

NONCONVEX OPTIMIZATION PROBLEMS INVOLVING THE EUCLIDEAN NORM: CHALLENGES, PROGRESS, AND OPPORTUNITIES*

ANATOLIY KUZNETSOV[†] AND NIKOLAOS V. SAHINIDIS^{†‡}

Abstract. The field of global optimization has advanced significantly over the past three decades. Yet, the solution of even small instances of many nonconvex optimization problems involving the Euclidean norm to global optimality remains beyond the reach of modern global optimization methods. These problems include numerous well-known and high-impact open research questions from a diverse collection of both fundamental and applied fields of science and engineering. In this review, we survey applications in which these problems arise, describe the sources of computational intractability, summarize existing solution methods, and identify promising research directions for future work. We also introduce `EuclidLib`, a library of instances of optimization problems of this type, to aid in performance benchmarking and algorithm development. The solution of all problems in `EuclidLib` to global optimality would represent a significant achievement for the field of global optimization and an important contribution to mathematics, science, and engineering.

Key words. spatial branch and bound, symmetry elimination, reverse convex, Euclidean norm

AMS subject classifications. 90-02, 90C26, 90C57, 90C59, 92E10, 74G65

1. Introduction. The field of global optimization is experiencing a surge of interest. Algorithms have advanced significantly since the turn of the century [20], leading to improved performance on benchmark libraries such as `MINLPLib` [23], and the number of available solvers, academic as well as commercial, is higher than ever [135, 109, 91, 13, 18, 17, 119, 177, 49, 55]. Nonetheless, compared to linear, mixed-integer, or quadratic programming, global optimization is not yet a mature technology. In this paper, we identify a class of global optimization problems arising from diverse applications which are particularly difficult to solve to global optimality. These problems take the form

$$\begin{aligned}
 (1.1) \quad & \min && f(x, y, z) \\
 & \text{s.t.} && g_i(\|x^i\|_2, y, z) \leq 0 && 1 \leq i \leq N \\
 & && h_{i,i'}(\|x^i - x^{i'}\|_2, y, z) \leq 0 && 1 \leq i < i' \leq N \\
 & && \phi_{ij}(\|x^i - a^j\|_2, y, z) \leq 0 && 1 \leq i \leq N, 1 \leq j \leq M \\
 & && \gamma(x, y, z) \leq 0 \\
 & && x \in \mathbb{R}^{Nd}, y \in \{0, 1\}^m, z \in \mathbb{R}^p
 \end{aligned}$$

where the variables x represent the positions of N points in \mathbb{R}^d , and additional binary variables y and real-valued variables z may also be present. The problem data also includes the fixed positions a^j of M objects in \mathbb{R}^d . We allow for nonconvexity in the objective function, the (possibly vector-valued) constraints g_i on the Euclidean norm of the points x^i , the constraints $h_{i,i'}$ on the Euclidean distances between points x^i and $x^{i'}$, the constraints ϕ_{ij} on the Euclidean distances between points x^i and a^j , and

*

Funding: This work was funded in part by the Air Force Office of Scientific Research under grant no. GR00022273.

[†]School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA.

[‡]H. Milton Stewart Department of Industrial and Systems Engineering, Georgia Institute of Technology, Atlanta, GA.(nikos@gatech.edu)

any other constraints γ . In the remainder of this paper, we will denote the Euclidean norm by $\|\cdot\|$, omitting the subscript for brevity.

Despite the assumptions on the structure of (1.1), a large number of optimization problems admit a formulation of this type. Problems related to geometry as well as distance-dependent physical phenomena are particularly well-represented. For example, the constraints of (1.1) can express non-overlap conditions in packing problems, potential energy fields as functions of the positions of charged particles, and the sum of squared regression error. Optimization problems of the form (1.1) are notoriously challenging to solve to provable global optimality. It is often difficult to find good solutions, as the number of local optima may be very large; for example, the number of local energy minima for atomic nanoclusters [37] and point charges on a sphere [26] is conjectured to grow at least exponentially in the number of items. Circle packing problems are also conjectured to have exponentially many local optima and may also have uncountably many stationary points which are not local optima [1]. This difficulty has motivated the development of a variety of specialized heuristic methods, such as tailored basin-hopping [166, 61, 133], particle swarm [173, 87], genetic [80, 50, 182, 146], neighborhood search [60, 38], and physics-inspired [68, 178, 183] methods. Improving the dual bound is similarly challenging due to the fact that the constraints g_i and h_{ij} in (1.1) are often reverse convex. To this end, efforts have been made to devise custom branch-and-bound algorithms for individual problems of the form (1.1) by exploiting specific problem structures [93, 36, 52, 169, 47, 125, 180, 59]. Yet, techniques to prove global optimality for these problems have only found success for small instances, and as we will show, the performance of general-purpose global optimization algorithms on problems remains prohibitively slow. In view of the fact that a number of well-known problems in mathematics, statistics, chemistry, physics, engineering, and operations research admit formulations of the form (1.1), enabling their solution to provable global optimality is of significant fundamental and practical interest. Moreover, the algorithmic techniques developed in the pursuit of this goal will likely be extensible to more general classes of optimization problems, such as (mixed-integer) quadratically constrained programs. Therefore, we believe that this area presents a fruitful opportunity for the mathematical optimization community.

The paper is organized as follows. In Section 2, we survey various applications across mathematics, science, and engineering in which nonconvex optimization problems involving the Euclidean norm arise. In Section 3, we introduce a new library of instances of optimization problems of this type, `EuclidLib`, and present and discuss the results of a computational study with modern global optimization solvers. In Section 4, we identify and illustrate challenging features of these problems which contribute to their computational intractability and survey existing techniques for addressing these challenges. We outline promising directions for future research efforts in Section 5. Finally, we provide concluding remarks in Section 6.

2. Applications and formulations. Many problems of fundamental and practical importance can be formulated as optimization problems with nonconvex constraints involving the Euclidean norm. A number of well-known open research questions belong to this category. Herein, we provide an exposition of the corresponding mathematical formulations grouped by their fields of origin. We remark that despite our grouping, many of these models have applications beyond the context in which they were first posed.

2.1. Mathematics and statistics.

The kissing number problem. A classic problem in geometry is to determine the maximum number of unit spheres in \mathbb{R}^d that can be positioned tangent to a central unit sphere without overlapping each other. This number is called the kissing number of dimension d , which we will denote by $KN(d)$. The terminology originates from the game of billiards, in which two adjacent rigid balls are said to kiss if they lie tangent to one another. Elementary arguments suffice to show that $KN(1) = 2$ and $KN(2) = 6$. However, the problem of determining $KN(3)$ is far from trivial, and was famously the subject of a dispute between Isaac Newton (who thought $KN(3) = 12$) and David Gregory (who thought $KN(3) = 13$) in the 17th century [154]. It was not until the 1950s that $KN(3)$ was shown to be 12 [140], and half a century later that $KN(4)$ was proved to be 24 [114]. To date, kissing numbers are only known for $d \in \{1, 2, 3, 4, 8, 24\}$, with lower and upper bounds known for other values of d . Applications of the kissing number problem include the design of transmission formats [2] and error-correcting codes [85], as well as the study of condensed matter phases [161]. The problem admits the following mathematical programming formulation [81]:

$$(2.1) \quad \begin{array}{ll} \max & \alpha \\ \text{s.t.} & \|x^i\|^2 = 4 \quad 1 \leq i \leq N \\ & \|x^i - x^j\|^2 \geq \alpha \quad 1 \leq i < j \leq N \end{array}$$

In this formulation, the central unit sphere is fixed to the origin, and the number of tangent spheres is fixed to N . If the optimal value $\alpha^* \geq 4$, it is possible to arrange N unit spheres tangent to a central unit sphere so that they do not overlap, from which it follows that $KN(d) \geq N$. On the other hand, if $\alpha^* < 4$, we have that $KN(d) < N$. $KN(d)$ can therefore be determined by solving a sequence of instances of problem (2.1). Alternatively, $KN(d)$ is given by the solution to the following mixed-integer formulation, once an upper bound \bar{d} on $KN(d)$ is known [96]:

$$(2.2) \quad \begin{array}{ll} \max & \sum_{i=1}^{\bar{d}} y_i \\ \text{s.t.} & \|x^i\|^2 = 4y_i \quad 1 \leq i \leq \bar{d} \\ & \|x^i - x^j\|^2 \geq 4y_i y_j \quad 1 \leq i < j \leq \bar{d} \\ & y_i \in \{0, 1\} \quad 1 \leq i \leq \bar{d} \end{array}$$

where the binary variables y indicate whether a sphere is chosen to be part of the configuration or not. Although a relaxation of (2.2) can give a valid upper bound on $KN(d)$ which is potentially tighter than \bar{d} , we remark that the most fruitful methods for computing upper bounds on $KN(d)$ have been *via* linear and semidefinite programming formulations. However, this is not the focus of the current paper; for a review, we direct the reader to [89], and more recent results are reported in [94]. Interestingly, the computational complexity of solving the kissing number problem is unknown [89].

The Euclidean Steiner tree problem. In the Euclidean Steiner tree problem, we are given a set of N points $\{a^1, \dots, a^N\}$ in \mathbb{R}^d , which must be connected by the shortest possible tree, as measured by the sum of edge lengths. In addition to the given points, which are known as terminals, we may introduce additional vertices called Steiner points, which has the potential to shorten the tree length. It is known that each Steiner point has degree three in a minimal Steiner tree, and that a Steiner tree contains at most $N - 2$ Steiner points [69]. If no Steiner points are allowed, the

problem reduces to the minimum spanning tree problem. A Euclidean Steiner tree is illustrated in Figure 1; note that Steiner points can coincide with terminals.

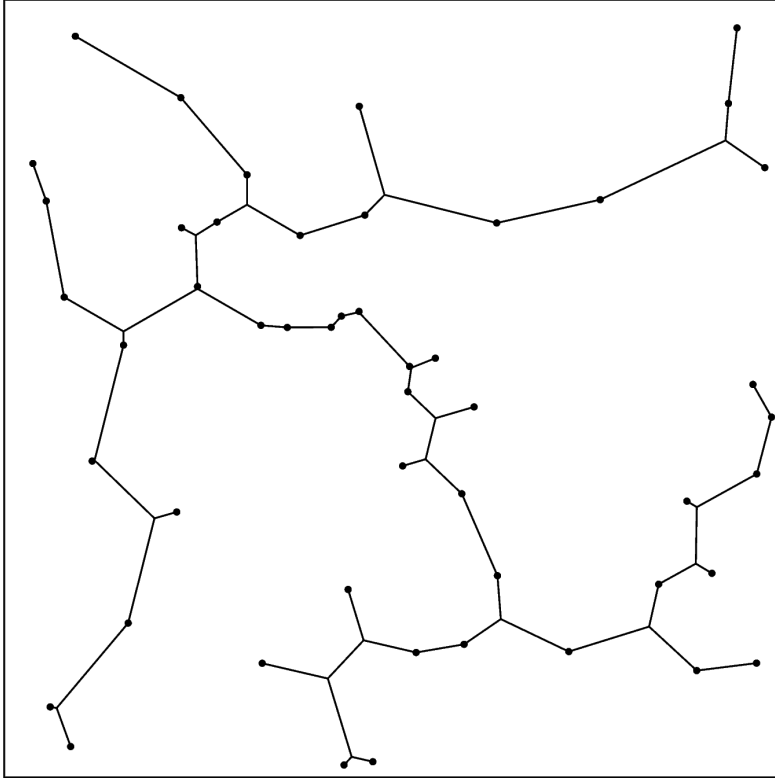


Fig. 1: Example of a Euclidean Steiner tree for a 50-terminal instance. Terminals are depicted as black dots. Plot generated using GeoSteiner 5.3 [77].

The Euclidean Steiner tree problem is a generalization of the Fermat-Torricelli problem of finding a point within a triangle such that the sum of distances from the point to the three vertices is minimal. For a review of the problem's history, we direct the reader to *e.g.*, [69, 41]. Its applications include the modeling of biomolecular systems [110, 148], the design of circuitry [184, 132], and the configuration of building components such as ducts and pipes [149]. It is known to be **NP**-hard [54], although for the two-dimensional case, algorithms such as GeoSteiner [180] perform well in practice [77]. For a recent survey of developments in the solution of the Euclidean Steiner tree problem in general dimension, see *e.g.*, [46].

Let $\mathcal{N} := \{1, \dots, N\}$ denote the index set of terminals, and $\mathcal{S} := \{1, \dots, N - 2\}$ denote the index set of possible Steiner points. Further, define $E_1 := \{(i, j) : i \in \mathcal{S}, j \in \mathcal{N}\}$ as the set of possible edges joining a terminal to a Steiner point, and $E_2 := \{(i, j) : i, j \in \mathcal{S}, i < j\}$ as the set of possible edges joining two Steiner points.

Then, the Euclidean Steiner tree problem admits the following formulation [48]:

$$\begin{aligned}
(2.3) \quad & \min \sum_{(i,j) \in E_1 \cup E_2} r_{ij} \\
& \text{s.t.} \quad \|a^j - x^i\| - M(1 - y_{ij}) \leq r_{ij} && (i,j) \in E_1 \\
& \quad \|x^i - x^j\| - M(1 - y_{ij}) \leq r_{ij} && (i,j) \in E_2 \\
& \quad \sum_{i \in \mathcal{S}} y_{ij} = 1 && j \in \mathcal{N} \\
& \quad \sum_{j \in \mathcal{N}} y_{ij} + \sum_{k \in \mathcal{S}, k < j} y_{ki} + \sum_{k \in \mathcal{S}, k > j} y_{ik} = 3 && i \in \mathcal{S} \\
& \quad \sum_{k \in \mathcal{S}, k < i} y_{ki} = 1 && i \in \mathcal{S} \setminus \{1\} \\
& \quad y_{ij} \in \{0, 1\}, r_{ij} \in \mathbb{R}_+ && (i,j) \in E_1 \cup E_2 \\
& \quad x^i \in \mathbb{R}^d && i \in \mathcal{S}
\end{aligned}$$

In (2.3), the variables r_{ij} model the Euclidean distances between points in the Steiner tree, the variables x^i are the positions of Steiner points, and the variables y_{ij} indicate whether edge (i, j) is part of the Steiner tree or not. The big- M constraints allow the variables r_{ij} to take a value of zero if the edge (i, j) is not part of the Steiner tree. A suitable value of big M can be derived based on the minimum spanning tree of the terminals [46]. Observe that the formulation (2.3) admits a convex continuous relaxation, namely a second-order cone program. Nevertheless, problem (2.3) is very challenging to solve to global optimality; even specialized branch-and-bound methods such as the SAMBA algorithm [47] are limited to instances with $d \leq 5$ and $N \leq 18$ [46].

The k -means clustering problem. An important problem in statistics and machine learning is to partition M data points a^j , $1 \leq j \leq M$, into k clusters in a way that minimizes a measure of the distance between each data point and the centroid x^i of the cluster to which it is assigned. When the objective is the squared Euclidean distance, this problem is known as the k -means clustering problem [95]. Other variants of this problem, *e.g.*, using the ℓ_1 norm instead of the Euclidean norm to reduce the influence of outliers, are also well-studied [138]. The k -means clustering problem is known to be **NP-hard** [3], even in two dimensions [97], and is solved heuristically in practice using algorithms belonging to the family of methods proposed in the 1950s and 1960s [128, 151]; for a recent review of algorithm variants, see [70]. The problem admits a mathematical programming formulation as follows [143]:

$$\begin{aligned}
(2.4) \quad & \min \sum_{i=1}^k \sum_{j=1}^M y_{ij} \|a^j - x^i\|^2 \\
& \text{s.t.} \quad \sum_{i=1}^k y_{ij} = 1 && 1 \leq j \leq M \\
& \quad y_{ij} \geq 0 && 1 \leq i \leq k, 1 \leq j \leq M
\end{aligned}$$

where the variable y_{ij} , which is always binary-valued at an optimal solution [143], models the assignment of data point j to cluster i . Cuong and Yen [155] characterized the set of global solutions to (2.4) as finite, and showed that standard heuristic algorithms may converge to points which are not even locally optimal. Rao [131] showed that, under an additional constraint on intra- and inter-cluster distances between data points, the problem has a reduction to set partitioning. Exact algorithms for (2.4) based on column generation [42, 4], customized branching [52, 36, 59], and semidefinite programming [125, 124] have been developed and have recently solved instances with up to 800 data points [124] to global optimality.

2.2. Chemistry and physics.

The molecular clustering problem. A problem of fundamental importance in chemical physics is to determine the minimum-energy configuration of N identical uncharged particles interacting by van der Waals forces. The term *van der Waals forces* refers to a combination of two physical effects. Firstly, as illustrated in Figure 2, instantaneous electron density fluctuations in orbitals induce dipoles in neighboring atoms, leading to momentary electrostatic attraction between nonpolar, uncharged particles [72]. This effect is called London dispersion.



Fig. 2: London dispersion: the formation of instantaneous dipoles due to electron density fluctuation.

Secondly, particles experience a strong repulsive force at short distances when electron clouds overlap [73]. The result of these two effects is that the energy of a pair of uncharged particles i and j can be expressed in terms of their Euclidean distance r_{ij} from one another, with a weak long-range attraction, a strong short-range repulsion, and an equilibrium distance. A popular model of van der Waals forces is the Lennard-Jones potential [75], usually expressed as

$$V_{LJ}(r_{ij}) = r_{ij}^{-6} (r_{ij}^{-6} - 2),$$

although variants with different coefficients and exponents also exist [142]. A second common model is the Morse potential [112], parameterized by a positive constant ρ ,

$$V_M(r_{ij}) = \exp(\rho(1 - r_{ij})) (\exp(\rho(1 - r_{ij})) - 2).$$

These potential functions are illustrated in Figure 3. When $\rho = 6$, the curvature of the Morse potential at the equilibrium distance is equal to that of the Lennard-Jones potential. When expressed in dimensionless form, the Lennard-Jones and Morse potentials have a minimum value of -1 at an inter-particle distance of $r_{ij} = 1$. Note that although these functions are quasiconvex when expressed in terms of the inter-particle distance r_{ij} , they are not quasiconvex when written in terms of the particle coordinates.

The Lennard-Jones and Morse potentials agree well with experimental energy measurements for systems such as noble gases and small molecules [186, 76]. Accordingly, they are ubiquitous in molecular simulations [172, 22] as well as theoretical studies of phenomena such as crystallization [86], protein folding [117], and melting [66]. The Morse potential has also been used to model the kinematic behavior of animal swarms [160, 15]. The bulk Lennard-Jones material is known to adopt a face-centered cubic and hexagonal close-packed lattice depending on temperature and pressure [163], and Morse lattices have been characterized as a function of ρ [24]. However, for nanoclusters too small to assemble into a repeating crystal lattice, determining the minimum-energy structure is an open question. The problem may be

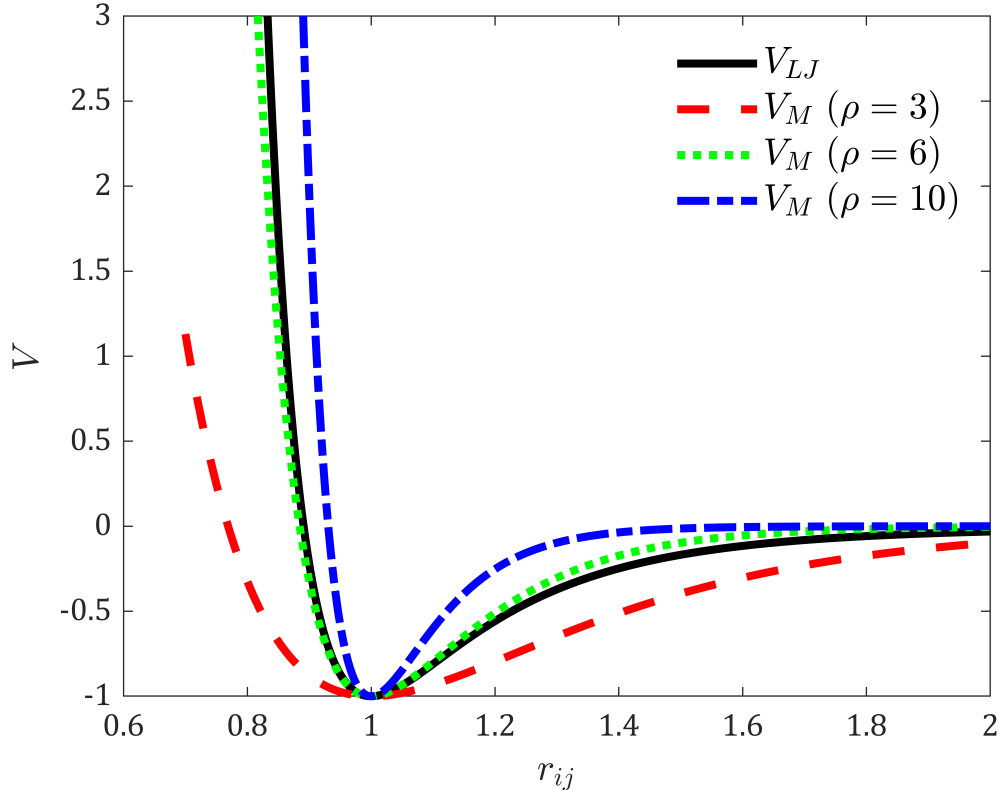


Fig. 3: Lennard-Jones and Morse potentials as a function of the Euclidean distance r_{ij} between particles i and j .

posed as follows:

$$(2.5) \quad \min_{x \in \mathbb{R}^{3N}} \sum_{i=1}^{N-1} \sum_{j=i+1}^N V(\|x^i - x^j\|)$$

where $V \in \{V_{LJ}, V_M\}$. Problem (2.5) was first posed by Hoare and Pal in 1971 for the Lennard-Jones potential [64]. As illustrated in Figure 4, the objective function of (2.5) is highly multimodal; this property has spurred the development of many minimization heuristics, including basin-hopping [166, 133], simulated annealing [178, 183], and genetic [182, 146] methods. Indeed, the number of stationary points of (2.5) is known to be bounded below by an exponential function of N [37], and the problem is known to be **NP**-hard [179]. A deterministic global optimization approach for (2.5) was explored in [98]; however, a non-physical choice of an algorithmic parameter invalidated optimality proofs (for example, for $N = 7$, [64] reports a solution better than the solution reported as the global minimum in [98]). The Cambridge Cluster Database [167] maintains a collection of putative optima for molecular clustering problems.

Laboratory experiments to characterize the structure of argon clusters have given results which are consistent with putative optima for Lennard-Jones clusters for most values of N between 13 and 150, with a number of notable exceptions at $N = 38, 75$,

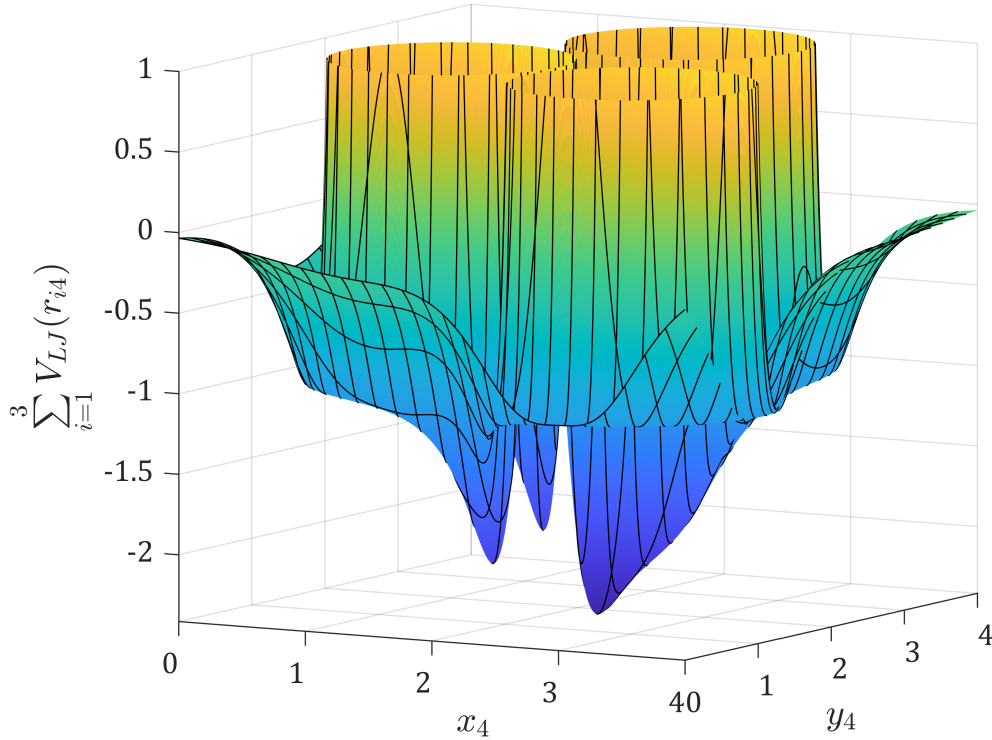


Fig. 4: Slice of the potential energy function of a 4-atom Lennard-Jones cluster in \mathbb{R}^2 with the first three atoms fixed to $(1.3, 1.5)$, $(3, 1)$, and $(2.3, 3)$.

76, 77, 102, 103 and 104 [9]. Similarly, Lennard-Jones cluster putative optima for $N = 38, 75$, and 101 disagree with experimentally determined structures for fullerene clusters [9]. The exact reason for these discrepancies is unknown. In light of the consistency between putative optima and experimentally determined structures for most clusters, and the fact that real 38- and 75-particle clusters of several materials differ from the putative optima, it is possible that some putative optima are not global.

The Thomson and Tammes problems. At the turn of the 20th century, before the development of quantum mechanics, the physicist J. J. Thomson proposed a model of the atom as a sphere of uniform positive charge whose electrons are classical negative point charges constrained to its boundary [159]. The positions of N electrons in this atomic model were postulated to minimize the overall Coulombic interaction energy:

$$(2.6) \quad \begin{aligned} \min_{x \in \mathbb{R}^{3N}} \quad & \sum_{i=1}^{N-1} \sum_{j=i+1}^N \|x^i - x^j\|^{-1} \\ \text{s.t.} \quad & \|x^i\| = 1 \quad 1 \leq i \leq N \end{aligned}$$

where length is scaled so that the atom has unit radius. Although this model of the atom has since been shown to be incorrect, it turns out that (2.6) has other important applications, such as in the complexity of solving polynomial equations [145], the

modeling of proteins on the surface of a spherical virus [107, 189, 71], and the study of particles at droplet interfaces [12]. Notably, the seventh of Smale’s eighteen mathematical problems [147] involves the approximate solution in polynomial time of (2.6), along with a variant in which the interaction potential is given by $-\log \|x^i - x^j\|$ rather than $\|x^i - x^j\|^{-1}$. Analogously to the molecular clustering problem, a number of heuristic minimization methods including basin-hopping [168], multistart local search [5], genetic algorithms [111], and simulated annealing [181] have been employed to find local minima for the Thomson problem, a catalogue of which can also be found at the Cambridge Cluster Database [167]. Provably global minima are known only for $N \in \{2, 3, 4, 6, 12\}$ [33] and $N = 5$ [141], the proof of the latter being published only in 2013; asymptotic bounds on the optimal value of (2.6) are given in [82, 104]. Due to its difficulty, several instances of the Thomson problem are included in the MINLPLib [23] benchmark set of optimization problems.

A closely related problem is to find the position N points on the surface of the unit sphere such that the closest distance between any two is maximized, which may be formulated in the following way:

$$(2.7) \quad \begin{aligned} \max \quad & L \\ \text{s.t.} \quad & L \leq \|x^i - x^j\| \quad 1 \leq i < j \leq N \\ & \|x^i\| = 1 \quad 1 \leq i \leq N \end{aligned}$$

Problem (2.7) is known as the Tammes problem, after the biologist who posed it in the context of the dispersion of pores on the surface of pollen grains [156]. Optimal solutions are known only for $N \leq 14$ and $N = 24$ [115].

2.3. Operations research.

Packing and cutting problems. The task of packing objects into a container without overlap, also known as nesting, is ubiquitous in operations research. Applications include loading items into shipping containers [188, 134], designing facility layouts [6], planning for additive manufacturing processes [83], designing cable bundles [152], task scheduling [27], radiosurgical treatment planning [171], and developing data visualizations [56]. The related problem of cutting parts from a stock of raw material finds applications in the manufacture of parts from textiles [57, 67] and sheet metal [127] and has connections to the well-known bin packing and cutting stock problems. For a recent comprehensive review of packing and cutting problems, see *e.g.*, [139]. Non-overlap constraints for general objects are typically expressed using phi-functions, which are functions defined for a pair of sets to be negative if the interiors of the two sets intersect [14]. Herein, we restrict ourselves to the problem of packing circles of given radii into a convex container for three reasons. Firstly, the phi-function for a pair of circles is the difference between the distance separating the circle centers and the sum of the radii, and therefore does not require a piecewise definition [31]. Secondly, more complicated objects may be approximated to arbitrary accuracy by a union of inscribed circles, reducing other packing problems to the packing of circles of unequal radii [74], as illustrated in Figure 5. Finally, even for this relatively simple packing problem, optimal solutions are only known for small instance sizes [169].

Given the radius r_i of each circle and a set X to which the circle centers are constrained, the problem may be stated as follows:

$$(2.8) \quad \begin{aligned} \max \quad & L \\ \text{s.t.} \quad & \|x^i - x^{i'}\|^2 \geq (Lr_i + Lr_{i'})^2 \quad 1 \leq i < i' \leq N \\ & x^i \in X \quad 1 \leq i \leq N \end{aligned}$$

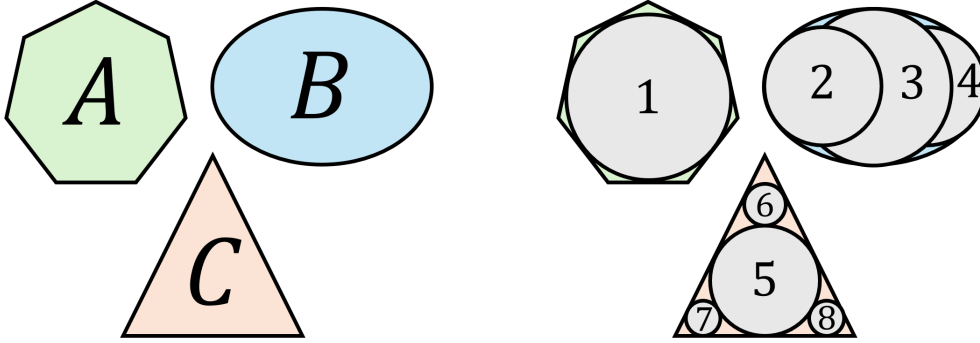


Fig. 5: The constraint that objects A , B and C cannot overlap can be approximated by the constraints that each circle in the sets $\{1\}$, $\{2, 3, 4\}$, and $\{5, 6, 7, 8\}$ cannot overlap any circle from another set.

The objective L can be thought of as a length scaling factor; if the optimal value $L^* \geq 1$ then it is possible to fit the circles inside the container. Problem (2.8) is known to be **NP-hard** [51]. A variety of heuristics have been developed for the circle packing problem [62]; the Packomania website [150] hosts the best known solutions for many commonly studied geometries. Exact algorithms based on custom branching [93, 170, 169], interval arithmetic [101, 102], as well as traditional geometric proofs with and without computer assistance [153] have succeeded in proving optimality for up to 39 identical circles in a square [153], and up to 11 circles of unequal radii in various containers [169].

Planar facility location problems. In a facility location problem, we are given the locations a^j of M customers and we seek to place N facilities optimally with respect to a metric such as cost or utility, which usually depends on the distance between customers and facilities. Although it is often realistic to model the set of candidate locations by vertices on a graph, it is common modeling practice to represent facility positions with continuous planar coordinates x^i in several situations, such as for so-called “greenfield” facility construction (*i.e.*, construction of a facility amidst undeveloped land), or for the location of items within a room of a building [11]. Moreover, for facilities such as cell towers [43], wireless sensors [53], or radioactive waste storage [32], quantities such as energy expenditure, coverage quality, and risk depend on the Euclidean distance from a facility. A classic planar facility location problem is to minimize the weighted sum of Euclidean distances from each facility to each customer:

$$(2.9) \quad \begin{aligned} \min \quad & \sum_{i=1}^N \sum_{j=1}^M w_{ij} \|x^i - a^j\| \\ \text{s.t.} \quad & x^i \in X \quad \quad \quad 1 \leq i \leq N \end{aligned}$$

where the weights $w_{ij} \in \mathbb{R}$ are fixed and the facility locations are constrained to lie in the set $X \subseteq \mathbb{R}^d$. When $N = 1$, $X = \mathbb{R}^d$, and all $w_{ij} = 1$, the solution to problem (2.9) is the geometric median of the customer locations a^j . In a well-studied special case of (2.9), called the Weber problem after the geographer who proposed it [174], we have $N = 1$ and $w_{ij} \in \mathbb{R}_+$. The Weber problem is a convex optimization problem and is readily solved using methods related to least-squares

algorithms [21, 121, 25, 176]. When weights are allowed to be either positive or negative, for example if some facilities are desirable while others are undesirable, the objective function of (2.9) is neither convex nor concave in general. However, it has an immediate representation as a difference of convex functions; global algorithms for its solution have been developed based on this property [28, 99]. We will refer to problem (2.9) as the planar p -median problem; note that this term is also sometimes used to refer to the related problem of minimizing the weighted sum of distances from each customer to the nearest facility [106], a problem related to clustering.

In a capacitated location-allocation variant of (2.9), the quantities w_{ij} are decision variables representing shipment quantities from each facility to each customer (with shipment costs assumed to be proportional to the squared Euclidean distance), each facility has a capacity c_i , and each customer has a demand d_j ; this problem may then be posed as follows [144]:

$$\begin{aligned}
 (2.10) \quad & \min \sum_{i=1}^N \sum_{j=1}^M w_{ij} \|x^i - a^j\|^2 \\
 & \text{s.t.} \quad \sum_{j=1}^M w_{ij} \leq c_i \quad 1 \leq i \leq N \\
 & \quad \sum_{i=1}^N w_{ij} = d_j \quad 1 \leq j \leq M \\
 & \quad x^i \in X \quad 1 \leq i \leq N \\
 & \quad w_{ij} \geq 0 \quad 1 \leq i < j \leq N
 \end{aligned}$$

The squared-distance dependence of the cost in (2.10) has been used to model systems such as transmission towers, whose power usage scales quadratically with their range [45]. The problem is **NP**-hard, and branch-and-bound algorithms have been introduced for its solution [144].

Most facility location models consider a benefit to customers that increases with proximity to facilities. However, in some cases, so-called obnoxious facilities must be placed in a way that minimizes disutility to customers [32]. For example, missile silos [44], power plants [35], landfills [113], and airports [175, 58] have been modeled in this way. Since the disutility caused by these facilities is typically a physical phenomenon such as radiation or noise, it is commonly expressed as a function of the Euclidean distance from the facility [126]. For example, inverse-square decay $f(r) = \alpha/r^2$ with $\alpha \geq 0$ [108] and exponential decay $f(r) = \alpha e^{-\beta r}$ with $\alpha, \beta \geq 0$ [164] have been used as disutility functions. Drezner and co-workers introduced the following formulation, in which we seek to maximize the smallest distance between any facility and any customer [40]:

$$\begin{aligned}
 (2.11) \quad & \max \quad L \\
 & \text{s.t.} \quad \|x^i - a^j\|^2 \leq L \quad 1 \leq i \leq N, 1 \leq j \leq M \\
 & \quad \|x^i - x^j\|^2 \geq D \quad 1 \leq i < j \leq N \\
 & \quad x^i \in X \quad 1 \leq i \leq N
 \end{aligned}$$

where D is a positive lower bound on inter-facility squared distances (with $D = 0$, the optimal solution is to place all facilities at the same point). Note that maximizing the smallest facility-community squared distance is equivalent to maximizing the smallest facility-community distance. As illustrated in Figure 6, this problem has many

local maxima and has been referred to as “extremely nonconvex” [78]. Correspondingly, a variety of heuristic methods, such as those based on Voronoi diagrams [40], integer programming formulations [78], multistart local search [39], and evolutionary algorithms [158], have been proposed. Exact algorithms [164, 175] have so far been limited to problems with less than 5 facilities.

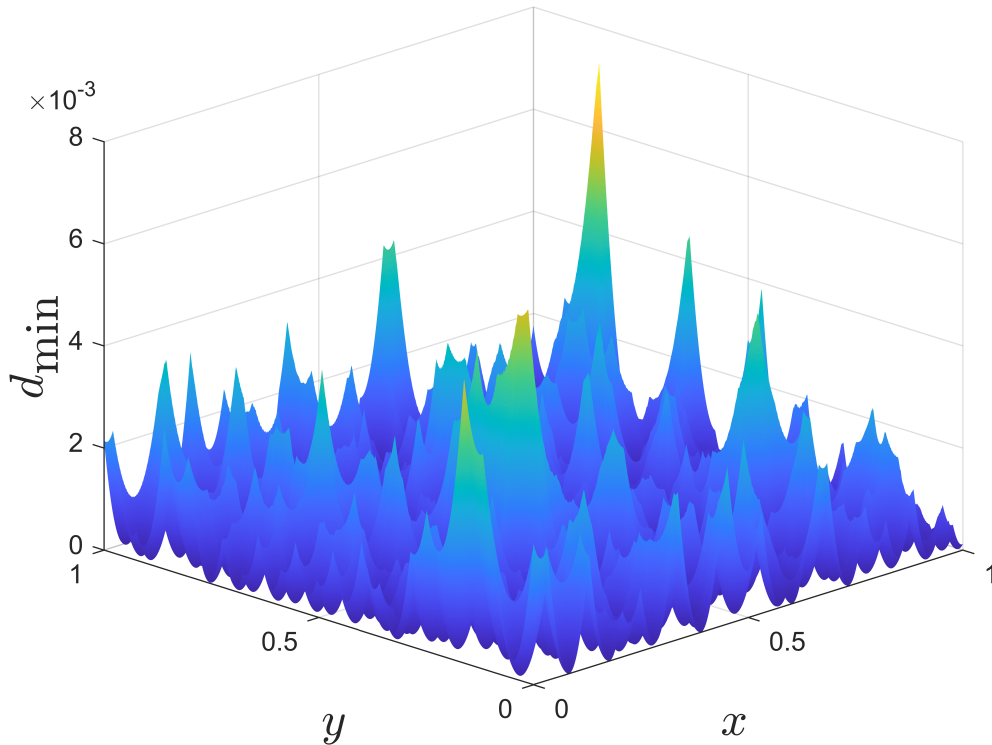


Fig. 6: Squared Euclidean distance to the nearest customer for an obnoxious facility location instance with 500 customers located within the unit square.

3. EuclidLib and a computational study. Despite the development of tailored global optimization algorithms for many of the problems introduced in Section 2, optimal solutions are typically known only for $N \ll 100$. As we will discuss in Section 4, the computational intractability of problems (2.1)-(2.11) stems in large part from their geometric and group structures. Therefore, we have compiled a library **EuclidLib** of instances of these problems to benchmark the performance of general-purpose global optimization solvers for this work and to assist in future studies of optimization problems involving the Euclidean norm.

Statistics for the **EuclidLib** instances are given in Table 2. The library comprises 1,352 instances in total, with an average of 6,395 variables (minimum: 5, maximum: 119,197) and 4,873 constraints (minimum: 1, maximum: 59,699). We sought to balance the number of instances of different problem types to ensure that **EuclidLib** would be an accurate measure of a global optimization algorithm’s performance on a variety of problems. The dimension d in which objects are embedded ranges from 2 to 10. For models of physical phenomena, d is 2 or 3. The number $|J|$ of fixed objects, such as data points or customer locations, ranges from 5 to 1000. The number N of ob-

jects whose positions are to be determined by solving the optimization problems ranges from 2 to 200 in most of the problems we chose, except for the kissing number and Euclidean Steiner tree problems, in which N does not vary independently from d . Although heuristic methods are routinely used to obtain locally optimal solutions for instances of many of these problems with $N \gg 100$, the problem of certifying global optimality even for $N \geq 25$ or so remains open for almost all problems considered herein. Therefore, the development of algorithms capable of solving all problems in `EuclidLib` to global optimality would represent a significant achievement for the field of global optimization, and would enable important contributions to mathematics, science, and engineering. In the remainder of this section, we describe the `EuclidLib` instances in more detail and present the performance of modern global optimization solvers in our computational benchmarking study. A repository containing all `EuclidLib` instances is maintained at <https://github.com/anatoliy-kuznetsov/EuclidLib>.

3.1. Description of instances. Formulation (2.1) for the kissing number problem can be transformed to a feasibility problem by adding the constraint $\alpha \geq 4$, where feasibility implies that $KN(d) \geq N$ and infeasibility implies that $KN(d) < N$. Therefore, we included instances of (2.1) with N ranging from the best known lower bound on $KN(d)$ to one above the best known upper bound on $KN(d)$. In this way, the solution of all kissing number problem instances in `EuclidLib` is sufficient to determine the kissing number for dimensions 2 through 10. In formulation (2.3) of the Euclidean Steiner tree problem, the number of Steiner points depends on the number of terminals, and not every Steiner point need be included in the tree. Although exact algorithms for Euclidean Steiner trees in general dimension are only capable of solving instances with fewer than 20 terminals at present [46], we included instances with up to 200 terminals, since it is common to consider Steiner tree problems on graphs containing hundreds or thousands of terminals [19], and the `GeoSteiner` algorithm is capable of solving problems of up to 10,000 terminals in two dimensions [77]. For the Euclidean Steiner tree, k -means clustering, and p -median problems, we generated synthetic instances using a uniform distribution for the points a^j representing terminals, data points, and customer locations, respectively. We restricted k -means clustering instances to no more than five dimensions. We remark that \mathbb{R}^5 is a relatively low dimension compared to that used in many applications; for example, data sets with over 1,500 features have been used in practice [29].

We chose molecular clustering problems with the Lennard-Jones potential as well as the Morse potential with parameter $\rho = 6$, which is commonly used to benchmark global optimization algorithms [167]. As mentioned in Section 2.2, discrepancies between experimentally observed cluster structures and putative minima of (2.5) have been observed for instances as small as $N = 38$ and up to $N = 104$. The solution of (2.5) for $N \leq 4$ is trivially to arrange all atoms equidistant from one another, but this is not possible in \mathbb{R}^3 for $N \geq 5$. Since the experiments described in [9] include clusters of up to 150 particles, we have included instances of (2.5) with $5 \leq N \leq 150$ in `EuclidLib`. Their solution to global optimality would settle a question which has been open for decades and would provide fundamental insight into the thermodynamics of small clusters of matter. Similarly, instances of the Thomson problem (2.6) with N up to 200 have long been used as part of global optimization benchmarks [23], but global optima remain unknown for the Thomson problem with $N > 12$ and for the Tammes problem with $N > 24$.

The problem of packing equal circles into a square is perhaps the most well-studied circle packing problem in two dimensions; yet, the largest instance whose

optimal solution is known is the 39-circle one. Moreover, specialized algorithms for this problem make simplifications such as domain reductions based on the container being square and the circles being of equal radius. In view of the many applications in which these assumptions do not hold, and the application of the packing of unequal circles to the approximate packing of general shapes, we have included the following instances with N up to 40: packing equal circles into the unit square, packing equal circles into the unit circle, packing circles with $r_i = i$ into a circle, and packing circles with $r_i = i^{-1/2}$ into a circle. The solution of these instances to global optimality will likely require the development of algorithms which are more generalizable to other optimization problems involving the Euclidean norm. Additionally, these geometries have been considered before in the global optimization community [169, 93] and putative optima are available on the Packomania website [150]. The facility location problems we have included in `EuclidLib` include the obnoxious facility location instances from [40], which have recently received attention in the global optimization community [78, 92] owing to their difficulty.

3.2. Computational benchmarking results. We assessed the performance of the global optimization solvers BARON [135], LindoGlobal [91], ANTIGONE [109], SCIP [17], and Gurobi [55] on `EuclidLib` instances using GAMS 46.4.0 on a machine with a 4 GHz processor, 5 GB RAM, and a time limit of 3600 s. The results are shown in Figure 7. The y -axis shows the cumulative percent of instances solved to global optimality (zero gap) by each solver. BARON [135] and SCIP [17] solve the most instances, 38, within the time limit. However, this figure represents just 2.9% of the test set. Indeed, only 73 instances (5.7%) are solvable by any solver within the time limit. For each solver, Table 1 shows the number of instances solved, the corresponding percentage of `EuclidLib` instances solved, the average number of variables and constraints in instances solvable by that solver within the time limit, and the geometric mean of solution times. Solver timeouts are counted as 3,600 s in calculating the geometric mean of solution times. Solvable instances have a mean of 42 variables, just 0.7% of the `EuclidLib` average, and 237 constraints, 4.9% of the `EuclidLib` average. These results indicate that only relatively small instances of `EuclidLib` problems are tractable for modern global optimization solvers.

Solver	Instances solved	Percent solved	Average # variables	Average # cons.	Geometric mean (s)
BARON 24.4.30	38	2.9%	65	62	2,891
SCIP 8.1	38	2.9%	12	422	3,080
Gurobi 11.0.1	28	2.1%	10	398	3,212
ANTIGONE 1.1	19	1.5%	14	311	3,280
LINDOGLOBAL 3.17P	15	1.1%	16	65	3,357

Table 1: Summary of computational results for `EuclidLib` instances.

As discussed in Section 1, `EuclidLib` problems are challenging from both the primal and dual “directions”. To assess whether improving the primal bound or the dual bound took longer in our study, we analyzed solver convergence for the instances solved to global optimality. The results are shown in Figure 8 for each individual solver. The x -axes show the fraction of time τ elapsed between the end of presolve routines and the end of the solution process. This scaling facilitates the comparison of solution progress between instances with different solution times. The y -axes show

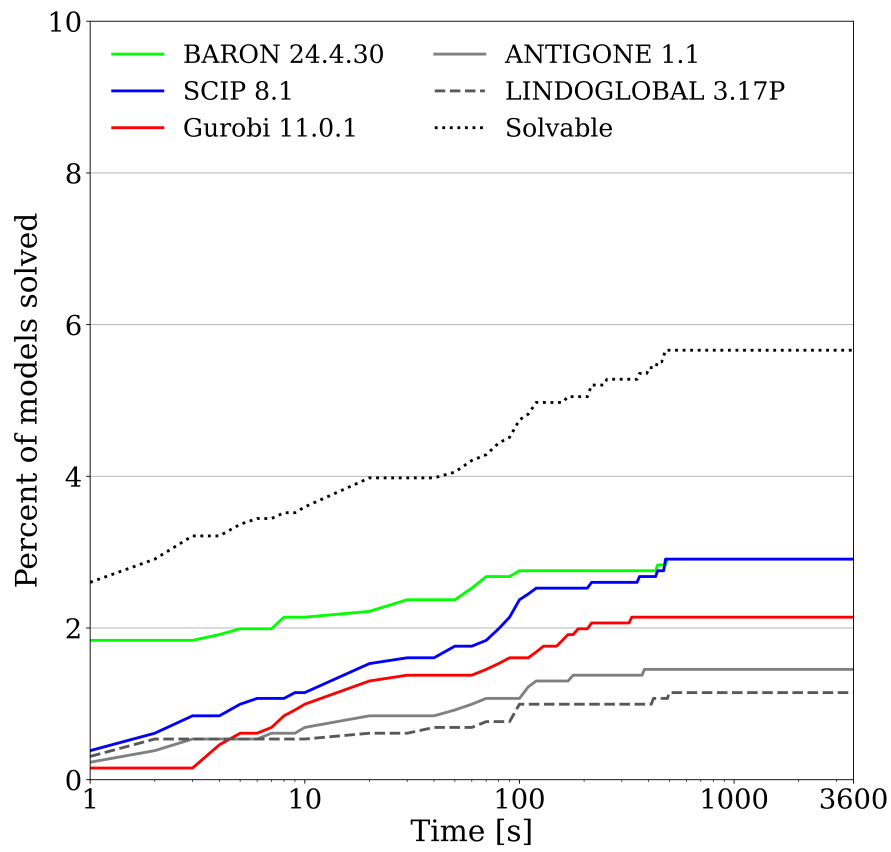


Fig. 7: Performance of global optimization solvers on the EuclidLib collection. Note the logarithmic scale on the x -axis.

Table 2: Statistics of EuclidLib instances. All instances are available online at <https://github.com/anatoliy-kuznetsov/EuclidLib> in GAMS, JuMP, and PyOMO formats.

Problem name	Formulation	$ J $	d	N	# of instances
Kissing number	(2.1)	—	$\{2, \dots, 10\}$	$\{LB(d), \dots, UB(d) + 1\}^1$	136
Euclidean Steiner tree	(2.3)	$\{5, 10, \dots, 195, 200\}$	$\{2, 3, 4, 5\}$	$ J - 2$	160
k -Means clustering	(2.4)	$\{100, 500, 1000\}$	$\{2, 3, 4, 5\}$	$\{2, \dots, 15\}$	168
Lennard-Jones clusters	(2.5) ²	—	3	$\{5, 6, \dots, 149, 150\}$	146
Morse clusters	(2.5) ³	—	3	$\{5, 6, \dots, 149, 150\}$	146
Thomson	(2.6)	—	3	$\{5, 6, \dots, 49, 50, 55, 60, \dots, 195, 200\}$	76
Tammes	(2.7)	—	3	$\{5, 6, \dots, 49, 50, 55, 60, \dots, 195, 200\}$	76
Circle packing	(2.8)	—	2	$\{2, \dots, 40\}$	156
p -Median	(2.9)	$\{100, 500, 1000\}$	2	$\{2, \dots, 25\}$	72
Capacitated p -median	(2.10)	$\{100, 500, 1000\}$	2	$\{2, \dots, 25\}$	72
Obnoxious facility location	(2.11) ⁴	$\{100, 500, 1000\}$	2	$\{2, \dots, 25\}$	144

¹ $LB(d)$ and $UB(d)$ refer to the best known lower and upper bounds for the kissing number in \mathbb{R}^d respectively. These values are:

d	$LB(d)$	$UB(d)$
2	6	6
3	12	12
4	24	24
5	40	44
6	72	78
7	126	134
8	240	240
9	306	363
10	510	553

²For Lennard-Jones clusters, $V(r_{ij}) = r_{ij}^{-6} (r_{ij}^{-6} - 2)$.

³For Morse clusters, $V(r_{ij}) = \exp(\rho(1 - r_{ij})) (\exp(\rho(1 - r_{ij})) - 2)$. In this work, we used the common choice $\rho = 6$.

⁴Consistent with [40], we used $D \in \{1/N, 1/(2N)\}$.

in the solver log file.

The profiles in Figure 8 show qualitatively that, on average, dual bounds are both initially weaker than primal bounds and also take longer to improve. Indeed, we observed that, for a significant fraction of instances, the optimal solution is found in local search during preprocessing, and almost all of the solution time is devoted to proving global optimality. Note that the specific shape of each profile in Figure 8, along with the scale of the y -axis, depends on a variety of factors such as the subset of instances solved, their relative solution times, and solver-specific parameters such as the strategies for tree exploration or preprocessing methods such as local search and bounds tightening. Therefore, we caution that these profiles should not be used to compare the performance of different solvers on metrics such as their relative quality of heuristics and relaxation methods. Instead, they are intended to show qualitatively that dual bound improvement is challenging for `EuclidLib` instances and therefore underscore the potential of stronger convex relaxations for this class of problems to accelerate the solution process.

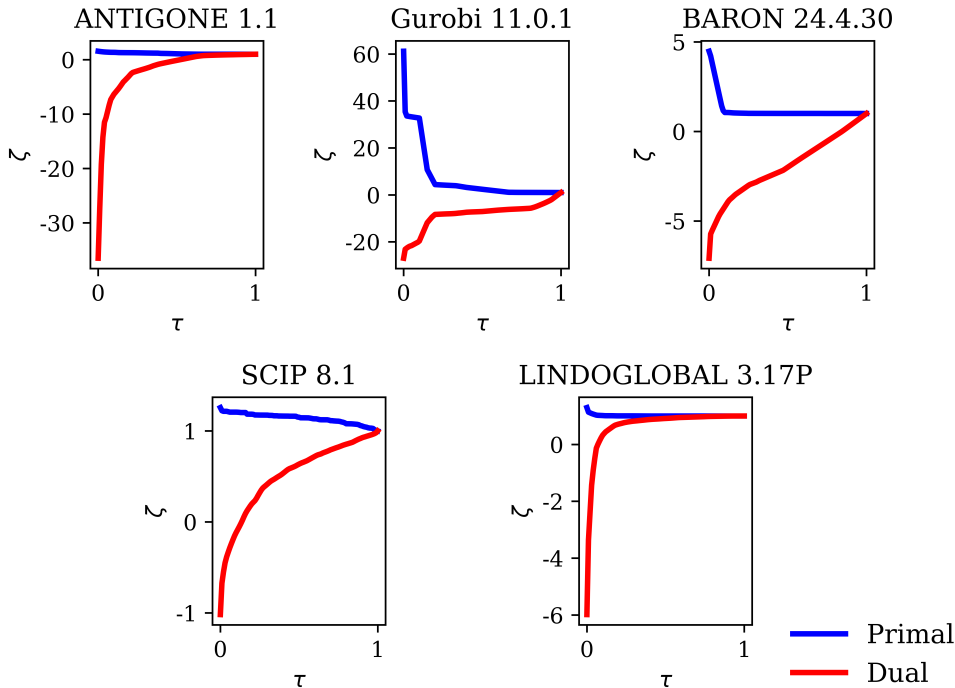


Fig. 8: Solution progress for `EuclidLib` instances solved to global optimality within the time limit, with scaled time on the x -axis and scaled objective value on the y -axis.

4. Challenges and progress. Herein, we highlight two features of `EuclidLib` problems which make them particularly challenging for global optimization methods based on a branch-and-bound framework. Firstly, due to the application areas from which they arise, many of these problems admit symmetric solutions; in particular, their symmetry group includes Euclidean transformations in addition to permutations. Secondly, many `EuclidLib` problems contain an inherent reverse convex structure

defined in terms of the Euclidean norm. Convex relaxations of these sets generated in the standard way are generally very weak. As shown in Section 3, these two characteristics together lead to very slow dual bound improvement, and subsequently, long solution times. In what follows, we elaborate further on these challenges and survey existing techniques, usually developed specifically for individual problems, for handling them.

4.1. Symmetry elimination. Symmetry elimination is an important aspect of branch-and-bound algorithms, often enabling the solution of otherwise intractable problems, and remains an active area of research [123]. A *symmetry* of an optimization problem $\min\{f(x) : x \in X \subseteq \mathbb{R}^n\}$ is a bijection $\pi : \mathbb{R}^n \rightarrow \mathbb{R}^n$ such that $\pi(X) := \{\pi(x) : x \in X\} = X$ and $f(\pi(x)) = f(x)$ for every $x \in X$ [120]. Let Π denote a set of symmetries, or symmetry group. Then, the *orbit* of a point $x \in X$ under Π is $\{\pi(x) : \pi \in \Pi\}$ [100]. In particular, if x is an optimal solution, then every solution in its orbit is an optimal solution. In practice, it is often the case at a low-depth node in a branch-and-bound tree that an optimal solution’s orbit intersects all child nodes. This fact prevents fathoming of large portions of the search tree and leads to enumeration of degenerate optimal solutions. Therefore, the goal of symmetry elimination methods for branch-and-bound algorithms is generally to reduce the domain X so the cardinality of its intersection with each orbit is as small as possible, ideally equal to one [123]. Achieving this goal is very difficult in practice, particularly for the problems in `EuclidLib`. One reason is that the application of symmetry-breaking inequalities for different orbits independently can make all optimal solutions infeasible. Some sufficient conditions for combining symmetry-breaking constraints for permutations of disjoint index sets are known [88, 90]. However, many problems in `EuclidLib` admit Euclidean symmetries (translation, rotation, and reflection) in addition to permutational symmetries, as noted in [88]. The question of necessary and sufficient conditions for the simultaneous breaking of multiple permutation orbits remains open, as does the breaking of permutation and Euclidean orbits.

Symmetry elimination methods can be categorized as either static (at the level of the formulation, or root node), or dynamic (at the level of each node in the branch-and-bound tree). Static symmetry elimination methods often include constraints which can be added directly to the formulation; their ease of implementation makes them accessible to the modeler. On the other hand, dynamic symmetry elimination methods typically require the implementation of a specialized algorithm at each node of the branch-and-bound tree but are usually more effective [90].

The most common types of static symmetry elimination constraints for problems in `EuclidLib` are the fixing of some variables and the imposition of an order on the positions x^1, \dots, x^N . As an illustrative example, consider the molecular clustering problem, (2.5). Since the potential energy of a cluster is defined only in terms of the pairwise Euclidean distances of identical atoms, the set of symmetries for this problem is the Cartesian product between the symmetric group S_N and the Euclidean group E_3 . In other words, permuting the atom numbers and applying translations, rotations, and reflections to the cluster preserve the domain and objective function. This group has infinite cardinality, but many of the translational and rotational symmetries can be broken by fixing the first atom to the origin, the second atom to the x -axis, and the third atom to the xy -plane [64]. Moreover, additional permutational symmetries can be eliminated by imposing an ordering $z_1 \leq z_2 \leq \dots \leq z_N$ on the z -coordinates of each atom. Bounds on the atomic coordinates can be derived from bounds d^L and d^U on interatomic squared distances at an optimal solution; for example, Yuhjtman [187]

showed that $d^L \geq 0.684^2$ and Blanc [16] showed that $d^U \leq N^2$. The molecular clustering formulation together with these constraints can then be written as

$$(4.1) \quad \begin{aligned} \min \quad & \sum_{i=1}^{N-1} \sum_{j=i+1}^N V(\sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}) \\ \text{s.t.} \quad & x_1 = y_1 = z_1 = y_2 = z_2 = z_3 = 0 \\ & z_i \leq z_{i+1} \quad 1 \leq i < N \\ & d^L \leq (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2 \leq d^U \quad 1 \leq i < j \leq N \\ & (x_i, y_i, z_i) \in [-\sqrt{d^U}, \sqrt{d^U}] \times [-\sqrt{d^U}, \sqrt{d^U}] \times [0, \sqrt{d^U}] \quad 1 \leq i \leq N \end{aligned}$$

However, both Euclidean and permutational symmetries remain in formulation (4.1). Consider the polyhedron formed by the convex hull of atomic positions at any solution, shown in Figure 9(a) for the triangular bipyramid, an optimal solution to (4.1) for $N = 5$. Formulation (4.1) enforces that three vertices of a face of this polyhedron should be embedded in the xy -plane, rotated and translated such that one is at the origin, one lies on the x -axis, and one lies in the xy -plane. Although these constraints make rotations of the polyhedron about the origin and translations without rotation infeasible, they do not restrict which faces can lie in the xy -plane. If not all faces are congruent, this leads to symmetric solutions, such as the one illustrated in Figure 9(b). In other words, many Euclidean transformations consisting of a translation composed with a rotation are not eliminated by this formulation. The atomic coordinates of these two solutions are given in Table 3.

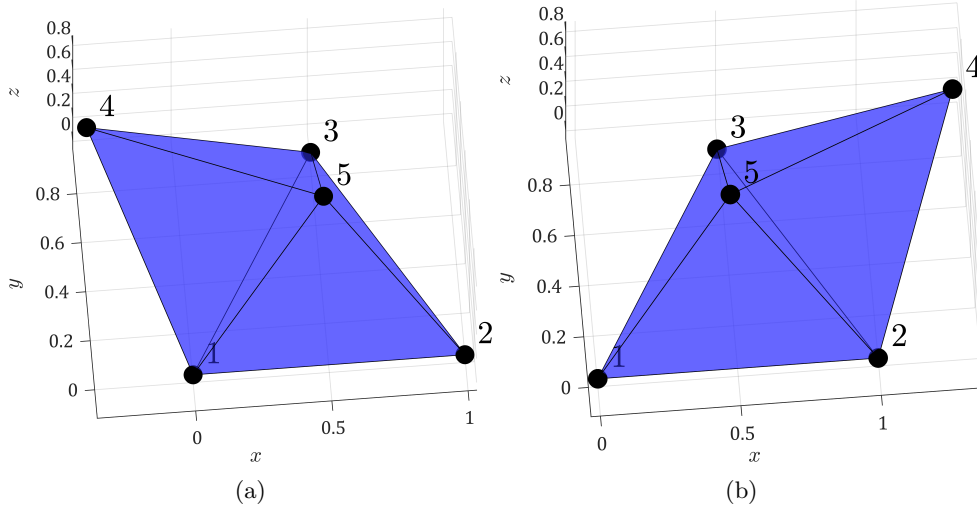


Fig. 9: Two symmetric solutions to the molecular clustering formulation (4.1) with symmetry elimination constraints.

By the above argument, given a solution to (4.1), one can estimate the cardinality of its orbit under Euclidean transformations as the number of triangles in a triangulation of the convex hull of the atomic positions, since the vertices of each triangle can be positioned in the xy -plane. For the putative optima with $5 \leq N \leq 150$, these values are plotted in Figure 10. In reality, these values are likely an underestimation

Atom	Solution (a)	Solution (b)
1	(0, 0, 0)	(0, 0, 0)
2	(0.997907, 0, 0)	(0.997907, 0, 0)
3	(0.502506, 0.866254, 0)	(0.495400, 0.866255, 0)
4	(-0.327898, 0.769087, 0.544798)	(1.325805, 0.769088, 0.544798)
5	(0.502507, 0.287377, 0.817197)	(0.495400, 0.287378, 0.817197)

Table 3: Atomic coordinates in symmetric solutions to (4.1).

of the number of symmetric solutions, since a polyhedral face with more than three vertices admits multiple triangulations.

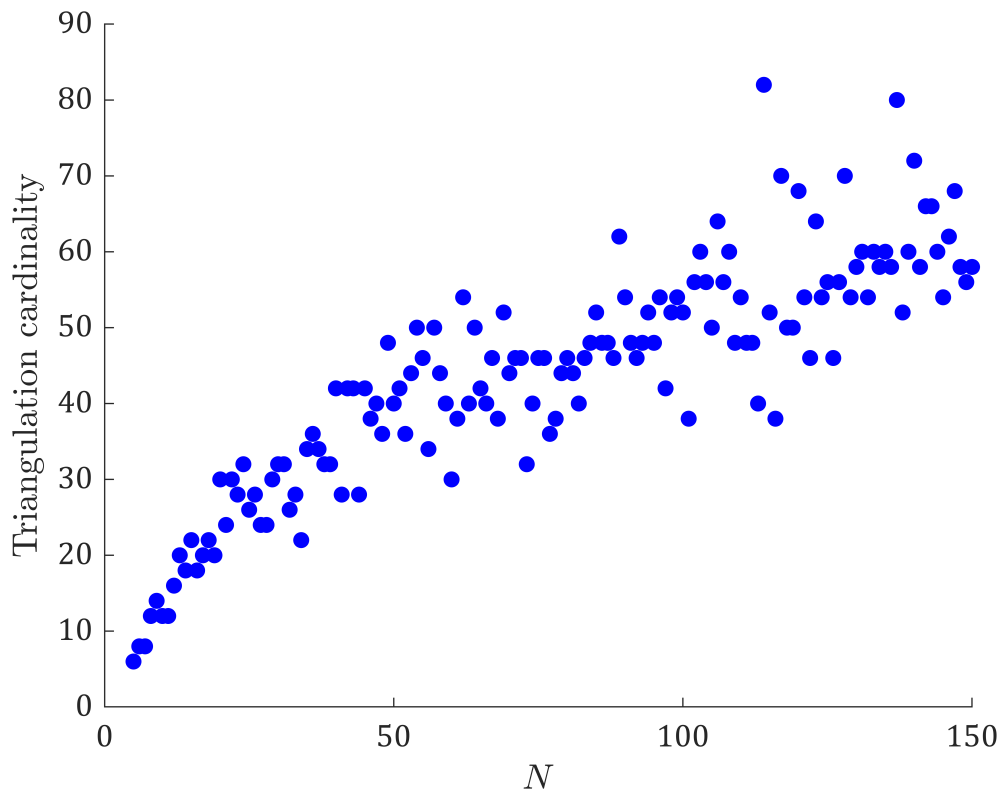


Fig. 10: Number of triangles in triangulations of the convex hulls of putative optima for the molecular clustering problem (4.1) with the Lennard-Jones potential. The strongest known symmetry elimination constraints enforce that three vertices of a facet of the polyhedron formed by atomic positions should be embedded within the xy -plane, but there are in general many choices of which facet.

Moreover, it may be the case that at a solution of (4.1), there exist subsets of vertices with equal z -coordinates. For example, the optimal solution of (4.1) with the Lennard-Jones potential and $N = 6$ is to arrange the atoms at the vertices of a regular octahedron. Then, if atoms 1, 2, and 3 lie in the xy -plane, it follows that

atoms 4, 5, and 6 lie in a plane parallel to it, and the permutation of their positions leads to multiple optimal solutions for (4.1). These symmetries are not accounted for in the quantities shown in Figure 10, so the number of symmetric solutions is likely even higher. Similar variable fixings and orderings have also been used for the circle packing problem [34], in the k -means clustering problem to order clusters by size [143], and in a transformed space for the solution of the Thomson problem [141].

Dynamic symmetry elimination methods have been employed, usually as part of a problem-specific algorithm, to simultaneously eliminate permutational and Euclidean symmetries in some of the problems in `EuclidLib`. For example, Locatelli and Raber [93] developed techniques for the problem of packing equal circles in a square,

$$(4.2) \quad \begin{aligned} \max \quad & r \\ \text{s.t.} \quad & (x_i - x_j)^2 + (y_i - y_j)^2 \geq 4r^2 \quad 1 \leq i < j \leq N \\ & 0 \leq x_i \leq 1, 0 \leq y_i \leq 1 \quad 1 \leq i \leq N \end{aligned}$$

An important step in their symmetry elimination method is to partition the square into a set of smaller squares constructed so that their diagonal is smaller than the largest radius r found so far; this idea was introduced in [122] and also employed in [118]. Then, by construction, at most one circle center can belong to any smaller square in an optimal solution. The algorithm proceeds by considering assignments of circle centers to squares, which can be thought of as a customized branching rule. Crucially, symmetric assignments of circle centers to squares can be pruned in a dynamic manner at each node. This idea is illustrated in Figure 11. First, each square is assigned a unique number. The exact numbering strategy is not important, as long as no two squares share a number. In [93], the square is partitioned into 4^m congruent subsquares, using the smallest value of m such that the condition on the diagonal length is satisfied. The numbering is defined recursively: all numbers in the lower left quadrant of a square are less than all numbers in the lower right quadrant, which in turn are less than all numbers in the upper left quadrant, which are less than all numbers in the upper right quadrant. This numbering scheme is shown in Figure 11(a). Without loss of generality, we can enforce the constraint that circle center i must belong to a lower-numbered square than circle $i + 1$, since any configuration of circles can be renumbered to satisfy this condition. Therefore, once the branch-and-bound node corresponding to the assignments shown in Figure 11(b) has been processed, the node shown in Figure 11(c) can be pruned. The same idea can be applied to nodes related by a Euclidean transformation to one already considered, as shown in Figure 11(d). Moreover, optimality conditions for this problem can be used to eliminate symmetric packings in which a circle is “loose” and may be translated without changing the objective value [129].

Not all `EuclidLib` problems admit Euclidean symmetries; for example, when problem (1.1) includes data a^j , such as in the Euclidean Steiner tree, k -means, and facility location problems, Euclidean isometries of the points x^i do not preserve the objective value in general. Nonetheless, an algorithm capable of detecting and automatically eliminating permutational and Euclidean symmetries simultaneously would likely lead to a significant speedup for `EuclidLib` problems that do have this group structure, including the molecular clustering, kissing number, Thomson, Tammes, and circle packing problems.

4.2. Construction of convex relaxations. The results in Section 3 indicate that standard methods used in global optimization solvers for the construction of convex relaxations typically lead to weak bounds for the problems in `EuclidLib`. As

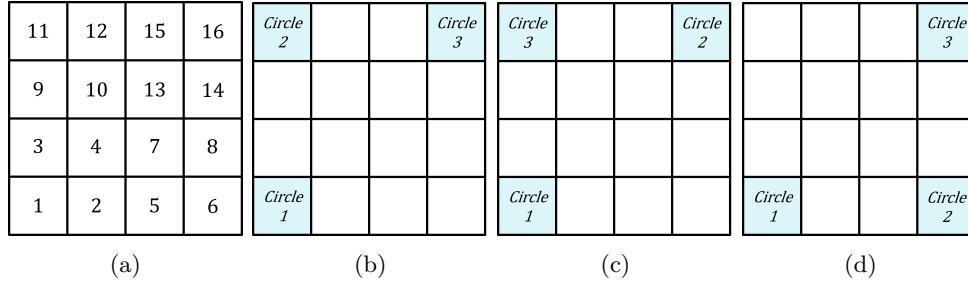


Fig. 11: Nodes in the tree of a custom branch-and-bound method for the problem (4.2) of packing equal circles in a square. By subdividing the square into numbered equal sub-squares such that at most one circle center can belong to each sub-square, Euclidean and permutational symmetries of the problem can be eliminated in a dynamic fashion.

we will show, this is partly due to a reverse convex structure inherent in many of these problems. Constructing a convex relaxation is commonly referred to as convexification. In this section, we define some requisite notions, illustrate the challenges in convexifying these problems, and survey techniques which are capable of generating stronger relaxations.

The terminology of reverse convex programming was introduced by Hillestad and Jacobsen in 1980 [63]. A constraint $f(x) \geq 0$ is called reverse convex when f is quasiconvex (*i.e.*, it has convex sublevel sets); the set $\{x : f(x) \geq 0\}$ described by constraint(s) of this form may also be referred to as reverse convex. Reverse convex sets are well-studied in the optimization literature, in part due to their applications in generating intersection cuts [8], a type of cutting plane based on a valid inequality for a reverse convex set. It is known that the convex hull of a reverse convex set is polyhedral [63], but the computation of high-quality convex relaxations of general reverse convex sets remains an active area of research [162]. For example, the set $\text{conv}\{x \in P : f(x) \geq 0\}$, where $\text{conv} S$ denotes the convex hull of a set S , P is a polytope, and f is a single quadratic function, was characterized only recently [136], and the question of convexifying the intersection of more than one such set is an important open question in the field of quadratic programming [116].

A common approach used within global optimization codes to convexify the set F described by multiple constraints $f_i(x) \geq 0$ is to convexify each constraint individually and to take the intersection of the resulting convex relaxations [105]. Relaxing constraints individually (single-row relaxation) yields a convex set containing F and is popular due to its ease of implementation and applicability to most functions which appear in optimization problems in practice. Since $\text{conv}(\cap_i F_i) \subseteq \cap_i \text{conv}(F_i)$, the relaxation quality can sometimes be significantly improved by the so-called simultaneous convexification of multiple constraints. Simultaneous convexification refers to the convexification of a set given by multiple constraints directly rather than by taking the intersection of convex relaxations of the individual constraints [157]. This approach has been described in the context of polynomial optimization [84] and quadratic bivariate functions [7] and was considered in a more general context in [10].

In the case of `EuclidLib` problems, single-row relaxations often lead to weak dual bounds even when the set described by each constraint is relaxed to its convex hull.

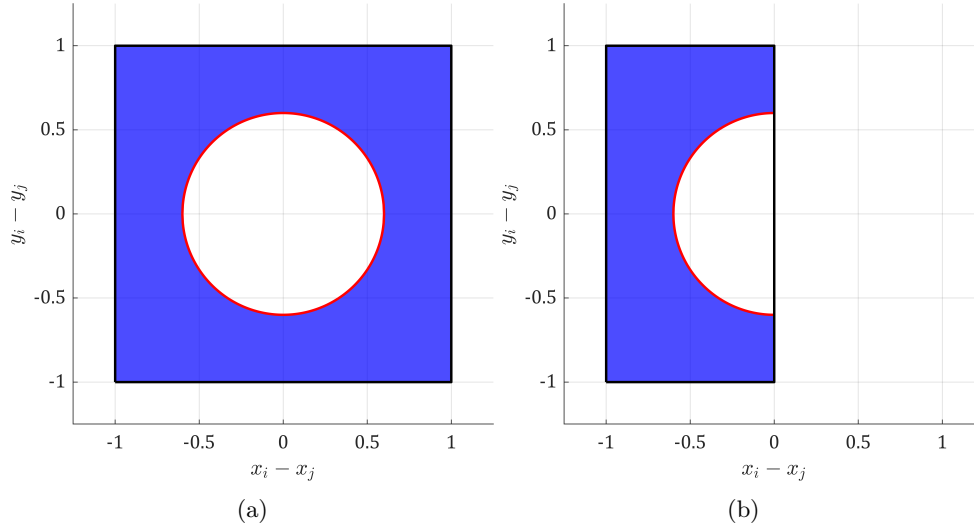


Fig. 12: Projection of the set $\{(x_i, y_i, x_j, y_j) : (x_i - x_j)^2 + (y_i - y_j)^2 \geq 0.36\}$ where (x_i, y_i) and (x_j, y_j) are constrained to the unit square with and without the symmetry elimination constraint $x_i \leq x_j$.

As an illustrative example, consider the circle packing problem in a unit square with identical radii (4.2), and suppose that an incumbent solution with objective value $r^* = 0.3$ has been found. Then, a non-overlap constraint satisfied by every optimal solution is

$$(x_i - x_j)^2 + (y_i - y_j)^2 \geq (2(0.3))^2 = 0.36.$$

At the root node, the centers of circles i and j are both constrained to the unit square, so by interval arithmetic, we can deduce that $(x_i - x_j, y_i - y_j) \in [-1, 1]^2$ in the absence of a symmetry elimination constraint enforcing $x_i \leq x_j$, and $(x_i - x_j, y_i - y_j) \in [-1, 0] \times [-1, 1]$ in the presence of such a constraint. The projection of the set described by the non-overlap constraint onto the $(x_i - x_j, y_i - y_j)$ plane is shown in blue in Figure 12 for these two situations. In both cases, the convex hull of this set is obtained by dropping the non-overlap constraint entirely. For this reason, convexifying (4.2) early in the branch-and-bound tree by relaxing each row separately can lead to very poor relaxations. This geometric structure is not unique to the circle packing problem and is a feature of any set of lower bounds on the Euclidean distances between points constrained to the same domain.

This fact is well known and has motivated the development of numerous strategies to ameliorate the poor quality of single-row relaxations. For example, Wang and Gounaris [170, 169] propose a branching scheme which generates three child nodes based on inscribing an equilateral triangle in the circle given by the non-overlap constraint with an orientation chosen to ensure the infeasibility of a relaxation solution. Then, the feasible set can be partitioned into three regions by branching on linear functions of coordinate differences instead of the usual strategy of branching on coordinates directly. This single-row relaxation strategy was successfully employed along with intersection cuts and a feasibility-based tightening technique to solve circle packing problems with unequal radii to global optimality [169]. In general, a polygon with

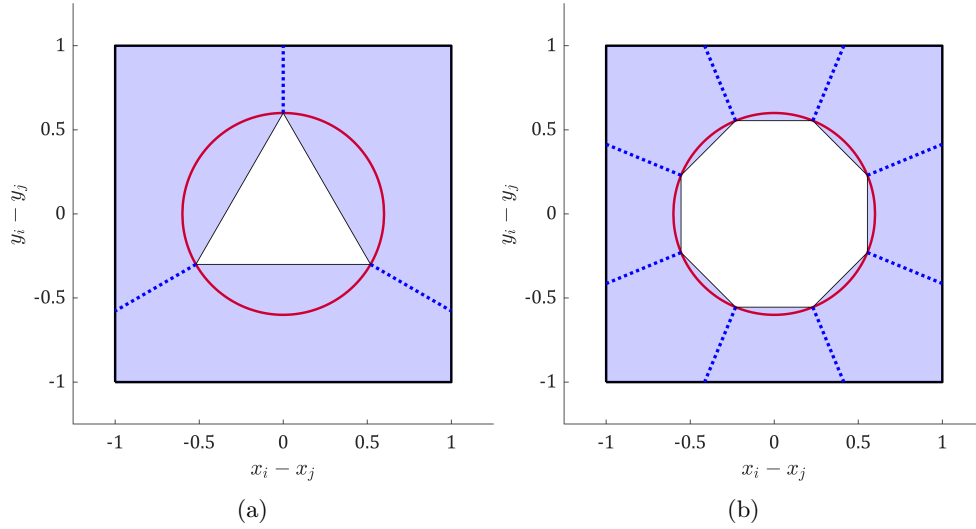


Fig. 13: Custom branching for a reverse convex constraint involving the Euclidean norm based on inscribed polygons. In panel (a), three child nodes are generated by a triangle, whereas in panel (b), eight child nodes are generated by an octagon. Boundaries between child nodes are depicted as blue dashed lines.

more vertices will yield a sharper convex relaxation of the reverse convex non-overlap constraint at the expense of generating more child nodes, as shown in Figure 13.

For the more well-studied case where all circles are of identical radius, simultaneous convexification techniques have been explored. For example, Khajavirad [79] derived sharper variable bounds for circle centers in (4.2) based on symmetry arguments and showed that facet-defining clique inequalities for the Boolean quadric polytope can be used to convexify non-overlap constraints for triplets of circles. The resulting root-node dual bounds were proven to be sharper than those obtained by a single-row relaxation. Though not presented as such, a simultaneous convexification method based on computational geometry techniques was used in [93] for optimality-based domain reduction. To illustrate this approach, consider three circle centers constrained to polytopes X_1 , X_2 , and X_3 , as shown in Figure 14, and suppose a feasible solution to (4.2) has been found with radius r^* . Then, one can calculate the set

$$R_2 = \{x \in X_2 : \|x - y\| < r^* \quad \forall y \in X_1\}$$

and compute the convex hull of $X_2 \setminus R_2$, which is polyhedral since $X_2 \setminus R_2$ is reverse convex [63]. The polytope $X'_2 := \text{conv}(X_2 \setminus R_2)$ can then be used to reduce X_3 by computing

$$\text{conv}(\{x \in X_3 : \|x - y\| < r^* \quad \forall y \in X'_2\})$$

which in turn can be used to further reduce X_1 , which can further reduce X'_2 and so on. In [93], this procedure, called the “wave effect”, was performed twice at each branch-and-bound node and enabled the solution to global optimality of instances of (4.2) up to $N = 39$ (on sub-GHz processors of the time).

Note that the problem of simultaneously convexifying multiple nonconvex con-

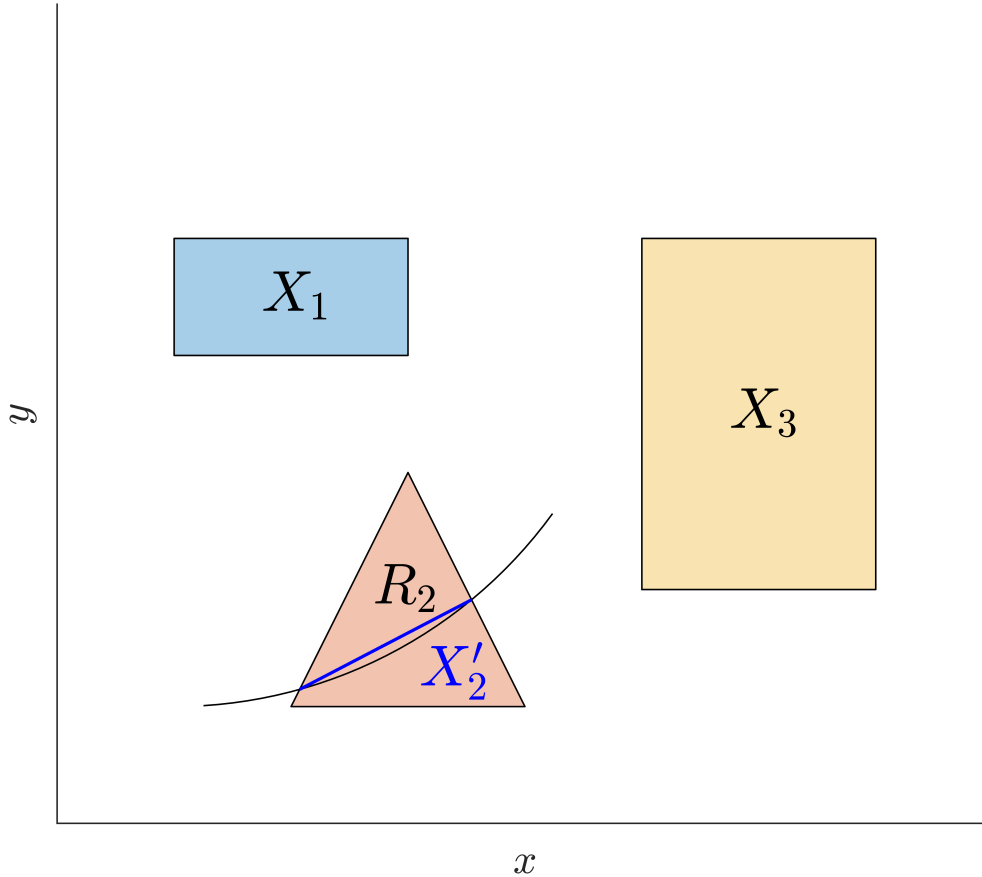


Fig. 14: Optimality-based domain reduction *via* simultaneous convexification.

straints is extremely challenging, which is intuitive since it is related to the problem of deciding the feasibility of a system of nonconvex constraints. The computational success of methods such as the ones described in this section points to the promise of simultaneous convexification, but the problem remains open in general.

5. Opportunities for future research. Considering the challenges outlined in Section 4, we have grouped promising avenues for future research into methods for symmetry elimination and methods for convexification. From the perspective of symmetry elimination, the most challenging problem types in `EuclidLib` are those which admit Euclidean as well as permutational symmetries, *i.e.*, the kissing number, molecular clustering, Thomson, Tammes, and circle packing problems. The symmetry groups of some of these, such as the circle packing problem [34] and kissing number problem [88], have been characterized. However, the most effective known way to eliminate symmetric solutions for these problems is by using custom branch-and-bound codes, which are time-consuming to develop and have limited generalizability. We envision a symmetry elimination algorithm capable of automatically computing symmetry groups for all problems in this class. Ideally, this method should be capable of eliminating all but one optimal solution without prior hard-coding of the instance geometry. In our view, one promising approach to this task is the use of cutting

planes based on fundamental domains of symmetry groups. Following the definition given in [123], given a set X , we say $F \subseteq X$ is a fundamental domain for X under the action of a group G if F contains one element from each orbit under G of each point $x \in X$. One well-known way to define fundamental domains is to make infeasible all elements of each orbit except for the one which minimizes a linear function α ; then, F can be described by the linear inequalities

$$(5.1) \quad \alpha^\top x \leq \alpha^\top g(x)$$

for each $g \in G$. The parameter α should be chosen so that each orbit has a unique minimizer, *i.e.*, the stabilizer of G with respect to α is the identity. In the context of a branch-and-bound algorithm, inequalities (5.1) can be added as cutting planes. The number of possible inequalities depends on the cardinality of G ; for Euclidean isometries, there are infinitely many. However, it may be possible to generate the most violated inequality efficiently by solving a convex optimization problem. For example, if G is a permutation group, the most violated inequality can be found by minimizing the right-hand side of (5.1) over the Birkhoff polytope, which is the convex hull of permutation matrices. Although the set of rotation matrices is nonconvex, its convex hull has been characterized [137] and efficient optimization over this set is an active area of research [185, 130] due to its applications in kinematics [30], computer graphics [103], and satellite positioning [165]. Rather than exactly solving an optimization problem for the most violated inequality (5.1), it may also be possible to solve it approximately and/or generate multiple such inequalities simultaneously. Symmetry detection graphs have also been recently explored for the elimination of symmetric solutions related by a reflection about the center of a box domain, with promising numerical results [65]. The characterization of symmetry groups of `EuclidLib` instances admitting Euclidean symmetries, descriptions of fundamental domains thereof, and algorithms for the efficient generation of valid inequalities for these fundamental domains are all open areas of research; considering the success of symmetry elimination methods in mixed-integer linear programming [123], we believe that these questions constitute a potentially fruitful direction for the community.

Apart from symmetry elimination, the other potentially impactful area for future research efforts is the simultaneous convexification of reverse convex sets defined in terms of the Euclidean norm. In the context of the circle packing problem, the advantages of convexifying multiple non-overlap constraints simultaneously has been shown both empirically [93] and theoretically [79]. Given the recent theoretical advances in the convexification of reverse convex quadratic sets [136, 116], and considering the very specific structure of the squared Euclidean norm as opposed to a general quadratic form, we believe that this challenge is within reach. From an algorithmic point of view, since many `EuclidLib` problems involve the placement of objects within \mathbb{R}^2 or \mathbb{R}^3 , it is our view that insights from computational geometry may be useful in the implementation of simultaneous convexification methods. For example, techniques from computational solid geometry, which is used to compute Boolean operations on solids for 3D modeling software such as computer-aided design programs, could be adapted to this task. Since the intersection of complements of spheres has a very natural Boolean representation, one possible approach to convexifying such a set could be to compute a “safe” mesh approximation (in the sense that it is guaranteed to contain the reverse convex set) and then compute the convex hull thereof using standard efficient algorithms for computing the convex hull of a finite number of points in \mathbb{R}^3 . This approach has the advantage of being extensible to account for linear constraints as well as other norms commonly considered for variants of `EuclidLib`

problems, such as the ℓ_1 norm, which appears in variants of the Steiner tree and planar facility location problems. It requires that the sphere centers be fixed rather than variable, a condition automatically satisfied when the Euclidean distance in question is that between a variable point x^i and a point a^j given as problem data, such as in the k -means or facility location problems. For problems in which $|J| = 0$ and there are no points a^j given as problem data, it is nonetheless possible to geometrically deduce and subsequently convexify reverse convex inequalities from linear constraints on each point x^i , as shown in Figure 14. To see this in general, observe that if X_i is a polytope with vertices v^k , and X_j is also a polytope, then the constraints $x^i \in X_i$ and $x^j \in X_j$, together with the reverse convex constraint $\|x^i - x^j\| \geq r^L$, imply that

$$x^j \in X_j \setminus \bigcap_k B_{r^L}(v^k),$$

where $B_r(x)$ denotes the closed ball of radius r centered at x , which follows from the fact that the maximum of a convex function over a polytope is attained at a vertex. This characterization could provide the basis for a geometric approach to the simultaneous convexification of reverse convex constraints involving the Euclidean distance between two variable points x^i .

6. Conclusions. Nonconvex optimization problems that involve the Euclidean norm arise in myriad contexts in mathematics, science, and engineering, are particularly challenging to solve to global optimality, and include well-known open problems. Although specialized algorithms have been developed over the years for their solution, with few exceptions, they have been limited to small instances. We have compiled a benchmarking library, `EuclidLib`, of instances of this type for use by the global optimization community and have conducted a computational study showing that these problems are currently beyond the reach of general-purpose global optimization solvers. We identified dual bound improvement as a key challenge and showed that the simultaneous presence of multiple symmetry groups as well as the geometric structure of reverse convex sets involving the Euclidean norm contribute to this difficulty. These shared problem structures make the development of symmetry elimination methods, such as those based on fundamental domains, and convexification methods, possibly incorporating insights from computational geometry, applicable to many of the problems within `EuclidLib`. The development of algorithms capable of solving all `EuclidLib` problems to global optimality would represent a remarkable achievement for the field of global optimization as well as a high-impact contribution to fundamental and applied knowledge in a variety of fields.

REFERENCES

- [1] B. ADDIS, M. LOCATELLI, AND F. SCHOEN, *Efficiently packing unequal disks in a circle*, *Operations Research Letters*, 36 (2008), pp. 37–42.
- [2] E. AGRELL AND M. KARLSSON, *Power-efficient modulation formats in coherent transmission systems*, *Journal of Lightwave Technology*, 27 (2009), pp. 5115–5126.
- [3] D. ALOISE, A. DESHPANDE, P. HANSEN, AND P. POPAT, *NP-hardness of Euclidean sum-of-squares clustering*, *Machine Learning*, 75 (2009), pp. 245–248.
- [4] D. ALOISE, P. HANSEN, AND L. LIBERTI, *An improved column generation algorithm for minimum sum-of-squares clustering*, *Mathematical Programming*, 131 (2012), pp. 195–220.
- [5] E. L. ALTSCHULER AND A. PÉREZ-GARRIDO, *Global minimum for Thomson’s problem of charges on a sphere*, *Physical Review E*, 71 (2005), p. 047703.
- [6] M. F. ANJOS AND M. V. C. VIEIRA, *Mathematical optimization approaches for facility layout problems: The state-of-the-art and future research directions*, *European Journal of Operational Research*, 261 (2017), pp. 1–16.

- [7] K. M. ANSTREICHER AND S. BURER, *Computable representations for convex hulls of low-dimensional quadratic forms*, *Mathematical Programming*, 124 (2010), pp. 33–43.
- [8] E. BALAS, *Intersection cuts—A new type of cutting planes for integer programming*, *Operations Research*, 19 (1971), pp. 19–39.
- [9] F. BALETTO AND R. FERRANDO, *Structural properties of nanoclusters: Energetic, thermodynamic, and kinetic effects*, *Reviews of Modern Physics*, 77 (2005), pp. 371–423.
- [10] M. BALLERSTEIN, *Convex Relaxations for Mixed-Integer Nonlinear Programs*, PhD thesis, ETH Zurich, 2013.
- [11] R. BATTA AND U. S. PALEKAR, *Mixed planar/network facility location problems*, *Computers & Operations Research*, 15 (1988), pp. 61–67.
- [12] A. R. BAUSCH, M. J. BOWICK, A. CACCIUTO, A. D. DINSMORE, M. F. HSU, D. R. NELSON, M. G. NIKOLAIDES, A. TRAVESSET, AND D. A. WEITZ, *Grain boundary scars and spherical crystallography*, *Science*, 299 (2003), pp. 1716–1718.
- [13] P. BELOTTI, J. LEE, L. LIBERTI, F. MARGOT, AND A. WÄCHTER, *Branching and bounds tightening techniques for non-convex MINLP*, *Optimization Methods and Software*, 24 (2009), pp. 597–634.
- [14] J. BENNELL, G. SCHEITHAUER, Y. STOYAN, AND T. ROMANOVA, *Tools of mathematical modeling of arbitrary object packing problems*, *Annals of Operations Research*, 179 (2010), pp. 343–368.
- [15] A. J. BERNOFF AND C. M. TOPAZ, *Nonlocal aggregation models: A primer of swarm equilibria*, *SIAM Review*, 55 (2013), pp. 709–747.
- [16] X. BLANC, *Lower bound for the interatomic distance in Lennard-Jones clusters*, *Computational Optimization and Applications*, 29 (2004), pp. 5–12.
- [17] S. BOLUSANI, M. BESANÇON, K. BESTUZHEVA, A. CHMIELA, J. DIONÍSIO, T. DONKIEWICZ, J. VAN DOORNBALLEN, L. EIFLER, M. GHANNAM, A. GLEIXNER, C. GRACZYK, K. HALBIG, I. HEDTKE, A. HOEN, C. HOJNY, R. VAN DER HULST, D. KAMP, T. KOCH, K. KOFLER, J. LENTZ, J. MANNS, G. MEXI, E. MÜHMER, M. E. PFETSCH, F. SCHLÖSSER, F. SERANO, Y. SHINANO, M. TURNER, S. VIGERSKE, D. WENINGER, AND L. XU, *The SCIP optimization suite 9.0*, 2024, <https://arxiv.org/abs/2402.17702>.
- [18] P. BONAMI, L. T. BIEGLER, A. R. CONN, G. CORNUÉJOLS, I. E. GROSSMANN, C. D. LAIRD, J. LEE, A. LODI, F. MARGOT, N. SAWAYA, AND A. WÄCHTER, *An algorithmic framework for convex mixed integer nonlinear programs*, *Discrete Optimization*, 5 (2008), pp. 186–204.
- [19] E. BONNET AND F. SIKORA, *The PACE 2018 parameterized algorithms and computational experiments challenge: The third iteration*, in *IPEC 2018*, Helsinki, Finland, 2018.
- [20] F. BOUKOUVALA, R. MISENER, AND C. A. FLOUDAS, *Global optimization advances in mixed-integer nonlinear programming, MINLP, and constrained derivative-free optimization*, *CDFO*, *European Journal of Operational Research*, 252 (2016), pp. 701–727.
- [21] J. BRIMBERG AND R. F. LOVE, *Global convergence of a generalized iterative procedure for the minimax location problem with l_p distances*, *Operations Research*, 41 (1993), pp. 1153–1163.
- [22] B. R. BROOKS, C. L. BROOKS III, A. D. MACKERELL JR., L. NILSSON, R. J. PETRELLA, B. ROUX, Y. WON, G. ARCHONTIS, C. BARTELS, S. BORESCH, A. CAFLISCH, L. CAVES, Q. CUI, A. R. DINNER, M. FEIG, S. FISCHER, J. GAO, M. HODOSCEK, W. IM, K. KUCZERA, T. LAZARIDIS, J. MA, V. OVCHINNIKOV, E. PACI, R. W. PASTOR, C. B. POST, J. Z. PU, M. SCHAEFER, B. TIDOR, R. M. VENABLE, H. L. WOODCOCK, X. WU, W. YANG, D. M. YORK, AND M. KARPLUS, *CHARMM: The biomolecular simulation program*, *Journal of Computational Chemistry*, 30 (2009), pp. 1545–1614.
- [23] M. R. BUSSIECK, A. S. DRUD, AND A. MEERAUS, *MINLPLib—A collection of test models for mixed-integer nonlinear programming*, *INFORMS Journal on Computing*, 15 (2003), pp. 114–119.
- [24] L. BÉTERMIN, *Minimizing lattice structures for Morse potential energy in two and three dimensions*, *Journal of Mathematical Physics*, 60 (2019), p. 102901.
- [25] P. H. CALAMAI AND A. R. CONN, *A stable algorithm for solving the multifacility location problem involving euclidean distances*, *SIAM Journal on Scientific and Statistical Computing*, 1 (1980), pp. 512–526.
- [26] M. CALEF, W. GRIFFITHS, AND A. SCHULZ, *Estimating the number of stable configurations for the generalized Thomson problem*, *Journal of Statistical Physics*, 160 (2015), pp. 239–253.
- [27] M. CARAMIA, S. GIORDANI, AND A. IOVANELLA, *Grid scheduling by on-line rectangle packing*, *Networks*, 44 (2004), pp. 106–119.
- [28] P. CHEN, P. HANSEN, B. JAUMARD, AND H. TUY, *Weber’s problem with attraction and repulsion*, *Journal of Regional Science*, 32 (1992), pp. 467–486.

- [29] X. CHEN, X. XU, J. Z. HUANG, AND Y. YE, *TW-k-means: Automated two-level variable weighting clustering algorithm for multiview data*, IEEE Transactions on Knowledge and Data Engineering, 25 (2013), pp. 932–944.
- [30] Y. CHEN, S. HUANG, AND R. FITCH, *Active SLAM for mobile robots with area coverage and obstacle avoidance*, IEEE/ASME Transactions on Mechatronics, 25 (2020), pp. 1182–1192.
- [31] N. CHERNOV, Y. STOYAN, AND T. ROMANOVA, *Mathematical model and efficient algorithms for object packing problem*, Computational Geometry, 43 (2010), pp. 535–553.
- [32] R. L. CHURCH AND Z. DREZNER, *Review of obnoxious facilities location problems*, Computers & Operations Research, 138 (2022), p. 105468.
- [33] H. COHN AND A. KUMAR, *Universally optimal distribution of points on spheres*, Journal of the American Mathematical Society, 20 (2007), pp. 99–148.
- [34] A. COSTA, L. LIBERTI, AND P. HANSEN, *Formulation symmetries in circle packing*, Electronic Notes in Discrete Mathematics, 36 (2010), pp. 1303–1310. ISCO 2010—International Symposium on Combinatorial Optimization.
- [35] K. M. CURTIN AND R. L. CHURCH, *A family of location models for multiple-type discrete dispersion*, Geographical Analysis, 38 (2006), pp. 248–270.
- [36] G. DIEHR, *Evaluation of a branch and bound algorithm for clustering*, SIAM Journal on Scientific and Statistical Computing, 6 (1985), pp. 268–284.
- [37] J. P. K. DOYE, D. J. WALES, AND M. A. MILLER, *Thermodynamics and the global optimization of Lennard-Jones clusters*, The Journal of Chemical Physics, 109 (1998), pp. 8143–8153.
- [38] M. DRAŽIĆ, C. LAVOR, N. MACULAN, AND N. MLADENVIĆ, *A continuous variable neighborhood search heuristic for finding the three-dimensional structure of a molecule*, European Journal of Operational Research, 185 (2008), pp. 1265–1273.
- [39] Z. DREZNER AND P. KALCZYNSKI, *Solving nonconvex nonlinear programs with reverse convex constraints by sequential linear programming*, International Transactions in Operational Research, 27 (2020), pp. 1320–1342.
- [40] Z. DREZNER, P. KALCZYNSKI, AND S. SALHI, *The planar multiple obnoxious facilities location problem: A Voronoi based heuristic*, Omega, 87 (2019), pp. 105–116.
- [41] D. DU, B. LU, H. NGO, AND P. M. PARDALOS, *Steiner tree problems*, Springer US, Boston, MA, 2009, pp. 3723–3736.
- [42] O. DU MERLE, P. HANSEN, B. JAUMARD, AND N. MLADENOVIC, *An interior point algorithm for minimum sum-of-squares clustering*, SIAM Journal on Scientific Computing, 21 (1999), pp. 1485–1505.
- [43] H. A. EISELT AND V. MARIANOV, *Mobile phone tower location for survival after natural disasters*, European Journal of Operational Research, 216 (2012), pp. 563–572.
- [44] E. ERKUT AND S. NEUMAN, *Comparison of four models for dispersing facilities*, INFOR: Information Systems and Operational Research, 29 (1991), pp. 68–86.
- [45] J. W. EYSTER AND J. A. WHITE, *Some properties of the squared Euclidean distance location problem*, AIIE Transactions, 5 (1973), pp. 275–280.
- [46] M. FAMPA, *Insight into the computation of Steiner minimal trees in Euclidean space of general dimension*, Discrete Applied Mathematics, 308 (2022), pp. 4–19.
- [47] M. FAMPA, J. LEE, AND W. MELO, *A specialized branch-and-bound algorithm for the Euclidean Steiner tree problem in n -space*, Computational Optimization and Applications, 65 (2016), pp. 47–71.
- [48] M. FAMPA AND N. MACULAN, *Using a conic formulation for finding Steiner minimal trees*, Numerical Algorithms, 35 (2004), pp. 315–330.
- [49] FICO, *FICO Xpress Optimizer Reference Manual*, 2024, <https://www.fico.com/en/products/fico-xpress-optimization>.
- [50] J. J. FLORES, J. MARTÍNEZ, AND F. CALDERÓN, *Evolutionary computation solutions to the circle packing problem*, Soft Computing, 20 (2016), pp. 1521–1535.
- [51] R. J. FOWLER, M. S. PATERSON, AND S. L. TANIMOTO, *Optimal packing and covering in the plane are NP-complete*, Information Processing Letters, 12 (1981), pp. 133–137.
- [52] K. FUKUNAGA, P. NARENDRA, AND W. KOONTZ, *A branch and bound clustering algorithm*, IEEE Transactions on Computers, 24 (1975), pp. 908–915.
- [53] T. FURUTA, M. SASAKI, F. ISHIZAKI, A. SUZUKI, AND H. MIYAZAWA, *A new clustering model of wireless sensor networks using facility location theory*, Journal of the Operations Research Society of Japan, 52 (2009), pp. 366–376.
- [54] M. R. GAREY, R. L. GRAHAM, AND D. S. JOHNSON, *The complexity of computing Steiner minimal trees*, SIAM Journal on Applied Mathematics, 32 (1977), pp. 835–859.
- [55] GUROBI OPTIMIZATION, LLC, *Gurobi Optimizer Reference Manual*, 2024, <https://www.gurobi.com>.

- [56] J. GÖRTLER, C. SCHULZ, D. WEISKOPF, AND O. DEUSSEN, *Bubble treemaps for uncertainty visualization*, IEEE Transactions on Visualization and Computer Graphics, 24 (2018), pp. 719–728.
- [57] K. HADJ SALEM, E. SILVA, J. F. OLIVEIRA, AND M. A. CARRAVILLA, *Mathematical models for the two-dimensional variable-sized cutting stock problem in the home textile industry*, European Journal of Operational Research, 306 (2023), pp. 549–566.
- [58] A. W. A. HAMMAD, A. AKBARNEZHAD, AND D. REY, *Sustainable urban facility location: Minimising noise pollution and network congestion*, Transportation Research Part E: Logistics and Transportation Review, 107 (2017), pp. 38–59.
- [59] P. HANSEN, B. JAUMARD, AND N. MLADENOVIC, *Minimum sum of squares clustering in a low dimensional space*, Journal of Classification, 15 (1998), pp. 37–55.
- [60] P. HANSEN AND N. MLADENOVIC, *J-means: A new local search heuristic for minimum sum of squares clustering*, Pattern Recognition, 34 (2001), pp. 405–413.
- [61] K. HE, M. HUANG, AND C. YANG, *An action-space-based global optimization algorithm for packing circles into a square container*, Computers & Operations Research, 58 (2015), pp. 67–74.
- [62] M. HIFI AND R. M'HALLAH, *A literature review on circle and sphere packing problems: Models and methodologies*, Advances in Operations Research, 2009 (2009), p. 150624.
- [63] R. J. HILLESTAD AND S. E. JACOBSEN, *Reverse convex programming*, Applied Mathematics and Optimization, 6 (1980), pp. 63–78.
- [64] M. HOARE AND P. PAL, *Physical cluster mechanics: Statics and energy surfaces for monatomic systems*, Advances in Physics, 20 (1971), pp. 161–196.
- [65] C. HOJNY, *Detecting and handling reflection symmetries in mixed-integer (nonlinear) programming*, 2024, <https://optimization-online.org/?p=26398>.
- [66] J. D. HONEYCUTT AND H. C. ANDERSEN, *Molecular dynamics study of melting and freezing of small Lennard-Jones clusters*, Journal of Physical Chemistry, 91 (1987), pp. 4950–4963.
- [67] X. HU, J. LI, AND J. CUI, *Greedy adaptive search: A new approach for large-scale irregular packing problems in the fabric industry*, IEEE Access, 8 (2020), pp. 91476–91487.
- [68] W. HUANG AND T. YE, *Quasi-physical global optimization method for solving the equal circle packing problem*, Science China Information Sciences, 54 (2011), pp. 1333–1339.
- [69] F. K. HWANG, D. S. RICHARDS, AND P. WINTER, *The Steiner tree problem*, North-Holland, Amsterdam, 1992.
- [70] A. M. IKOTUN, A. E. EZUGWU, L. ABUALIGAH, B. ABUHALJA, AND J. HEMING, *K-means clustering algorithms: A comprehensive review, variants analysis, and advances in the era of big data*, Information Sciences, 622 (2023), pp. 178–210.
- [71] A. IORIO AND S. SEN, *Scar-driven shape-changes of virus capsids*, Central European Journal of Biology, 3 (2008), pp. 380–387.
- [72] J. N. ISRAELACHVILI, *6—van der Waals forces*, in Intermolecular and Surface Forces (Third Edition), Academic Press, San Diego, third edition ed., 2011, pp. 107–132.
- [73] J. N. ISRAELACHVILI, *7—repulsive steric forces, total intermolecular pair potentials, and liquid structure*, in Intermolecular and Surface Forces (Third Edition), Academic Press, San Diego, third edition ed., 2011, pp. 133–149.
- [74] D. R. JONES, *A fully general, exact algorithm for nesting irregular shapes*, Journal of Global Optimization, 59 (2014), pp. 367–404.
- [75] J. E. JONES AND S. CHAPMAN, *On the determination of molecular fields.—I. From the variation of the viscosity of a gas with temperature*, Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character, 106 (1924), pp. 441–462.
- [76] S. Y. JOSHI AND S. A. DESHMUKH, *A review of advancements in coarse-grained molecular dynamics simulations*, Molecular Simulation, 47 (2021), pp. 786–803.
- [77] D. JUHL, D. M. WARME, P. WINTER, AND M. ZACHARIASEN, *The GeoSteiner software package for computing Steiner trees in the plane: An updated computational study*, Mathematical Programming Computation, 10 (2018), pp. 487–532.
- [78] P. KALCZYNSKI AND Z. DREZNER, *Extremely non-convex optimization problems: The case of the multiple obnoxious facilities location*, Optimization Letters, 16 (2022), pp. 1153–1166.
- [79] A. KHAJAVIRAD, *The circle packing problem: A theoretical comparison of various convexification techniques*, 2024, <https://arxiv.org/abs/2404.03091>.
- [80] K. KRISHNA AND M. NARASIMHA MURTY, *Genetic k-means algorithm*, IEEE Transactions on Systems, Man, and Cybernetics, Part B (Cybernetics), 29 (1999), pp. 433–439.
- [81] S. KUCHERENKO, P. BELOTTI, L. LIBERTI, AND N. MACULAN, *New formulations for the kissing number problem*, Discrete Applied Mathematics, 155 (2007), pp. 1837–1841. 3rd Cologne/Twente Workshop on Graphs and Combinatorial Optimization.

- [82] A. B. J. KUIJLAARS AND E. B. SAFF, *Asymptotics for minimal discrete energy on the sphere*, Transactions of the American Mathematical Society, 350 (1998), pp. 523–528.
- [83] J. A. D. A. L. J. P. ARAÚJO, E. ÖZCAN AND M. BAUMERS, *Analysis of irregular three-dimensional packing problems in additive manufacturing: A new taxonomy and dataset*, International Journal of Production Research, 57 (2019), pp. 5920–5934.
- [84] J. B. LASSERRE, *Global optimization with polynomials and the problem of moments*, SIAM Journal on Optimization, 11 (2001), p. 796–817.
- [85] J. LEECH AND N. SLOANE, *Sphere packings and error-correcting codes*, Canadian Journal of Mathematics, 23 (1971), pp. 718–745.
- [86] M. LEWIN AND X. BLANC, *The crystallization conjecture: A review*, EMS Surveys in Mathematical Sciences, 2 (2015), pp. 255–306.
- [87] H. LI, H. HE, AND Y. WEN, *Dynamic particle swarm optimization and k-means clustering algorithm for image segmentation*, Optik, 126 (2015), pp. 4817–4822.
- [88] L. LIBERTI, *Symmetry in mathematical programming*, in Mixed Integer Nonlinear Programming, New York, NY, 2012, Springer New York, pp. 263–283.
- [89] L. LIBERTI, *Mathematical programming bounds for kissing numbers*, in Optimization and Decision Science: Methodologies and Applications, A. Sforza and C. Sterle, eds., Cham, 2017, Springer International Publishing, pp. 213–222.
- [90] L. LIBERTI AND J. OSTROWSKI, *Stabilizer-based symmetry breaking constraints for mathematical programs*, Journal of Global Optimization, 60 (2014), pp. 183–194.
- [91] Y. LIN AND L. SCHRAGE, *The global solver in the LINDO API*, Optimization Methods and Software, 24 (2009), pp. 657–668.
- [92] M. LOCATELLI, *A new approach to the multiple obnoxious facility location problem based on combinatorial and continuous tools*, Optimization Letters, 18 (2024), pp. 873–887.
- [93] M. LOCATELLI AND U. RABER, *Packing equal circles in a square: A deterministic global optimization approach*, Discrete Applied Mathematics, 122 (2002), pp. 139–166.
- [94] F. C. MACHADO AND F. M. DE OLIVEIRA FILHO, *Improving the semidefinite programming bound for the kissing number by exploiting polynomial symmetry*, Experimental Mathematics, 27 (2018), pp. 362–369.
- [95] J. MACQUEEN, *Some methods for classification and analysis of multivariate observations*, in Proceedings of the fifth Berkeley symposium on mathematical statistics and probability, vol. 1, Oakland, CA, USA, 1967, pp. 281–297.
- [96] N. MACULAN, P. MICHELON, AND J. M. SMITH, *Bounds on the kissing numbers in R^n : mathematical programming formulations*, tech. report, University of Massachusetts Amherst, 1996.
- [97] M. MAHAJAN, P. NIMBORKAR, AND K. VARADARAJAN, *The planar k-means problem is NP-hard*, in WALCOM: Algorithms and Computation, Berlin, Heidelberg, 2009, Springer Berlin Heidelberg, pp. 274–285.
- [98] C. D. MARANAS AND C. A. FLOUDAS, *A global optimization approach for Lennard-Jones microclusters*, The Journal of Chemical Physics, 97 (1992), pp. 7667–7678.
- [99] C. D. MARANAS AND C. A. FLOUDAS, *A Global Optimization Method For Weber’s Problem With Attraction And Repulsion*, Springer US, Boston, MA, 1994, pp. 259–285.
- [100] F. MARGOT, *Exploiting orbits in symmetric ILP*, Mathematical Programming, 98 (2003), pp. 3–21.
- [101] M. C. MARKÓT, *Interval methods for verifying structural optimality of circle packing configurations in the unit square*, Journal of Computational and Applied Mathematics, 199 (2007), pp. 353–357.
- [102] M. C. MARKÓT AND T. CSENDES, *A reliable area reduction technique for solving circle packing problems*, Computing, 77 (2006), pp. 147–162.
- [103] H. MARON, N. DYM, I. KEZURER, S. KOVALSKY, AND Y. LIPMAN, *Point registration via efficient convex relaxation*, ACM Transactions on Graphics, 35 (2016), pp. 1–12.
- [104] A. MARTÍNEZ-FINKELSHTEIN, V. MAYMESKUL, E. A. RAKHMANOV, AND E. B. SAFF, *Asymptotics for minimal discrete Riesz energy on curves in R^d* , Canadian Journal of Mathematics, 56 (2004), p. 529–552.
- [105] G. P. MCCORMICK, *Computability of global solutions to factorable nonconvex programs: Part I—Convex underestimating problems*, Mathematical Programming, 10 (1976), pp. 147–175.
- [106] N. MEGIDDO AND K. J. SUPOWIT, *On the complexity of some common geometric location problems*, SIAM Journal on Computing, 13 (1984), pp. 182–196.
- [107] D. MEHTA, J. CHEN, D. Z. CHEN, H. KUSUMAATMAJA, AND D. J. WALES, *Kinetic transition networks for the Thomson Problem and Smale’s seventh problem*, Physical Review Letters, 117 (2016), p. 028301.

- [108] E. MELACHRINOUDIS AND T. P. CULLINANE, *Locating an undesirable facility with a minimax criterion*, European Journal of Operational Research, 24 (1986), pp. 239–246.
- [109] R. MISENER AND C. A. FLOUDAS, *ANTIGONE: Algorithms for continuous / integer global optimization of nonlinear equations*, Journal of Global Optimization, 59 (2014), pp. 503–526.
- [110] R. P. MONDAINI, *The Steiner Tree Problem and its Application to the Modelling of Biomolecular Structures*, Springer Berlin Heidelberg, Berlin, Heidelberg, 2008, pp. 199–219.
- [111] J. R. MORRIS, D. M. DEAVEN, AND K. M. HO, *Genetic-algorithm energy minimization for point charges on a sphere*, Physical Review B, 53 (1996), pp. R1740–R1743.
- [112] P. M. MORSE, *Diatomic molecules according to the wave mechanics. II. Vibrational levels*, Physical Review, 34 (1929), pp. 57–64.
- [113] A. T. MURRAY, R. L. CHURCH, R. A. GERRARD, AND W. TSUI, *Impact models for siting undesirable facilities*, Papers in Regional Science, 77 (1998), pp. 19–36.
- [114] O. R. MUSIN, *The kissing number in four dimensions*, Annals of Mathematics, 168 (2008), pp. 1–32.
- [115] O. R. MUSIN AND A. S. TARASOV, *The Tammes problem for $N = 14$* , Experimental Mathematics, 24 (2015), pp. 460–468.
- [116] G. MUÑOZ AND F. SERRANO, *Maximal quadratic-free sets*, Mathematical Programming, 192 (2022), pp. 229–270.
- [117] A. NEUMAIER, *Molecular modeling of proteins and mathematical prediction of protein structure*, SIAM Review, 39 (1997), pp. 407–460.
- [118] K. J. NURMELA AND P. R. J. OSTERGÅRD, *More optimal packings of equal circles in a square*, Discrete & Computational Geometry, 22 (1999), pp. 439–457.
- [119] OCTERACT, *Octeract Engine Reference Manual*, 2024, <https://octeract.gg/>.
- [120] J. OSTROWSKI, *Using symmetry to optimize over the Sherali–Adams relaxation*, Mathematical Programming Computation, 6 (2014), pp. 405–428.
- [121] M. L. OVERTON, *A quadratically convergent method for minimizing a sum of Euclidean norms*, Mathematical Programming, 27 (1983), pp. 34–63.
- [122] R. PEIKERT, D. WÜRTZ, M. MONAGAN, AND C. DE GROOT, *Packing circles in a square: A review and new results*, in System Modelling and Optimization, Berlin, Heidelberg, 1992, Springer Berlin Heidelberg, pp. 45–54.
- [123] M. E. PFETSCH AND T. REHN, *A computational comparison of symmetry handling methods for mixed integer programs*, Mathematical Programming Computation, 11 (2019), pp. 37–93.
- [124] V. PICCIALLI, A. RUSSO RUSSO, AND A. M. SUDOSO, *An exact algorithm for semi-supervised minimum sum-of-squares clustering*, Computers & Operations Research, 147 (2022), p. 105958.
- [125] V. PICCIALLI, A. M. SUDOSO, AND A. WIEGELE, *SOS-SDP: An exact solver for minimum sum-of-squares clustering*, INFORMS Journal on Computing, 34 (2022), pp. 2144–2162.
- [126] F. PLASTRIA, *Optimal location of undesirable facilities: A selective overview*, Belgian Journal of Operations Research, Statistics, and Computer Science, 36 (1996), pp. 109–127.
- [127] Y. K. D. V. PRASAD, S. SOMASUNDARAM, AND K. P. RAO, *A sliding algorithm for optimal nesting of arbitrarily shaped sheet metal blanks*, International Journal of Production Research, 33 (1995), pp. 1505–1520.
- [128] J. PÉREZ-ORTEGA, N. N. ALMANZA-ORTEGA, A. VEGA-VILLALOBOS, R. PAZOS-RANGEL, C. ZAVALA-DÍAZ, AND A. MARTÍNEZ-REBOLLAR, *The k-means algorithm evolution*, in Introduction to Data Science and Machine Learning, K. Sud, P. Erdogmus, and S. Kadry, eds., IntechOpen, Rijeka, 2019, ch. 5.
- [129] U. RABER, *Nonconvex All-Quadratic Global Optimization Problems: Solution Methods, Application and Related Topics*, PhD thesis, University of Trier, 1999.
- [130] A. RAMACHANDRAN, K. SHU, AND A. L. WANG, *Hidden convexity, optimization, and algorithms on rotation matrices*, 2024, <https://arxiv.org/abs/2304.08596>.
- [131] M. R. RAO, *Cluster analysis and mathematical programming*, Journal of the American Statistical Association, 66 (1971), pp. 622–626.
- [132] G. ROBINS AND A. ZELIKOVSKY, *Handbook of Algorithms for Physical Design Automation*, Auerbach Publications, New York, NY, 2019, ch. 24, pp. 487–508.
- [133] G. G. RONDINA AND J. L. F. DA SILVA, *Revised basin-hopping Monte Carlo algorithm for structure optimization of clusters and nanoparticles*, Journal of Chemical Information and Modeling, 53 (2013), pp. 2282–2298.
- [134] M. RUAN, C. SHEN, J. TANG, C. QI, AND S. QIU, *A double traveling salesman problem with three-dimensional loading constraints for bulky item delivery*, IEEE Access, 9 (2021), pp. 13052–13063.
- [135] N. V. SAHINIDIS, *BARON: A general purpose global optimization software package*, Journal

- of Global Optimization, 8 (1996), pp. 201–205.
- [136] A. SANTANA AND S. S. DEY, *The convex hull of a quadratic constraint over a polytope*, SIAM Journal on Optimization, 30 (2020), pp. 2983–2997.
- [137] J. SAUNDERSON, P. A. PARRILO, AND A. S. WILLSKY, *Semidefinite descriptions of the convex hull of rotation matrices*, SIAM Journal on Optimization, 25 (2015), pp. 1314–1343.
- [138] A. SAXENA, M. PRASAD, A. GUPTA, N. BHARILL, O. P. PATEL, A. TIWARI, M. J. ER, W. DING, AND C. LIN, *A review of clustering techniques and developments*, Neurocomputing, 267 (2017), pp. 664–681.
- [139] G. SCHEITHAUER, *Introduction to Cutting and Packing Optimization: Problems, Modeling Approaches, Solution Methods*, Springer Nature, Cham, Switzerland, 2018.
- [140] K. SCHÜTTE AND B. L. VAN DER WAERDEN, *Das problem der dreizehn kugeln*, Mathematische Annalen, 125 (1953), pp. 325–334.
- [141] R. E. SCHWARTZ, *The five-electron case of Thomson’s problem*, Experimental Mathematics, 22 (2013), pp. 157–186.
- [142] P. SCHWERDTFEGGER AND D. J. WALES, *100 Years of the Lennard-Jones Potential*, Journal of Chemical Theory and Computation, 20 (2024), pp. 3379–3405.
- [143] H. D. SHERALI AND J. DESAI, *A global optimization RLT-based approach for solving the hard clustering problem*, Journal of Global Optimization, 32 (2005), pp. 281–306.
- [144] H. D. SHERALI AND C. H. TUNCBILEK, *A squared-Euclidean distance location-allocation problem*, Naval Research Logistics, 39 (1992), pp. 447–469.
- [145] M. SHUB AND S. SMALE, *Complexity of Bezout’s theorem: III. Condition number and packing*, Journal of Complexity, 9 (1993), pp. 4–14.
- [146] F. T. SILVA, M. X. SILVA, AND J. C. BELCHIOR, *A new genetic algorithm approach applied to atomic and molecular cluster studies*, Frontiers in Chemistry, 7 (2019), pp. 1–21.
- [147] S. SMALE, *Mathematical problems for the next century*, The Mathematical Intelligencer, 20 (1998), pp. 7–15.
- [148] J. M. SMITH, *Steiner Minimum Trees in E3: Theory, Algorithms, and Applications*, Springer New York, New York, NY, 2013, pp. 3179–3259.
- [149] J. M. SMITH AND J. S. LIEBMAN, *Steiner trees, Steiner circuits and the interference problem in building design*, Engineering Optimization, 4 (1979), pp. 15–36.
- [150] E. SPECHT, *Packomania*. <http://www.packomania.com/>.
- [151] D. STEINLEY, *K-means clustering: A half-century synthesis*, British Journal of Mathematical and Statistical Psychology, 59 (2006), pp. 1–34.
- [152] K. SUGIHARA, M. SAWAI, H. SANO, D. KIM, AND D. KIM, *Disk packing for the estimation of the size of a wire bundle*, Japan Journal of Industrial and Applied Mathematics, 21 (2004), pp. 259–278.
- [153] P. G. SZABÓ, M. C. MARKÓT, AND T. CSENDES, *Global Optimization in geometry—Circle packing into the square*, Springer US, Boston, MA, 2005, pp. 233–265.
- [154] G. G. SZPIRO, *Newton and the kissing problem*, Maths Plus Magazine, (2003), <https://plus.maths.org/content/newton-and-kissing-problem>.
- [155] J. Y. T. H. CUONG AND N. D. YEN, *Qualitative properties of the minimum sum-of-squares clustering problem*, Optimization, 69 (2020), pp. 2131–2154.
- [156] P. M. L. TAMMES, *On the origin of number and arrangement of the places of exit on the surface of pollen-grains*, Recueil des travaux botaniques néerlandais, 27 (1930), pp. 1–84.
- [157] M. TAWARMALANI, *Inclusion certificates and simultaneous convexification of functions*. Working paper, 2010, <https://optimization-online.org/2010/09/2722/>.
- [158] A. TERAN-SOMOHANO AND A. E. SMITH, *Locating multiple capacitated semi-obnoxious facilities using evolutionary strategies*, Computers & Industrial Engineering, 133 (2019), pp. 303–316.
- [159] J. J. THOMSON, *XXIV. On the structure of the atom: An investigation of the stability and periods of oscillation of a number of corpuscles arranged at equal intervals around the circumference of a circle; with application of the results to the theory of atomic structure*, The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science, 7 (1904), pp. 237–265.
- [160] C. M. TOPAZ, A. J. BERNOFF, S. LOGAN, AND W. TOOLSON, *A model for rolling swarms of locusts*, The European Physical Journal Special Topics, 157 (2008), pp. 109–157.
- [161] S. TORQUATO, *Perspective: Basic understanding of condensed phases of matter via packing models*, Journal of Chemical Physics, 149 (2018), p. 020901.
- [162] E. TOWLE AND J. LUEDTKE, *Intersection disjunctions for reverse convex sets*, Mathematics of Operations Research, 47 (2022), pp. 297–319.
- [163] A. TRAVESSET, *Phase diagram of power law and Lennard-Jones systems: Crystal phases*, The Journal of Chemical Physics, 141 (2014), p. 164501.

- [164] H. TUY, F. AL-KHAYYAL, AND F. ZHOU, *A D.C. optimization method for single facility location problems*, Journal of Global Optimization, 7 (1995), pp. 209–227.
- [165] G. WAHBA, *A least squares estimate of satellite attitude*, SIAM Review, 7 (1965), pp. 409–409.
- [166] D. J. WALES AND J. P. K. DOYE, *Global optimization by basin-hopping and the lowest energy structures of Lennard-Jones clusters containing up to 110 atoms*, The Journal of Physical Chemistry A, 101 (1997), pp. 5111–5116.
- [167] D. J. WALES, J. P. K. DOYE, A. DULLWEBER, M. P. HODGES, F. Y. NAUMKIN, F. CALVO, J. HERNÁNDEZ-ROJAS, AND T. F. MIDDLETON, *The Cambridge Cluster Database*, 2004, <http://www-wales.ch.cam.ac.uk/CCD.html>.
- [168] D. J. WALES AND S. ULKER, *Structure and dynamics of spherical crystals characterized for the Thomson problem*, Physical Review B, 74 (2006), p. 212101.
- [169] A. WANG AND C. E. GOUNARIS, *On tackling reverse convex constraints for non-overlapping of unequal circles*, Journal of Global Optimization, 80 (2021), pp. 357–385.
- [170] A. WANG, C. L. HANSELMAN, AND C. E. GOUNARIS, *A customized branch-and-bound approach for irregular shape nesting*, Journal of Global Optimization, 71 (2018), pp. 935–955.
- [171] J. WANG, *Packing of unequal spheres and automated radiosurgical treatment planning*, Journal of Combinatorial Optimization, 3 (1999), pp. 453–463.
- [172] J. WANG, R. M. WOLF, J. W. CALDWELL, P. A. KOLLMAN, AND D. A. CASE, *Development and testing of a general amber force field*, Journal of Computational Chemistry, 25 (2004), pp. 1157–1174.
- [173] Y. WANG, J. LV, L. ZHU, AND Y. MA, *Crystal structure prediction via particle-swarm optimization*, Physical Review B, 82 (2010), p. 094116.
- [174] A. WEBER AND C. J. FRIEDRICH, *Alfred Weber’s theory of the location of industries*, University of Chicago Press, 1929.
- [175] S. B. WELCH, S. SALHI, AND Z. DREZNER, *The multifacility maximin planar location problem with facility interaction*, IMA Journal of Management Mathematics, 17 (2008), pp. 397–412.
- [176] E. WIESZFELD, *Sur le point pour lequel la somme des distances de n points donnés est minimum*, Tohoku Mathematical Journal, First Series, 43 (1937), pp. 355–386.
- [177] M. E. WILHELM AND M. D. STUBER, *EAGO.jl: Easy advanced global optimization in Julia*, Optimization Methods and Software, 37 (2022), pp. 425–450.
- [178] L. T. WILLE, *Minimum-energy configurations of atomic clusters: New results obtained by simulated annealing*, Chemical Physics Letters, 133 (1987), pp. 405–410.
- [179] L. T. WILLE AND J. VENNIK, *Computational complexity of the ground-state determination of atomic clusters*, Journal of Physics A: Mathematical and General, 18 (1985), p. L419.
- [180] P. WINTER AND M. ZACHARIASEN, *Euclidean Steiner minimum trees: An improved exact algorithm*, Networks, 30 (1997), pp. 149–166.
- [181] Y. XIANG AND X. G. GONG, *Efficiency of generalized simulated annealing*, Physical Review E, 62 (2000), pp. 4473–4476.
- [182] Y. XIANG, H. JIANG, W. CAI, AND X. SHAO, *An efficient method based on lattice construction and the genetic algorithm for optimization of large Lennard-Jones clusters*, The Journal of Physical Chemistry A, 108 (2004), pp. 3586–3592.
- [183] G. XUE, *Molecular conformation on the CM-5 by parallel two-level simulated annealing*, Journal of Global Optimization, 4 (1994), pp. 187–208.
- [184] J. YAN AND Z. CHEN, *Electromigration-aware rectilinear Steiner tree construction for analog circuits*, in APCCAS 2008 - 2008 IEEE Asia Pacific Conference on Circuits and Systems, 2008, pp. 1692–1695.
- [185] H. YANG AND L. CARLONE, *A quaternion-based certifiably optimal solution to the Wahba problem with outliers*, in Proceedings of the IEEE/CVF International Conference on Computer Vision (ICCV), October 2019.
- [186] D. YIN AND A. D. MACKERELL JR., *Combined ab initio/empirical approach for optimization of Lennard-Jones parameters*, Journal of Computational Chemistry, 19 (1998), pp. 334–348.
- [187] S. A. YUHJTMAN, *A sensible estimate for the stability constant of the Lennard-Jones potential*, Journal of Statistical Physics, 160 (2015), pp. 1684–1695.
- [188] E. E. ZACHARIADIS, C. D. TARANTILIS, AND C. T. KIRANOUDIS, *Integrated distribution and loading planning via a compact metaheuristic algorithm*, European Journal of Operational Research, 228 (2013), pp. 56–71.
- [189] R. ZANDI, D. REGUERA, R. F. BRUINSMA, W. M. GELBART, AND J. RUDNICK, *Origin of icosahedral symmetry in viruses*, Proceedings of the National Academy of Sciences, 101 (2004), pp. 15556–15560.