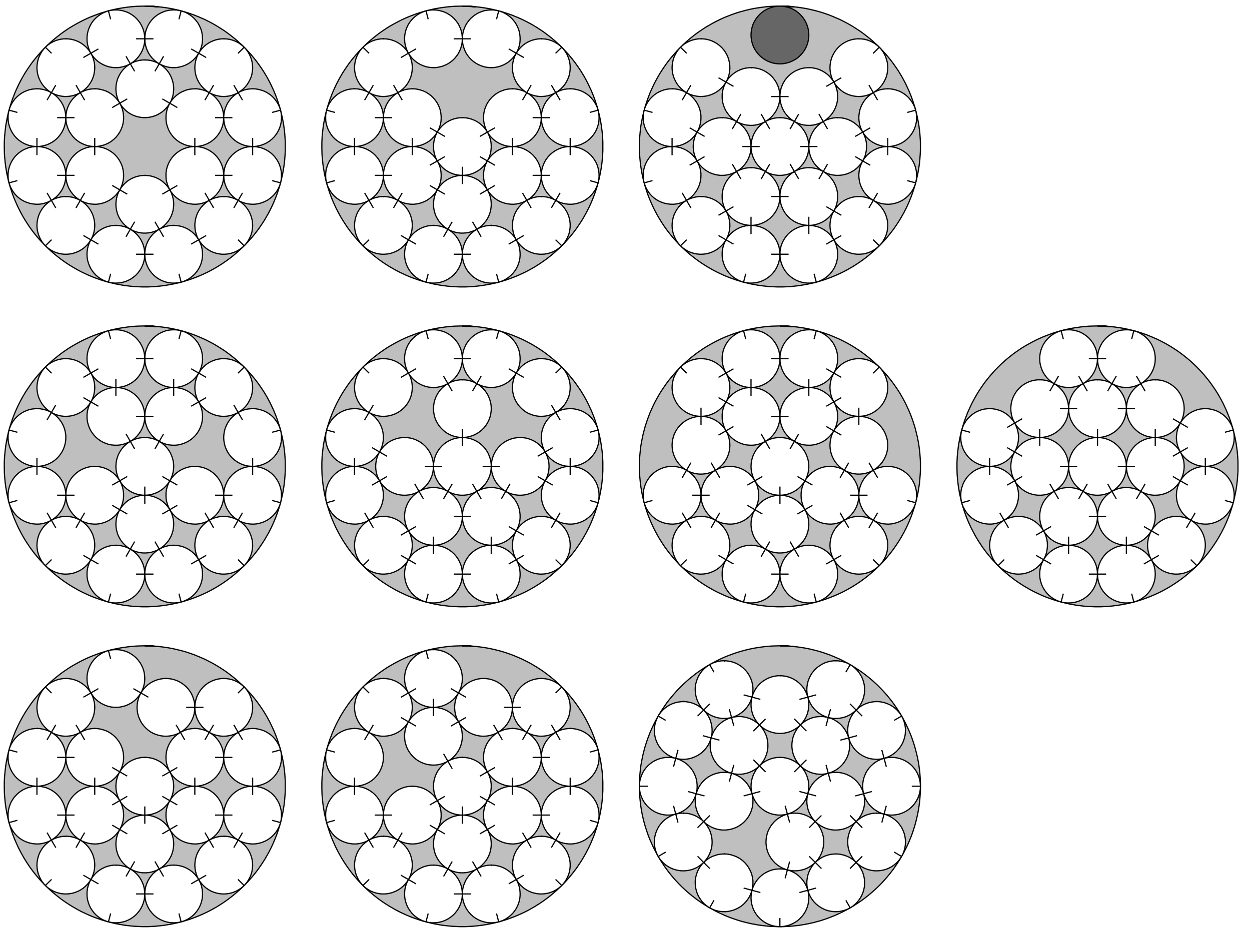
Stochastic Optimization Methods in Sphere Packing and Covering Problems in Discrete Geometry and Coding Theory

Kari J. Nurmela



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Dissertation for the degree of Doctor of Technology to be presented with due permission for public examination and debate in Auditorium N at Helsinki University of Technology (Espoo, Finland) on the 12th of December, 1997, at 12 o'clock noon.

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ISBN 952-90-9460-4 (with Appendix)
ISBN 952-90-9461-2 (without Appendix)

printed by Picaset Oy, November 1997

Cover: The picture shows the best currently known packings of 18 equal circles in a circle. All ten packings have equal density, and it is conjectured that exactly these packings are all the optimal packings of 18 circles.

Contents

Preface

This thesis is a result of the work carried out at the Digital Systems Laboratory of Helsinki University of Technology during 1992–1997. I am very grateful to the head of the laboratory, Prof. Leo Ojala, for making this work possible.

My special thanks go to my thesis instructor, Dr. Patric Östergård, without whom this work would never have been realized. He has co-authored several papers of this thesis and he has continuously given immeasurably valuable comments and guidance throughout my work.

It was a true pleasure to co-author one of the papers in this thesis with Prof. Ronald Graham and Dr. Boris Lubachevsky. I thank Emil Aaltonen Foundation, Tekniikan edistämissäätiö (the Foundation of Technology), Vilho, Yrjö, and Kalle Väisälä Foundation, and Helsinki Graduate School in Computer Science and Engineering (HeCSE) for their financial support during this work.

Espoo, November 1997

Kari J. Nurmela

List of Publications

This thesis consists of a summary and the following publications:

[P1] K. J. Nurmela and P. R. J. Östergård, Upper bounds for covering designs by simulated annealing, *Congressus Numerantium* **96** (1993), 93–111.

[P2] K. J. Nurmela, Minimum-energy point charge configurations on a circular disk, Research Report **A43**, Digital Systems Laboratory, Helsinki University of Technology.

[P3] K. J. Nurmela and P. R. J. Östergård, Packing up to 50 equal circles in a square, *Discrete & Computational Geometry* **18** (1997), 111–120.

[P4] R. L. Graham, B. D. Lubachevsky, K. J. Nurmela, and P. R. J. Östergård, Dense packings of congruent circles in a circle, *Discrete Mathematics*, to appear.

[P5] K. J. Nurmela, M. K. Kaikkonen, and P. R. J. Östergård, New constant weight codes from linear permutation groups, *IEEE Transactions on Information Theory* **43** (1997), 1623–1630.

Paper [P2] was written without co-authors. The other papers were written partly by the author; in [P5] Nurmela is the main author.

The computer programs which yielded the results in the papers [P1], [P3], [P5] were written (and mainly designed) by the author, some of the programs in [P5] by M. K. Kaikkonen. In paper [P4] the repulsion-force approach as well as the numerical solving of the systems of equations and the rigidity check of the packings were designed and programmed by the author.

1 Introduction

In 1611 Johannes Kepler claimed that no arrangement of spheres of equal radius in 3-space has density greater than that of the face-centered cubic lattice. This claim is known as the Kepler conjecture [29] and it is generally regarded still as unsettled, although numerous attempts of proof have been made (see, e.g. [30] and the discussion in [29]). The Kepler conjecture is an example of a *sphere packing* problem which for centuries has resisted mathematicians' attempts of finding a proof.

In two dimensions the densest packing of circles is known; it is the hexagonal lattice in the plane. However, when the area in the plane is finite, the densest packings are known only in special cases. The problem of packing circles into different geometrical shapes has received much attention since the seminal work of Fejes Tóth [21]. Much work has been done on packing circles on the surface of a sphere, in a square, in a circle, and even in an equilateral triangle. Results and references to earlier work can be found in [16, 27, 28, 50, 54], [P3], and [P4].

The space where we pack spheres does not have to be Euclidean, or even continuous. If we take the points in an n-dimensional Hamming space, an important problem is to find as many points as possible in that space that have mutual Hamming distance at least d. The resulting collection of points is an error-correcting code, which is able to correct up to $\lfloor (d-1)/2 \rfloor = e_{\max}$ errors. Error-correcting codes are essentially points in a Hamming space spread so that the spheres of radius $e_{\max}$ around the points have no overlap. The class of error-correcting codes that is investigated in this thesis is that of constant weight codes, where each word has equal weight.

The dual of the packing problem is the covering problem. Whichever problem we consider, we have a set of points and a collection of objects which cover some of the points. Now we are interested in finding the maximum number of objects such that no point is covered more than once (densest packing), or the minimum number of objects such that each point is covered at least once (thinnest covering).

Not surprisingly, also covering of various geometrical shapes has received attention in discrete geometry [42, 45, 72–74, 82]. Coding theoretical examples are covering codes [14], where each point of a Hamming space is included in at least one of the spheres. In this thesis we consider the covering analogue of constant weight codes, covering designs, where each word of given weight in the Hamming space is covered by at least one block of the design.

In addition to their theoretical significance many of the packing and covering problems have direct every-day practical applications. For example if we want to pack as many equal milk bottles as possible in a given box, or produce stamped parts from a coil of metal so that the amount of scrap is minimized, we are facing geometrical packing problems.

In discussions of applications of covering designs, two fields are generally mentioned. They can be used as lottery systems (see, e.g. [48, 55]) and for error-trapping decoding (see [12]). The size (and price) of the lottery system should be as low as possible and we are searching for the thinnest covering. In the case of error-trapping decoding the number of blocks in the covering design gives the complexity of the decoding procedure; this justifies the importance of finding minimal covering designs.

Error-correcting codes were developed to correct errors in noisy communication channels. When the errors are random and independent, we can use *block codes* where a block of message symbols is encoded into a codeword. If the mutual distance between the codewords is large enough, then we can retrieve the original codeword from the received, slightly distorted codeword by simply looking up the codeword that is closest to the received word. To use the bandwidth of the channel as efficiently as possible a densest packing is needed.

2 Circle Packings in the Plane

Problems of packing congruent circles in different geometrical shapes in the plane were raised in the 1960s, and many results—mainly for small packings—were obtained. Excellent sources of results and open problems are [16, 21]. The development of new, effective optimization algorithms for packing problems and the ever-increasing performance of computing systems have recently brought these problems into focus again; computer-aided methods can now be used to construct good large packings.

In this thesis we have concentrated on two circle packing problems that have received a lot of attention in the past, namely packing circles in a square and in a larger circle. These problems can be geometrically expressed as follows: Determine $r_n^{\square}$ and $r_n^{\bigcirc}$, the maximum radius of n non-overlapping circles in a unit square and unit circle, respectively.

In some cases (for example when packing circles in a regular polygon, in a larger circle in the plane, or on the surface of a sphere) the circle packing problem can be stated as that of spreading *points*, i.e., we try to find a configuration of points in the given region such that the minimum mutual distance between the points is as large as possible. If we denote a point configuration by $S = \{\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_n\}$, then the function to be maximized is

$$d(S) = \min\left\{\|\mathbf{s}_i - \mathbf{s}_j\| : 1 \leq i < j \leq n\right\}. \tag{1}$$

In this thesis we use this formulation of the circle packing problems. When packing n circles in a square or in a circle, we denote the maximum values of (1) by $d_n^{\square}$ and $d_n^{\bigcirc}$, respectively, and have the following relation between $r_n^{\square}$ and $d_n^{\square}$:

$$r_n^{\square} = \frac{d_n^{\square}}{2(d_n^{\square} + 1)}.$$

An analogous relation holds between $r_n^{\bigcirc}$ and $d_n^{\bigcirc}$.

A packing corresponding to $d_n^{\square}$ (or $d_n^{\bigcirc}$) is called an *optimal* packing. Optimality of circle packings in a square and in a circle has been proved only for some small values of n and for some n where the optimal packing has a nice structure (see Sections 2.4 and 2.5 for more detailed results). Even if we for larger values of n are not able to find the exact values of $d_n^{\square}$ and $d_n^{\bigcirc}$, we can still try to find as good packings as possible, thereby lower-bounding $d_n^{\square}$ and $d_n^{\bigcirc}$.

In 1961 Oler proved a theorem [57] that implies the following corollary: if X is a compact convex subset of the Euclidean plane, then the number of points with mutual distance at least 1 is at most

$$\frac{2}{\sqrt{3}}A(X) + \frac{1}{2}P(X) + 1,$$

where $A(X)$ is the area and $P(X)$ is the perimeter of the convex subset. This corollary can be used to obtain asymptotically tight upper bounds on $d_n^{\square}$ and d_n°.

2.1 Repulsion Force Method

Our first packing method [P3], [P4] is closely related to that of [13] and [35]. The difficulty with (1) when trying to apply an efficient local optimization algorithm is that (1) is not smooth, and, furthermore, most of the first derivatives of the function are zero almost everywhere in the feasible region. To overcome these difficulties, we instead of maximizing (1) minimize the objective function

$$E(S) = \sum_{1 \le i < j \le n} \left(\frac{\lambda}{\|\mathbf{s}_i - \mathbf{s}_j\|^2} \right)^m, \tag{2}$$

where λ is a scaling factor to prevent numerical overflows (it is adjusted during the optimization to keep the values of E suitably scaled) and m is a positive integer. Each point is constrained inside the container area, i.e., a unit square or circle. To make the optimization problem unconstrained we use a simple coordinate transformation [P3], [P4].

Equation (2) can be seen as a potential energy function of the point configuration when there are repulsion forces between the points. Different optimization problems are obtained depending on the value of m, which controls the strength of the repulsion forces (see [46]). The optima of (2) approximate those of (1) in the sense that as m tends to infinity, only the shortest distance between the points becomes significant. The energy function (2) is twice continuously differentiable except where two points coincide.

A packing is formed by first finding a local optimum of (2) using a relatively low value of m [P3]. Then the value of m is increased and the optimization step is repeated. If the value of m is not increased too much, the local optima of consecutive approximations (2) are close to each other, so this optimization step is usually relatively fast. Finally, when m is relatively large, a local optimum of (2) is usually close to a local optimum of (1) [P3].

There is a trade-off when selecting the initial value of m: a small m gives faster convergence to the first local optimum but then some good local optima of (1) may be lost.

2.2 Billiards Simulation

In addition to the method described in Section 2.1 we use another packing algorithm in [P4] (see [P4] for a rough comparison of the performance of the algorithms). In this algorithm the hard disks or *billiards* model of computational physics is employed.

Consider a set S of points spread randomly in the unit circle. We draw circles of diameter d around each point in that set so that the circles do not overlap. Now imagine that we relax the configuration S and let the circles, which can also be thought of as hard disks, move and experience elastic collisions between each other and the area boundary. The initial velocities are chosen randomly.

The computer algorithm used in [P4] simulates the movement and collisions of the disks. The computations are implemented in an efficient, event-driven fashion where the algorithm proceeds directly from one collision to another [38].

During the simulation the radius of the disks is slowly increased, and as a result the disks have less and less room to move around. At some point the movement is totally blocked and we have a local maximum of (1).

In some cases we can make the packing algorithms faster by concentrating only on the packings having certain symmetries and thus reducing the number of variables; a simple example of this technique can be found in [50]. However, while most of the smaller (optimal or conjecturally optimal) packings have symmetries, it seems that when the number of circles is increased, the best currently known packings are more and more rarely symmetric.

In this thesis the billiards approach was used only when packing circles in a circle. Packings in a square by this method were searched in [28], and a few packings of [P3] were improved. Some "families" of packings are also listed in [28], but one very natural and important infinite family is missing; it is described in [54], where the optimality of an infinite subset of this family is conjectured.

2.3 Tightening the Packings

Both methods discussed in Sections 2.1 and 2.2 can give the coordinates of the circles in the packing only with finite precision. To become convinced that we have the correct structure of the packing and to get more accurate numerical values for the locations of the circles we construct a system of nonlinear equations corresponding to the contacts between the circles and between the circles and the boundary. That system is then solved numerically to a desired accuracy.

We first sort all the distances between the points into increasing order and find the location where the distance shows sudden increase. The distances up to this location are assumed to be equal, and points very close to the boundary are assumed to be on the boundary. We then form a system of equations from these assumptions, see Figure 1, where each small bar denotes a contact between two circles or between one circle and the area boundary. Often there are more equations than unknowns in the system, especially when the packing is symmetric. In the system of equations directly corresponding to the packing in Figure 1 there are 93 variables and 120 equations.

In some cases the system of equations corresponding to the structure of a packing has been reduced to a polynomial equation—of one variable—that has a zero at the diameter of the circles [17]. Large irregular packings have so complex polynomials that there is little hope of explicitly constructing them. In practice the diameter of the circles of a large packing can be solved in radicals only in special cases.

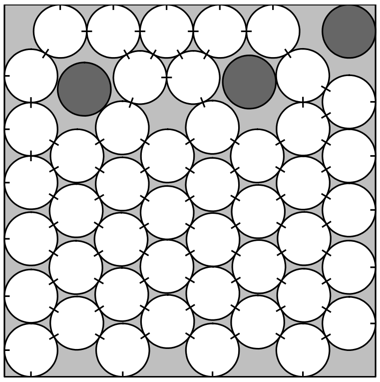

Figure 1: A packing of 49 circles in a square.

Previous research has revealed that there are good circle packings in an equilateral triangle and in a square with very narrow gaps between the circles or between a circle and the boundary [27, 44], [P3]. This is why the equations are solved using a very high computational resolution [P3], [P4].

Finding a numerical solution to the system of equations corresponding to the proposed structure of the packing does not guarantee that the structure exists, because of the finite precision in calculations. By using arbitrary precision arithmetic we can make the probability of non-existence very small, thus we are relatively confident about the existence of a packing whenever we manage to numerically solve the system of equations with a high precision. However, the solution might exist and yet, the packing might not be *rigid*; that is, there might exist a continuous movement of a subset of circles (different from the rotation of the entire assembly when the containing area is a circle), such that no circles overlap or penetrate the boundary.

Numerical evidence for the rigidity of the packings in a circle in [P4] was obtained as follows. We solved the system of equations several times with different initial solutions which were obtained by rotating and slightly perturbing the solution obtained from one of the packing algorithms. Each time the algorithm converged to the same solution (up to a rotation) with a very high precision. If the packing were not rigid, infinitely many different solutions would have existed in some neighborhood of the first solution, and it would be highly improbable that the algorithm would converge every time to the same solution (within the very high computational resolution that was used).

2.4 Circle Packings in a Square

For up to 9 circles, the problem of packing circles in a square was solved in the 1960s by Graham, Meir, and Schaer; the proofs of these cases have been reported in [41, 65, 67, 70]. The proofs for $n \leq 5$ are easy, whereas the cases $n = 6, 8, 9$ require more elaborate mathematical tools. In [65] it is mentioned that the packing of 7 circles has been proven optimal, but the proof has never been published. A computational proof for $n = 7$ can be found in [52].

For $n \geq 10$, only the optimal packings of 14, 16, 25, and 36 circles have been proved by hand (see [79], [78], [80], and [32], respectively); some of those proofs are disputable.

The best currently known packing in Figure 1 for $n = 49$ found in [P3] concludes the proof that for $n = k^2$, the square lattice packings are optimal exactly for $n \leq 36$. This disproves a conjecture of Wengerodt (who found denser packings for $n \geq 64$) that the square lattice packings are optimal for $n \leq 49$; see [16] and its references. An open question stated in [16] is whether there are any values of n such that $d_n = d_{n+1}$. In view of the results in [P3] we conjecture that there are no such n.

Recently, de Groot *et al.* [18] used computers to find good packings for $n \leq 22$. They were later even able to give a computer proof of optimality for the best packings with up to 20 circles [17,58]. In particular, this ended a series of articles on packings of 10 circles (and conjectures about the optimality of the respective packings); see [24,66,68,75] and some further references in [18]. The proofs involve extensive use of computers; as of today this is about as far as we can come with that approach. The proof method of de Groot *et al.* has been further developed in [52].

2.5 Circle Packings in a Circle

Kravitz [36] was, to our knowledge, the first to consider the problem of packing n congruent circles in a circle. In [36] packings of up to 19 circles are given without any optimality proofs. Graham [26] and Pirl [60] independently proved optimality of packings of up to 7 and 10 circles, respectively. Pirl also presented good packings of up to 19 circles; some of these packings (for $n = 14$, 16, 17) were later improved by Goldberg [25], who also gave a packing of 20 circles. Goldberg's packing of 17 circles was further improved by Reis [62], who extended the range of n to 25. The packing of $n = 25$ is improved in [P4]. Recently, Melissen [40] proved optimality for the case $n = 11$. One family of good packings has been reported in [39].

A peculiarity of the 18-circle case is that the best known packings of 18 circles have the same $d_n^{\bigcirc}$ as the best known packing of 19 circles. There are at least 10 different, equally dense packings of 18 circles. It is conjectured that these 10 packings are exactly the optimal packings of 18 circles in a circle [P4].

The case of 6 circles is analogous to that of 18 circles; different packings can be obtained from the 7-circle packing by removing and reordering circles. There are more than one optimal packing also for $n = 11$.

In [P3] it was conjectured that $d_n^{\square} > d_{n+1}^{\square}$ for all $n \geq 2$. For packings in a circle a similar claim is not true; an optimal packing of 6 circles is obtained from the optimal packing of 7 circles by removing one circle.

Optimal circle packings in an equilateral triangle are known for $n = k(k+1)/2; k = 1, 2, \ldots$ (the triangular numbers) [56]. It has been conjectured that $d_{n-1}^{\triangle} = d_n^{\triangle}$ for all these values of n [27]. Here $d_n^{\triangle}$ is the largest possible value of (1) when the points are confined to an equilateral triangle with sides of unit length. When packing circles in a circle no other similar situations are known or conjectured except when $n = 7$ and $n = 19$. Finally, no infinite family of (conjecturally) optimal circle packings is known in a circle.

2.6 Electrostatic Minimization on a Circular Disk

Thomson's problem is a well-studied (see [P2] for references) optimization problem where one tries to find a minimum-energy configuration of n equal point charges on the surface of a sphere (or, equivalently, in a sphere [10]). This corresponds to minimizing (2) with $m = 1$, i.e., the potential is Coulombic. Several tables of solutions to Thomson's problem have appeared in the literature, see [P2]. A continuously updated table is available electronically through Neil Sloane's World Wide Web home page currently at <URL:http://www.research.att.com/~njas/> (note that the address of the page has changed from the one given in ref. [46] in [P2]).

The question what is the minimum-energy configuration of n equal point charges on a *circular disk* was raised in 1985 by Berezin [3]. It appeared that in the optimal configuration not all the charges are located on the circle boundary when $n \geq 12$ (for proofs of this fact, see [31, 43, 63, 77]).

In fact, finding optimal point charge configurations on a circular disk is a difficult multimodal optimization problem. In the literature we can find several examples where a locally optimal configuration was conjectured globally optimal (see [P2] for references). Physical experiments related to this problem were made in [59] (parallel bar magnets on an airbed) and in [7] (small conductive charged balls).

When the number of charges approaches infinity, the problem tends to the well-known problem of charge distribution over a conducting disk [49]. On a conducting circular disk of unit radius the charge density is proportional to $(1 - r^2)^{-1/2}$, where r is the distance from the center of the disk [61].

Since [81] no more tables or figures of (conjecturally) optimal charge configurations have been published. In this thesis we partially fill that gap in the literature by presenting configurations of up to 80 charges [P2]. In [P2] we use several stochastic global optimization methods. The best performance was obtained by a multi-level single linkage algorithm [64]. Our algorithm employs a special heuristic distance function which is used to prevent multiple optimization runs from initial solutions that are close to each other. That way the solution space is explored more thoroughly when only a limited number of optimization runs can be used.

It is possible to consider other than Coulombic potentials when searching for optimal configurations in a sphere or on a circular disk [4–6, 9, 10, 76]. Leech [37] showed that on the surface of the sphere the only configurations which are in equilibrium under all laws of repulsion forces are those that have a rotational symmetry about every diameter through points of the system, see also [46].

It is interesting to find out which configurations on a disk are in equilibrium under *any* law of repulsion. In [P2] we prove the following theorem (analogous to that in [37]) that characterizes all such configurations. By "law of repulsion" we mean a repulsive force between two points that only depends on the distance between the points, i.e., the magnitude of the force between $\mathbf{p}_i$ and $\mathbf{p}_j$ is $v(\|\mathbf{p}_i - \mathbf{p}_j\|)$, where $v(d)$ is any function such that $v(d) \geq 0$ for all $d \geq 0$.

Theorem 1 *The configurations of $n \geq 2$ points on a circular disk that are in equilibrium under any law of repulsion are exactly*

1. n points evenly spaced on the disk boundary, and

2. $n-1$ points evenly spaced on the disk boundary and one point in the center of the disk. In this case we require $n > 2$.

Using the theorem we find out that the best configurations of $n \leq 16$ charges in [P2] are equilibrium configurations under any law of repulsion. They are also locally optimal circle packings, but of them only the configurations of up to 6 charges, all of type 1 in Theorem 1, are at the same time globally optimal circle packings (see [P4] and its references). When $n = 6$ there exists another globally optimal packing of circles that is not a globally optimal charge configuration. It is conjectured that the optimal circle packings and charge configurations are different for all $n > 6$ [P2].

3 Covering Designs and Constant Weight Codes

Packing and covering problems of discrete geometry have direct applications in coding theory. For example a packing of circles on the surface of a sphere is a spherical code [15]. However, the solution space of the packings or coverings does not have to be continuous. In this thesis we consider two well known coding theoretical structures, covering designs and constant weight codes (packing designs), which both can be defined by a suitable covering or packing in a space whose points are constant weight words in an n-dimensional Hamming space $\{0,1\}^n$.

3.1 Definitions and Basic Results

Let $v \geq k \geq t$ and $v \geq m \geq t$. A $t-(v,m,k,\lambda)$ *covering design* is a pair $(X,\mathcal{A})$, where X is a set of v elements (called *points*) and $\mathcal{A}$ is a multiset of k-subsets of X (called *blocks*), such that every m-subset of X intersects at least λ members of $\mathcal{A}$ in at least t points.

We define

$$C_\lambda(v,m,k,t) = \min\{|\mathcal{A}| : \text{there is a } t-(v,m,k,\lambda) \text{ covering design } (X,\mathcal{A})\}.$$

For example let $X = \{0,1,\ldots,8\}$. Now the three blocks (or k-sets) {0123, 3456, 5678} are a $2-(9,4,4,1)$ covering design. However, this design is not a minimal covering design, because $\{0123, 4567\}$ has also the required covering property. Clearly, a single 4-set will not suffice. Therefore, $C_1(9,4,4,2) = 2$.

Covering designs are here defined in a very general sense. Most of the published results on covering designs have concerned the case $m = t$ (see [47] for an excellent survey). Some results on the case $m > t$ exist [1,2,71]; in those papers $\lambda = 1$, and the notation $B(t,k,m,v) = C_1(v,m,k,t)$ is used.

A well-known result for covering designs with $m = t$ is the Schönheim lower bound [69]:

Theorem 2

$$C_\lambda(v,t,k,t) \geq \left\lceil \frac{v}{k} \left\lceil \frac{v-1}{k-1} \cdots \left\lceil \frac{v-t+1}{k-t+1}\lambda \right\rceil \cdots \right\rceil \right\rceil.$$

While similar theorem is not known for $m > t$, we can use the following simple volume bound.

Theorem 3

$$C_\lambda(v,m,k,t) \geq \left\lceil \frac{\lambda\binom{v}{m}}{\sum_{i=t}^{\min(k,m)} \binom{k}{i}\binom{v-k}{m-i}} \right\rceil.$$

Our definition of *packing* designs is analogous to that of covering designs: a $t-(v,m,k,\lambda)$ packing design is a pair $(X,\mathcal{A})$, where X is a set of v elements and $\mathcal{A}$ is a multiset of k-subsets of X, such that every m-subset of X intersects *at most* λ members of $\mathcal{A}$ in at least t points. Let

$$D_\lambda(v,m,k,t) = \max\{|\mathcal{A}| : \text{there is a } t-(v,m,k,\lambda) \text{ packing design } (X,\mathcal{A})\}.$$

If $\lambda = 1$, a design is a packing design if and only if the distance between the blocks (the number of points belonging to exactly one of the blocks) is at least $d = 2m - 4t + 2k + 2$. From this follows [P1] that we can without loss of generality assume that $t = m$.

Constant weight codes are $t-(v,m,k,1)$ packing designs. The notation $A(n,d,w) = D_1(n, w-d/2+1, w, w-d/2+1)$ is used in the literature [8], [P5] to denote the maximum number of binary words of length n and weight w that have mutual distance at least d (because the words have constant weight, the distance d can always be taken even).

An important upper bound for the size of constant weight codes is the first Johnson bound [8], which is the smallest bound obtained by iterating the inequalities

$$\begin{aligned} A(n,d,w) &\leq \left\lfloor \frac{n}{w} A(n-1,d,w-1) \right\rfloor, \\ A(n,d,w) &\leq \left\lfloor \frac{n}{n-w} A(n-1,d,w) \right\rfloor \end{aligned}$$

until a trivial bound (as defined in [8]) can be applied.

If a design simultaneously is both a packing and a covering design, it is called a *t-design*. *Steiner systems* are t-designs with $\lambda = 1$. 2-designs are generally referred to as *balanced incomplete block designs* (BIBDs).

3.2 Local Search Algorithms

In this thesis we have used two stochastic combinatorial optimization algorithms, simulated annealing [11, 33] and tabu search [23]. Both of them can be classified as local search algorithms: we start from some initial solution, then repeatedly slightly change the current solution according to some rules, until, hopefully, a solution is found that meets our demands.

Both algorithms require that we define the set of feasible solutions (solution space) and a cost function that ranks the solutions. In addition to that we need to specify a neighborhood structure in the solution space to define which solutions are neighbors to each other. From the neighborhood of a solution we obtain the set of *moves* applicable to that solution.

In simulated annealing we take randomly one of the neighbors of the current solution. If the solution is better than or equal to the current solution, we take that as the new current solution. If the solution is inferior to the current solution, we still accept the change with probability $\exp(-\Delta/T)$, where Δ is the difference between the cost of the proposed new solution and the cost of the current solution (assuming minimization of the cost function; maximization can be obtained by reversing the sign of Δ). The *temperature* T is decreased slowly during the optimization run.

In tabu search we start with an initial solution and move to the best allowed solution in the neighborhood of the current solution. To prevent looping around a local optimum, a tabu list is used. A history based tabu list prevents the inverses of the latest few moves from being used.

A great advantage of the local search algorithms is that because at every iteration the solution is changed only slightly, we often can calculate the *change* of cost very quickly.

When the solution space is large, the search may take too much time. In such cases we can restrict the solution space by assuming certain symmetries of the solution. For example we can specify an automorphism group of the solution before the search and thus greatly reduce the solution space [P5]. However, most often it is not known if a solution with the desired automorphism group exists.

3.3 Searching Covering Designs by Simulated Annealing

To apply the simulated annealing algorithm to searching for covering designs we have to specify the cost function and the neighborhood. In [P1] we use the cost function

$$\mathrm{cost}(S) = \sum_{x \in X_m} \max\left(0, \lambda - |\{y \in S : |x \cap y| \geq t\}|\right), \tag{3}$$

where S is the multiset of blocks representing the current solution and X_m is the family of all m-subsets of the set X of v points. If (3) reaches zero, we have a covering design.

The most natural neighborhood structure is as follows. Suppose we have a solution S. Then we can make another solution by first selecting one of the k-sets belonging to S, and by replacing a point in this k-set by a point not belonging to this k-set. We define *the neighborhood of* S as the set of all solutions obtained from S by one such change. To calculate cost changes quickly we rely on an extensive tabulation of neighborhood and covering data [P1], [51]. The computer program `cover` [51], [P1], which implements this scenario, has been used by several mathematicians and lottery system constructors since its publication in 1993.

3.4 Searching Constant Weight Codes by Tabu Search

Several recent papers have discussed the problem of finding good constant weight codes and a variety of optimization methods have been applied [19, 20, 34]. Unfortunately, a search without limitations on the structure of the code does not work well if we are searching for a large code; in such cases, we can predefine a structure (automorphism group) of the code to facilitate the search. This approach has resulted in almost 40 new codes in [P5] (cf. [8]). The codes in [P5] give improved lower bounds on $A(n, d, w)$ (see Section 3.1).

Given a permutation group, its orbits on the w-element subsets of the n coordinates partition all words of weight w. Following the terminology in [P5], an orbit is called *feasible* if any two words of the orbit are distance at least d apart. Two (or more) feasible orbits are said to be *compatible* if any two words in their union are distance at least d apart.

To construct codes, we first compute all feasible orbits for given code parameters and then employ a tabu search based heuristic to find a compatible collection of these orbits that has as many words as possible. This leads to an optimization problem of finding the largest clique in a graph with weighted vertices, which generally is NP-complete [22]. However, our tabu search strategies seem to provide good results within reasonable time in the problem instances of [P5].

Several different neighborhoods, tabu lists, and cost functions have been used in [P5]. Selection of a suitable search strategy depends on the number of different sizes of feasible orbits, the total number of feasible orbits, and the amount of available computing resources.

In some cases the search can be made easier by making a good guess about the structure of the code. For example, we may require that the code consists of orbits of only one size, or we can require that a certain orbit or codeword must be included in the code. These restrictions usually allow us to discard a majority of orbits before the search.

Occasionally, additional words from orbits that are not feasible can be added to the final code. Of course, after adding those words the resulting code is no more invariant under permutations of the group that was used in the search.

By shortening the codes found by tabu search we can get other lower bounds on $A(n, d, w)$. The averaging formulas

$$\begin{aligned} A(n-1, d, w-1) &\geq \lceil wA(n, d, w)/n \rceil, \\ A(n-1, d, w) &\geq \lceil (n-w)A(n, d, w)/n \rceil \end{aligned}$$

always hold [8], but in some cases a better bound can be reached by explicitly counting the number of 1s and 0s in different positions.

Methods similar to those in [P5] can also be used in search of covering designs, when the design size is so large that search without structure (as described in Section 3.3) cannot be applied successfully. Instead of single words, we consider orbits of codewords [53].

4 Conclusions

This thesis gives new methods for finding good solutions to several classical problems in discrete geometry and coding theory. In this thesis computers have played a central role, and furthermore, stochastic optimization algorithms have been the main tool to new results. Each problem is formulated as an optimization problem, and while the problems may seem diverse, it turns out that they share a common background. The multitude of different solution methods reflects the difficulty of the problems.

We have showed that stochastic optimization methods can successfully be used to construct several different mathematical structures, for which general effective construction methods are not known. Purely mathematical constructions often give valuable insight into the structure of the constructed object. Computational methods are very useful in that they can give important knowledge regarding effectiveness of the best construction methods. If better solutions than previously known ones can be found by a computer search, this gives justification for further efforts to develop more sophisticated construction methods. Also, by investigating the structure of a computer-constructed object we sometimes can invent new construction methods or gather deeper understanding of the structure of the computer-constructed object.

Of the problems studied in this thesis, the search for constant weight codes [P5] turned out to be especially successful. Even though constant weight codes have been extensively studied and numerous different construction methods are known [8], almost 40 new codes, better than previously known, were found by the optimization methods of [P5]. It is very probable that by considering automorphism groups not used in [P5] some further new codes can be found by the same search methods.

When searching for covering designs by simulated annealing in [P1], our approach works well with designs that are not very large. The success in [P5] motivates using automorphism groups also in search of covering designs, a work in progress [53] at the moment.

In the literature, packings of n circles in a square or in a circle have been earlier published only for relatively small values of n. Articles [P3] and [P4] extend the values of n to 50 and 65, respectively. These packings (when the improvements in [28] are included) can be used as reference packings for future research.

One aim of studying circle packings in the plane is to find good families of packings; they can be used to construct good lower bounds on the densities of packings for any n. In an equilateral triangle there is an infinite family of packings where each packing is optimal (see Section 2.5). No such families are known in a circle, and based on the results in [P4] it may be that no such families exist (at least no clear pattern is visible in the packings of [P4]). In a square, one such family has been conjectured optimal [54], but the values of n in the family are relatively sparse ($n = 2, 12, 120, 1512, \ldots$).

Of the circle packings in [P4], especially interesting are those that are also locally optimal configurations of other potential functions. As an example of a different potential function, in [P2] we searched for optimal point charge configurations on a circular disk. In addition to providing the first comprehensive table of configurations and their energies of up to 80 charges, we found all configurations that are locally optimal under *any* potential; these configurations have either "maximal symmetry" (no other configuration having larger symmetry group with the same number of charges exists) or "almost maximal symmetry" (only one configuration having larger symmetry group exists).

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