n : k \geq b^{t/c}\}) \leq 4 \exp\left(-\frac{b^{t/c'}}{8n}\right)$$

with the constants c and c', where $c = 2c'$.

Now suppose $b\lambda > 1$. Then

$$Top(k) = \sum_{i=1}^{\lceil \log_b k \rceil} (b\lambda)^i = \frac{1}{1-\lambda} \cdot b\lambda \frac{(b\lambda)^{\lceil \log_b k \rceil} - 1}{b\lambda - 1} \leq C_1(b, \lambda)(b\lambda)^{\log_b k},$$

where $C_1(b, \lambda)$ is a constant depending only on b and λ. The inequality $K \cdot Top(k)/(1 - \lambda) \geq t$, using that $(b\lambda)^{\log_b k} = k^{\log_b (b\lambda)}$, implies the inequality

$$k \geq \left(\frac{t}{C_2(b, \lambda)}\right)^{\frac{1}{\log_b (b\lambda)}}.$$

This in turn implies

$$\mathbf{P}(|L(X) - med(L)| \geq t) \leq 2\mu^n(\{X \in \Omega^n : K \cdot Top(k)/(1 - \lambda) \geq t\}) \leq$$

$$2\mu^n(\{X \in \Omega^n : k \geq (t/C_2(b, \lambda))^{\frac{1}{\log_b (b\lambda)}}\}) \leq 4 \exp\left(-\frac{t^{2/\log_b (b\lambda)}}{C_3 n}\right)$$

for $b\lambda > 1$.

Since $\int \mathbf{P}(Z \geq t)\ dt = \mathbf{E}Z$ for any random variable Z, integrating these inequalities over the non-negative reals produces an upper bound for $\mathbf{E}|L(X) - med(L)| \geq |\mathbf{E}L(X) - med(L)|$. Hence, we can derive concentration inequalities for the probability $\mathbf{Pr}(|L(X) - \mathbf{E}L(X)| \geq t)$. In the next section we will look at some important special cases.

It is particularly interesting to consider the case $\lambda = 1/2$, since it relates the functionals in question on an HST with functionals on the unit cube of some dimension. When $b = 2^d$ for some positive integer d, the HST approximates the d-dimensional unit cube in Euclidean space.

Let us first consider the case $b = 2$: we encounter such a tree T when approximating the $[0, 1]$ interval. For this case $b\lambda = 1$, and therefore $Top(k) = O(\log_2 k)$. One can show (using, e.g., numerical approximation) that

$$\begin{aligned} |\mathbf{E}L(X) - med(L)| &\leq \int_{t\geq 0} \mathbf{Pr}(|L(X) - med(L)| \geq t)\ dt \\ &\leq 4 \int_{t\geq 0} \exp\left(-\frac{2^{t/c}}{8n}\right)\ dt \\ &= \Theta(\log_2 n). \end{aligned}$$

Consequently, we have

$$\mathbf{Pr}(|L(X) - \mathbf{E}L(X)| \geq t + C\log_2 n) \leq 4\exp\left(-\frac{2^{t/c}}{8n}\right).$$

Since $\mathbf{E}L(X) = O(\log_2 n)$, this means that we don't have an especially useful concentration result for this special case. Inspecting cases, one finds the following inequality for the case $b = 2$ and $\lambda = 1/2$:

$$\mathbf{Pr}(|L(X) - \mathbf{E}L(X)| \geq t) \leq 8 \exp\left(-\frac{2^{t/c}}{8n}\right),$$

where c is a real constant. While the constants can be improved somewhat (partly due to the fact that the constants are not the best possible for this case), this inequality allows $L(X)$ to be spread out over an interval of length $\Theta(\mathbf{E}L(X))$. However, the probability of $L(X)$ falling outside this interval is very small: even a deviation of $C \log\log n$ results in a probability less than $1/n$.

On the other hand, the bounds that we have derived will provide very good concentration inequalities for the case $b > 2$. As above, we need to estimate an integral to get a bound for $|\mathbf{E}L(X) - med(L)|$:

$$\begin{aligned} |\mathbf{E}L(X) - med(L)| &\leq 4 \int_{t \geq 0} \exp\left(-\frac{t^{2/\log_b(b\lambda)}}{C_3 n}\right) dt \\ &= \Theta(\sqrt{\mathbf{E}L(X)}), \end{aligned}$$

as can be shown by numerical approximation.

We thus have the following concentration inequality:

$$\mathbf{Pr}(|L(X) - \mathbf{E}L(X)| \geq t) \leq 8 \exp\left(-\frac{t^{2/\log_b(b/2)}}{c'n}\right),$$

where c' is a real constant. Notice $\log_b(b/2) < 1$; thus, whenever $\lambda = 1/2$ and $b \geq 3$, the exponent of t above is larger than 2. In other words, in these cases all the considered monochromatic optimization problems exhibit sub-gaussian behavior.

The case $b = 2^d$ can be used to approximate the L-functional in the d-dimensional unit cube. In general, when $b = 2^d$ the inequality has the following form:

$$\mathbf{Pr}(|L(X) - \mathbf{E}L(X)| \geq t) \leq 8 \exp\left(-\frac{t^{2d/(d-1)}}{c''n}\right),$$

for some real constant c''.

2.7 Application to problems on random point sets from $[0,1]^d$

Let us finish by considering these problems on the Euclidean hypercube $[0,1]^d$. As described in the introduction, we can break the hypercube into s parts (with s a power of 2) along every dimension, giving us a set of s^d smaller hypercubes. We now build an HST with branching factor 2^d, edge weight ratio 1/2, and s^d leaves. (The implied depth is $\log_{2^d}(s^d) = \log_2 s$.) Each leaf corresponds to one of the small hypercubes. The structure of the tree is such that the root corresponds to the whole hypercube, its children correspond to the 2^d hypercubes obtained by breaking it in half along every dimension, etc.

A point set W is chosen i.i.d. uniformly, and we wish to know the expected cost of the minimum matching, spanning tree, or tour. We can translate the point set into a leaf set as follows: Each point is contained in one of the s^d small hypercubes. Move each point to the center of its hypercube. The distances in the HST dominate the distances between the centered points, so that the cost of the optimal solution to the HST problem dominates the cost of the optimal solution to the point problem.

We introduced some error when we centered the points, but this error can be made to vanish by increasing s. Although the tree becomes deeper, the *effective* height of the tree is capped at $\log_b n$: this is the number that appears in our results. Thus the error is negligible, and our results on the monochromatic HST problems give upper bounds for the corresponding problems on point sets.

Theorem 2.28 *Fix a dimension $d \geq 2$, and let W be a set of points chosen i.i.d. uniformly from $[0,1]^d$. The expected costs of the monochromatic minimum matching, MST, and TSP tour on W are*

$$O\left(n^{(d-1)/d}\right).$$

Proof: Transforming the problem into an HST problem, we obtain an HST with $b = 2^d$ and $\lambda = 1/2$. Its effective height is $\log_b n = \log_{2^d} n$. By Theorems 2.7, 2.12, and 2.17, the cost of the optimal solution to the HST problem is $\Theta(\sum_{k=1}^{\log_b n}(b\lambda)^k)$. Here, $b\lambda = 2^{d-1}$, so the dominant term in the series is $(2^{d-1})^{\log_{2^d} n}$. Using the identity $a^{\log b} = b^{\log a}$, we obtain

$$(2^{d-1})^{\log_{2^d} n} = n^{\log_{2^d} 2^{d-1}} = n^{(d-1)/d},$$

the desired bound. □

(If we repeat this process for $d = 1$, we have $b\lambda = 1$ and the summation evaluates to $\log_2 n$, a weak result.)

Our upper bounds for $d \geq 2$ are, in fact, tight; see, e.g., Yukich [58], who proves (by a different method) that $n^{(d-1)/d}$ is a tight bound for all $d \geq 1$. Our inequalities from the previous section apply here, but only from above. They do not prove concentration, then, but rather show that our upper bound holds with extremely high probability.

2.8 Conclusion

We began by showing how the Euclidean hypercube $[0,1]^d$ can be embedded into a hypertorus on $[0,2]^d$ and then approximated by a balanced HST. Once this embedding has been done, numerous problems about point sets on $[0,1]^d$ can be re-expressed as problems about multisets of the leaves of the HST.

We showed tight bounds on the monochromatic matching problem, MST problem, and TSP on balanced HSTs. The expected optimal cost for each problem is on the order of $\sum_{k=1}^{h}(b\lambda)^k$, where $h = \min(\delta, \log_b n)$. From our tight concentration results, we know that with high probability, an optimal solution to these problems will have a cost close to the expected cost.

Along the way, we presented the lifting lemma, a useful tool in tightening the bounds on our solutions. We saw that the $(\log_b n)$-th level of the tree is "special" in a sense that is hard to pin down precisely. This level of the tree has an average (in expectation) of one point per node; for the matching problem, this situation gives the worst case, but for the MST problem the relationship is not as clear. In the next chapter, we consider the bichromatic versions of these problems, and the lifting lemma will become crucial.

3. Bichromatic MST and TSP on HSTs

3.1 Introduction

Monochromatic problems on HSTs have natural generalizations to bichromatic problems. Instead of considering a single n-element multiset of leaves, we now have two n-element multisets, which we generally call the "red" set and the "blue" set, denoting these by R and B. Links between the leaves — matches in a matching problem, and edges in the MST problem and TSP — are now allowed only between points of different colors. We assume that the reader has already read Chapter 2.

The bichromatic matching problem emerges naturally in many areas. It is often termed the *earth-mover's distance*: if we view each red point as a load and each blue point as a site, the optimal bichromatic matching gives the most efficient way (minimizing total distance) to move each load to a distinct site. Beyond its obvious logistical uses, bichromatic matching finds uses in such diverse areas of computer science as image retrieval [26], hashing schemes [27], wireless network routing [49], and subtree isomorphism problems [32].

Abrahamson et al. [1, 2] solved the bichromatic matching problem on HSTs, showing that the optimal matching has a cost of $\Theta\left(\sqrt{n} \cdot \sum_{i=1}^{h} (\sqrt{b}\lambda)^i\right)$, where $h = \min(\delta, \log_b n)$. We will extend their results to cover the bichromatic MST problem and the bichromatic TSP. For the sake of completeness, we will also give a short proof of the bound for the matching problem. The following observation will be crucial; the reader may find it intuitive, but we state it here to refer to it later.

Observation 3.1 *Let $\mathcal{P}$ be a monochromatic problem and $\mathcal{P}'$ be the corresponding bichromatic problem. Writing $\mathcal{P}(W)$ for the cost of the optimal solution to $\mathcal{P}$ on the point set W, and writing $\mathcal{P}'(R, B)$ for the cost of optimal solution to $\mathcal{P}'$ on the sets*

R and B, we have

$$\mathcal{P}(R \cup B) \leq \mathcal{P}'(R, B).$$

Note that a bichromatic problem with $|R| = |B| = n$ will give rise to a monochromatic problem on a multiset of size $2n$. Defining $h = \min(\delta, \log_b n)$ and $h' = \min(\delta, \log_b(2n))$, we see $h' \leq h + \log_b 2$. If $b\lambda > 1$, the optimal cost for one of our monochromatic problems on $2n$ points will thus have a lower bound of $\Omega\left(\sum_{k=1}^{h}(b\lambda)^k\right)$ and an upper bound of

$$O\left(\sum_{k=1}^{h'}(b\lambda)^k\right) = O\left(\sum_{k=1}^{h+log_b 2}(b\lambda)^k\right) = (b\lambda)^{\log_b 2} \cdot O\left(\sum_{k=1-\log_b 2}^{h}(b\lambda)^k\right),$$

so that the cost is still $\Theta\left(\sum_{k=1}^{h}(b\lambda)^k\right)$. If $b\lambda < 1$, taking extra terms of the sequence does not change its asymptotic cost. If $b\lambda = 1$, the cost becomes $\Theta\left(\log_b n + \log_b 2\right) = \Theta(\log_b n)$. In every case, then, we see that the cost of an optimal solution on $2n$ points is the same, up to a constant factor, as the cost of an optimal solution on n points. In fact, for any constant $K \geq 1$, the optimal cost for one of our monochromatic problems on Kn points remains $\Theta\left(\sum_{k=1}^{h}(b\lambda)^k\right)$: the factor $(b\lambda)^{\log_b 2} = 2^{1+\log_b \lambda}$ becomes $(b\lambda)^{\log_b K} = K^{1+\log_b \lambda}$, which is still a constant.

After settling these problems for HSTs, we will consider the bichromatic MST problem and TSP on point sets in the Euclidean hypercube $[0,1]^d$. By relying on Observation 3.1 and on previously known results about monochromatic problems (see Yukich, [58]), we can obtain novel bounds on these two problems for $d \geq 3$.

3.2 Definitions of problems

The bichromatic versions of our problems are defined very similarly to the monochromatic cases. We first choose two submultisets of the leaves of H; let us call these R'

and B'. We define G to be the complete bipartite graph with two n-element color classes R and B, where, as before, R will contain every element of R', B will contain every element of B', and, if necessary, we index the multiple copies of the leaves. The weight of an edge is again determined by the distance between its the endpoints in H. Since G is bipartite, every edge that will be included in the solution of any of the optimization problems above will be a red-blue edge. For completeness, we list these problems more formally below.

Bichromatic Minimum Matching Problem (MMP'): The minimum matching on V has cost given by

$$\min_{M \subseteq G} \sum_{e \in M} |e|,$$

where $|e|$ denotes the weight of the edge e and the minimum is taken over all possible perfect bichromatic matchings M of G.

Bichromatic Travelling Salesman Problem (TSP'): A bichromatic tour is a simple cycle that visits each vertex of V exactly once and alternates colors along each edge. The minimum tour length is given by

$$\min_{T \subseteq G} \sum_{e \in T} |e|,$$

where the minimum is taken over all bichromatic tours T.

Bichromatic Minimum Spanning Tree Problem (MST'): The minimum bichromatic spanning tree cost is given by

$$\min_{F \subseteq G} \sum_{e \in F} |e|,$$

where the minimum is taken over all bichromatic spanning trees F.

One can also consider K-partite versions of these problems for arbitrary $K > 2$, where a pair of points is allowed to be joined if and only if the two points are of different colors. It turns out that the K-chromatic minimum spanning tree problem behaves much like the bichromatic version; we will have more to say about this at the end of the chapter. We have not pursued the K-chromatic matching problem or TSP.

3.3 Behavior of the discrepancy

Our proof for the bichromatic TSP relies on a kind of random variable to which we will refer as *discrepancy*. Recall that a binomial variable $Binomial(n, p)$ is one of the form $Y_1+Y_2+\ldots+Y_n$, where $P(Y_i = 1) = p$ and $P(Y_i = 0) = 1-p$ for every $1 \leq i \leq n$, with the Y_i's independent. For a vertex v in level ℓ of an HST, the discrepancy has the form $|R(v) - B(v)|$, where $R(v)$ and $B(v)$, the numbers of red and blue points in v's subtree, are independent variables with distribution $Binomial(n, 1/b^\ell)$. We can, if we like, view the discrepancy as the outcome of a random walk. Let us start at zero on the number line, and at each turn, we move left with probability $p \leq 1/2$, move right with probability p, and stay put with probability $1 - 2p$. After n turns, our distance from the origin is given by the discrepancy.

We now consider its expected behavior. We prove two bounds: one will be useful in the case of a star tree, while the other will be used in the bound for general HSTs.

Lemma 3.2 *Let X be the difference of two i.i.d. $Binomial(n, p)$ variables. For fixed p,*

$$\mathbf{E}|X| = \Theta(\sqrt{n}).$$

Lemma 3.3 *Let X be the difference of two i.i.d. $Binomial(n, p)$ variables, with $n \geq 1/p$ and $p \leq 1/2$. Then*

$$\sqrt{Cnp} \leq \mathbf{E}|X| \leq \sqrt{2np}$$

for some constant $C > 0$.

Proof (of both lemmata): We denote by $\mathbf{D}Y$ the standard deviation of the random variable Y. From elementary probability, we recall

$$0 \leq \mathbf{Var}|X| = \mathbf{E}|X|^2 - (\mathbf{E}|X|)^2 = \mathbf{E}X^2 - (\mathbf{E}|X|)^2 = (\mathbf{D}X)^2 - (\mathbf{E}|X|)^2,$$

and $\mathbf{E}|X| \leq \mathbf{D}X$. Since $\mathbf{D}X = \sqrt{2np(1-p)}$, the upper bounds on $\mathbf{E}|X|$ follow.

The lower bound will take more work. Recall Hölder's inequality,

$$\mathbf{E}|YZ| \leq (\mathbf{E}|Y|^q)^{1/q} \cdot (\mathbf{E}|Z|^r)^{1/r} \text{ when } 1/q + 1/r = 1.$$

Setting $Y = |X|^{2/3}, Z = |X|^{4/3}, q = 3/2, r = 3$, we obtain $\mathbf{E}|X|^2 \leq (\mathbf{E}|X|)^{2/3}(\mathbf{E}|X|^4)^{1/3}$, and thus

$$\mathbf{E}|X| \geq \frac{(\mathbf{E}X^2)^{3/2}}{\sqrt{\mathbf{E}X^4}}.$$

By definition, we can write X as the sum $X_1 + X_2 + \ldots + X_n$, where the X_i's are i.i.d. with

$$X_i = \begin{cases} 1 & \text{with probability } p(1-p), \\ -1 & \text{with probability } p(1-p), \\ 0 & \text{with probability } p^2 + (1-p)^2. \end{cases}$$

It is clear that $\mathbf{E}X^2 = 2np(1-p)$.

Consider the expansion $X^4 = (X_1 + X_2 + \ldots + X_n)^4$. Any term with an odd power of an X_i, such as $X_1^3 X_2$ or $X_1^2 X_2 X_3$, will have zero expectation, by independence and the fact $\mathbf{E}X_i = \mathbf{E}X_i^3 = 0$. Thus the only terms with nonzero expectation will be the terms X_i^4 and $X_i^2 X_j^2$ with $i \neq j$. Since $\mathbf{E}X_i^4 = \mathbf{E}X_i^2 = 2p(1-p)$ and

$\mathbf{E}X_i^2X_j^2 = \mathbf{E}X_i^2 \cdot \mathbf{E}X_j^2 = 4p^2(1-p)^2$ for $i \neq j$, we have

$$\mathbf{E}X^4 = \sum_{i=1}^{n} X_i^4 + 6\sum_{i\neq j} \mathbf{E}X_i^2X_j^2 = 2np(1-p) + 24n(n-1)p^2(1-p)^2 = \Theta(n^2).$$

Thus

$$\mathbf{E}|X| \geq \frac{(\mathbf{E}X^2)^{3/2}}{\sqrt{\mathbf{E}X^4}} = \frac{[2np(1-p)]^{3/2}}{\sqrt{\Theta(n^2)}} = \Omega(\sqrt{n}),$$

proving Lemma 3.2. Note that without the $2np(1-p)$ term in the denominator, this function would behave as $\sqrt{Cnp(1-p)}$. To see when the $24n(n-1)p^2(1-p)^2$ term will dominate, we set

$$np(1-p) \leq 24n(n-1)p^2(1-p)^2$$

and obtain

$$1 \leq 24(n-1)p(1-p).$$

For $n \geq 2$ we have $2(n-1) \geq n$, and for $p \leq 1/2$ (as it always is for us) we have $p(1-p) \geq p/2$; thus $1 \leq np$ will imply $1 \leq 4(n-1)p(1-p)$. When $n \geq 1/p$, then, this bound is at least $\sqrt{Cnp}$, and Lemma 3.3 is proved. $\square$

Remark 3.4 *For a vertex in level ℓ of the tree, $p = 1/b^\ell$; thus when $\ell \leq \log_b n$, we have $n \geq 1/p$.*

3.4 Bichromatic TSP

In this section, we will show that the expected TSP cost on two n-element multisets R and B is on the order of $\sqrt{n} \cdot \sum_{i=1}^{h}(\sqrt{b}\lambda)^i$, where $h = \min(\delta, \log_b n)$.

We start by considering the case when F is a star tree with edge weight λ. Let n red points and n blue points be uniformly distributed at random among the leaves of F. We will call a leaf *easy* if it has been assigned equal numbers of red and blue points; otherwise, we will call the leaf *hard*. Note that a hard leaf can be either monochromatic or bichromatic.

Our optimal tour is produced by the following algorithm:

1. Connect the points at every easy leaf into a path that begins at a red point and ends at a blue point. These paths have zero cost.

2. Connect the paths at the easy leaves into one long red-blue path. If there are k easy leaves, the total cost of this is $(k-1)\lambda$.

3. At each hard leaf, find the longest possible red-blue path, depending on whether we have more red or more blue points.

   Since one color outnumbers the other, each of these paths can have the same color at both its endpoints. We delete the inner points of all such paths, leaving only the two same-colored endpoints. Hence, after this process, some points are isolated, while the other points are all arranged into a long path.

4. Connect the isolated points into a long red-blue path, and then glue the two long paths together to get the traveling salesman tour.

This algorithm can easily be extended to find the optimal TSP tour for general HSTs (not just star trees). To this end, it is useful to consider a version that works when the numbers of red and of blue points are different. In such a case, we can only have a path of minimum cost, hence, in Steps 3 and 4 one has to modify the method to first connect as many isolated red-blue points together into a red-blue path as possible, and then connect this long path to the path containing the points of the easy leaves.

Let us now apply Lemma 3.2 to the problem of finding the expected TSP cost for a star tree. Let us write R_i for the number of red points assigned to leaf l_i, and similarly B_i for the number of blue points. Then X in Lemma 3.2 will be $R_i - B_i$ for the leaf l_i. As described initially, we make as long a path as possible in each leaf; these paths have zero cost. Our task is now to connect these paths into a tour.

If $R_i \neq B_i$, our tour must visit the leaf exactly $|R_i - B_i| + 1$ times. If $R_i = B_i$, the cost depends on whether R_i and B_i are zero or not. If they are, then there is no cost; if not, the leaf must be visited once. Therefore, the cost contributed by leaf l_i is either $|R_i - B_i|$ or $|R_i - B_i| + 1$.

The extra $+1$ poses no problem. By Observation 3.1, the cost of the optimal *monochromatic* tour is less than or equal to the cost of the optimal bichromatic tour. Thus we can add the cost of the monochromatic tour to the bichromatic tour and only increase its cost by a constant factor. Since $\mathbf{E}|R_i - B_i| = \Theta(\sqrt{n})$ by Lemma 3.2, we have

Proposition 3.5 *Let R and B be two multisets of size n of the leaves of the star tree F with b leaves and all edge weights 1. Consider b fixed, and assume that n is large. The expected cost of the optimal bichromatic tour on R and B is $\Theta(\sqrt{n})$.*

The case of a general HST can be handled similarly, this time using Lemma 3.3. Let v be a non-leaf vertex in the HST. As described above, we make as long a path as possible in the subtree rooted at v. The endpoints of this path must now look upward to connect to the rest of the tour, as must the leftover points that were not incorporated into the path.

Let the number of red (resp. blue) points assigned to a non-leaf node v be $R(v)$ (resp. $B(v)$). If $R(v) \neq B(v)$, our tour must enter v's subtree exactly $|R(v) - B(v)| + 1$ times. If $R(v) = B(v)$, then the cost depends on whether their value is zero or not: if it is zero, then there is no cost, while if the value is nonzero, the subtree must be entered once. Thus the cost contributed by v is either $|R(v) - B(v)|$ or $|R(v) - B(v)| + 1$.

As before, the extra $+1$ does not matter: using Observation 3.1, we can add the cost of the monochromatic tour to the bichromatic tour, and the only effect will be to increase its cost by a constant factor.

Theorem 3.6 *Let R and B be two n-element multisets taken independently from the leaves of the HST $H(b, \delta, \lambda)$. Consider b and λ fixed, and define $h = \min(\delta, \log_b n)$. The expected cost of the optimal bichromatic tour on R and B is*

$$\Theta\left(\sqrt{n} \cdot \sum_{i=1}^{h} (\sqrt{b}\lambda)^i\right).$$

Proof: Let v be a node in level $\ell \leq h$. By Lemma 3.3 and Remark 3.4, the expected contribution of v to the cost of the tour is $\Theta(\lambda^\ell \cdot \sqrt{n/b^\ell}) = \Theta((\lambda/\sqrt{b})^\ell \cdot \sqrt{n})$. The total cost of level ℓ, obtained by multiplying by b^ℓ, is therefore $\Theta((\sqrt{b}\lambda)^\ell \cdot \sqrt{n})$; summing up over levels $1, 2, \ldots, h$ and adding in the cost of the monochromatic MST gives us bounds on the cost of the portion of the tour above level h: the lower bound is

$$\Omega\left(\sqrt{n} \cdot \sum_{i=1}^{h} (\sqrt{b}\lambda)^i\right),$$

while the upper bound is

$$O\left(\sqrt{n} \cdot \sum_{i=1}^{h} (\sqrt{b}\lambda)^i + \sum_{i=1}^{h} (b\lambda)^i\right).$$

But in fact

$$\sum_{i=1}^{h} (b\lambda)^i = O\left(\sqrt{n} \cdot \sum_{i=1}^{h} (\sqrt{b}\lambda)^i\right),$$

because $b^i \leq \sqrt{n \cdot b^i}$ for $i \leq h$. (The inequality simplifies to $b^i \leq n$; recall $b^h = n$.) We have shown, then, that the expected cost of the tour above level h is

$$\Theta\left(\sqrt{n} \cdot \sum_{i=1}^{h} (\sqrt{b}\lambda)^i\right).$$

If $h = \delta$ we are done. If instead $h = \log_b n$, we must first lift the points to level h; the cost of the lifting is $O((b\lambda)^h)$, but as above, $(b\lambda)^h = O\left(\sqrt{n} \cdot \sum_{i=1}^{h} (\sqrt{b}\lambda)^i\right)$, so that the lifting does not increase the asymptotic cost. $\square$

3.5 Bichromatic matching revisited

If we lean on the results from the previous section, we can easily re-derive the bichromatic matching result from [1] and [2].

When we considered monochromatic matching, we spoke in terms of the number of transits at each node v in the tree. For bichromatic matching, we should instead think about the points that must be sent up from v. Suppose the subtree rooted at v contains $R(v)$ red points and $B(v)$ blue points. We can form $\min(R(v), B(v))$ matches within this subtree, but $|R(v) - B(v)|$ of the points must look for matches outside this subtree. The parent edge of v must therefore be used $|R(v) - B(v)|$ times. If v is in level $\ell \leq h$ of the HST, this edge has weight λ^ℓ, so that the contribution of v to the matching cost is $\lambda^\ell \cdot |R(v) - B(v)|$. By Lemma 3.3 with $p = 1/b^\ell$, the expectation of this cost is $\Theta(\lambda^\ell \cdot \sqrt{n/b^\ell})$. The entire cost of level ℓ is

$$b^\ell \cdot \Theta(\lambda^\ell \cdot \sqrt{n/b^\ell}) = \Theta(\sqrt{n} \cdot (\sqrt{b}\lambda)^\ell).$$

Adding over all the levels from 1 to h, we obtain a bound of

$$\Theta\left(\sqrt{n} \cdot \sum_{k=1}^{h} (\sqrt{b}\lambda)^k\right)$$

for the tree edges above level h that are used in the matching. Thus

Lemma 3.7 *Let R and B be two multisets of size n of the leaves of the HST $H(b, \delta, \lambda)$. Consider b and λ fixed, and define $h = \min(\delta, \log_b n)$. In an optimal bichromatic* *matching on R and B, the total cost of the edges needed above level h of the tree is*

$$\Theta\left(\sqrt{n}\cdot\sum_{k=1}^{h}(\sqrt{b}\lambda)^k\right).$$

Theorem 3.8 ([1, 2]) *Let R and B be two multisets of size n of the leaves of the HST $H(b,\delta,\lambda)$. Consider b and λ fixed, and define $h = \min(\delta, \log_b n)$. Then the expected cost of the optimal bichromatic matching on R and B is*

$$\Theta\left(\sqrt{n}\cdot\sum_{k=1}^{h}(\sqrt{b}\lambda)^k\right).$$

Proof: If $h = \delta$, the above argument shows the theorem to be true. Suppose instead $h = \log_b n$. By Lemma 3.7, the cost is lower-bounded by $\Omega(\sqrt{n}\cdot\sum_{k=1}^{h}(\sqrt{b}\lambda)^k)$. To show the upper bound, we lift the points to level h. The cost of this lifting is $O((b\lambda)^h)$, but since $(b\lambda)^h = O(\sqrt{n}\cdot(\sqrt{b}\lambda)^h)$, the total cost remains $O(\sqrt{n}\cdot\sum_{k=1}^{h}(\sqrt{b}\lambda)^k)$. $\square$

3.6 Bichromatic MST

It turns out that the bichromatic MST problem is substantially different from the bichromatic TSP and matching problem; for this reason, we have saved its discussion for last. This difference appears even in the simple example of a star tree. Consider the following problem: F is a star tree centered at r and has l leaves, $x_1, x_2, \ldots, x_l$, with l even. Assume that at half the leaves x_i there are $s > 1$ red points and one blue point, and at each of the other leaves there are s blue points and one red point. We stipulate that the distance of two points residing at the same leaf is zero, and the distance between any other pair of points is one. It is easy to see that the optimal cost for the bichromatic TSP is $(s-1)l$, while the optimal bichromatic spanning tree we will have a total weight of merely $l-1$.

Of course, our example has not shown anything about the expected behavior of the bichromatic MST problem. Nonetheless, it turns out that on average, the optimal bichromatic MST is lighter than the bichromatic TSP tour. Let R and B be two multisets of n points chosen uniformly at random from the leaves of an HST $H(b, \delta, \lambda)$. In this section, we will show that the expected cost of the MST is on the order of $\sum_{k=1}^{h}(b\lambda)^k$, where $h = \min(\delta, \log_b n)$. This result is somewhat unexpected, since it differs from our other bichromatic results and coincides with our monochromatic results.

To form the bichromatic MST, we must connect each red point r_i to its nearest blue neighbor, and similarly, we must connect each blue point b_i to its nearest red neighbor. Since these two cases are symmetric, we will assume without loss of generality that we are concerned with connecting a red point r_i to a blue neighbor. We will write $N(r_i)$ for the closest opposite-colored point in the tree. (In fact, more than one point may be the "closest"; we can disambiguate by making $N(r_i)$ the leftmost closest point.) It is evident that $N(r_i)$ is the blue point p that minimizes the height of the highest node $\mathcal{H}$ in the path from r_i to p. If p is at the same leaf as r_i, the cost will be zero. Otherwise, if $\mathcal{H}$ is in level ℓ, the cost of the path from r_i to $\mathcal{H}$ will be $\lambda^{\ell+1} + \lambda^{\ell+2} + \ldots + \lambda^{\delta} < \lambda^{\ell+1}/(1-\lambda)$, while the cost of the path from $\mathcal{H}$ to p will be the same. Therefore, the cost that r_i contributes to the MST is between $2\lambda^{\ell+1}$ and $2\lambda^{\ell+1}/(1-\lambda)$.

We can illustrate this process by coloring the nodes of the MST as follows. We color a node violet if it has both red and blue points in its subtree. If it has no points in its subtree, we leave the node white. Otherwise, the node is colored red or blue, depending on which color of points appears in its subtree. See Figure 3.1 for an example (the colors are represented by the letters R, B, V, W). The cost of the bichromatic MST is then obtained by finding the cost from each point p_i to its nearest (ancestral) violet node $V(p_i)$.

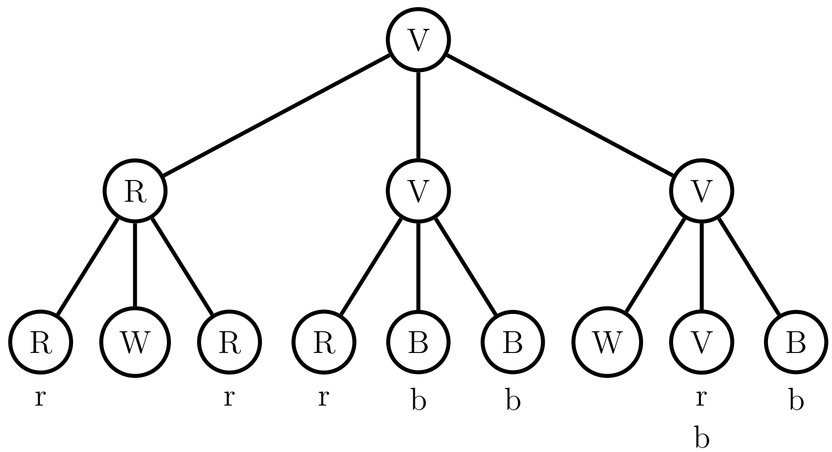


Figure 3.1: Four red points and four blue points are distributed among the leaves of an HST with $b = 3$ and $\delta = 2$. Lowercase letters represent points; uppercase letters represent the node colors. R = red, B = blue, V = violet, W = white (blank)

There is a caveat with this formulation: the resulting structure may not be connected. (This will occur, for example, when each subtree of the root receives n/b red points and n/b blue points.) As before, we will include the edges of the *monochromatic* MST on $R \cup B$ as part of the bichromatic MST. The cost of the monochromatic MST does not increase the asymptotic cost of the bichromatic MST, since the former is easily seen to cost no more than the latter by Observation 3.1.

We can now state

Proposition 3.9 *Let R and B be two uniformly and independently chosen multisets of n leaves from the HST $H(b, \delta, \lambda)$. The expected cost of the bichromatic MST on R and B is*

$$\Theta(\mu + n \cdot \mathbf{E}[\mathcal{C}(b, \delta, \lambda, n)]),$$

where $\mathcal{C}(b, \delta, \lambda, n)$ is the cost of the path from a point p to its lowest violet ancestor in H, and μ is the expected cost of the monochromatic MST of $R \cup B$.

Note that the distribution of $\mathcal{C} = \mathcal{C}(b, \delta, \lambda, n)$ is the same for every point in $R \cup B$.

(They are not, however, independent.) We determine $\mathbf{E}[\mathcal{C}]$ by calculating explicitly the distribution of $\mathcal{C}$. Let the first red point r_1 be located, without loss of generality, at the leftmost leaf L of the HST. We define the function $P(m, n, i, j)$ to be the probability that the smallest element of an n-element randomly chosen submultiset of $\{1, \ldots, m\}$ falls in the range $i, \ldots, j$. Then

- the probability that its leaf L is violet is the probability that one of the blue points is also located at L, which is $P(b^\delta, n, 1, 1) = 1 - (1 - 1/b^\delta)^n$.
- The probability that L is not violet, but its parent *is* violet, is the probability that L has no blue point but one of its siblings does. This probability is $P(b^\delta, n, 2, b)$.
- The probability that L and its parent are not violet, but its grandparent *is* violet, is $P(b^\delta, n, b+1, b^2)$, etc., etc.

Lemma 3.10

$$P(m, n, i, j) = \frac{(m - i + 1)^n - (m - j)^n}{m^n}.$$

Proof: One can visualize the elements of the multiset as lattice points in the n-dimensional cube with edge length m. Then the total number of points is m^n. The chosen points must belong to a sub-cube with edge length $m - i + 1$; however, we have to discard those lattice points that have only large entries. These lattice points belong to a sub-cube of volume $(m - j)^n$. $\square$

In general, the probability that the red point will have its lowest violet ancestor in the ℓ-th level from the *bottom* of the tree, $1 \leq \ell \leq \delta$, is

$$\begin{aligned} P(b^\delta, n, b^{\ell-1} + 1, b^\ell) &= \frac{(b^\delta - b^{\ell-1})^n - (b^\delta - b^\ell)^n}{(b^\delta)^n} \\ &= (1 - b^{(\ell-\delta)-1})^n - (1 - b^{\ell-\delta})^n. \end{aligned}$$

Clearly $P(b^\delta, n, b^{\ell-1}+1, b^\ell) \leq (1-b^{(\ell-\delta)-1})^n$. Under stronger conditions, a similar lower bound (Lemma 3.12 below) also holds. Before we prove it, we make a brief digression to talk about the behavior of the expression $(1 \pm r/n)^n$ for r fixed. It is well known that it approaches $e^{\pm r}$ as $n \to \infty$. But since our earlier results did not rely on n going to infinity, we would like to avoid that here as well. Fortunately, the expression is bounded between exponentials even for relatively small values of n.

Proposition 3.11 *Let $r > 0$. Then for $n > r$,*

$$e^{r/2} < (1+r/n)^n < e^r,$$

and for $n > 3r$,

$$e^{-3r/2} < (1-r/n)^n < e^{-r}.$$

Proof: The upper bounds follow from the elementary inequality $1+y < e^y$ for $y \neq 0$. (The simplest proof: The expression $e^y - (1+y)$ has its unique global minimum at $y = 0$, shown by taking derivatives. The value of this minimum is 0.)

Now we show the lower bounds. We use the Taylor series

$$\ln(1-x) = -x - x^2/2 - x^3/3 - x^4/4 - \ldots,$$

which is valid for $-1 \leq x < 1$.

$$\begin{aligned} n \cdot \ln(1+r/n) &= n \cdot (r/n - r^2/2n^2 + r^2/3n^3 - r^4/4n^4 + \ldots) \\ &> n \cdot (r/n - r^2/2n^2) \\ &= r - r^2/2n. \end{aligned}$$

Simplifying $r - r^2/2n > r/2$ shows that it is equivalent to $n > r$. Thus, for $n > r$, we have $n \cdot \ln(1 + r/n) > r/2$. Exponentiating both sides gives the first statement.

Similarly,

$$\begin{aligned} n \cdot \ln(1 - r/n) &= n \cdot (-r/n - r^2/2n^2 - r^3/3n^3 - \ldots) \\ &> n \cdot (-r/n - r^2/n^2 - r^3/n^3 - \ldots) \\ &= n \cdot \frac{-r/n}{1 - r/n} \\ &= \frac{rn}{r - n}. \end{aligned}$$

Simplifying $rn/(r - n) > -3r/2$, assuming $n > r$, shows that it is equivalent to $n > 3r$. Thus for $n > 3r$, we have $n \cdot \ln(1 - r/n) > -3r/2$. Exponentiating both sides gives the second statement. □

We now turn our attention back to the lower bound on $P(b^\delta, n, b^{\ell-1} + 1, b^\ell)$.

Lemma 3.12 *When $\delta \leq \log_b n$ and $n > 1$,*

$$P(b^\delta, n, b^{\ell-1} + 1, b^\ell) \geq 1/5 \cdot (1 - b^{(\ell-\delta)-1})^n.$$

Proof: For brevity, we write $z = b^{\ell-\delta}$. The smallest that z can be is $b^{-\delta} \geq b^{-\log_b n} = 1/n$ — that is, z cannot be smaller than $1/n$.

Consider the fraction $\frac{1 - z}{1 - z/b}$. It is less than 1, and its value increases as z decreases. Thus

$$\left(\frac{1 - z}{1 - z/b}\right)^n \leq \frac{(1 - 1/n)^n}{(1 - 1/bn)^n} \leq \frac{e^{-1}}{e^{-3/2b}} = e^{3/2b-1} \leq e^{-1/4} < 4/5.$$

(We have used Proposition 3.11 to show $(1 - 1/bn)^n \geq e^{-3/2b}$. Notice that $n > 1$ implies $n > 3/b$.)

So

$$(1 - z)^n \leq 4/5 \cdot (1 - z/b)^n,$$

and

$$(1 - z/b)^n - (1 - z)^n \geq 1/5 \cdot (1 - z/b)^n.$$

□

Accordingly, given $\delta \leq \log_b n$, we have

$$\begin{aligned}
\mathbf{E}[\mathcal{C}(b, \delta, \lambda, n)] &= \Theta\Big(0 \cdot P(b^\delta, n, 1, 1) + 2\lambda^\delta/(1-\lambda) \cdot P(b^\delta, n, 2, b) + \\
&\quad 2\lambda^{\delta-1}/(1-\lambda) \cdot P(b^\delta, b, b+1, b^2) + \\
&\quad 2\lambda^{\delta-2}/(1-\lambda) \cdot P(b^\delta, n, b^2+1, b^3) + \\
&\quad \ldots + 2\lambda^1/(1-\lambda) \cdot P(b^\delta, n, b^{\delta-1}+1, b^\delta)\Big) \\
&= \Theta\left(\sum_{\ell=1}^{\delta} 2\lambda^{(\delta-\ell)+1}/(1-\lambda) \cdot (1 - b^{(\ell-\delta)-1})^n\right) \\
&= 2\lambda^\delta \cdot \Theta\left(\sum_{\ell=1}^{\delta} \lambda^{1-\ell} \cdot (1 - b^{(\ell-\delta)-1})^n\right)
\end{aligned}$$

for fixed b and λ. Our next task is to show that the expression $\Theta\left(\sum_{\ell=1}^{\delta} \lambda^{1-\ell} \cdot (1 - b^{(\ell-\delta)-1})^n\right)$ is bounded between constants.

Lemma 3.13 *Let $b \geq 2$ and $\lambda < 1$ be fixed, let $\delta \leq \log_b n$, and let $n > 4\ln(1/\lambda)$. Define $a_\ell = \lambda^{1-\ell} \cdot (1 - b^{(\ell-\delta)-1})^n$. Then there is a constant C such that*

$$\frac{a_\ell}{a_{\ell+1}} \geq \frac{1}{\lambda}$$

for all $\ell \in \{C, \ldots, \delta\}$.

Proof: Defining $z = b^{\ell-\delta}$ as above, we have

$$\begin{aligned}\frac{a_\ell}{a_{\ell+1}} &= \lambda\left(\frac{1-z/b}{1-z}\right)^n \\ &\geq \lambda\left(\frac{1-z/2}{1-z}\right)^n \\ &= \lambda\left(1+\frac{z/2}{1-z}\right)^n \\ &\geq \lambda\left(1+\frac{z}{2}\right)^n.\end{aligned}$$

When $z > (8\ln(1/\lambda))/n$, we have

$$\left(1+\frac{z}{2}\right)^n > \left(1+\frac{4\ln(1/\lambda)}{n}\right)^n > e^{2\ln(1/\lambda)} = \frac{1}{\lambda^2};$$

thus $\left(1+\frac{z}{2}\right)^n \geq \frac{1}{\lambda^2}$, and we have $a_\ell/a_{\ell+1} \geq 1/\lambda$.

We have shown that the inequality $a_\ell/a_{\ell+1} \geq 1/\lambda$ can fail to hold only when $z \leq (8\ln(1/\lambda))/n$. We need to see what this means in terms of ℓ:

$$\begin{aligned}z &\leq \frac{8\ln(1/\lambda)}{n} \\ &\Downarrow \\ b^{\ell-\delta} &\leq \frac{8\ln(1/\lambda)}{n} \\ &\Downarrow \\ \ell-\delta &\leq \log_b\frac{8\ln(1/\lambda)}{n} \\ &\Downarrow \\ \ell &\leq \log_b\frac{8\ln(1/\lambda)}{n} + \delta \\ &\leq \log_b\frac{8\ln(1/\lambda)}{n} + \log_b n \\ &= \log_b(8\ln(1/\lambda)).\end{aligned}$$

Thus $a_\ell/a_{\ell+1} \geq 1/\lambda$ is true with the possible exceptions of when $\ell = 1, 2, \ldots,$ $\log_b(8\ln(1/\lambda))$. Set $C = \log_b(8\ln(1/\lambda)) + 1$. □

We next consider the behavior of the expression $n \cdot (1 - 1/b^\delta)^n$. It will be more convenient to substitute $z = b^\delta$.

Lemma 3.14 *Let $z \geq 1$ and $n > 0$. Then*

$$n \cdot (1 - 1/z)^n < z.$$

Proof: If $z = 1$ the proof is trivial, so let us assume $z > 1$. Dividing and taking roots, we obtain the equivalent statement $1 - 1/z < \sqrt[n]{z/n}$. We will prove

$$1 - \frac{1}{z} \leq e^{-1/z} < e^{-1/ez} \leq \sqrt[n]{\frac{z}{n}}.$$

The first inequality of these three follows from the well-known fact $1 + y \leq e^y$, here taking $y = -1/z$. The second is equally simple, since $a < b$ implies $e^a < e^b$; take $a = -1/z$ and $b = -1/ez$.

Only the third inequality remains to be proved. We will show that the minimum value of $\sqrt[n]{z/n} = (z/n)^{1/n}$ as a function of n (considering z constant) is $e^{-1/ez}$. Several manipulations will make this task easier. First, set $x = 1/n$. Then

$$(z/n)^{1/n} = (zx)^x,$$

where $x \in (0, \infty)$. It is equivalent to minimize its logarithm,

$$\ln(zx)^x = x \ln zx = x \ln x + x \ln z.$$

This expression has derivative

$$1 + \ln x + \ln z;$$

the derivative is zero when $x = 1/ez$. This value of x does, in fact, give a minimum, since the second derivative $1/x$ is positive. We conclude that the minimum value of $(zx)^x$ is

$$(z/ez)^{1/ez} = e^{-1/ez},$$

as desired. $\square$

Corollary 3.15 *Let $b \geq 2$ and $\lambda < 1$ be fixed, and let $\delta \leq \log_b n$. Then*

$$n \cdot \sum_{\ell=1}^{\delta} \lambda^{1-\ell} \cdot (1 - b^{(\ell-\delta)-1})^n = O(b^\delta).$$

Proof: Let n be sufficiently large. We define $a_\ell = \lambda^{1-\ell} \cdot (1 - b^{(\ell-\delta)-1})^n$. Notice $a_1 = (1 - b^{-\delta})^n$. By Lemma 3.14 with $z = b^\delta$, we have $n \cdot a_1 < b^\delta$. For $\ell > 1$, we have $(1 - b^{(\ell-\delta)-1})^n < (1 - b^{-\delta})^n$, so that $n \cdot a_\ell < \lambda^{1-\ell} \cdot b^\delta$.

Set C as in Lemma 3.13. We see that each of the first C terms $n \cdot a_1, \ldots, n \cdot a_C$ is at most $\lambda^{-C} \cdot b^\delta$, so their sum is at most $C\lambda^{-C} b^\delta$. For $\ell > C$, we have $a_{\ell+1}/a_\ell \leq \lambda$, so that the sum $n \cdot \sum_{\ell=C+1}^{\delta} a_\ell$ converges faster than a geometric series with common ratio λ; this part of the sum is at most $C\lambda^{-C} b^\delta/(1-\lambda)$. Both of these quantities are $O(b^\delta)$. $\square$

At long last, we can bound the value of $\mathbf{E}[n \cdot \mathcal{C}(b, \delta, \lambda, n)]$:

Proposition 3.16 *For $\delta \leq \log_b n$,*

$$\mathbf{E}[n \cdot \mathcal{C}(b, \delta, \lambda, n)] = O((b\lambda)^\delta).$$

Proof:

$$\begin{aligned}
\mathbf{E}[n \cdot \mathcal{C}(b,\delta,\lambda,n)] &= n \cdot 2\lambda^{\delta} \cdot \Theta\left(\sum_{\ell=1}^{\delta} \lambda^{1-\ell} \cdot (1 - b^{(\ell-\delta)-1})^{n}\right) \\
&= n \cdot 2\lambda^{\delta} \cdot O(b^{\delta}/n) \qquad \text{(by the previous Corollary)} \\
&= O(\lambda^{\delta} b^{\delta}).
\end{aligned}$$

□

Applying this result to Proposition 3.9 gives our main result for the bichromatic MST.

Theorem 3.17 *Let R and B be two uniformly chosen multisets of n leaves from the HST $H(b,\delta,\lambda)$. The expected cost of the bichromatic MST on R and B is*

$$\Theta\left(\sum_{i=1}^{h} (b\lambda)^{i}\right),$$

where $h = \min(\delta, \log_b n)$.

This is the same (up to constant factors depending on b and λ) as the expected cost for the monochromatic MST on $R \cup B$.

Proof: Suppose $\delta \leq \log_b n$. By Proposition 3.9, the expected cost is $\Theta\left(\mathbf{E}[n \cdot \mathcal{C}(b,\delta,\lambda,n)] + \sum_{i=1}^{\delta}(b\lambda)^{i}\right)$; by Observation 3.1, it is $\Omega\left(\sum_{i=1}^{\delta}(b\lambda)^{i}\right)$. We need only to show $\mathbf{E}[n \cdot \mathcal{C}(b,\delta,\lambda,n)] = O\left(\sum_{i=1}^{\delta}(b\lambda)^{i}\right)$. But by the previous Proposition, $\mathbf{E}[n \cdot \mathcal{C}(b,\delta,\lambda,n)] = O((b\lambda)^{\delta})$, and the last term in the summation is $(b\lambda)^{\delta}$. Thus the total cost is also $O\left(\sum_{i=1}^{\delta}(b\lambda)^{i}\right)$.

If $\delta > \log_b n$, we lift the points up to level $\log_b n$. By the above argument, the expected cost of the bichromatic MST on the lifted points is $\Theta\left(\sum_{i=1}^{\log_b n}(b\lambda)^{i}\right)$. The lifting cost is $\Theta((b\lambda)^{\log_b n})$, and as before, such a term is already present in the summation. □

3.7 Application to problems on random point sets from $[0,1]^d$

As with the monochromatic problems, we can apply the results of this chapter to bichromatic problems on random point sets taken from the unit hypercube. Let R and B be two n-element point sets chosen i.i.d. uniformly from $[0,1]^d$. We are interested in the bichromatic minimum spanning tree and the optimal bichromatic tour on R and B.

Recall that our result for the bichromatic MST (Theorem 3.17) is the same as for the monochromatic problems. Thus

Lemma 3.18 *Fix a dimension $d \geq 2$, and let R and B be two sets of points chosen i.i.d. uniformly from $[0,1]^d$. The expected cost of the bichromatic MST on R and B is $O\left(n^{(d-1)/d}\right)$.*

But by Observation 3.1 and the $\Theta(n^{(d-1)/d})$ bound [58] on the monochromatic problems, the expected cost of the bichromatic MST is also $\Omega\left(n^{(d-1)/d}\right)$, and thus

Theorem 3.19 *Fix a dimension $d \geq 2$, and let R and B be two sets of points chosen i.i.d. uniformly from $[0,1]^d$. The expected cost of the bichromatic MST on R and B is $\Theta\left(n^{(d-1)/d}\right)$.*

We can derive a similar result for the bichromatic TSP.

Theorem 3.20 *Fix a dimension $d \geq 3$, and let R and B be two sets of points chosen i.i.d. uniformly from $[0,1]^d$. The expected cost of the bichromatic TSP tour on R and B is*

$$\Theta\left(n^{(d-1)/d}\right).$$

Proof: The lower bound follows from Observation 3.1 and the $\Theta(n^{(d-1)/d})$ bound on the monochromatic problem; we proceed to prove the upper bound. Transforming the problem into an HST problem, we obtain an HST with $b = 2^d$ and $\lambda = 1/2$. Its effective height is $\log_b n = \log_{2^d} n$. By Theorem 3.6, the cost of the optimal solution to the HST problem is

$$\begin{aligned}
\Theta\left(\sqrt{n} \cdot \sum_{k=1}^{\log_b n} (\sqrt{b}\lambda)^k\right) &= \Theta\left(\sqrt{n} \cdot (\sqrt{2^d} \cdot 1/2)^{\log_{2^d} n}\right) \\
&= \Theta\left(\sqrt{n} \cdot n^{\log_{2^d}(\sqrt{2^d} \cdot 1/2)}\right) \\
&= \Theta(n^{(d-1)/d}).
\end{aligned}$$

This is also an upper bound on the point problem. □

For bichromatic matching, this result appears in [1] and [2]. To the best of our knowledge, the results for the bichromatic MST problem and TSP are novel.

For $d < 3$ we can derive weaker results. When $d = 1$ the summation is constant and we obtain an upper bound of $O(\sqrt{n})$. This bound is known to be tight for bichromatic matching (see [1]). When $d = 2$, we have $\sqrt{b}\lambda = 1$ and obtain a bound of $O(\sqrt{n}\log n)$. This exceeds the tight bound $\Theta(\sqrt{n \log n})$ found for bichromatic matching by Ajtai et al. [3] by a factor of $\sqrt{\log n}$.

We are not limited to the d-dimensional hypercube, either. One can apply similar reasoning to other spaces (fractal spaces are a natural choice). We may pursue such courses in the future, but we will not consider them here.

3.8 Conclusion

We showed tight bounds on the bichromatic MST problem and TSP on balanced HSTs; we also revisited the bichromatic matching problem from [1] and [2]. The expected optimal cost for the TSP (and for the matching problem) is on the order of $\sqrt{n} \cdot \sum_{k=1}^{h} (\sqrt{b}\lambda)^k$, where $h = \min(\delta, \log_b n)$. On the other hand, the MST has expected cost on the order of $\sum_{k=1}^{h} (b\lambda)^k$. It is surprising that the bichromatic matching and TSP problems should behave so similarly to each other, yet so differently from the bichromatic MST problem. Moreover, the bichromatic MST problem has the same solution cost as the monochromatic problems we considered in Chapter 2.

Since the monochromatic and bichromatic MST problems had the same cost, one might naturally wonder what will happen for a K-chromatic MST problem with $K \geq 3$. For any fixed *even* value of K, a simple argument shows that the expected cost remains $\Theta\left(\sum_{k=1}^{h}(b\lambda)^k\right)$. Let us say we have K multisets (color classes) of n points, denoted $W_1, W_2, \ldots, W_K$, and we wish to form the MST T_K in which every edge connects points in two different color classes. By Observation 3.1, the cost of this MST exceeds the cost of the monochromatic MST T_1. On the other hand, we can group the color classes into two equal-sized multisets — say, $R = W_1 \cup W_3 \cup W_5 \cup \ldots W_{K-1}$ and $B = W_2 \cup W_4 \cup W_6 \cup \ldots \cup W_K$ — and find the bichromatic MST T_2 for R and B. The cost of T_2 must exceed the cost of T_K, since T_2 is a K-chromatic spanning tree for the W_i's. In summary, we have

$$c_1 \cdot Cost(T_1) \leq Cost(T_K) \leq c_2 \cdot Cost(T_2),$$

where c_1 and c_2 are constants depending only on K, b, and λ. Thus the cost of T_K is $\Theta\left(\sum_{k=1}^{h}(b\lambda)^k\right)$. We note that the constants c_1 and c_2 are not too extreme: T_1 is built on a multiset of Kn points, so c_1 is at most $K^{1+\log_b \lambda}$. Meanwhile, T_2 is built on $K/2$ multisets of $2n$ points, so c_2 is at most $(K/2)^{1+\log_b 2}$.

We can make a similar, but less slick, argument for odd values of K. If we take $R = W_1$ and $B = W_2 \cup W_3 \cup W_4 \cup \ldots \cup W_K$, it makes sense to ask about the bichromatic MST on R and B, even though the sets are of different size. Our proof for the bichromatic MST can be extended to apply to the case of sets of unequal size. Each red point must be linked to a blue point, but now we have *more* than n blue points, so it will be easier for each red point. The constants hidden by the Θ-notation will change.

We ended the chapter by applying our HST results to the bichromatic MST problem and TSP on uniformly chosen point sets from the Euclidean hypercube $[0,1]^d$. We showed that the bichromatic MST has cost $\Theta(n^{(d-1)/d})$ for $d \geq 2$. The bichromatic TSP tour also has this cost for $d \geq 3$. In smaller dimensions, our results are too weak to give a tight bound. Our preceding argument about the K-chromatic MST problem on HSTs also transfers to the K-chromatic MST problem on point sets in $[0,1]^d$: that is, for fixed $d \geq 2$ and $K \geq 2$, the expected K-chromatic MST cost on K random sets of n points taken i.i.d. uniformly from $[0,1]^d$ is $\Theta(n^{(d-1)/d})$. Here, again, the constants hidden by the Θ-notation are reasonable: the hidden factors are $K^{(d-1)/d}$ and $(K/2)^{(d-1)/d}$.

The bichromatic problems do not offer tight concentration inequalities like the ones we derived for the monochromatic problems in Section 2.6, since a bichromatic version of Lemma 2.24 is lacking. Since the deviation after the first level is already $\Omega(\sqrt{n})$, we cannot hope for sub-gaussian behavior. The most we can say is that a change at one point changes the length of the red-blue matching by at most one unit (the diameter of T is a constant, and after normalization it is one unit). If we now apply Azuma's inequality, we obtain

$$\mathbf{P}(|M(X) - \mathbf{E}M(X)| \geq t) \leq 2\exp\left(-\frac{t^2}{2n}\right).$$

This is clearly weaker than the very strong concentration results we obtained for the monochromatic matching problems.

4. Problems on hypergraphs

4.1 Introduction

A *graph* $G = (V, E)$ is a combinatorial structure consisting of a *vertex set* V and an *edge set* E. The vertex set can be any finite set. The edge set is a list of unordered pairs of the vertices; if two vertices u and v have an edge $\{u, v\}$ present in the set, we say that u and v are *connected*. We do not allow a vertex to be connected to itself. Many real-world problems involving transportation and communication have natural and straightforward representations as graph problems.

The concept of a graph can be generalized to a *hypergraph*: here every edge is a subset of V, not necessarily a pair. If every edge has the same cardinality K, we say that the hypergraph is *K-uniform*; for example, a 2-uniform graph is the same thing as a graph (by our definition above). The *degree* of a vertex v is the number of edges to which v belongs. We say a hypergraph is *d-regular* if every vertex has degree d. We call a graph *uniform* when it is K-uniform for some K; we use the term *regular* similarly.

Many graph and hypergraph problems are NP-hard; assuming P $\neq$ NP, the optimal solutions to these problems cannot be found in polynomial time. However, under special circumstances, one may find a polynomial-time *approximation algorithm* to produce a nearly optimal solution. We have already seen an NP-hard problem: the travelling salesman problem (TSP), considered in Chapters 2 and 3, is one of the best known and most studied. For graphs G whose edge weights obey the triangle inequality, several polynomial-time approximation algorithms for the TSP are known. An early one appearing in Rosenkrantz et al. [41] finds a solution whose weight is at most twice the weight of the optimal solution. Since the minimum spanning tree of

G weighs less than the optimal TSP tour, we can traversing the MST T of G and eliminate duplicate visits, yielding a tour of weight at most 2 times the weight of T. A refinement of this algorithm due to Christofides [15] improves the ratio to 1.5: we find the optimal matching M on the vertices of odd degree in T, and traverse the edges of $M \cup T$. The optimal matching has weight at most half the weight of the optimal tour.

We emphasize that these TSP approximation algorithms only apply when the edge weights of G obey the triangle inequality; for general graphs, even approximating the TSP solution within a constant factor is NP-hard.

The previous algorithms are made possible by the relationships between the solutions to the different graph problems: the MST (which is computable in polynomial time) provides an approximation to the TSP (which is not, given P $\neq$ NP). Later, Christofides noticed that a tour on an even number of vertices consists of two matchings, and thus uses the optimal matching (computable in polynomial time) to form part of a tour.

In situations where no such relation is forthcoming, we may make recourse to the *probabilistic method* [6], in which we generate a candidate solution at *random* and show that it is satisfactory. We can choose a target size and show that with positive probability, our candidate is a valid solution; another way is to bound the expected size of our candidate solution. Solutions to the *independent set problem*, another NP-hard problem and a subject of this chapter, can be found in this way. We call attention to our Theorems 4.13 and 4.17, novel results.

This chapter is laid out as follows. We first review the independent set problem on hypergraphs, looking at the Caro-Wei and Caro-Tuza lower bounds on the sizes of independent sets. We then develop an algebraic form of Caro-Tuza that closely resembles the form of Caro-Wei. Next, we introduce the *triple-free set problem* on hypergraphs. From there we formulate a conjecture about independent sets in a certain type of 3-uniform hypergraph; this conjecture is related to the no-three-in-line problem, a lattice problem that we will examine in Chapter 5.

4.2 The independent set problem

An independent set I of a hypergraph $H = (V, E)$ is a subset of V such that for all $e \in E$, we have $e \not\subseteq I$. For a graph ($K = 2$), an independent set is a subset of V that contains no pair of neighbors. The *independent set problem* is to find the largest independent set in a given hypergraph. As mentioned above, this problem is NP-hard. The *independence number* of H, denoted $\alpha(H)$, is the size of the largest independent set; as one might expect, calculating this number is also NP-hard.

We will apply the probabilistic method to the problem of bounding the independence number of a uniform hypergraph. We start with the simplest case, a graph. A theorem due independently to Caro [13] and to Wei [56] states that for a graph $G = (V, E)$ with vertices of respective degrees $d_1, d_2, \ldots, d_n$,

$$\alpha(G) \geq \sum_{i=1}^{n} \frac{1}{d_i + 1}.$$

This quantity is in fact the expected size of the independent set constructed by the following algorithm (due to Boppana; see [6]). Let σ be a random permutation of V. We construct an independent set $I(G)$ by considering the vertices in σ in order, adding each vertex to the set if none of its neighbors precedes it in σ. The probability of v_i being added is thus $1/(d_i + 1)$, the same as the probability that v_i precedes in σ all its neighbors in G. Adding over the v_i gives the result.

From the proof, it is straightforward to produce a deterministic algorithm that generates an independent set of this size. We will start with an empty set I and add vertices to it one by one. Notice that when we add a vertex v to I, all of its neighbors become ineligible for inclusion in I. This constraint suggests the following process for generating an independent set of a graph G: select a vertex v, add v to I, delete v and its neighbors from G, and repeat. To choose v, we employ the Caro-Wei estimate. Let us write $CW(G)$ to denote the Caro-Wei estimate for $\alpha(G)$, and let us define G_i to be the subgraph of G induced by removing v_i and its neighbors. We have

$$CW(G) \leq 1 + \frac{1}{n}\sum_{i=1}^{n} CW(G_i),$$

so that choosing the vertex v_i that maximizes $CW(G_i)$ will induce an independent set of size at least $1 + CW(G_i) \geq CW(G)$. Repeating this process recursively on G_i will give us the desired independent set of G.[1]

Caro and Tuza [14] later generalized this result to K-uniform hypergraphs, and Thiele [54] extended it further to general hypergraphs. Caro and Tuza proved

Theorem 4.1 (Caro-Tuza) *For $K \geq 2$, let $H = (V, E)$ be a K-uniform hypergraph whose vertices $v_1, v_2, \ldots, v_n$ have respective degrees $d_1, d_2, \ldots, d_n$. Then $\alpha(H)$ obeys*

$$\alpha(H) \geq \sum_{i=1}^{n} p_K(d_i),$$

where

$$p_K(d) = \prod_{j=1}^{d}\left(1 - \frac{1}{(K-1)j+1}\right).$$

When $K = 2$ the probability function simplifies to $p_2(d) = 1/(d+1)$. For $K = 3$, we

[1] An alternate method: at each step, set v to be the vertex with the highest degree (in the remaining graph, i.e., ignoring vertices that have already been removed), and remove v. Repeat until every vertex has degree 0; the resulting graph forms an independent set. It is a simple, but lengthy, matter of arithmetic to show that such a choice maintains the expectation of the Caro-Wei estimate.

have the elegant closed form

$$p_3(d) = \frac{4^d \cdot (d!)^2}{(2d+1)!}.$$

This result is the optimal bound on the random permutation algorithm.

4.3 Proof of Caro-Tuza for $K = 3$

In this section, we prove

Theorem 4.2 (Caro-Tuza for 3-uniform hypergraphs) *For $K \geq 2$, let $H = (V, E)$ be a 3-uniform hypergraph whose vertices $v_1, v_2, \ldots, v_n$ have respective degrees $d_1, d_2, \ldots, d_n$. Then $\alpha(H)$ obeys*

$$\alpha(H) \geq \sum_{i=1}^{n} p(d_i),$$

where

$$p(d) = \prod_{j=1}^{d} \left(1 - \frac{1}{2j+1}\right) = \frac{2}{3} \cdot \frac{4}{5} \cdots \frac{2d}{2d+1}.$$

The function $p(d)$ will emerge from consideration of a particular set of sequences. Let $\mathbb{S}_m$ be the set of the $2m+1$ symbols $\{x, y_1, y_1', y_2, y_2', \ldots, y_m, y_m'\}$. It consists of the symbol x together with m pairs of symbols $\{y_i, y_i'\}$ for $i = 1, \ldots, m$. We will say that for a given i, the symbols y_i and y_i' are *complements*. We call a permutation of $\mathbb{S}_m$ *valid* if for each pair $\{y_i, y_i'\}$, one of the elements of the pair comes after x. We consider m to be fixed for the rest of this section.

Lemma 4.3 *The number of valid permutations of $\mathbb{S}_m$ is $4^m \cdot (m!)^2$.*

Proof: Let us index the positions by $0, 1, \ldots, 2m$. The position of x must be from 0 to m. Let us consider the number of valid permutations with x at position k. The portion preceding x must have k elements, and for each i, it can only contain at most one of y_i and y_i'. There are $\frac{m!}{(m-k)!}$ possibilities for this portion that use only non-primed symbols. Since we can replace (or not) each symbol with its complement, there are $2^k \cdot \frac{m!}{(m-k)!}$ possibilities altogether. The part after x can be any arrangement of the remaining $2m-k$ symbols, so there are $(2m-k)!$ possibilities there. We conclude that the total number of valid permutations is

$$\begin{aligned}\sum_{k=0}^{m} 2^k \cdot \frac{m!}{(m-k)!} \cdot (2m-k)! &= \sum_{k=0}^{m} 2^k \cdot m! \binom{2m-k}{m} m! \\ &= (m!)^2 \cdot \sum_{k=0}^{m} 2^k \cdot \binom{2m-k}{m} \\ &= (m!)^2 \cdot 4^m,\end{aligned}$$

where the final substitution is justified by Lemma B.5 (see Section B.3). □

Lemma 4.4 *The probability that a uniformly chosen random permutation σ of $\mathbb{S}_d$ is valid is*

$$p(d) = \frac{4^d \cdot (d!)^2}{(2d+1)!}.$$

Proof: By Lemma 4.3, there are $4^d \cdot (d!)^2$ permutations in which x precedes an element of each pair, and each of these permutations is equally likely to appear in σ. There are $(2d+1)!$ total permutations of these symbols; dividing gives the statement of the lemma. □

Note that this expression for $p(d)$ is equal to the one given in Theorem 4.2.

Remark 4.5 *We note in passing the similarity between $p(d)$ and the formula for the d-th Catalan number,*

$$C_d = \binom{2d}{d} / (d+1) = \frac{(2d)!}{(d!)^2(d+1)}.$$

Suppose a vertex $v \in V$ of degree d has a *disjoint neighborhood* — that is, it has exactly $2d$ neighboring vertices, because none of its neighbors appears in more than one edge incident on v. Lemma 4.4 already gives us the probability that v will be placed into the independent set: this probability is $p(d)$. To see this, identify v with the symbol x, and for edge $e_i = \{v, u_i, w_i\}$ incident on v, identify $\{u_i, w_i\}$ with the complement pair $\{y_i, y_i'\}$. Then the valid permutations of $\mathbb{S}_d$ correspond precisely to the permutations of v and its neighbors in which v precedes a vertex in each of its incident edges. As a result, we have

Theorem 4.6 *Let H be a 3-uniform hypergraph whose vertices have degrees $d_1, d_2, \ldots, d_n$, and each of whose vertices has a disjoint neighborhood. Then*

$$\mathbf{E}|I| = \sum_{i=1}^{n} p(d_i).$$

Our goal now is to generalize this to vertices with non-disjoint neighborhoods. A nice monotonicity result enables us to carry this out.

Let $T = \{s_1, s_2, \ldots, s_{|T|}\}$ be a partition of $\mathbb{S}_m - \{x\}$ into non-empty sets such that no set s_i contains both an element y_k and its complement y_k'. We define a permutation of $T \cup \{x\}$ to be a rearrangement of these sets with x included in the permutation.[2] We permute only the sets, not the elements that they contain. To illustrate, for $T = \{\{y_1, y_2'\}, \{y_1'\}, \{y_2\}\}$, the permutations of $T \cup \{x\}$ are

$$x\{y_1, y_2'\}\{y_1'\}\{y_2\}$$
$$\{y_1'\}x\{y_1, y_2'\}\{y_2\}$$
$$\{y_1, y_2'\}\{y_2\}x\{y_1'\}$$
$$\{y_1'\}\{y_1, y_2'\}\{y_2\}x$$

etc.

[2]We include x in the permutations but exclude it from T. We do this in order to simplify the arithmetic for the lemmata of this section.

The number of permutations of $T \cup \{x\}$ is $(|T|+1)!$

Given $s_i, s_j \in T$, we say that s_i and s_j are *conflicting* if for some k, we have $\{y_k, y'_k\} \subseteq s_i \cup s_j$. That is, s_i and s_j conflict with each other if one contains the complement of an element in the other. Note that by construction, s_i never conflicts with itself. If two sets are not conflicting, we will call them *compatible*. We define a *valid* permutation of $T \cup \{x\}$ to be a permutation of $T \cup \{x\}$ in which no pair of conflicting sets appears before x. These definitions match those given for $\mathbb{S}_m$; indeed, $\mathbb{S}_m$ is equivalent to the base partition $T_0 = \{\{y_1\}, \{y'_1\}, \ldots, \{y_m\}, \{y'_m\}\}$.

Let us define $\mathcal{P}(T)$ to be the set of non-conflicting subsets of T. Then

Lemma 4.7 *The number of valid permutations of $T \cup \{x\}$ is*

$$\sum_{S \in \mathcal{P}(T)} |S|! \cdot (|T| - |S|)!$$

Proof: We arrange S to the left of x and $T - S$ to the right of x. This gives us $|S|! \cdot (|T| - |S|)!$ valid permutations for each S. $\square$

We can form a new partition T' by merging two non-conflicting sets $s_1, s_2 \in T$ into a new set $s_1 \cup s_2$. It is clear that there will be some relationship between the valid permutations of T and those of T', but the relationship is fairly complex. Let us partition $\mathcal{P}(\{s_3, s_4, \ldots, s_{|T|}\})$ into three sets $\mathcal{P}_0(T), \mathcal{P}_1(T), \mathcal{P}_2(T)$. Those sets compatible with s_1 and s_2 will be placed into $\mathcal{P}_2(T)$; those compatible with neither will be placed into $\mathcal{P}_0(T)$; and the rest of the sets will be placed into $\mathcal{P}_1(T)$. Thus a set in $\mathcal{P}_i(T)$ is compatible with exactly i of $\{s_1, s_2\}$.

Let us define $N(T)$ to be the number of valid permutations of $T \cup \{x\}$, and similarly for $N(T')$.

Lemma 4.8 $N(T) = L_1(T) + L_2(T) + L_3(T) + L_4(T)$ *and* $N(T') = L_5(T) + L_6(T)$, *where*

$$\begin{aligned}
L_1(T) &= \sum_{S \in \mathcal{P}_0(T) \cup \mathcal{P}_1(T) \cup \mathcal{P}_2(T)} |S|! \cdot (|T| - |S|)! \\
L_2(T) &= \sum_{S \in \mathcal{P}_1(T)} (|S|+1)! \cdot (|T| - 1 - |S|)! \\
L_3(T) &= 2 \cdot \sum_{S \in \mathcal{P}_2(T)} (|S|+1)! \cdot (|T| - 1 - |S|)! \\
L_4(T) &= \sum_{S \in \mathcal{P}_2(T)} (|S|+2)! \cdot (|T| - 2 - |S|)!
\end{aligned}$$

$$\begin{aligned}
L_5(T) &= \sum_{S \in \mathcal{P}_0(T) \cup \mathcal{P}_1(T) \cup \mathcal{P}_2(T)} |S|! \cdot (|T| - 1 - |S|)! \\
L_6(T) &= \sum_{S \in \mathcal{P}_2(T)} (|S|+1)! \cdot (|T| - 2 - |S|)!
\end{aligned}$$

Proof: First consider $N(T)$. Each S in $\mathcal{P}_0(T) \cup \mathcal{P}_1(T) \cup \mathcal{P}_2(T)$ can be permuted $|S|!$ ways without s_1 or s_2, yielding $|S|! \cdot (|T| - |S|)!$ valid permutations. Furthermore, each S in $\mathcal{P}_1(T)$ can be permuted with exactly one of $\{s_1, s_2\}$, yielding $(|S|+1)! \cdot (|T| - 1 - |S|)!$ extra permutations. Finally, each S in $\mathcal{P}_2(T)$ can be permuted with either of s_1 and s_2, yielding $2 \cdot (|S|+1)! \cdot (|T| - 1 - |S|)!$ extra permutations, or with *both* s_1 and s_2, yielding $(|S|+2)! \cdot (|T| - 2 - |S|)!$ extra permutations. The sum of these four quantities yields $N(T)$.

The reasoning for $N(T')$ is similar, but now s_1 and s_2 have been merged into $s_1 \cup s_2$. (Note $|T'| = |T| - 1$.) Each S in $\mathcal{P}_0(T) \cup \mathcal{P}_1(T) \cup \mathcal{P}_2(T)$ can be permuted $|S|!$ ways, but now only the elements of $\mathcal{P}_2(T)$ can be permuted with the new set $s_1 \cup s_2$, and $S \cup \{s_1 \cup s_2\}$ can be permuted $(|S|+1)!$ ways. $\square$

Proposition 4.9

$$(|T|+1) \cdot N(T') \geq N(T).$$

Proof: By Lemma 4.8, we have $(|T|+1)\cdot N(T')-N(T) = (|T|+1)\cdot(L_5(T)+L_6(T))-(L_1(T)+L_2(T)+L_3(T)+L_4(T))$; we will show that this quantity is nonnegative. To make it clearer, we will perform the evaluation piecemeal.

$$\begin{aligned}
(|T|+1)\cdot L_6(T) - L_4(T) &= \sum_{S\in\mathcal{P}_2(T)} (|S|+1)!\cdot(|T|-2-|S|)!\cdot(|T|+1) - \\
&\quad \sum_{S\in\mathcal{P}_2(T)} (|S|+2)!\cdot(|T|-2-|S|)! \\
&= \sum_{S\in\mathcal{P}_2(T)} (|S|+1)!\cdot(|T|-1-|S|)! \\
&= L_3(T)/2. \\
(|T|+1)\cdot L_5(T) - L_1(T) &= \sum_{S\in\mathcal{P}_0(T)\cup\mathcal{P}_1(T)\cup\mathcal{P}_2(T)} |S|!\cdot(|T|-1-|S|)!\cdot(|T|+1) - \\
&\quad \sum_{S\in\mathcal{P}_0(T)\cup\mathcal{P}_1(T)\cup\mathcal{P}_2(T)} |S|!\cdot(|T|-|S|)! \\
&= \sum_{S\in\mathcal{P}_0(T)\cup\mathcal{P}_1(T)\cup\mathcal{P}_2(T)} (|S|+1)!\cdot(|T|-1-|S|)! \\
&= \sum_{S\in\mathcal{P}_0(T)} (|S|+1)!\cdot(|T|-1-|S|)! + \\
&\quad \sum_{S\in\mathcal{P}_1(T)} (|S|+1)!\cdot(|T|-1-|S|)! + \\
&\quad \sum_{S\in\mathcal{P}_2(T)} (|S|+1)!\cdot(|T|-1-|S|)! \\
&= L_2(T) + L_3(T)/2 + \sum_{S\in\mathcal{P}_0(T)} (|S|+1)!\cdot(|T|-1-|S|)! \\
&\geq L_2(T) + L_3(T)/2.
\end{aligned}$$

Therefore

$$
\begin{aligned}
& (|T|+1)\cdot(L_5(T)+L_6(T)) - (L_1(T)+L_2(T)+L_3(T)+L_4(T)) \\
= \; & [(|T|+1)\cdot L_6(T) - L_4(T)] + [(|T|+1)\cdot L_5(T) - L_1(T)] - L_2(T) - L_3(T) \\
\geq \; & (L_3(T)/2) + (L_2(T) + L_3(T)/2) - L_2(T) - L_3(T) \\
= \; & 0.
\end{aligned}
$$

□

Define $P(T)$ to be the probability that a random permutation of $T \cup \{x\}$ is valid, and let T' be a permutation obtained by merging two non-conflicting sets of T. Clearly $P(T) = N(T)/(|T|+1)!$ and $P(T') = N(T')/|T|!$

Corollary 4.10

$$P(T') \geq P(T).$$

Proof: Dividing the conclusion of Proposition 4.9 by $(|T|+1)!$, we obtain

$$\frac{N(T')}{|T|!} \geq \frac{N(T)}{(|T|+1)!},$$

i.e., $P(T') \geq P(T)$. □

Remark 4.11 *Lemma 4.8, Proposition 4.9 and Corollary 4.10 can also be made to apply to K-uniform hypergraphs with $K > 3$, provided we change the definition of $\mathbb{S}_m$ and valid sets accordingly. The analogue of Lemma 4.4 must, however, use more sophisticated counting methods than those that we have used here.*

Theorem 4.12 *Let $H = (V, E)$ be a 3-uniform hypergraph, and let σ be a (uniformly) random permutation of V. For $v \in V$ with degree d, the probability that v precedes, in σ, a vertex in each of its incident edges is at least $p(d)$.*

Proof: Let us denote the edges incident on v by $e_1, e_2, \ldots, e_k$. We will identify the vertices in e_i with the symbols y_i and y_i', and we identify v with the symbol x. Define the base partition $T_0 = \{\{y_1\}, \{y_1'\}, \ldots, \{y_d\}, \{y_d'\}\}$ of $\mathbb{S}_d - \{x\}$. We represent shared vertices between edges by merging the corresponding sets. For example, if y_1 and y_2' represent the same vertex, we merge the sets that contain y_1 and y_2'. Note that these merges will never create a conflicting set, since that would mean one of the edges of H has cardinality 2.

We perform these merges one at a time, creating a sequence of partitions $T_0, T_1, T_2, \ldots, T_c$. The partition T_c represents the actual vertex set, and every valid permutation of $T_c \cup \{x\}$ represents a permutation of v and its neighbors that will cause v to precede one vertex in each of its incident edges. By Lemma 4.4, $P(T_0) = p(d)$, since the (valid) permutations of $T_0 \cup \{x\}$ are simply the (valid) permutations of $\mathbb{S}_m$. By Corollary 4.10, $P(T_i) \geq P(T_{i-1})$ for each i. We conclude that $P(T_c) \geq p(d)$, so that with probability at least $p(d)$, the vertex v will precede one vertex in each of its incident edges. $\square$

We are finally in a position to prove Theorem 4.2.

Proof of Theorem 4.2: Let σ be a random permutation of V, and build I as described in the introduction. By Theorem 4.12, the probability that v_i will be added to the set is at least $p(d_i)$. Therefore, $\mathbf{E}|I|$ is at least $\sum_{i=1}^{n} p(d_i)$, and some σ yields an independent set I of at least this size. $\square$

K-uniform hypergraphs (for $K > 2$) pose a problem when we want to derandomize the algorithm: when we add v_i to I and remove it from H, we cannot now remove its neighbors. We are left, in effect, with a non-uniform hypergraph, in which some edges will have cardinality K and others $K - 1$.[3] We can avoid this difficulty by running the algorithm in reverse: iterate through the permutation σ backwards, removing the

[3]For a (2-)graph this was not a problem, since the edges generated were of cardinality 1, meaning that the incident vertices can never be taken into the independent set.

vertex v_i from the graph if and only if it has an edge incident on it. When we remove v_i, all its incident edges dissolve. When the algorithm is done, an independent set will remain whose expected size is at least the number given by Caro-Tuza. This algorithm can be derandomized as above (see also [14] and [54]).

4.4 Algebraic bounds on $\alpha(H)$

Based on the Caro-Tuza result, we have found what we believe to be novel results on $\alpha(H)$ for K-uniform hypergraphs H. We begin by handling the simplest case of $K = 3$. For convenience, we will write $p(\cdot)$ to mean $p_3(\cdot)$.

Theorem 4.13 *Let H be a 3-uniform hypergraph, and let $d_1, d_2, \ldots, d_n$ be the degrees of its vertices, with $n > 0$. Then*

$$\alpha(H) > \frac{\sqrt{\pi}}{2} \cdot \sum_{i=1}^{n} \frac{1}{\sqrt{d_i + 1}}.$$

The proof is as follows. Recall Wallis' formula,

$$\frac{\pi}{2} = \prod_{i=1}^{\infty} \frac{2 \cdot \lceil i/2 \rceil}{2 \cdot \lfloor i/2 \rfloor + 1} = \frac{2}{1} \cdot \frac{2}{3} \cdot \frac{4}{3} \cdot \frac{4}{5} \cdot \frac{6}{5} \cdot \frac{6}{7} \cdot \frac{8}{7} \cdot \frac{8}{9} \cdot \frac{10}{9} \cdot \frac{10}{11} \cdots.$$

Let W_k denote the product of the first k fractions in the formula as written above. Thus $W_1 = \frac{2}{1}$, $W_2 = \frac{2}{1} \cdot \frac{2}{3}$, etc.

Remark 4.14 *Normally Wallis' formula is given as*

$$\prod_{i=1}^{\infty} \frac{(2i)^2}{(2i-1)(2i+1)},$$

giving partial products $W_2, W_4, \ldots$, but we will find the prior version more convenient.

The difference in grouping does not change its convergence properties, since

$$\lim_{k\to\infty} \frac{W_{2k+1}}{W_{2k}} = 1;$$

as a result, the sequence $\{W_1, W_3, W_5, \ldots\}$ *has the same limit as the sequence* $\{W_2, W_4, W_6, \ldots\}$.

Proposition 4.15 $W_k < \frac{\pi}{2}$ *for even* k*, and* $W_k > \frac{\pi}{2}$ *for odd* k.

Proof: Let k be even. The next two factors in the product have the forms $\frac{i}{i-1}$ and $\frac{i}{i+1}$; their product is greater than 1. The same is true for the next two, the next two after them, etc. Letting R be the product of *all* these pairs of factors, we have $R > 1$. Since $W_k \cdot R = \frac{\pi}{2}$, it follows that $W_k < \frac{\pi}{2}$.

Similarly, when k is odd, each subsequent pair of factors has the form $\frac{i-1}{i}$ and $\frac{i+1}{i}$, whose product is less than 1. Thus the product of the remaining pairs, R, is less than 1. Since $W_k \cdot R = \frac{\pi}{2}$, we have $W_k > \frac{\pi}{2}$. □

Theorem 4.16

$$\frac{\sqrt{\pi}}{2\sqrt{d+1}} < p(d) < \frac{\sqrt{\pi}}{2\sqrt{d+1/2}}.$$

Note the tightness of this bound.

Proof:

$$\begin{aligned} p(d) &= \frac{(2^d \cdot d!)^2}{(2d+1)!} \\ &= \frac{2^2 \cdot 4^2 \cdot 6^2 \cdots (2d)^2}{1 \cdot 2 \cdot 3 \cdots (2d+1)} \\ &= \frac{2 \cdot 4 \cdot 6 \cdots (2d)}{1 \cdot 3 \cdot 5 \cdots (2d+1)}, \end{aligned}$$

because each even factor in the denominator had a counterpart in the numerator.

Squaring and multiplying by $2d+1$,

$$p(d)^2 \cdot (2d+1) \quad = \quad \frac{2\cdot 2\cdot 4\cdot 4\cdot 6\cdot 6\cdots(2d)\cdot(2d)}{1\cdot 3\cdot 3\cdot 5\cdot 5\cdot\cdots(2d-1)\cdot(2d-1)\cdot(2d+1)} = W_{2d} < \frac{\pi}{2}$$

by Proposition 4.15.

Similarly,

$$p(d)^2 \cdot (2d+2) \quad = \quad \frac{2\cdot 2\cdot 4\cdot 4\cdot 6\cdot 6\cdots(2d)\cdot(2d)\cdot(2d+2)}{1\cdot 3\cdot 3\cdot 5\cdot 5\cdot\cdots(2d+1)\cdot(2d+1)} = W_{2d+1} > \frac{\pi}{2}.$$

Thus

$$\begin{aligned}
\frac{\pi}{2(2d+2)} &< p(d)^2 < \frac{\pi}{2(2d+1)} \\
\frac{\sqrt{\pi}}{\sqrt{4d+4}} &< p(d) < \frac{\sqrt{\pi}}{\sqrt{4d+2}} \\
\frac{\sqrt{\pi}}{2\sqrt{d+1}} &< p(d) < \frac{\sqrt{\pi}}{2\sqrt{d+1/2}}.
\end{aligned}$$

□

The proof of Theorem 4.13 follows from applying the lower bound in Theorem 4.16 to the Caro-Tuza theorem.

What about when $K > 3$? It is known (see [19]) that for each $K > 1$, some positive constant c_K satisifies

$$\alpha(H) \geq c_K \cdot \frac{1}{(d_i+1)^{1/(K-1)}}.$$

For the case $K = 3$, we were fortunate to find that the probability given by Caro-Tuza has a connection to Wallis' formula. When $K = 4$, for instance, we instead obtain the product

$$p_4(d) = \frac{3}{4}\cdot\frac{6}{7}\cdot\frac{9}{10}\cdots\frac{3d}{3d+1} = \frac{3^d \cdot d!}{4\cdot 7\cdot 10\cdots(3d+1)},$$

whose corresponding constant is not so easy (perhaps impossible) to express in a closed form. As we will see, these constants can be *approximated* quite closely.

Theorem 4.17 *Let H be a K-uniform hypergraph for $K \geq 3$, and let $d_1, d_2, \ldots, d_n$ be the degrees of its vertices, with $n > 0$. Then*

$$\alpha(H) > e^{-\gamma/(K-1)} \cdot \sum_{i=1}^{n} \frac{1}{(d_i+1)^{1/(K-1)}},$$

where $\gamma = 0.5772\ldots$ is the Euler-Mascheroni constant.

The proof is as follows. For general $K \geq 2$, we have

Proposition 4.18

$$\lim_{d\to\infty} p_K(d) \cdot (d+1)^{1/(K-1)} = e^{h(K-1)},$$

where

$$h(z) = \frac{1}{z} \cdot \sum_{i=2}^{\infty} \frac{(-1)^i \cdot \zeta(i)}{i} \cdot \left(\frac{1}{z^{i-1}} - 1\right)$$

and ζ is the Riemann zeta function.

Thus for fixed K,

$$p_K(d) \sim \frac{e^{h(K-1)}}{d^{1/(K-1)}}.$$

Proof: We can rewrite $p_K(d) \cdot (d+1)^{1/(K-1)}$ as $\prod_{i=1}^{d} a_i$, where

$$\begin{aligned} a_i &= \frac{(K-1)i}{(K-1)i+1} \cdot \left(\frac{i+1}{i}\right)^{1/(K-1)} \\ &= \left(1 + \frac{1}{(K-1)i}\right)^{-1} \cdot \left(1 + \frac{1}{i}\right)^{1/(K-1)}. \end{aligned}$$

Then

$$\begin{aligned}
\log a_i &= \frac{1}{K-1} \cdot \log\left(1+\frac{1}{i}\right) - \log\left(1+\frac{1}{(K-1)i}\right) \\
&= \frac{1}{K-1} \cdot \sum_{j=1}^{\infty} \frac{(-1)^{j+1}}{j \cdot i^j} - \sum_{j=1}^{\infty} \frac{(-1)^{j+1}}{j \cdot ((K-1)i)^j} \\
&= \frac{1}{K-1} \cdot \sum_{j=2}^{\infty} \frac{(-1)^{j+1}}{j \cdot i^j} - \sum_{j=2}^{\infty} \frac{(-1)^{j+1}}{j \cdot ((K-1)i)^j},
\end{aligned}$$

since the terms for $j = 1$ cancel out. These were the troublesome terms, since they belong to the harmonic series, which does not converge.

The next step is to calculate $\sum_{i=1}^{\infty} \log a_i$, but we must be careful. The series for $\log a_i$ converges absolutely when $i > 1$ but *not* when $i = 1$. We must therefore handle that series differently.

$$
\begin{aligned}
\sum_{i=1}^{\infty} \log a_i &= \sum_{i=1}^{\infty} \left(\frac{1}{K-1} \cdot \sum_{j=2}^{\infty} \frac{(-1)^{j+1}}{j \cdot i^j} - \sum_{j=2}^{\infty} \frac{(-1)^{j+1}}{j \cdot ((K-1)i)^j} \right) \\
&= \sum_{i=1}^{\infty} \left(\sum_{j=2}^{\infty} \left(\frac{(-1)^{j+1}}{(K-1) \cdot j \cdot i^j} - \frac{(-1)^{j+1}}{j \cdot ((K-1)i)^j} \right) \right) \\
&= \sum_{j=2}^{\infty} \left(\frac{(-1)^{j+1}}{(K-1) \cdot j} - \frac{(-1)^{j+1}}{j \cdot (K-1)^j} \right) \\
&\qquad + \sum_{i=2}^{\infty} \sum_{j=2}^{\infty} \left(\frac{(-1)^{j+1}}{(K-1) \cdot j \cdot i^j} - \frac{(-1)^{j+1}}{j \cdot ((K-1)i)^j} \right) \\
&= \sum_{j=2}^{\infty} \frac{(-1)^{j+1}}{j} \left(\frac{1}{K-1} - \frac{1}{(K-1)^j} \right) \\
&\qquad + \sum_{i=2}^{\infty} \sum_{j=2}^{\infty} \frac{(-1)^{j+1}}{j \cdot i^j} \left(\frac{1}{K-1} - \frac{1}{(K-1)^j} \right) \qquad (1) \\
&= \sum_{j=2}^{\infty} \frac{(-1)^{j+1}}{j} \left(\frac{1}{K-1} - \frac{1}{(K-1)^j} \right) \\
&\qquad + \sum_{j=2}^{\infty} \sum_{i=2}^{\infty} \frac{(-1)^{j+1}}{j \cdot i^j} \left(\frac{1}{K-1} - \frac{1}{(K-1)^j} \right) \qquad (2) \\
&= \sum_{j=2}^{\infty} \left(\frac{(-1)^{j+1}}{j} \left(\frac{1}{K-1} - \frac{1}{(K-1)^j} \right) \right. \\
&\qquad \left. + \sum_{i=2}^{\infty} \frac{(-1)^{j+1}}{j \cdot i^j} \left(\frac{1}{K-1} - \frac{1}{(K-1)^j} \right) \right) \\
&= \sum_{j=2}^{\infty} \left(\sum_{i=1}^{\infty} \frac{(-1)^{j+1}}{j \cdot i^j} \left(\frac{1}{K-1} - \frac{1}{(K-1)^j} \right) \right) \\
&= \sum_{j=2}^{\infty} \frac{(-1)^{j+1}}{j} \left(\sum_{i=1}^{\infty} \frac{1}{i^j} \left(\frac{1}{K-1} - \frac{1}{(K-1)^j} \right) \right) \\
&= \sum_{j=2}^{\infty} \frac{(-1)^{j+1}}{j} \left(\frac{1}{K-1} \cdot \sum_{i=1}^{\infty} \frac{1}{i^j} - \frac{1}{(K-1)^j} \cdot \sum_{i=1}^{\infty} \frac{1}{i^j} \right) \\
&= \sum_{j=2}^{\infty} \frac{(-1)^{j+1}}{j} \left(\frac{\zeta(j)}{K-1} - \frac{\zeta(j)}{(K-1)^j} \right) \\
&= \frac{1}{K-1} \cdot \sum_{j=2}^{\infty} \frac{(-1)^{j+1} \cdot \zeta(j)}{j} \left(1 - \frac{1}{(K-1)^{j-1}} \right) \\
&= h(K-1).
\end{aligned}
$$

We have repeatedly used the identity $\sum_{k=1}^{\infty}(x_k + y_k) = (\sum_{k=1}^{\infty} x_k) + (\sum_{k=1}^{\infty} y_k)$, which is valid whenever the sums $\sum_{k=1}^{\infty} x_k$ and $\sum_{k=1}^{\infty} y_k$ are finite. To get from (1) to (2), switching the summations for i and j, we used the fact that the double sum is absolutely convergent (in fact, $\sum_{i=2}^{\infty}\sum_{j=2}^{\infty} 1/(j \cdot i^j) = 1 - \gamma$).

Exponentiating, we conclude $\prod_{i=1}^{\infty} a_i = \exp(h(K-1))$. □

As was the case for $K = 3$, our asymptotic bound also yields a lower bound:

Proposition 4.19

$$p_K(d) \cdot (d+1)^{1/(K-1)} > e^{h(K-1)}.$$

Thus

$$p_K(d) > \frac{e^{h(K-1)}}{(d+1)^{1/(K-1)}}.$$

Proof: We will show that each factor a_i (from the proof of Proposition 4.18) is less than 1; as a result, the partial products will decrease toward the limit given in Proposition 4.18. The statement $a_i < 1$ is equivalent to

$$\frac{(K-1)i}{(K-1)i+1} \cdot \left(\frac{i+1}{i}\right)^{1/(K-1)} < 1,$$

from which we obtain

$$\left(\frac{(K-1)i}{(K-1)i+1}\right)^{K-1} \cdot \frac{i+1}{i} < 1,$$

and

$$((K-1)i)^{K-1} \cdot (i+1) < ((K-1)i+1)^{K-1} \cdot i.$$

This latter statement is easily shown to be true. The left-hand side equals $(K-1)^{K-1} \cdot i^K + (K-1)^{K-1} \cdot i^{K-1}$. The expansion of the right-hand side will contain (among others) the terms $(K-1)^{K-1} \cdot i^K$ and $\binom{K-1}{1} \cdot (K-1)^{K-2} \cdot i^{K-2} \cdot i$. Thus the right-hand side exceeds the left-hand side. $\square$

Since for a K-uniform hypergraph H we have $\alpha(H) \geq \sum_{i=1}^{n} p_K(d_i)$, Theorem 4.1 and Proposition 4.19 now let us state

Theorem 4.20 *For $K \geq 3$, let $H = (V, E)$ be a K-uniform hypergraph whose n vertices $v_1, v_2, \ldots, v_n$ (with $n > 0$) have respective degrees $d_1, d_2, \ldots, d_n$. Then*

$$\alpha(H) > e^{h(K-1)} \cdot \sum_{i=1}^{n} \frac{1}{(d_i + 1)^{1/(K-1)}}.$$

(For $K = 2$ we must replace "$>$" with "$\geq$".)

Proof of Theorem 4.17: The identity $\sum_{i=2}^{\infty} (-1)^i \cdot \zeta(i)/i = \gamma$ lets us rewrite $h(z)$ as

$$\frac{1}{z} \cdot \left[\left(\sum_{i=2}^{\infty} \frac{(-1)^i \cdot \zeta(i)}{i \cdot z^{i-1}} \right) - \gamma \right].$$

The parenthesized summation is an alternating series whose terms are descending in magnitude; thus the sign of the limit is the same as its first term, which is positive. We thereby have

$$h(K-1) > -\frac{\gamma}{K-1},$$

which together with Theorem 4.20 proves Theorem 4.17. $\square$

Using the fact $\zeta(2) = \pi^2/6$ (Euler's solution to the Basel problem), we can bound $h(z)$ fairly tightly. The summation is at most $\pi^2/(12z)$, giving us:

Corollary 4.21

$$-\frac{\gamma}{z} < h(z) < -\frac{\gamma}{z} + \frac{\pi^2}{12z^2}.$$

($\pi^2/12 = 0.8224...$)

The bound in Corollary 4.21 is tighter than the obvious bound $h(z) < 0$, since

$$-\frac{\gamma}{z} + \frac{\pi^2}{12z^2} = \frac{\pi^2 - 12\gamma z}{12z^2}$$

is negative for $z \geq 2$.

The results of this section have been published in February 2012 as [16].

Remark 4.22 *Why would we believe, in the first place, that such an argument is true? The following simple argument (adapted from Alon and Spencer, [6, Chapter 1]; see also [47]) shows that for a K-uniform hypergraph H with average vertex degree $\delta \geq 1$, we have $\alpha(H) \geq (1 - 1/K) \cdot n/\delta^{1/(K-1)}$. We construct a set S of vertices at random by choosing each vertex independently with probability p, whose value is yet to be determined. An edge e_i will have a violation (all of its vertices will be in S) with probability $1/p^K$; to fix the violation, we will remove one of the vertices of e_i from S. This process gives us an independent set of expected size at least $np - mp^K$. Given the (reasonable) assumption[4] $m \geq n/K$ (equivalent to $\delta \geq 1$), this quantity is maximized when $p = (n/mK)^{1/(K-1)}$, giving an independent set of size*

$$\frac{n^{1+1/(K-1)}}{m^{1/(K-1)}} \cdot \frac{1}{K^{1/(K-1)}} \cdot \left(1 - \frac{1}{K}\right).$$

Since $m = \delta n/K$, we have

$$\alpha(H) \geq \frac{n}{\delta^{1/(K-1)}} \cdot \left(1 - \frac{1}{K}\right).$$

Theorems 4.13 and 4.17 are best applied for graphs with large degrees. For small degrees the approximation is too slack (consider a 3-uniform hypergraph on n vertices

[4]This condition is needed to ensure that p is a valid probability, i.e., less than or equal to one.

and *no* edges: Theorem 4.13 gives $\alpha(H) > n\sqrt{\pi}/2)$. For larger degrees, the approximation is quite close. It is curious that the worst value of the constant occurs for $K = 3$.

We comment briefly that the result of Caro-Tuza (Theorem 4.1) and Thiele's result in [54] are the best in general — in the former case, the best given the degree sequence $\{d_i\}$; in the latter, the best given the degree matrix D. Tighter bounds are possible given tighter constraints on the hypergraph. For instance, a bipartite graph G has $\alpha(G) \geq \lceil n/2 \rceil$, and we see that this bound is tight from the graph $K_{\lceil n/2 \rceil, \lfloor n/2 \rfloor}$. For a triangle-free[5] graph G of average degree $\delta > 0$, we have

$$\alpha(G) \geq (1 - f(\delta)) \cdot \frac{n \log \delta}{\delta},$$

where $f(\delta) \to 0$ as $\delta \to \infty$. This bound is due to Ajtai, Komlós, and Szemerédi [5], who showed the order of magnitude, and Shearer [44], who subsequently showed that the leading constant can be taken to be $1 - o(1)$.

4.5 The K-tuple-free set problem

The estimate of Caro and Tuza gives a lower bound on the expected size of the independent set generated by the random permutation algorithm. This estimate is in fact tight when the hypergraph H is *linear*: a linear hypergraph is one in which every pair u, v of distinct vertices belongs to at most one edge. For a given vertex v and its neighborhood $N(v)$, every vertex in $N(v)$ shared between more than one edge increases the probability of v being chosen; we would like to take advantage of this fact.

This phenomenon becomes especially apparent when, as in the next chapter, we

[5] A graph is said to be *triangle-free* if it contains no subgraph isomorphic to K_3. In such a graph, no pair u, v of adjacent vertices has a common neighbor.

deal with points and collinearity. We will construct hypergraphs using lattice points for the vertices and collinear triples as the edges. A set of N collinear points gives rise to $\binom{N}{3}$ collinear triples, and each pair along this line will belong to $N-2$ edges. It would be nice to increase the Caro-Tuza estimate, in anticipation of the sharing that will occur between the edges.

Toward this end, we introduce[6] the *K-tuple-free set problem.* A K-tuple-free set of a hypergraph $H = (V, E)$ is a subset F of V such that for each $e \in E$, we have $|e \cap F| < K$ — in words, F contains at most $K-1$ vertices from every edge.[7] For $K = 2$ we will say *pair-free*, and for $K = 3$ we will say *triple-free*. We will write $\beta_K(H)$ to denote the size of the largest K-tuple-free subset of H.

Let H be a linear[8] hypergraph and let v be one of its vertices. Let us say that v has degree d, and its incident edges $e_1, e_2, \ldots, e_d$ have respective cardinalities $C_1, C_2, \ldots, C_d$. We will set $s_i = C_i - 1$, so that s_i is the number of vertices aside from v in e_i. We denote $\sum_{i=1}^{d} s_i$ by $\sigma_s(v)$.

We first consider the case $K = 2$. The probability that v will be chosen before any of its neighbors is $1/(\sigma_s(v) + 1)$, so that we have

$$\beta_2(H) \geq \sum_{i=1}^{n} \frac{1}{\sigma_s(v_i) + 1}.$$

This is in fact the same quantity as we would get if we split every edge in E into 2-edges[9] and apply Caro-Wei to the resulting graph. It is a consequence of the fact that every 2-graph is linear.

The case $K = 3$ is more interesting. We obtain

[6] As far as we know, this problem has not been considered before.

[7] For comparison, note that the condition $|e \cap F| < |e|$ would instead redefine the independent-set problem.

[8] We suspect that this condition is not necessary, but we are not sure.

[9] This is done by creating a 2-edge for every pair of vertices in E.

Theorem 4.23

$$\beta_3(H) \geq \sum_{i=1}^{n} \frac{\sum_{a=0}^{d_i} a! \cdot (\sigma_s(v_i) - a)! \cdot \mathcal{C}_a(s_1(v_i), \ldots, s_{d_i}(v_i))}{(\sigma_s(v_i) + 1)!},$$

where $\mathcal{C}_a(s_1, \ldots, s_d)$ is the coefficient of x^a in the expansion of the product

$$(s_1 x + 1)(s_2 x + 1) \cdots (s_d x + 1).$$

This formula is admittedly unwieldy; for the case where every vertex has degree d and every edge has cardinality $s+1$, we can simplify it considerably. In this case $C_a = \binom{d}{a} \cdot s^a$, hence

Corollary 4.24

$$\beta_3(H) \geq \frac{n \cdot d! \cdot [(s-1)d]!}{(sd+1)!} \cdot \sum_{a=0}^{d} \binom{sd-a}{d-a} s^a.$$

When $s = 2$ the summation simplifies to 4^d (see Section B.3), and we obtain

$$\beta_3(H) \geq \frac{n \cdot (d!)^2 \cdot 4^d}{(2d+1)!};$$

this bound is the same as the one that Caro-Tuza gives for 3-uniform hypergraphs of regular degree d.

To demonstrate the difference in these estimates, we will consider a simple problem in which every vertex will have the same degree. Let p be prime, and take the $p \times p$ lattice square $\{1, \ldots, p\}^2$. How many points can we select such that no three points lie on a modular line $\pmod{p}$? In Section 5.2 we will see a deterministic construction that gives $p-1$ points, but for now, let us consider a random solution: we will order the points randomly and insert points into a set whenever it will not cause a conflict. How many points will be placed into the set?

Let us first see what Caro-Tuza has to tell us. Let q be one of the points in the lattice. Every pair of points lies on exactly one modular line,[10] and each modular line contains exactly p points. The number of collinear triples to which q belongs is therefore

$$\frac{(p^2-1)(p-2)}{2}$$

exactly. We will denote this quantity by Δ_p. The Caro-Tuza bound is

$$\frac{p^2 \cdot (\Delta_p!)^2 \cdot 4^{\Delta_p}}{(2\Delta_p+1)!};$$

because of the large numbers involved, when $p > 5$ we approximate this by

$$\frac{p^2\sqrt{\pi}}{2\sqrt{\Delta_p+1}}.$$

(The error here is negligible; see Theorem 4.16.)

On the other hand, we can apply Corollary 4.24 with $s = p-1$ and $d = p+1$. These values are such because each modular line passes through p points (cardinality p) and each point belongs to $p+1$ modular lines ($d = p+1$). We compare these results in Table 4.1. There is no clear trend present, although the results for Corollary 4.24 are always larger than those for Caro-Tuza.

We remark briefly on the summation in Corollary 4.24. The summation is listed in the Online Encyclopedia of Integer Sequences [33] as approaching

$$\frac{s}{2(s-1)} \cdot \left(\frac{s^s}{(s-1)^{s-1}}\right)^d$$

[10] This was our reason for using a prime size; for a composite size the situation is much more complicated.

Table 4.1: A comparison of the results of Caro-Tuza and Corollary 4.24 for an example problem.

p	**Caro-Tuza**	**Corollary 4.24**	**difference**
3	3.66	3.66	0
5	3.65	4.04	0.40
7	3.95	4.45	0.50
11	4.61	5.20	0.59
13	4.92	5.53	0.61
17	5.51	6.14	0.63
19	5.78	6.42	0.64
23	6.30	6.94	0.64
29	6.99	7.65	0.66
31	7.22	7.87	0.65
101	12.72	13.39	0.67
113	13.44	14.11	0.67

from above. This permits us to rewrite the corollary as

$$\beta_3(H) \geq \frac{n}{(sd+1)\cdot\binom{sd}{d}} \cdot \left(\frac{s^s}{(s-1)^{s-1}}\right)^d .$$

4.6 Proof of Theorem 4.23

Our proof goes along the same lines as the proof of Caro-Tuza presented earlier. Let us consider a single vertex v and its $\sigma_s(v)$ neighbors. There are $(\sigma_s(v)+1)!$ orderings of these vertices. For v to be placed into the triple-free set, we need it to be the case that at most one vertex from each edge $e_1, e_2, \ldots, e_d$ occurs before v in the ordering. Put another way, if we define c_i $(i = 1, \ldots, d)$ to be the number of vertices in edge e_i occurring before v, we need $c_i \in \{0, 1\}$ for all i.

Let us temporarily fix values for $c_1, c_2, \ldots, c_d$. The question now becomes: How many orderings are there in which, for all i, exactly c_i vertices from s_i occur before v?

We can break the ordering down to the form AvB, where A is the sequence of vertices before v, and B is the sequence after v. The length of A must be $\Sigma_c = \sum_{i=1}^{d} c_i$. The number of unordered sets of vertices that can comprise A is $\prod_{i=1}^{d} s_i^{c_i}$. Each of these sets can be ordered in $\Sigma_c!$ ways. The remaining vertices in B can be ordered in $(\sigma_s(v) - \Sigma_c)!$ ways. Therefore, the number of orderings in which exactly c_i vertices from s_i occur before v, for all i, is

$$\left(\prod_{i=1}^{d} s_i^{c_i}\right) \cdot \Sigma_c! \cdot (\sigma_s(v) - \Sigma_c)!$$

Fix a value of a from among $0, 1, 2, \ldots, n$. The number of valid orderings for which $\Sigma_c = a$ is

$$\begin{aligned}
&\sum_{\substack{c_1, c_2, \ldots, c_d \in \{0,1\} \\ c_1 + c_2 + \ldots + c_d = a}} \left(\left(\prod_{i=1}^{d} s_i^{c_i}\right) \cdot a! \cdot (\sigma_s(v) - a)!\right) \\
= \quad & a! \cdot (\sigma_s(v) - a)! \cdot \sum_{\substack{c_1, c_2, \ldots, c_d \in \{0,1\} \\ c_1 + c_2 + \ldots + c_d = a}} \prod_{i=1}^{d} s_i^{c_i} \\
= \quad & a! \cdot (\sigma_s(v) - a)! \cdot \mathcal{C}_a(s_1, \ldots, s_d).
\end{aligned}$$

The theorem follows. □

4.7 A conjecture on 3-uniform hypergraphs with bounded degrees and pair-degrees

The no-three-in-line problem (see Section 5.2) inspired us to make the following conjecture. Let us define the *pair-degree* of two distinct vertices $u, v \in V(H)$, written $\gamma(u, v)$, to be the number of edges containing both u and v. The *maximum pair-degree* of H is the maximum of $\gamma(u, v)$ over all distinct vertex pairs (u, v).

Conjecture 4.25 *Let H be a 3-uniform hypergraph on n vertices with maximum vertex degree $\leq n \log n$ and maximum pair-degree $\leq \sqrt{n} - 2$. Then $\alpha(H) \geq \lfloor 1.6\sqrt{n} \rfloor$.*

It can be shown that the hypergraph induced by the no-three-in-line problem (see Section 5.2) on the $\sqrt{n} \times \sqrt{n}$ lattice fits the hypothesis of this conjecture. The condition on the pair-degree is obvious, since any line can only pass through $\sqrt{n}$ of the lattice points; the bound on the (individual) degrees is shown by Zhang [59]. A proof of this conjecture would demonstrate a better bound for the no-three-in-line problem than the best bound currently known (due to [25]). We believe that both of the conditions, the one on the degree and the one on the pair-degree, are necessary. If we relax the condition on the degree, then the problem considered previously on the $p \times p$ lattice disproves the conjecture: each vertex has pair-degree $p - 2 = \sqrt{n} - 2$, but we can only select $p + 2 = \sqrt{n} + 2$ points (see Section 5.2). Experimental results suggest that relaxing the pair-degree condition will also cause the conjecture to fail.

We do not yet know how to prove this conjecture, but we have good reason to believe it is true. We have run experiments on randomly generated[11] hypergraphs for $n = 9, 16, 25, 36$, and we have never seen the conjecture fail for these sizes. Unfortunately, we have to try every vertex subset of size $\lfloor 1.6\sqrt{n} \rfloor$; we have not found a reasonable algorithm that reliably generates an independent set of this size. Furthermore, any significant tightening of the conclusion of the conjecture makes it fail (for example, replacing the pair-degree $\sqrt{n} - 2$ with $\sqrt{n} - 1$, or increasing the constant 1.6 to 1.7). This sensitivity leads us to believe that the conjecture holds for all such hypergraphs and not just for most of them.

We have not encountered any result of this ilk in the literature; most strengthenings of the Turán and Caro-Wei bounds rely on the hypergraph H containing no small cycles. Here we make no such assumption: on the contrary, the hypergraph

[11] according to the Erdös-Rényi model

induced by the $\sqrt{n} \times \sqrt{n}$ lattice has large numbers of 2-cycles. It is our hope that the condition on the pair-degree can be applied, instead of the absence of small cycles, to similar effect.

Another difficulty is that most of these results are given in Ω-notation, without an explicit constant. For the conjecture to be applicable to the no-three-in-line problem, we need the constant in the conjecture to be greater than 1.5. There is also the question of *why* 1.6 works; our best guess is that it has something to do with $\log_2 3 \approx 1.584$.

4.8 Conclusion

In this chapter, we examined the independent set problem and some results related to it. We stated the Caro-Wei bound and gave a short proof of it; then, we moved on to the Caro-Tuza bound and proved it for the case $K = 3$. We showed (for general K) a consequence of Caro-Tuza that had not previously appeared in the literature.

We introduced the *triple-free set problem* on hypergraphs and showed that, while it can be reduced to a standard independent set problem, the bound obtained for the independent set problem is slightly less than the bound on the original triple-free set problem. We also stated a bound that applies to the triple-free set problem on linear hypergraphs. We ended with a conjectured lower bound on the independence number of a specifically structured 3-uniform hypergraph, with an eye toward applying the result to the no-three-in-line problem. Unfortunately, we have not been able to prove the conjecture. If someone proves it in the future, it will immediately imply an improved bound for the no-three-in-line problem.

5. Packing problems in lattices

The d-dimensional lattice of width n is the set of points $\{1, 2, \ldots, n\}^d$. There is a rich literature on packing problems in such lattices. In our exposition we focus the greatest part of our attention on the no-three-in-line problem, because it has, arguably, been studied the most, and because we have several ideas as to how the current optimal bound can be improved. We will then proceed to other problems in the literature, before finally outlining the generalizations of these problems which we intend to address.

5.1 Preliminaries

Many of these questions are concerned with lines passing through lattice points. In the plane, the general form of a line is $ax + by + c = 0$, with one of a, b nonzero. This line has slope $-a/b$; if this slope is written in lowest terms as c/d, the number of lattice points lying on the line is at most $\lceil n/\max(|c|, |d|) \rceil$. To simplify things later, we will define the *characteristic* of a line as the quantity $\max(|c|, |d|)$. The number of lines with characteristic C is $\leq 4\Phi(C)$, where Φ is Euler's totient function:

$$\Phi(n) = |\{m : m \in \{1, \ldots, n\},\ m \text{ and } n \text{ are relatively prime}\}|.$$

Most of the time we will use the obvious bound $\Phi(n) \leq n$.

We can also define the characteristic of lines in three or more dimensions. Let d be the dimension. A line ℓ through two lattice points can be specified by a lattice point P and a difference vector δ such that $P + \delta$ is also a lattice point. Without loss of generality we can assume $\mathrm{GCD}(\delta_1, \delta_2, \ldots, \delta_d) = 1$. Then the characteristic of ℓ is $\max(|\delta_1|, |\delta_2|, \ldots, |\delta_d|)$, and the number of points of the $n \times n \times \cdots \times n$ lattice lying on ℓ is at most $\lceil n/\max(|\delta_1|, |\delta_2|, \ldots, |\delta_d|)\rceil$.

5.2 The no-three-in-line problem

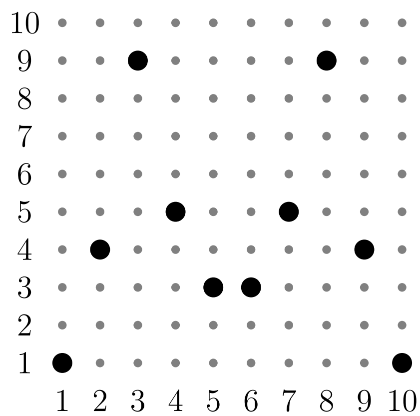
One of the oldest open lattice problems is the no-three-in-line problem, due to Dudeney [18]: *How many points can be chosen from the $n \times n$ lattice with no three collinear?* The obvious upper bound is $2n$, and a simple construction of Erdős shows that we can choose $(1 - o(1)) \cdot n$ points. The optimum must therefore lie somewhere in between. Hall et al. [25] improved this bound to $(1.5 - o(1)) \cdot n$, but no advances have been made since then.

Erdős observed (cf. [42, Appendix]) that the set $S_p = \{(x, x^2 \bmod p)\}_{x=1}^{p-1}$ contains no three collinear points. (This follows from the fact that in the set $\{(x, y) : y \equiv x^2 \pmod{p}\} \subseteq \mathbb{Z}^2$, any set of three collinear points must contain two congruent points; see Section B.1 for the proof.) Figure 5.1a depicts this set for $p = 11$. Given n, we set p to be the largest prime not exceeding n, and we take S_p for our subset. The size of this subset is therefore $p - 1 = (1 - o(1)) \cdot n$.

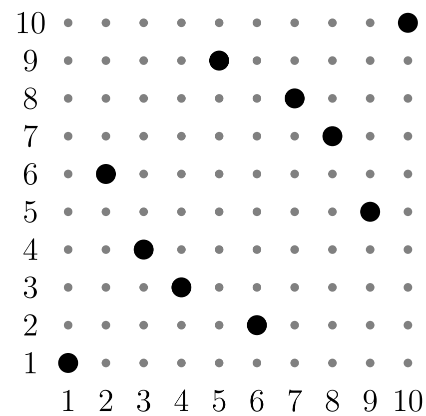
Remark 5.1 *This construction is quite versatile; for example, as observed in [6], it can be applied to Heilbronn's triangle problem [42] to yield a set of n points in the unit square with minimum triangle area $\geq (1 - o(1))/2n^2$. Again, take the set S_p. Since no three points are collinear, no triangle has area zero; thus the minimum triangle area is at least $1/2$, because the area of the triangle $(x_1, y_1), (x_2, y_2), (x_3, y_3)$ is*

$$\frac{1}{2}\left|\det \begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{bmatrix}\right|$$

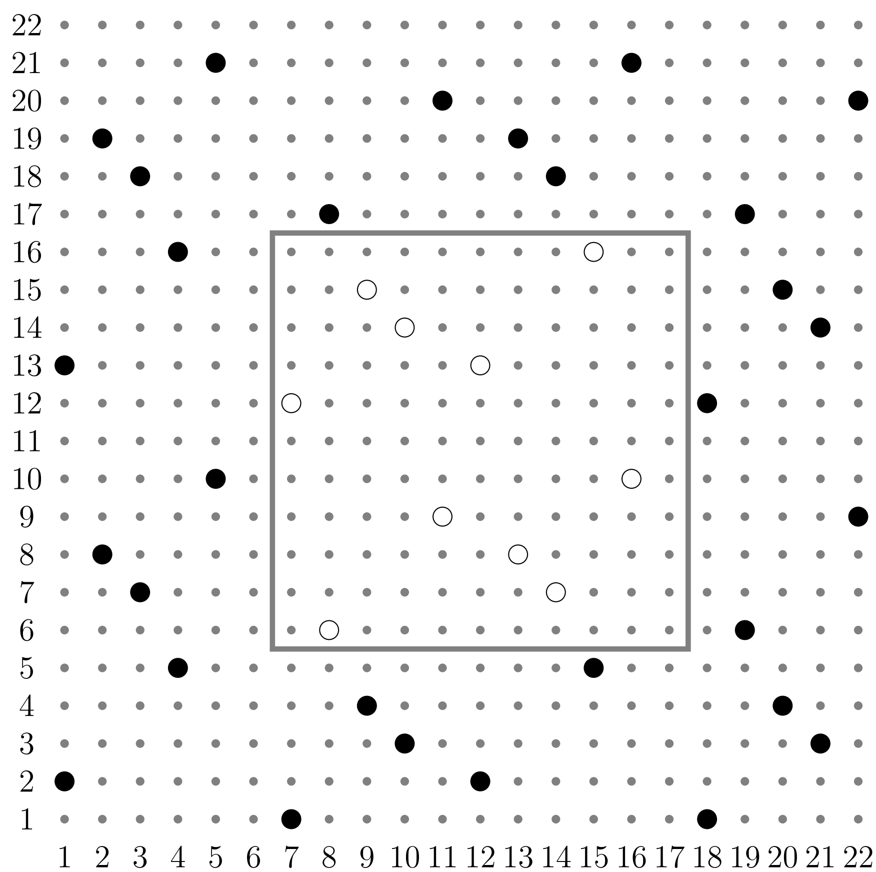
and the determinant is a nonzero integer. Dividing these points by p will place them within $[0, 1]^2$ and maintains a minimum triangle area of $1/2p^2$.



(a)



(b)



(c)

Figure 5.1: No-three-in-line arrangements. (a) The points $(x, x^2 \bmod 11)$ for $x = 1, \ldots, 10$. (b) The points in $\{1, \ldots, 10\}^2$ satisfying $xy \equiv 1 \pmod{11}$. (c) The construction of Hall et al. [25] for $p = 11$. The initial set is $\{(x, y) : x, y \in \{1, \ldots, 22\}, (x+5)y \equiv 1 \pmod{11}\}$. The central points are removed as shown, leaving 30 points in a 22×22 lattice.

The construction of Hall et al. used a similar principle: the set $S'_p = \{(x, y) : xy \equiv 1 \pmod{p}\} \subseteq \mathbb{Z}^2$ also has the property that any set of three collinear points must contain two congruent points (see Section B.2). See Figure 5.1b for an example of such a set; these sets bear a clear resemblance to permutation matrices. By choosing a $2p \times 2p$ region of the plane (which contains $4(p-1)$ points) and throwing out $p-1$ points, we obtain a set of $3(p-1)$ points in $\{1, \ldots, 2p\}^2$ in which no three points are collinear. (Figure 5.1c gives an example.) This ratio tends to 1.5 as $n \to \infty$.

Some simple heuristics appear to give a better ratio than 1.5; these are explained in the next section.

These constructions also give a solution to the related problem of choosing points from the $p \times p$ lattice (for p prime) so that no three lie on a *modular* line. We can show that these solutions are nearly optimal: Without loss of generality, let us say $(0, 0)$ belongs to the set. Each other point (x_i, y_i) forms a line with $(0, 0)$ of slope y_i/x_i, and so the modular line has slope $y_i x_i^{-1}$ (the inverse is taken mod p) unless $x_i = 0$, in which case the slope is ∞. The different points must give different slopes, since otherwise three points will be collinear mod p. The possible slopes are $0, 1, \ldots, p-1$ and ∞, a total of $p+1$ slopes. Thus there can be at most $p+2$ points in the arrangement, and our construction generates a set whose size is only 3 less than this.

Pór and Wood [36] showed that for the 3-dimensional analogue of the no-three-in-line problem, the set $\{(x, y, (x^2 + y^2) \bmod p) : x, y = 1, \ldots, p-1\}$, which contains $(p-1)^2$ points, has no three points collinear, as long as $p \equiv 3 \pmod{4}$.

5.3 Heuristic results for the no-three-in-line problem

We have found four algorithms that yield better results for the no-three-in-line problem than the best currently known; we are, however, at a loss to explain why they work. Recall that the best known bound is $(1.5 - o(1)) \cdot n$. We conjecture that the first algorithm gives a bound of $(1.51 - o(1)) \cdot n$; the second algorithm gives a bound of $1.623n$ for $n > 1$; the third gives a bound of $1.6n$ for $n > 1$; and the fourth gives a bound of $1.51n$ for $n > 1$.

The first is a simple greedy algorithm. The most straightforward greedy algorithm — consider each point in order, adding each to the set unless it causes a conflict — performs poorly, yielding a set of size around $1.35n$. Curiously, a minor modification, listed below as Algorithm 1, yields greatly improved results.

Algorithm 1 The checkerboard algorithm.

$S \leftarrow \{\}$
for $x = 1$ **to** n **do**
    for $y = 1$ **to** n **do**
        if $x + y$ is *even* and the point (x, y) is not collinear with any two points of S **then**
            $S \leftarrow S \cup \{(x, y)\}$
for $x = 1$ **to** n **do**
    for $y = 1$ **to** n **do**
        if $x + y$ is *odd* and the point (x, y) is not collinear with any two points of S **then**
            $S \leftarrow S \cup \{(x, y)\}$
return S

We call this the checkerboard algorithm because if we treat the lattice points as the squares of an $n \times n$ checkerboard, we can imagine this process as considering all the black squares in order, then all the red squares in order. The sizes of the generated sets are shown in Figure 5.2; for $1000 \leq n \leq 23000$, the size exceeds $1.51n$. There appears to be a limit around 1.525.

The second algorithm considers the number of "free" points in the arrangement, i.e., the number of points that have not been eliminated by points already chosen.

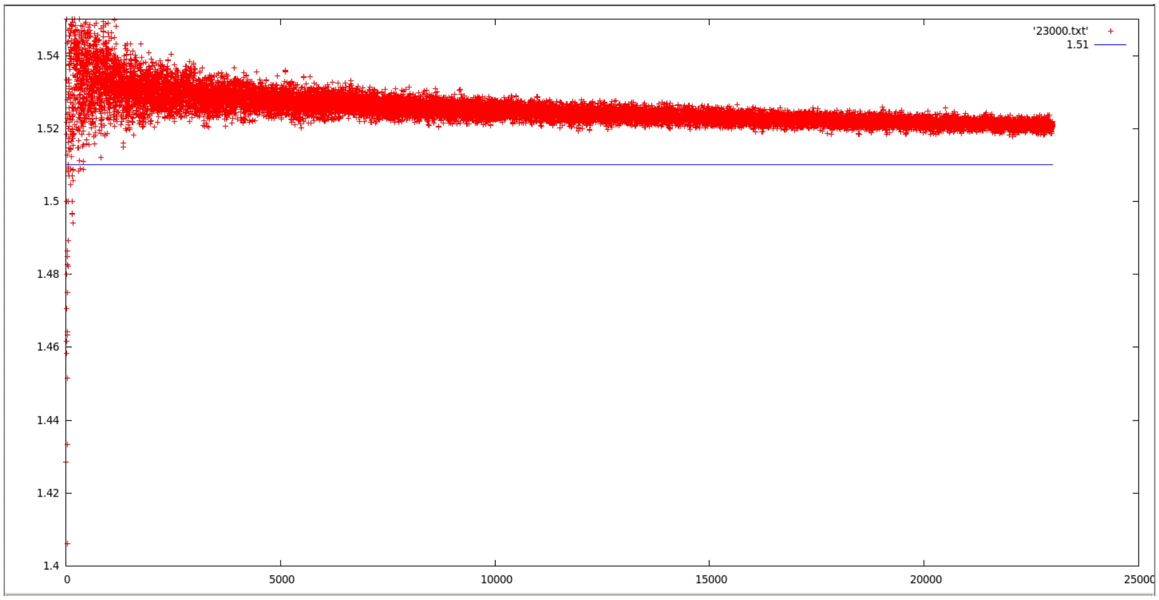


Figure 5.2: Results for the checkerboard algorithm. The horizontal axis shows the value of n; the vertical axis shows the ratio of the size of the subset to n.

Let us define $free(S)$ to be the set of free points left after choosing all those in S; we say that p is free if and only if $p \notin S$ and p is not collinear with any two points in S. We will add points to S that keep the size of $free(S)$ as high as possible, for as long as possible. See the listing for Algorithm 2.

Algorithm 2 The max-free algorithm.

1: $S \leftarrow \{\}$
2: **while** $free(S) \neq \{\}$ **do**
3: $\quad p \leftarrow \operatorname*{argmax}_{q \in free(S)} |free(S \cup \{q\})|$ /* break ties arbitrarily */
4: $\quad S \leftarrow S \cup \{p\}$
5: **return** S

The max-free algorithm reliably generates point sets of size $> 1.62n$; the sizes are

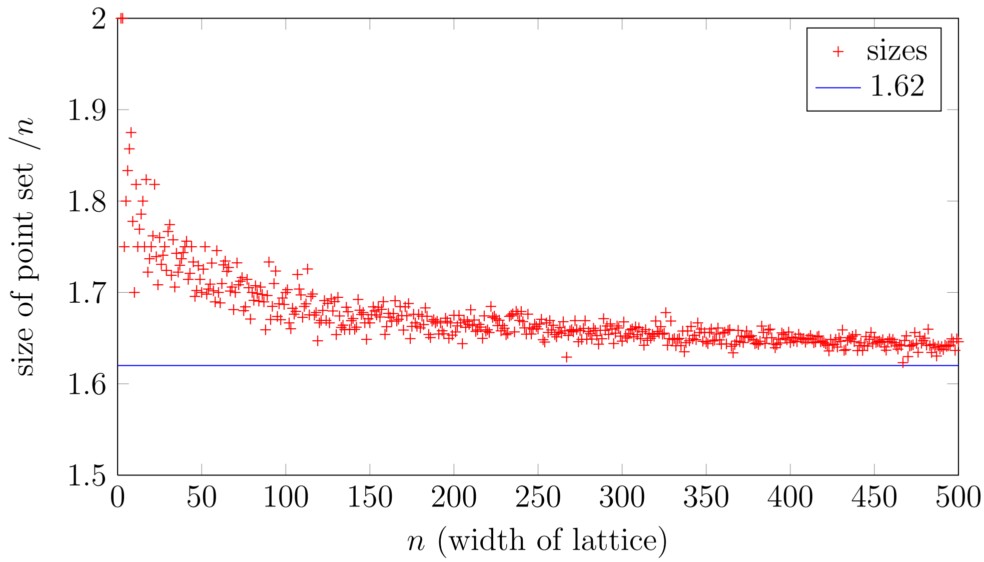


Figure 5.3: Results for the max-free algorithm.

shown in Figure 5.3 for $2 \leq n \leq 500$.

The third algorithm employs expectation minimization. Given a set of points S, we can compute in polynomial time the expected number of collinear triples that will arise if we complete S randomly — that is, while the size of S is less than $2n$, we choose a random point not already in S and add it to S. The algorithm picks the point that minimizes this quantity. We stop when it chooses a point that would cause S to have three collinear points; at this point, no further improvement is possible. Results are given in Figure 5.4 for $n \leq 42$; for $n > 1$ we see that the point set generated is of size greater than $1.6n$.

This E-M algorithm, while producing good results, runs quite slowly, since at every step it must consider many triples; the first two algorithms only need to consider pairs of points already placed in the set. Note well that the usual justification for E-M does not apply here, since the expected number of collinear triples is quite large.[1] Each

[1] It is in excess of $8n$ when n is large.

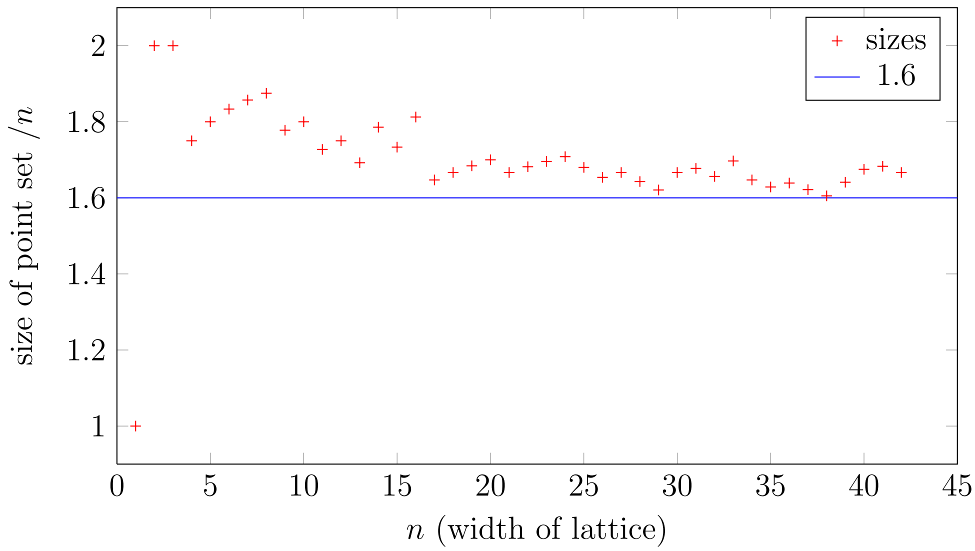


Figure 5.4: Results for the E-M algorithm.

step reduces this expectation considerably, but we do not understand why.

The fourth and final algorithm we will consider here is related to the second, but applies the idea in reverse. We start with a full $n \times n$ grid; at each iteration, we remove one point. The point removed is the one that belongs to the greatest number of collinear triples in the remaining configuration. We were inspired to try this by [4], in which Ajtai et al. start with a triangle-free graph G, remove certain vertices to create G', and then apply the Turán estimate $\alpha \geq n/(\delta+1)$ to this reduced graph. Perhaps a similar strategy can be applied to the no-three-in-line problem, through a judicious choice of point removals. Results are given in Figure 5.5 for $n \leq 40$; for $n > 1$ we see that the point set generated is of size $> 1.51n$.

5.4 "Strong" configurations

We observe that most of the complexity of the configurations in [25] (recall Figure 5.1c) stems from the collinear triples that occur on the lines of slope ± 1. If we

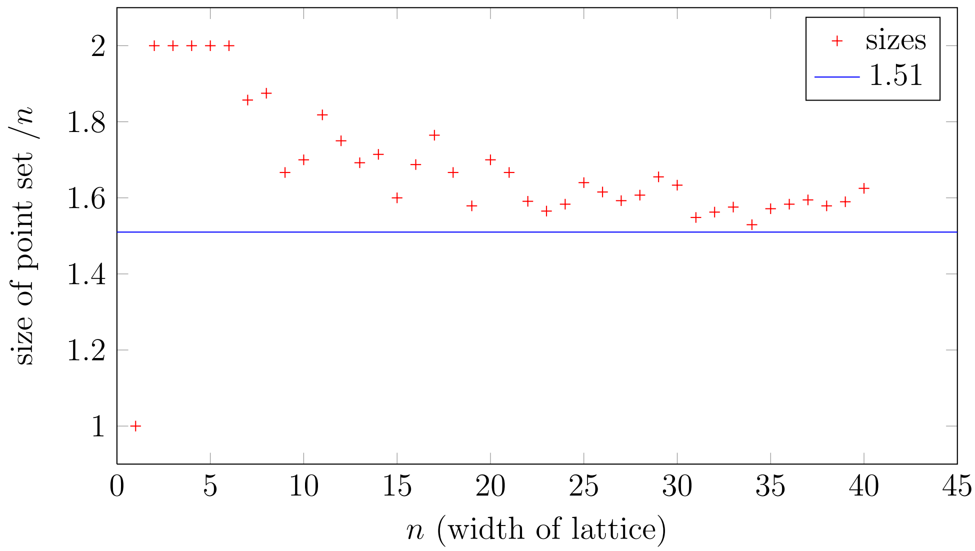


Figure 5.5: Results for the reduction algorithm.

could create a similar (and large enough) configuration that avoids the difficulties along these diagonals, we would have an improved solution to the no-three-in-line problem. We dub these "strong" configurations.

Definition 5.2 *A* strong $n \times n$ configuration *is a subset of* $\{1, \ldots, n\}^2$ *in which*

1. *every row and every column contains at most one point;*
2. *every modular line* (mod n) *passes through at most two points; and*
3. *every modular line* (mod n) *of slope* ± 1 *passes through at most one point.*

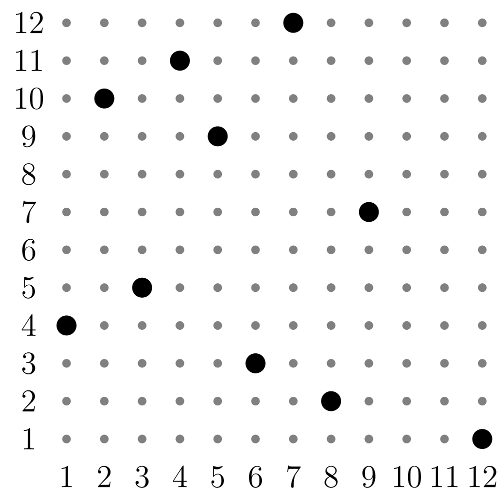
Figure 5.6 demonstrates the utility of such a configuration. In (a) we see a strong 12×12 configuration containing 10 points. In (b) we have tiled four copies of this configuration side by side; it creates a no-three-in-line subset of the 24×24 lattice containing 40 points, a ratio of $5/3 \approx 1.67$. The fact that this configuration has no three collinear points is not hard to see: we need two of the points on the line to be congruent, but this induces a line of slope $0, \infty$, or ± 1, and these lines can only contain two points.

The parabolic construction (Figure 5.1a) satisfies condition 1 but not 2 or 3. The hyperbolic construction (Figure 5.1b) satisfies conditions 1 and 2 but not 3. We can satisfy the third condition by starting with a modular hyperbola and removing half of its points. Each point (except those on the main diagonals) has three mirror images, and the four together form a rectangle; removing an opposite pair of points eliminates the problem with the modular lines of slope ± 1. This only leaves $(p-1)/2$ points, however; our experiments suggest that this is close to optimal for prime p. For composite sizes we may have more luck. Unfortunately the brute-force search takes a long time, and we have only been able to run it for n from 1 to 26. The best results (containing more than $3n/4$ points) occur for $n = 12$ and $n = 20$. The optimal configuration for $n = 12$ was already shown in Figure 5.6; that for $n = 20$ is shown in Figure 5.7. For the sake of completeness we present all the maximum sizes of the strong $n \times n$ configurations for $n = 1, \ldots, 26$ in Table 5.1.

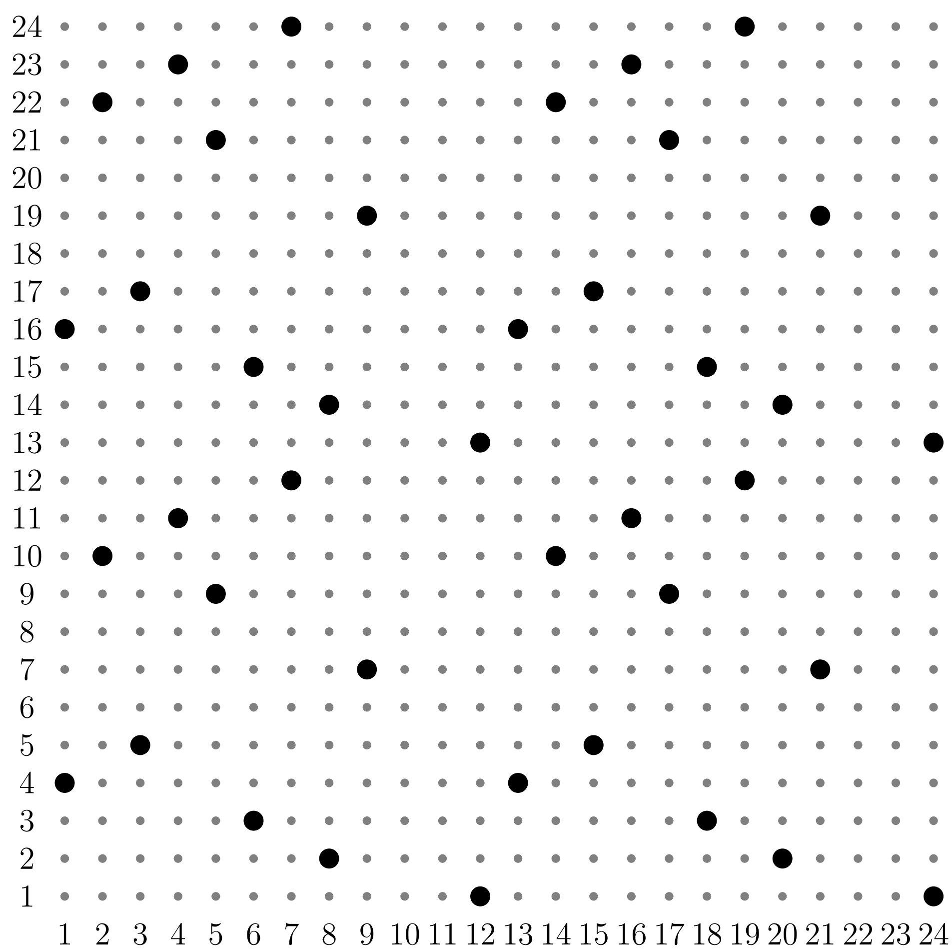
We conjecture that large strong configurations exist for n of the form $4p$, where p is an odd prime. It may be possible that they exist only for certain small values of n and that no general construction exists, but we do not think it likely.

5.5 Other packing problems

A problem related to the no-three-in-line problem was considered by Thiele [53]: *How many points can be chosen from the $n \times n$ lattice with no four points co-circular?* Here we consider four collinear points to lie on a circle of infinite radius (zero curvature). Again the optimum is known to be $\Theta(n)$, but the optimal constant is not known. Thiele's construction, yielding $(1/4 - o(1)) \cdot n$ points, is as follows. Let $S''_p = \{(x, x^2 \bmod p)\}_{x=1}^{\lfloor p/4 \rfloor}$. Four points $(x_1, y_1), \ldots, (x_4, y_4)$ are co-circular if and only



(a)



(b)

Figure 5.6: (a) A strong 12×12 configuration containing 10 points. (b) Tiling four copies of (a) creates a no-three-in-line packing of 40 points into the 24×24 lattice.

Table 5.1: The maximum sizes of strong $n \times n$ configurations for n from 1 to 26.

n	**maximum size**	**ratio**
1	1	1.000
2	1	0.500
3	1	0.333
4	2	0.500
5	2	0.400
6	4	0.667
7	4	0.571
8	5	0.625
9	4	0.444
10	7	0.700
11	6	0.545
12	**10**	**0.833**
13	7	0.538

n	**maximum size**	**ratio**
14	10	0.714
15	10	0.667
16	10	0.625
17	10	0.588
18	12	0.667
19	10	0.526
20	**16**	**0.800**
21	14	0.667
22	14	0.636
23	13	0.565
24	17	0.708
25	17	0.680
26	16	0.615

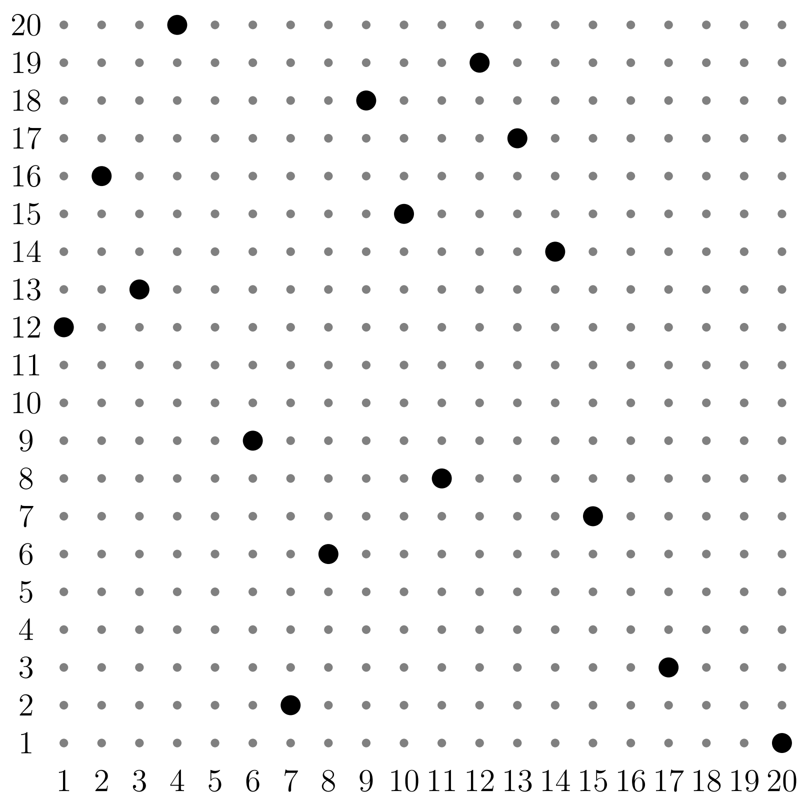


Figure 5.7: A strong 20×20 configuration containing 16 points.

if the determinant

$$\begin{vmatrix} 1 & x_1 & y_1 & x_1^2 + y_1^2 \\ 1 & x_2 & y_2 & x_2^2 + y_2^2 \\ 1 & x_3 & y_3 & x_3^2 + y_3^2 \\ 1 & x_4 & y_4 & x_4^2 + y_4^2 \end{vmatrix}$$

is zero. But since $y_i \equiv x_i^2 \pmod{p}$, this determinant simplifies mod p to

$$(x_1 + x_2 + x_3 + x_4) \cdot \prod_{i<j} (x_j - x_i),$$

which is nonzero mod p.

Erdős and Guy [21] considered the problem of selecting k points from an $n \times n$ lattice such that every pair of these points determines a distinct distance. A simple argument gives $k \leq n$; their paper presents a construction that provides, given $\epsilon > 0$, a configuration of $n^{2/3-\epsilon}$ lattice points for sufficiently large n. We now review their proof. (Later results by Thiele and Lefmann [30, 52] improved the bound to $\Omega(n^{2/3})$.)

First let us see why k cannot exceed n. In the $n \times n$ lattice there are at most $\binom{n+1}{2}$ distinct distances — this is the number of unordered pairs of $\{0, 1, \ldots, n-1\}$ with repetition. A set of k points determines $\binom{k}{2}$ distances; since none of these distances can be zero and they must all be distinct, we have

$$\binom{k}{2} < \binom{n+1}{2},$$

so that $k < n + 1$.

We now turn to proving the lower bound of $n^{2/3-\epsilon}$. Their proof is constructive and uses an elegant greedy algorithm. We start with an empty point set. Inductively, suppose k points have already been chosen. We will show that when $k < n^{2/3-\epsilon}$, there is still another point available. In order to avoid duplicating a distance, the new point cannot sit a distance d away from another point, where d is the distance between any two points already in the set (we call this condition A); and the new point cannot be equidistant from two already-chosen points (condition C). These conditions ensure that the resulting point set has distinct distances. To obtain the lower bound, we enforce an additional condition: no two lines should lie on a line of characteristic $< n^{1/3}$ (condition B).[2]

Let us suppose now that k points have been chosen: are any points still available? This will be the case when the number of eliminated and chosen points is less than n^2: let us count these points. To count the number of points eliminated by condition A, we note that these points lie on the circles centered at the k points with radii defined by the $\binom{k}{2}$ pairs of points. A circle centered at a lattice point passes through at most $n^{c_1/\log\log n}$ points of an $n \times n$ lattice (see Section B.4); therefore condition A eliminates at most $k\binom{k}{2}n^{c_1/\log\log n} \leq \frac{k^3}{2} \cdot n^{c_1/\log\log n}$ points. This quantity also accounts for the points already chosen, since when $k > 1$, each point lies on one of these circles.

We turn now to condition B. If a line ℓ has slope a/b, a line perpendicular to ℓ will have slope $-b/a$; the line ℓ and the perpendicular have the same characteristic. Each point in the set therefore excludes at most

$$\sum_{i=1}^{n^{1/3}} 4\Phi(i) \cdot \frac{n}{i} = 4n \sum_{i=1}^{n^{1/3}} \frac{\Phi(i)}{i} \leq 4n^{4/3}$$

points. Altogether, the k points exclude at most $4k \cdot n^{4/3}$ points.

Let us now consider condition C. There are $\binom{k}{2}$ pairs of points; the bisector of each pair has characteristic $\geq n^{1/3}$, so that each bisector passes through at most $n^{2/3}$ points. The bisectors therefore exclude

$$\binom{k}{2} \cdot n^{2/3} \leq \frac{k^2 n^{2/3}}{2}$$

[2]Our odd lettering was chosen to match the order of explanation in Erdős and Guy's paper.

points.

Adding these together, the total number of chosen and excluded points is at most

$$\frac{k^3}{2} \cdot n^{c_1/\log\log n} + 4k \cdot n^{4/3} + \frac{k^2 n^{2/3}}{2},$$

which is less than n^2 for $k < n^{2/3-\epsilon}$.

We conclude our review of lattice packing problems with a problem in higher dimensions. Riddell [40] considered a particular d-dimensional generalization of the no-three-in-line problem: *How many points can be chosen from the d-dimensional lattice hypercube of width n with no n points collinear?* The sets of n collinear points have a very restricted form: if we denote a set of n collinear points by $z_1, z_2, \ldots, z_n$ and write $z_i = (z_{i1}, z_{i2}, \ldots, z_{in})$, then for the sequence $(z_{1j}, z_{2j}, \ldots, z_{nj})$ formed from the j-th coordinate of each point, we have either

$$z_{1j} = z_{2j} = \ldots = z_{nj}$$

or

$$(z_{1j}, z_{2j}, \ldots, z_{nj}) = (1, 2, \ldots, n)$$

or

$$(z_{1j}, z_{2j}, \ldots, z_{nj}) = (n, n-1, \ldots, 1).$$

Riddell observed that for a fixed integer r, the set of points containing exactly r 1's contains no points fitting these descriptions, and thus contains no subset of n collinear points. The number of points in this set is easily shown to be

$$\binom{d}{r}(n-1)^{n-d};$$

this quantity is maximized when $r = \lfloor d+1 \rfloor / n$, giving a lower bound (when $d > \max\{2(n-2), (n+8)/2\}$) of

$$\frac{1}{e^{3/2}\sqrt{2\pi}} \cdot \frac{n^{d+1}}{\sqrt{d(n-1)}}.$$

Generally speaking, algorithms for generating solutions to lattice packing problems follow one of three paradigms:

1. Greedy algorithms, as in the distinct slopes problem discussed above [21].

2. The application of some mathematical structure to the problem, yielding a declarative description (a construction) of the solution. Oftentimes, modular constructions are used for this purpose (e.g., [25, 53]); Riddell's is a different kind of example [40]. Here, there is required some fortuitous insight into the problem; certain problems do not lend themselves to such neat solutions.

3. Optimization of expectation (E-M), where we seek simultaneously to maximize the number of chosen points and minimize the number of conflicts.

Of our heuristics in Section 5.3, the checkerboard algorithm embodies principle #1 here, while our E-M algorithm clearly follows #3.

5.6 Generalizations

We now consider generalizations of the no-three-in-line and no-four-on-circle problems to higher dimensions:

Problem 5.3

How many points can be chosen from $\{1, \ldots, n\}^d$ *with no three points collinear?*

Problem 5.4

How many points can be chosen from $\{1, \ldots, n\}^d$ *with no* K *points collinear?*

Problem 5.5

How many points can be chosen from $\{1, \ldots, n\}^d$ *with no four points co-circular?*

Here we are allowing d and K to vary, whereas [25] and [53] considered only the case $d = 2$ (and for [25], $K = 3$).

The structures of these problems readily lend themselves to hypergraph representations. For Problem 5.3, we can represent each triple of collinear points as an edge in a 3-uniform hypergraph. For Problem 5.4, we can represent each K-tuple of collinear points as an edge in a K-uniform hypergraph. For Problem 5.5, we can represent each 4-tuple of co-circular points as an edge in a 4-uniform hypergraph. Each problem induces a hypergraph whose vertex set is the point set $\{1, \ldots, n\}^d$ and whose edge set is the set of conflicting point tuples. The main difficulty is to bound effectively the degrees of the vertices in these graphs. Geometric reasoning will give us these bounds, which we can then apply in Theorem 4.17 to find a lower bound on the independence number.

Let us first examine Problem 5.3. Let P be a point in the d-dimensional $n \times n \times \cdots \times n$ lattice, with $n > 1$. For every other point P', there is a line $\ell(P')$ passing through it and P. There are $n^d - 1$ choices for P' and then, for each P', at most $n - 2$ other points along the line $\ell(P')$. This process accounts for two copies of each (unordered) pair of points that is collinear with P; the number of collinear triples containing P is therefore no greater than $(n^d - 1) \cdot (n - 2)/2$, meaning we have a hypergraph on n^d vertices with maximum degree $\leq (n^d - 1) \cdot (n - 2)/2 \leq n^{d+1}/2$. Substituting into Theorem 4.13 gives

$$\alpha(H) > \frac{\sqrt{\pi}}{2} \cdot \frac{n^d}{\sqrt{n^{d+1}/2}} = \sqrt{\frac{\pi}{2}} \cdot n^{(d-1)/2}.$$

Theorem 5.6 *For $n > 1$, there is a subset S of the d-dimensional $n \times n \times \cdots \times n$ lattice such that*

$$|S| > \sqrt{\frac{\pi}{2}} \cdot n^{(d-1)/2}$$

and S contains no set of three collinear points.

We now turn our attention to Problem 5.4. As before, let P be a point in the d-dimensional $n \times n \times \cdots \times n$ lattice. For every other point P', there is a line $\ell(P')$ passing through it and P. There are $n^d - 1$ choices for P' and then, for each P', at most $n-2$ other points along the line $\ell(P')$. From these $n-2$ points, there are $\binom{n-2}{K-2}$ sets of $K-2$ points. The number of collinear triples is therefore bounded from above by

$$(n^d - 1) \cdot \binom{n-2}{K-2} / (K-1) \leq \frac{(n^d - 1) \cdot (n-2)^{K-2}}{(K-2)! \cdot (K-1)} \leq \frac{n^{d+K-2}}{(K-1)!}.$$

Substituting into Theorem 4.17 gives

$$\alpha(H) > e^{-\gamma/(K-1)} \cdot \frac{n^d}{\sqrt[K-1]{n^{d+K-2}}} \cdot \sqrt[K-1]{(K-1)!}$$

We must now simplify this expression.

Lemma 5.7 $\sqrt[m]{m!} > m/e$.

Proof: Using the fact that Stirling's approximation is a lower bound on the factorial, we obtain

$$\begin{aligned} \sqrt[m]{m!} &> \sqrt[m]{\sqrt{2\pi m} \cdot \left(\frac{m}{e}\right)^m} \\ &= \sqrt[2m]{2\pi m} \cdot \frac{m}{e} \\ &> \frac{m}{e}. \end{aligned}$$

$\square$

Thus $\sqrt[K-1]{(K-1)!} > (K-1)/e$. We also have

$$\frac{n^d}{\sqrt[K-1]{n^{d+K-2}}} = n^{d-d/(K-1)-1-1/(K-1)} = n^{(d-1)\cdot(K-2)/(K-1)}.$$

We conclude

Theorem 5.8 *For $n > K-1$, there is a subset S of the d-dimensional $n \times n \times \cdots \times n$ lattice such that*

$$|S| > (K-1)e^{-1-\gamma/(K-1)} \cdot n^{(d-1)\cdot(1-1/(K-1))}$$

and S contains no set of K collinear points.

Let us finish by looking at Problem 5.5. Let P be a point in the d-dimensional $n \times n \times \cdots \times n$ lattice. We will build a 4-uniform hypergraph which has an edge for every cocircular 4-tuple of points in the lattice. Let P' and P'' be two other points in the lattice. (If P, P', and P'' are collinear, we can say either that there is no circle passing through them, or that the line passing through them is a circle of zero curvature. We will say the latter.) The plane determined by these three points contains at most n^2 points, and a circle can only pass through $2n$ of these. Thus, every point will have degree at most $\binom{n^d}{2} \cdot 2n < n^{2d+1}$. We conclude

Theorem 5.9 *There is a subset S of the d-dimensional $n \times n \times \cdots \times n$ lattice such that*

$$|S| > e^{-\gamma/3} \cdot n^{(d-1)/3}$$

and S contains no set of four cocircular points.

5.7 Conclusions

The first part of this chapter focused on the no-three-in-line problem in the $n \times n$ lattice. We saw some heuristics that give better results than the best-known construction, due to Hall et al. [25]. Unfortunately, we have not been able to provide a proof for any of these experimental results. It is still heartening to know that better results are likely possible; perhaps someone will be able to prove the efficacy of one of the algorithms presented here. The max-free algorithm seems the best candidate, since it gives substantially better results than [25], while its process closely resembles the independent set algorithms that we touched on in Chapter 4.

We attempted to extend the no-three-in-line problem to higher dimensions; our generalizations were listed as Problems 5.3 and 5.4. Our result for the first problem, listed as Theorem 5.6, is disappointing, since the analogous problems in 2 and 3 dimensions lead us to expect that we can choose $\Theta(n^{d-1})$ points. The exponent we obtained is instead $(d-1)/2$. Our second result is a little better: the exponent that we obtained in Theorem 5.8 is $(d-1)\cdot(1-1/(K-1))$, which is close to $d-1$ when K is large.

We have had difficulty finding other bounds with which to compare the bounds in this section. Brass et al. [12, Chapter 10] mention that few bounds are known beyond the trivial bounds, but we are not sure what qualifies as "trivial" in their eyes. If we take $d = K$ in Theorem 5.8, we obtain an exponent of $d-2$; this compares unfavorably with Brass and Knauer [11], who demonstrated an exponent of $d-1$.

6. Concluding remarks

We have come to the end of our material. Our investigations into optimization problems on HSTs were quite successful, as we derived several new results. For the monochromatic matching problem, MST problem, and TSP, we proved that the expected cost of an optimal solution for a randomly chosen multiset of n leaves is $\Theta(\sum_{k=1}^{h}(b\lambda)^k)$, where $h = \min(\delta, \log_b n)$. Turning to the bichromatic problems, we discovered that the bichromatic MST problem obeys the same bound, while the cost of the optimal tour for the bichromatic TSP is $\Theta(\sqrt{n}\cdot\sum_{i=1}^{h}(\sqrt{b}\lambda)^i)$. This latter bound is the same as the one found by Abrahamson et al. [1, 2] for the bichromatic matching problem. The lifting lemma proved vital to the bichromatic proofs; we anticipate that many more researchers may make use of this lemma in the future.

One might wonder, apart from the mathematics, why the bounds for the bichromatic MST and TSP are so different. We can offer only a rough idea: In the TSP, each node is attached to two other nodes (its neighbors in the tour), while in a spanning tree, each node can be attached to many other nodes. Thus we should expect the TSP to behave more like the matching problem, and we should expect the bichromatic MST problem to behave less like it.

Noting that the monochromatic and bichromatic MST problems had the same bound, we briefly considered the K-chromatic MST problem for $K \geq 3$. For fixed even values of K, we showed that the asymptotic bounds for the bichromatic MST also apply to the K-chromatic MST problem; the only change is in the leading constants, which now depend on K. In fact there is no need for K to be even (and it would be quite surprising if the parity of K affected our result!). We can recast a K-chromatic problem into a bichromatic problem as follows. Let $W_1, W_2, \ldots, W_K$ be our K multisets of leaves. We form the bichromatic problem by calling W_1 our red set and calling $W_2 \cup W_3 \cup W_K$ our blue set. Even though the red set and the blue set have different sizes, our proof for the bichromatic MST still holds: each red point must still reach out to a blue point, and it will be *easier* with a larger blue set.

We have not determined what happens in the K-chromatic matching problem or TSP. This may be a fruitful area for future research. We anticipate that the matching problem and TSP will again have the same solution. To prove a bound the way we have in this thesis, one must first figure out how to extend our notion of discrepancy to more than two colors.

We ended our look at HSTs by deriving novel bounds on the bichromatic problems on unit hypercubes. We showed that for sufficiently high dimension d, the cost of the optimal solutions to the bichromatic matching problem, MST problem, and TSP obey the asymptotic bound $\Theta(n^{(d-1)/d})$. This bound was proved by sandwiching the cost between previous known bounds on the monochromatic problems [58] and the upper bound obtained by the HST approximation.

Let us now turn to our investigations into hypergraph problems. We concentrated on the independent set problem on uniform hypergraphs. Here, we were able to apply a result of Caro and Tuza [14] to obtain a bound resembling Caro and Wei's bound [13, 56]. Our result is a natural consequence of Caro-Tuza, but it did not appear to have been published previously. The novel results of Chapter 4 (to be specific, Theorems 4.13 and 4.17) were published in February 2012 as [16].

We proceeded to explain an alternative formalism to the independent set problem, naming this alternative formalism the *K-tuple-free set problem*. In this problem, we are given a hypergraph $H = (V, E)$, and we wish to find a subset $I \subseteq V$ such that no K vertices of I appear in an edge in E. While problems of this form can easily be turned into independent set problems, this transformation sacrifices some of the properties of the original hypergraph. We may be able to derive better bounds by tackling the problem directly. Unfortunately, our results for $K = 3$ (the *triple-free set problem*) were not very impressive. It would be nice to know what happens for larger values of K.

At the end of the chapter, we outlined a conjecture about the independence number of a certain type of 3-uniform hypergraph. Again, our motivation here was that a proof of this conjecture would improve the best-known bound for the no-three-in-line problem. Unfortunately we did not manage to prove the conjecture, but we have great reason to believe it is true. If it is true, it would imply that the structure of the $n \times n$ lattice is not as important to the no-three-in-line problem as initially suspected; rather, the most important properties of the graph are the degrees of its vertices and the pair-degrees of its vertex pairs.

Appendix C contains some material that we developed late in the writing of this thesis. It presents an interesting new algorithm for generating independent sets. We have been unable to find proofs of its efficacy (we explain this in the appendix), but we have managed to find several small examples for which our algorithm outdoes other simple algorithms.

We finished off by considering several packing problems in point lattices. We devoted the most attention to the no-three-in-line problem in the plane, coming up with several heuristics that improve the best-known bound due to Hall et al. [25]. Unfortunately we could not come up with a proof for any of these heuristics. We also considered three generalizations of the no-three-in-line problem to higher dimensions, leaning on the results of Chapter 4 to derive our bounds. These bounds are smaller than we would like, but we have been unable to find other results with which to compare our bounds.

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[1] "On the order of magnitude of the number of divisors of an integer."

Appendix A. Notation

$\mathbf{Pr}[A]$	the probability of the event A
$\mathbf{E}X$	the expected value of the random variable X
$\mathbf{D}X$	the standard deviation of X
$\mathbf{Var}X$	the variance of X

Recall

$$\mathbf{Var}X = \mathbf{E}(X - \mathbf{E}X)^2 = \mathbf{E}X^2 - (\mathbf{E}X)^2$$

and $\mathbf{D}X = \sqrt{\mathbf{Var}X}$.

e	Euler's constant $2.718281828\ldots$, the base of the natural logarithm
$\log x$	the natural logarithm (to the base e) of x
γ	the Euler-Mascheroni constant $0.5772156649\ldots$
$\lfloor x \rfloor$	the greatest integer less than or equal to x
$\lceil x \rceil$	the least integer greater than or equal to x

We will sometimes write $\exp(x)$ to mean e^x.

Appendix B. Postponed proofs

To maintain the flow of the main text, we have waited until now to give proofs of some statements given or used earlier. The AM-GM inequality (Section B.5) was not used in the main text, but instead is used in Section B.4.

B.1 Modular parabola

We can follow the derivation of the quadratic formula to obtain

Theorem B.1 *The quadratic congruence* $ax^2 + by + c \equiv 0 \pmod{p}$*, with* $a \not\equiv 0 \pmod{p}$*, has the precise solutions*

$$x \equiv \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \pmod{p};$$

if $b^2 - 4ac$ *is a quadratic non-residue, there is no solution.*

An immediate consequence is

Corollary B.2 *A quadratic congruence with nonzero quadratic coefficient has at most two solutions* mod p*.*

Let $S_{p,k} = \{(x, y) : x, y \in \mathbb{Z}, y \equiv kx^2 \pmod{p}\}$. We say two points $(x_1, y_1), (x_2, y_2) \in S_p$ are *congruent* if $x_1 \equiv x_2$ and $y_1 \equiv y_2 \pmod{p}$.

Here we show

Theorem B.3 *Let* $k \not\equiv 0 \pmod{p}$*. If three points* $(x_1, y_1), (x_2, y_2), (x_3, y_3) \in S_{p,k}$ *are collinear, two of them are congruent.*

Proof: Suppose the line ℓ passes through two points of S_p. This line has the form $ax + by = c$, where $a, b, c \in \mathbb{Z}$ and $a, b \not\equiv 0 \pmod{p}$. This implies $ax + by \equiv c$

(mod p). Substituting $y \equiv kx^2$, we obtain a quadratic congruence; by Corollary B.2, there are at most two values of x that satisfy it. Therefore two of the x_i, say x_1 and x_2, must be congruent. Since $y_1 \equiv x_1^2 \equiv x_2^2 \equiv y_2$, we have that (x_1, y_1) and (x_2, y_2) are congruent. $\square$

B.2 Modular hyperbola

Let $S'_{p,k} = \{(x, y) : x, y \in \mathbb{Z}, xy \equiv k \pmod{p}\}$.

Theorem B.4 *Let $k \not\equiv 0 \pmod{p}$. If three points $(x_1, y_1), (x_2, y_2), (x_3, y_3) \in S'_{p,k}$ are collinear, two of them are congruent.*

The **proof** resembles the previous one. Suppose the line ℓ passes through two points of S_p. This line has the form $ax + by = c$, where $a, b, c \in \mathbb{Z}$ and $a, b \not\equiv 0 \pmod{p}$. Multiplying by x, we obtain $ax^2 + bk \equiv cx$; by Corollary B.2, there are at most two values of x that satisfy it. Therefore two of the x_i, say x_1 and x_2, must be congruent. Since $y_1 \equiv x_1^2 \equiv x_2^2 \equiv y_2$, we have that (x_1, y_1) and (x_2, y_2) are congruent. $\square$

B.3 A combinatorial lemma

In Section 4.5 we claimed $\sum_{a=0}^{d} \binom{2d-a}{d-a} 2^a = 4^d$. Note that this summation is the same as $\sum_{a=0}^{d} \binom{2d-a}{d} 2^a$. We now show

Lemma B.5

$$\sum_{a=0}^{d} \binom{2d-a}{d} 2^a = 4^a.$$

Proof: Let $f(d)$ equal the summation. Clearly $f(0) = 4^0$. Then for $d > 0$, assuming $f(d-1) = 4^{d-1}$, we have

$$\begin{aligned}
f(d) &= \sum_{a=0}^{d-1} 2^a \cdot \binom{2d-a-1}{d} + \sum_{a=0}^{d} 2^a \cdot \binom{2d-a-1}{d-1} \\
&= \sum_{a=1}^{d} 2^{a-1} \cdot \binom{2d-a}{d} + \sum_{a=-1}^{d-1} 2^{a+1} \cdot \binom{2d-a-2}{d-1} \\
&= \left(-\frac{1}{2} \cdot \binom{2d}{d} + \sum_{a=0}^{d} 2^{a-1} \cdot \binom{2d-a}{d}\right) + \sum_{a=-1}^{d-1} 2^{a+1} \cdot \binom{2(d-1)-a}{d-1} \\
&= \left(-\frac{1}{2} \cdot \binom{2d}{d} + \frac{1}{2} \cdot f(d)\right) + \left(\binom{2d-1}{d-1} + \sum_{a=0}^{d-1} 2^{a+1} \cdot \binom{2(d-1)-a}{d-1}\right) \\
&= \left(-\frac{1}{2} \cdot \binom{2d}{d} + \frac{1}{2} \cdot f(d)\right) + \left(\binom{2d-1}{d-1} + 2 \cdot f(d-1)\right) \\
&= \frac{1}{2} \cdot f(d) + 2 \cdot 4^{d-1},
\end{aligned}$$

implying $f(d) = 4^d$. $\square$

B.4 Lattice points on a circle

In Section 5.5 we made reference to a result concerning the number of lattice points on a circle:

Theorem B.6 *A circle centered on a lattice point passes through at most $n^{C/\log\log n}$ points of the $n \times n$ lattice, where C is a universal constant.*

For every $\epsilon > 0$, this number is $o(n^\epsilon)$.

There are two elements to the proof. The first is the relation between the divisor function $d(n)$ and the number of ways to write n as the sum of two squares. Every expression of n in the form $x^2 + y^2$ induces a factorization of n into two Gaussian integers; for instance,

$$13 = 3^2 + (-2)^2$$

corresponds to the factorization

$$13 = (3 - 2i)(3 + 2i).$$

A number whose prime factorization over the real integers is $p_1^{a_1} \cdots p_k^{a_k}$ will have at most $8(a_1 + 1)(a_2 + 1) \cdots (a_k + 1) = 8d(n)$ factorizations into two Gaussian integers. (To see where the 8 comes from, notice that we can also write 13 as $[U(3-2i)](3+2i)$ or $[U(3 + 2i)](3 - 2i)$ where $U \in \{1, i, -1, -i\}$.) The number of ways to write n as the sum of two squares is thus $\leq 8d(n)$. Naturally, we have glossed over the finer points in this argument; a good treatment of the Gaussian integers and their unique factorization can be found in [35, Chapter 1].

The second element is the bound on $d(n)$. Wigert [57] showed that $d(n)$ obeys

$$d(n) < n^{C/\log \log n}$$

for $n \geq 3$. We are going to provide a new (as far as we know) proof of this theorem. Surprisingly little of it has to do with number theory — the bulk of the proof is algebraic in nature. To simplify things, we will use ln to denote the natural logarithm and log to denote the logarithm to the base $2^{1/3}$ (we will explain later this odd choice of base).

If n has the prime factorization $p_1^{a_1} \cdots p_k^{a_k}$, with $p_1 < p_2 < \ldots < p_k$ and all $a_i \geq 1$, then $d(n) = (a_1 + 1) \cdots (a_k + 1)$. We prove here that for $n \geq 3$ and for some constant c,

$$d(n) < n^{c/\ln \ln n}.$$

This result was first proved by Wigert around 1907; Wigert also found that the optimal value for c approaches $\ln 2$ as $n \to \infty$. Our proof does not determine c.

Some preliminaries:

Lemma B.7 *For integer $k \geq 1$ and for some constant C, the function $f(k) = k \ln\ln(k+1) - \sum_{i=1}^{k} \ln\ln(i+1)$ obeys $f(k) < Ck$.*

Proof: We show that for all k greater than some k_0, we have $f(k+1)-f(k) < 1$. This will show f to obey $f(k) < k+D$ for some D; we then choose C so that $Ck > k+D$.

$$\begin{aligned} f(k+1)-f(k) &= (k+1)\ln\ln(k+2) - \sum_{i=1}^{k+1} \ln\ln(i+1) \\ &\quad -k\ln\ln(k+1) + \sum_{i=1}^{k} \ln\ln(i+1) \\ &= k(\ln\ln(k+2) - \ln\ln(k+1)). \end{aligned}$$

Recall $\frac{d}{dx}\ln\ln x = \frac{1}{x\ln x}$. By l'Hôpital's rule, the limit as $k \to \infty$ is

$$\begin{aligned} & \lim_{k\to\infty} \frac{\ln\ln(k+2) - \ln\ln(k+1)}{1/k} \\ = & \lim_{k\to\infty} \frac{\frac{1}{(k+2)\ln(k+2)} - \frac{1}{(k+1)\ln(k+1)}}{-1/k^2} \\ = & \lim_{k\to\infty} k^2 \cdot \frac{(k+2)\ln(k+2) - (k+1)\ln(k+1)}{(k+1)(k+2)\ln(k+1)\ln(k+2)} \\ = & \lim_{k\to\infty} k^2 \cdot \frac{\ln(k+2) - (k+1)\ln\left(\frac{k+2}{k+1}\right)}{(k+1)(k+2)\ln(k+1)\ln(k+2)} \\ = & \lim_{k\to\infty} \frac{k^2\ln(k+2)}{(k+1)(k+2)\ln(k+1)\ln(k+2)} - \lim_{k\to\infty} \frac{k^2(k+1)\ln\left(\frac{k+2}{k+1}\right)}{(k+1)(k+2)\ln(k+1)\ln(k+2)} \\ = & \ 0 - \lim_{k\to\infty} \frac{k^2\ln\left(1+\frac{1}{k+1}\right)}{(k+2)\ln(k+1)\ln(k+2)}. \end{aligned}$$

Examination of the Taylor series for $\ln(1+x)$ gives us $0 < \ln(1+x) < x$ for $0 < |x| < 1$. Therefore $k^2\ln\left(1+\frac{1}{k+1}\right)$ is between 0 and $\frac{k^2}{k+1}$. Since $\lim_{k\to\infty} \frac{0}{(k+2)\ln(k+1)\ln(k+2)}$ and $\lim_{k\to\infty} \frac{k^2/(k+1)}{(k+2)\ln(k+1)\ln(k+2)}$ are both 0, we have $\lim_{k\to\infty} \frac{k^2\ln\left(1+\frac{1}{k+1}\right)}{(k+2)\ln(k+1)\ln(k+2)} = 0$. Thus $f(k+1)-f(k) \to 0$. For some k_0, then, $k > k_0$ implies $f(k+1)-f(k) < 1$. $\square$

We will also use the well-known arithmetic mean-geometric mean inequality:

Lemma B.8 (AM-GM inequality) *For $x_1, x_2, \ldots, x_n > 0$,*

$$\frac{x_1 + x_2 + \ldots + x_n}{n} \geq \sqrt[n]{x_1 x_2 \cdots x_n},$$

with equality if and only if $x_1 = x_2 = \ldots = x_n$.

For completeness, we present a proof of this inequality in the following section.

Now, the main proof. We prove first that $d(n) < n^{c/\log\log n}$, where $\log x$ denotes the logarithm to the base $2^{1/3}$. Solving for c, we find that this statement is equivalent to

$$(\log_n d(n)) \cdot \log\log n < c;$$

let us evaluate the left-hand side. Since $n = p_1^{a_1} \cdots p_k^{a_k}$, we have $\log n = a_1 \log p_1 + \ldots + a_k \log p_k$. Also, $\log_n d(n) = \frac{\log d(n)}{\log n} = \frac{\log(a_1+1)+\ldots+\log(a_k+1)}{a_1 \log p_1 + \ldots + a_k \log p_k}$. The left-hand side therefore evaluates to

$$(\log(a_1+1) + \ldots + \log(a_k+1)) \cdot \frac{\log(a_1 \log p_1 + \ldots + a_k \log p_k)}{a_1 \log p_1 + \ldots + a_k \log p_k}.$$

The function $\frac{\log x}{x}$ has its maximum at $x = e$ and goes to zero, so that $3 \leq x \leq y$ implies $\frac{\log x}{x} \geq \frac{\log y}{y}$. Thus

$$(\log(a_1+1) + \ldots + \log(a_k+1)) \cdot \frac{\log(a_1 \log p_1 + \ldots + a_k \log p_k)}{a_1 \log p_1 + \ldots + a_k \log p_k}$$

$$\leq (\log(a_1+1) + \ldots + \log(a_k+1)) \cdot \frac{\log(a_1 \log 2 + \ldots + a_k \log(k+1))}{a_1 \log 2 + \ldots + a_k \log(k+1)} \equiv f(a_1, \ldots, a_k),$$

since replacing p_i with $i+1$ can only lower the value of the denominator, but the denominator remains at least 3. We proceed to bound $f(a_1, \ldots, a_k)$.

Let us write

$$f(a_1, \ldots, a_k) \equiv g(a_1, \ldots, a_k) \cdot \frac{\log(h(a_1, \ldots, a_k))}{h(a_1, \ldots, a_k)}.$$

Let $v = h(a_1, \ldots, a_k)$; note $v \geq \log(k+1)!$. We now consider the problem of maximizing $g(b_1, \ldots, b_k)$ subject to the constraint $h(b_1, \ldots, b_k) = v$ and $b_i > -1$; clearly, for the optimal b_i's, the value $f(b_1, \ldots, b_k)$ will be an upper bound on $f(a_1, \ldots, a_k)$. We rewrite the constraint $b_1 \log 2 + \ldots + b_k \log(k+1) = v$ as

$$(b_1 + 1) \log 2 + \ldots + (b_k + 1) \log(k+1) = v + \log(k+1)!$$

and replace the objective function $(b_1 + 1) \cdots (b_k + 1)$ with an equivalent objective $((b_1+1)\log 2) \cdots ((b_k+1)\log(k+1)))$. If we write $x_i = (b_i+1)\log(i+1)$, we can see that we are maximizing the geometric mean $\sqrt[k]{x_1 \cdots x_n}$ subject to a constraint on the arithmetic mean, where the x_i's are taken from the positive reals; by Lemma B.8, the geometric mean is maximized (and is in fact equal to the arithmetic mean) when the x_i's are made equal. Therefore g is maximized when $x_1 = x_2 = \ldots = x_k = \frac{v+\log(k+1)!}{k}$, giving

$$b_i = \frac{v + \log(k+1)!}{k \log(i+1)}.$$

We have $h(b_1, \ldots, b_k) = v$ and $g(b_1, \ldots, b_n) = k \log \frac{v+\log(k+1)!}{k} - \sum_{i=1}^{k} \log\log(i+1)$. Substituting $v = y \cdot \log(k+1)!$, and using the facts $\frac{1}{2} k \log(k+1) \leq \log(k+1)! \leq$

$k \log(k+1)$ and $y \geq 1$, we obtain

$$
\begin{aligned}
f(b_1, \ldots, b_k) &= \left(k \log \frac{(y+1)\log(k+1)!}{k} - \sum_{i=1}^{k} \log\log(i+1)\right) \cdot \frac{\log y + \log\log(k+1)!}{y \log(k+1)!} \\
&\leq (k \log((y+1)\log(k+1)) - \sum_{i=1}^{k} \log\log(i+1)) \cdot \frac{\log y + \log k + \log\log(k+1)}{\frac{1}{2} yk \log(k+1)} \\
&= 2\left(\log(y+1) + \log\log(k+1) - \frac{1}{k}\sum_{i=1}^{k} \log\log(i+1)\right) \\
&\quad \times \frac{\log y + \log k + \log\log(k+1)}{y \log(k+1)} \\
&= 2\Bigg(\frac{\log(y+1)\log y}{y\log(k+1)} + \frac{\log(y+1)\log k}{y \log(k+1)} + \frac{\log(y+1)\log\log(k+1)}{y\log(k+1)} \\
&\quad + (\log\log(k+1) - \frac{1}{k}\sum_{i=1}^{k} \log\log(i+1)) \cdot \frac{\log y + \log k + \log\log(k+1)}{y\log(k+1)}\Bigg).
\end{aligned}
$$

It is easily seen that $\frac{\log(y+1)\log y}{y\log(k+1)}$, $\frac{\log(y+1)\log k}{y\log(k+1)}$, $\frac{\log(y+1)\log\log(k+1)}{y\log(k+1)}$, and $\frac{\log y + \log k + \log\log(k+1)}{y\log(k+1)}$ are bounded by constants (independent of k and y) for $y \geq 1$. A constant bound on the value of $(\log\log(k+1) - \frac{1}{k}\sum_{i=1}^{k} \log\log(i+1))$ would prove the entire expression to be bounded. It is equivalent to bound instead $(\ln\ln(k+1) - \frac{1}{k}\sum_{i=1}^{k} \ln\ln(i+1))$, since

$$
\begin{aligned}
\log\log(k+1) - \frac{1}{k}\sum_{i=1}^{k} \log\log(i+1) &= \log\left(\frac{\ln(k+1)}{\ln 2^{1/3}}\right) - \frac{1}{k}\sum_{i=1}^{k} \log\left(\frac{\ln(i+1)}{\ln 2^{1/3}}\right) \\
&= \log\ln(k+1) - \log\ln 2^{1/3} \\
&\quad - \frac{1}{k}\sum_{i=1}^{k} \log\ln(i+1) + \log\ln 2^{1/3} \\
&= \frac{\ln\ln(k+1) - \frac{1}{k}\sum_{i=1}^{k}\ln\ln(i+1)}{\ln 2^{1/3}}.
\end{aligned}
$$

Lemma B.7 shows that the numerator is bounded.

Finally we show that for sufficiently large n, we have $n^{c/\log\log n} \leq n^{c/\ln\ln n}$. We need to show that $\ln\ln n \leq \log\log n$:

$$\begin{aligned}
\log\log n &= \log\left(\frac{\ln n}{\ln 2^{1/3}}\right) \\
&= \log\ln n - \log\ln 2^{1/3} \\
&= \frac{\ln\ln n}{\ln 2^{1/3}} - \log\left(\frac{1}{3}\ln 2\right) \\
&= \frac{3}{\ln 2}\cdot\ln\ln n - \log\left(\frac{1}{3}\ln 2\right),
\end{aligned}$$

which is $\geq \ln\ln n$ for n larger than some N_0. To make the statement of the theorem hold for the integers from 3 to N_0, we can increase c to a large enough value.

The proof of Theorem B.6 is now complete. $\square$

B.5 Proof of the AM-GM inequality

By induction, we assume that the inequality has been shown for n. We now prove it for $n+1$. For $y > 0$, define

$$f(y) = \frac{x_1 + x_2 + \ldots + x_n + y}{n+1} - (x_1 x_2 \cdots x_n \cdot y)^{1/(n+1)}.$$

Our ultimate goal is to show $f(x_{n+1}) \geq 0$.

Let y^* be the location of the critical point of f. We set the derivative to zero and solve:

$$
\begin{aligned}
0 &= f'(y) \\
&= \frac{1}{n+1} - \frac{1}{n+1} \cdot y^{-n/(n+1)} \cdot (x_1 x_2 \ldots x_n)^{1/(n+1)} \\
&\Downarrow \\
1 &= y^{-n/(n+1)} \cdot (x_1 x_2 \ldots x_n)^{1/(n+1)} \\
&\Downarrow \\
1 &= y^{-n} \cdot (x_1 x_2 \ldots x_n)^{1} \\
&\Downarrow \\
y &= (x_1 x_2 \ldots x_n)^{1/n}.
\end{aligned}
$$

Thus $y^* = (x_1 x_2 \ldots x_n)^{1/n}$, the geometric mean of $\{x_1, \ldots, x_n\}$, is the only critical point of f. Since $f''(y) = \frac{(x_1 x_2 \ldots x_n)^{1/(n+1)}}{n+1} \cdot \frac{n}{n+1} \cdot y^{-n/(n+1)-1}$ is always positive, f has its unique minimum at y^*.

What is the *value* of this minimum? Let us see.

$$
\begin{aligned}
f(x_{n+1}) \geq f(y^*) &= \frac{x_1 + x_2 + \ldots + x_n + (x_1 x_2 \cdots x_n)^{1/n}}{n+1} - \\
&\quad (x_1 x_2 \cdots x_n \cdot (x_1 x_2 \ldots x_n)^{1/n})^{1/(n+1)} \\
&= \frac{x_1 + x_2 + \ldots + x_n}{n+1} + \frac{(x_1 x_2 \cdots x_n)^{1/n}}{n+1} - ((x_1 x_2 \cdots x_n)^{(n+1)/n})^{1/(n+1)} \\
&= \frac{x_1 + x_2 + \ldots + x_n}{n+1} + \frac{(x_1 x_2 \cdots x_n)^{1/n}}{n+1} - (x_1 x_2 \cdots x_n)^{1/n} \\
&= \frac{x_1 + x_2 + \ldots + x_n}{n+1} - ((x_1 x_2 \cdots x_n)^{1/n}) \cdot \frac{n}{n+1} \\
&= \frac{n}{n+1} \cdot \left(\frac{x_1 + x_2 + \ldots + x_n}{n} - (x_1 x_2 \cdots x_n)^{1/n} \right).
\end{aligned}
$$

By the inductive hypothesis, the expression inside the parentheses is ≥ 0. Thus the inequality is proved. To prove the statement about equality, note that for $f(x_{n+1}) = 0$ to hold, we need

$$f(x_{n+1}) = f(y^*)$$

and

$$\frac{x_1 + x_2 + \ldots + x_n}{n} - (x_1 x_2 \cdots x_n)^{1/n} = 0.$$

By the inductive hypothesis, the latter holds if and only if $x_1 = x_2 = \ldots = x_n$. Then the former holds if and only if $x_{n+1} = y^* = (x_1 x_2 \cdots x_n)^{1/n} = x_1$. $\square$

Appendix C. Variations on Caro-Wei

This material is still in rough form. I had these ideas in mid-March 2012, long after the previous chapters were written. My goals (what I hope to prove) are given in the conclusion.

C.1 Introduction

Caro [13] and Wei [56] found the following lower bound on the independence number of a graph G.

Theorem C.1 (Caro-Wei [13, 56]) *Let G be a graph on n vertices whose respective degrees are $d_1, d_2, \ldots, d_n$. Then*

$$\alpha(G) \geq \sum_{i=1}^{n} \frac{1}{d_i + 1}.$$

Proof: (after [6]) Let σ be a (uniformly) random permutation on $V(G)$. We insert a vertex v_i into the set if and only if v_i precedes all of its neighbors in the ordering determined by σ. Clearly, the probability that v_i does so is $1/(1+d_i)$. Then the expected number of vertices put into the independent set is given by the above formula. □

Selkow [43] came up with a stronger formula using the degrees of v_i and the degrees of v_i's neighbors. Let us write $N_G(v)$ to denote the neighborhood of v in G.

Theorem C.2 (Selkow [43]) *Let G be a graph on n vertices whose respective degrees are $d_1, d_2, \ldots, d_n$. Then*

$$\alpha(G) \geq \sum_{i=1}^{n} \left(\frac{1}{d_i + 1}\right) \left(1 + \left(\frac{d_i}{d_i + 1} \,\Delta \sum_{v_j \in N_G(v_i)} \frac{1}{d_j + 1}\right)\right),$$

where Δ *is the proper subtraction operator:*

$$a \; \Delta \; b = \max(a - b, 0).$$

Let's look again at Theorem C.1, supposing now that we also know the neighbor degrees for each vertex. Our observation here is that the permutation σ does not have to be constructed with uniform probabilities. We can instead assign probabilities $p_1, p_2, \ldots, p_n$ to each vertex. Every time we choose a new vertex for the set, the vertex v_i is chosen with probability proportional to p_i.

Example: suppose we have three vertices v_1, v_2, v_3, and we use $p_1 = 4/7, p_2 = 2/7, p_3 = 1/7$. Then our first vertex is p_1 with probability $4/7$; v_2 with probability $2/7$; and v_3 with probability $1/7$. Suppose our first chosen vertex is v_2; this leaves v_1 and v_3 still to be chosen. In the next round, v_1 is chosen with probability $(4/7)/(4/7+1/7) = 4/5$, and v_3 is chosen with probability $(1/7)/(1/7 + 4/7) = 1/5$.

The p_i's can, in fact, be any positive numbers; the division described above will always give numbers in the range $(0, 1)$. Multiplying or dividing every p_i by the same value has no effect on the set generated by the algorithm.

Theorem C.3 *Let* G *be a graph on* n *vertices, and let* $p_1, p_2, \ldots, p_n > 0$*. Then*

$$\alpha(G) \geq \sum_{i=1}^{n} \frac{p_i}{\sum_{v_j \in N_G(v_i)} p_j}.$$

Proof: Follow the proof of Theorem C.1, but form the permutation according to the values of the p_i's. That is, denoting by V' the set of vertices not yet chosen, $v_i \in V'$ is chosen next with probability

$$\frac{p_i}{\sum_{v_j \in V'} p_j}.$$

The probability that v_i is chosen before all its neighbors is

$$\frac{p_i}{\sum_{v_j \in N_G(v_i)} p_j}.$$

$\square$

If we set $p_i = 1$ for all i, we obtain the Caro-Wei bound. Perhaps some different choices for the p_i's will give better results. It makes sense to prefer to choose vertices that have low degrees, while avoiding vertices with high degrees. So let's set $p_i = 1/d_i$ for $d_i > 0$, or 1 for $d_i = 0$. If any vertex has degree 0, we can just put it in the independent set automatically. So we will assume $d_i > 0$. Plugging these values into Theorem C.3, we obtain

Theorem C.4 *Let G be a graph on n vertices whose respective degrees are $d_1, d_2, \ldots, d_n > 0$. Then*

$$\alpha(G) \geq \sum_{i=1}^{n} \frac{1/d_i}{\sum_{v_j \in N_G(v_i)} 1/d_j}.$$

We will say "the expectation for v_i" to refer to the i-th term in this summation.

We can try different settings for the p_i's; the problem is that it is not easy to see which ones are better than others. I am fairly confident that Theorem C.4 always gives a bound better than or equal to Caro-Wei, but I don't have a proof yet. I will therefore demonstrate a quick example. The end of Selkow's paper uses the example of a star tree on $n+1$ nodes (1 central node and n outer nodes). For this graph, Caro-Wei gives a bound of approximately $n/2$, since every node but one has degree 1. Selkow says that his bound gives approximately $3n/4$. What does our bound give? The expectation for the central node is nearly zero. But the expectation for an outer node is $(1/1)/(1/1 + 1/n) = 1 - 1/(n+1)$. Since we have n outer nodes, we have $\alpha(G) \geq n - n/(n+1)$. This is within 1 of the optimal value. In fact, since the independence number is an integer, we must round the value anyway; rounding it up gives n exactly.

Certain graphs give all these formulas problems. Consider a cycle on n vertices. Caro-Wei gives $n/3$. Our formula must give the same, since every degree in the graph is the same. Notice, though, that this bound is attained for a graph consisting of a set of 3-cycles; any improvement to this formula would have to assume something else about the graph (such as assuming that the graph is connected).

C.2 Take the p_i's to the extremes

We can generalize Theorem C.4 further:

Theorem C.5 *Let G be a graph on n vertices whose respective degrees are $d_1, d_2, \ldots, d_n > 0$. Then for any value of k,*

$$\alpha(G) \geq \sum_{i=1}^{n} \frac{1/d_i^k}{\sum_{v_j \in N_G(v_i)} 1/d_j^k}.$$

It appears that the estimate increases as k increases. If this is so, the best estimate of this form is obtained by letting $k \to \infty$. Then the contribution of a vertex v is as follows:

- If v has a lower degree than all of its neighbors, v contributes 1.
- If v has a higher degree than one of its neighbors, v contributes 0.
- Otherwise, v contributes $1/(m+1)$, where m is the number of v's neighbors that have degree equal to v.

Let's look at this graph:

```
A-----B  B-----A
|     | /     /
|     |/     /
B-----C-----B
     / \
    /   \
   B     B
    \   /
     \ /
      A
```

Caro-Wei gives $\alpha \geq 3\frac{1}{7}$. Let's see what Selkow's formula gives. For vertex C, the contribution is still 1/7. Each vertex A still contributes 1/3. The contribution for each vertex B increases slightly to $1/3 \cdot (1 + (2/3 - 1/2 - 1/7)) = 43/126$. The grand total is $3\frac{4}{21}$, which is little improvement over the Caro-Wei estimate.

What if we apply Theorem C.5? Each A contributes 1/3; each B contributes 1/2; and C contributes 0. The total is 4. Quite an improvement! We suspect that Theorem C.5, with $k \to \infty$, is the best possible bound on α given only the vertex degrees and neighbor degrees.

C.3 An iterative algorithm

Since any positive values are permissible for the p_i's, we can try to modify them to increase the bound. For a fixed graph G, let us define functions $f_1, f_2, \ldots, f_n$ on the p_i's. Each f_i takes as input the vector $[p_1, p_2, \ldots, p_n]^T$ and outputs the expectation for v_i, that is, $p_i / \sum_{v_j \in N_G(v_i)} p_j$. Now define a vector-valued function $f : \mathbb{R}^n \to \mathbb{R}^n$ by

$$f(x) = [f_1(x), f_2(x), \ldots, f_n(x)]^T.$$

We call this the *adjacency function*.

We should give an example here. Suppose the graph is a chain of three nodes: v_1—v_2—v_3. Then the adjacency function is

$$f\left(\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}\right) = \begin{bmatrix} x_1/(x_1+x_2) \\ x_2/(x_1+x_2+x_3) \\ x_3/(x_2+x_3) \end{bmatrix}.$$

Suppose we initially use $x^{(0)} = [1/n, 1/n, \ldots, 1/n]$. Apply f to $x^{(0)}$ to obtain $x^{(1)}$. Continue this process, obtaining a sequence $x^{(0)}, x^{(1)}, \ldots, x^{(k)}, \ldots$. Each vector is the result of applying Theorem C.3 to the p-values given by the previous vector; the sum of any of these vectors, then, is a lower bound on the independence number of G. In fact, we use the expectations from one algorithm as the probabilities for the next algorithm.

Eventually the sequence reaches an equilibrium. Typically the equilibrium will have every element 0 or 1; in this case, the independent set is evident. We run into a problem with certain graphs, though, such as the cycle on n vertices. Here, we will have $x^{(1)} = [1/3, 1/3, \ldots, 1/3]$, and it remains the same on every subsequent step. This is an unstable equilibrium; the problem is that an optimal independent set must favor some set of vertices over the other, but the probabilities are equal to start with. To eliminate this situation, we can apply a small perturbation to every $x^{(k)}$ before applying f in the next step. (In fact, this perturbation may not be necessary in an implementation; I noticed that floating-point error seems to have the same effect. Also, we may only need the perturbation on the first step in the algorithm, not at every step.)

We see a stable equilibrium when we run the algorithm on a complete graph K_n. Here, the sequence of vectors remains the same, except for the perturbations involved.

This seems to be saying that the relative ordering of these vertices does not matter, since we can only choose one of them anyway.

I suspect that without perturbations, $\sum_i x_i^{(k+1)} \geq \sum_i x_i^{(k)}$ for all k. If so, then this algorithm is guaranteed to give a larger bound than Caro-Wei, since $\sum_i x_i^{(1)}$ is equal to the Caro-Wei bound.

We have a curious situation here that adding edges to the graph can, in fact, help the algorithm out! Suppose again that we have a complete cycle on n vertices, this time with n even. If we do not use perturbations, it remains stuck at a suboptimal solution. If we add an edge between two opposite vertices, then their probabilities will be lower. This drives up the probabilities of their neighbors, then *their* neighbors decrease in probability, and so on. We approach a state $[0, 1, 0, 1, \ldots]$ or $[1, 0, 1, 0, \ldots]$.

The perturbations also give us a convenient stopping point. If we ever have $\sum_i x_i^{(k+1)} < \sum_i x_i^{(k)}$, it must be because the perturbations pushed the sum down. As long as there is still an improvement to be made, the perturbations cannot have such a strong effect; therefore, we can interpret a decrease as a hint that there is no gain to be had from continuing on.

C.4 Comparison to greedy algorithms

Let us call the algorithm from the above section Algorithm I. There are two well-known greedy algorithms for building independent sets:

— Algorithm II: Find a vertex of highest degree in the graph and remove it. Repeat until every vertex has degree zero; the remainder is the independent set.

— Algorithm III: Take a vertex v of lowest degree, put it into the independent set, then remove v and its neighbors from the graph.

Algorithm II is a derandomization of Caro-Wei; Algorithm III is not, but often gives good results. Our goal in this section is to show that Algorithm I outperforms these two algorithms in certain cases. Let us first look at Algorithm II. We consider a cycle C_{3n} on $3n$ vertices, ordered on the cycle as $v_1, v_2, \ldots, v_{3n}$. One possible course of Algorithm II is that it chooses to remove $v_1, v_4, v_7, \ldots, v_{3n-2}$. The remaining graph only has n independent vertices. This is a poor result, since there is an independent set of size $\lfloor 3n/2 \rfloor$. Algorithm I will find such a set. Suppose we apply an initial perturbation of ϵ to v_1. Now v_1 has initial probability $1/3n + \epsilon$, while the other vertices have initial probability $1/3n$. One iteration will increase the value for v_1 and drive down the values of its neighbors. The effect ripples out, causing an alternating of values, high-low-high-low-etc. Eventually the values will converge to alternating zeroes and ones. This is demonstrated below for a cycle on 9 vertices.

v_1	v_2	v_3	v_4	v_5	v_6	v_7	v_8	v_9
1.010	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.336	0.332	0.333	0.333	0.333	0.333	0.333	0.333	0.332
0.336	0.332	0.334	0.333	0.333	0.333	0.333	0.334	0.332
0.336	0.331	0.334	0.333	0.333	0.333	0.333	0.334	0.331
0.336	0.331	0.334	0.333	0.333	0.333	0.333	0.334	0.331
0.337	0.330	0.335	0.333	0.333	0.333	0.333	0.335	0.330
0.338	0.330	0.336	0.332	0.334	0.334	0.332	0.336	0.330
0.339	0.329	0.336	0.332	0.334	0.334	0.332	0.336	0.329
0.340	0.328	0.337	0.331	0.334	0.334	0.331	0.337	0.328
0.342	0.326	0.339	0.330	0.334	0.334	0.330	0.339	0.326
0.344	0.324	0.340	0.329	0.335	0.335	0.329	0.340	0.324
0.347	0.321	0.343	0.328	0.335	0.335	0.328	0.343	0.321
0.350	0.318	0.345	0.326	0.336	0.336	0.326	0.345	0.318
0.355	0.314	0.349	0.324	0.337	0.337	0.324	0.349	0.314
0.362	0.308	0.354	0.321	0.338	0.338	0.321	0.354	0.308
0.370	0.301	0.360	0.317	0.339	0.339	0.317	0.360	0.301
0.380	0.292	0.368	0.312	0.341	0.341	0.312	0.368	0.292
0.395	0.281	0.379	0.305	0.343	0.343	0.305	0.379	0.281
0.413	0.266	0.393	0.297	0.346	0.346	0.297	0.393	0.266
0.437	0.248	0.411	0.287	0.350	0.350	0.287	0.411	0.248
0.468	0.227	0.434	0.274	0.355	0.355	0.274	0.434	0.227
0.508	0.201	0.464	0.258	0.361	0.361	0.258	0.464	0.201
0.558	0.171	0.503	0.238	0.368	0.368	0.238	0.503	0.171
0.620	0.139	0.551	0.215	0.378	0.378	0.215	0.551	0.139
0.690	0.106	0.609	0.188	0.389	0.389	0.188	0.609	0.106
0.765	0.075	0.675	0.158	0.403	0.403	0.158	0.675	0.075
0.835	0.050	0.743	0.128	0.418	0.418	0.128	0.743	0.050
0.893	0.031	0.807	0.099	0.434	0.434	0.099	0.807	0.031
0.936	0.018	0.861	0.074	0.449	0.449	0.074	0.861	0.018
0.964	0.010	0.904	0.054	0.462	0.462	0.054	0.904	0.010

It is approaching [1, 0, 1, 0, 0.5, 0.5, 0, 1, 0]. The values 0.5 mean that either v_5 or v_6 can be added to the independent set.

Another example is the following graph:

```
A--B--C--B--A
    |
    |
    B
    |
    |
    A
```

Algorithm II removes vertex C at the first iteration. The remaining graph has only 3 independent vertices. Algorithm I without perturbations generates the following values:

A	B	C
1.000	1.000	1.000
0.500	0.333	0.250
0.600	0.308	0.200
0.661	0.278	0.178
0.704	0.249	0.176
0.739	0.220	0.191
0.770	0.192	0.224
0.801	0.162	0.281
0.832	0.130	0.367
0.865	0.098	0.485
0.898	0.068	0.623
0.930	0.043	0.755
0.956	0.025	0.855
0.975	0.013	0.921
0.986	0.007	0.958

We see that the value for C decreases initially, but it rebounds and eventually approaches 1.

To evaluate Algorithm III, let us look at our original graph again:

```
A-----B  B-----A
|     | /     /
|     |/     /
B-----C-----B
     / \
    /   \
   B     B
    \   /
     \ /
      A
```

Here, every vertex except the central one has degree 2. Algorithm III may therefore choose all the A vertices, eliminating the B vertices. Then vertex C can be chosen, giving an independent set of size 4.

When we run Algorithm I without perturbations on this graph, we obtain the following values:

A	B	C
1.000	1.000	1.000
0.333	0.333	0.143
0.333	0.412	0.067
0.288	0.507	0.026
0.221	0.617	0.009
0.152	0.729	0.002
0.094	0.825	0.001

Clearly it favors the B vertices, giving an independent set of size 6. We can extend this example to n loops; Algorithm I will give $2n$ independent vertices, but Algorithm III may give only $n + 1$.

C.5 Conclusion

I want to prove the following statements, or at least one of them:

Conjecture C.6 *For a given graph G, the quantity in Theorem C.5 increases as k increases.*

Conjecture C.7 *Each iteration of Algorithm I increases the value of $\sum_i x_i$.*

The first conjecture implies that the bound in Theorem C.5 is always an improvement on Caro-Wei. When we have $k = 0$, the bound is equal to the Caro-Wei bound. When we have $k = 1$, the bound is the same as that in Theorem C.4. Thus the bound for $k \to \infty$ would be an improvement on both.

The second conjecture is necessary to show that Algorithm I is actually a good way to generate independent sets. It makes sense, but there does not seem to be an easy proof (either probabilistic or algebraic).

Vita

Thomas A. Plick was born in Philadelphia, Pennsylvania in 1984. As an undergraduate student, he dual-majored in mathematics and computer science, receiving his bachelor's degree from La Salle University (in Philadelphia) in 2006. He began his studies at Drexel University in 2006, earning his master's degree in computer science in 2009. He earned his Ph.D. from Drexel in 2012.

While at Drexel, he served as a teaching assistant for the graduate and undergraduate algorithms classes from 2007 until 2012. He won the Department of Computer Science's Outstanding Teaching Assistant Award in 2012.

His first paper, "A note on the Caro-Tuza bound on the independence number of uniform hypergraphs" [16], was published in February 2012. Another paper, "Optimal random matchings, tours, and spanning trees in hierarchically separated trees" [17], was submitted for publication in the spring of 2012.