The Kissing Number Problem: A New Result from Global Optimization

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Abstract

Determining the maximum number of D-dimensional spheres of radius r that can be adjacent to a central sphere of radius r is known as the Kissing Number Problem (KNP). The problem has been solved for 2 and 3 dimensions. The smallest open case is 4 dimensions: a solution with 24 spheres is known, and an upper bound of 25 has been found. We present a new nonlinear mathematical programming model for the solution of the KNP. This problem is solved using a quasi Monte Carlo variant of a multi level single linkage algorithm for global optimization. The numerical results indicate that the solution of the KNP is 24 spheres, and not 25.

1 Introduction

When rigid balls touch each other, in technical terms, they “kiss”. This is the etimology of the term “kissing number”. In mathematical terms, the *kissing number* in D dimensions is the number of D-spheres of radius R that can be arranged around a central D-sphere of radius R so that each of the surrounding spheres touches the central one without overlapping. Determining the maximum kissing number in various dimensions has become a well-known problem in Combinatorial Geometry.

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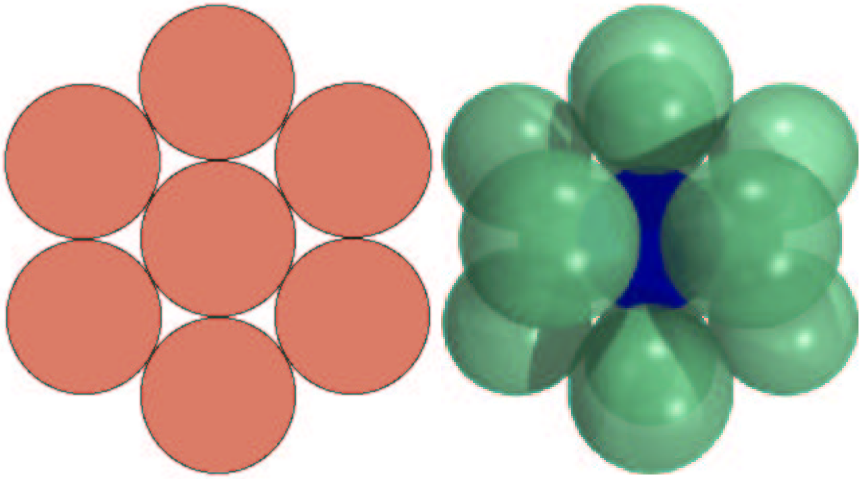

Fig. 1. The problem in $\mathbb{R}^2$ (a) and $\mathbb{R}^3$ (b)

In $\mathbb{R}^2$ the result is trivial: the maximum kissing number is 6 (Fig. 1, a). The situation is far from trivial in $\mathbb{R}^3$. The problem earned its fame because, according to Newton, the maximum kissing number in 3D is 12, whereas according to his contemporary fellow mathematician David Gregory, the maximum kissing number in 3D is 13 (this conjecture was stated without proof). This question was settled, at long last, more than 250 years after having been stated, when J. Leech finally proved that the solution in 3D is 12 [1]. The question for the 4-dimensional case is still open. A best known solution is 24, and the tightest upper bound is 25 [2]. In this paper, we propose a mathematical programming approach to settle the question. The continuous nonconvex optimization models we shall propose are not dissimilar, in nature, from those found in [3]. However, whereas that paper carried the infamous sentence "the solution of the above programs remains an open question" in its conclusion, in this paper we report the numerical solution of this problem. Our results seem to indicate the solution should be 24. We derived this result by using a general-purpose global optimization software [4] that includes both a stochastic method [5] and a deterministic one [6]. Methodologically speaking, neither method produces an output that is equivalent to a mathematical proof. We are offering strong numerical evidence that seems to point out that the solution of the maximum kissing problem in 4 dimensions is 24.

2 The model

The formulation we propose is a special case of a more general formulation found in [3]. As has been said above, we know a feasible solution with 24 spheres around a central one, and we know that 25 spheres is a tight upper bound. We maximize a decision variable α, bounded by the interval $[0, 1]$, which represents the degree of separation of the 25-sphere configuration being tested, subject to the necessary geometric constraints. Since the constraints are nonconvex, there may be multiple local minima. If the global optimization of the model determines that the global maximum is at $\alpha = 1$, then there is enough space for 25 balls, otherwise the kissing number is 24. The geometric variables $x^i = (x_1^i, x_2^i, x_3^i, x_4^i)$, $1 \le i \le 25$, determine the position of the center of the i-th sphere around the central one. The following formulation was used:

$$\begin{aligned} \max \quad & \alpha && && (1)\\ \text{s.t.} \quad & ||x^i||^2 = 4 && \forall i \le 25 && (2)\\ & ||x^i - x^j||^2 \ge 4\alpha && \forall i < j \le 25 && (3) \end{aligned}$$

3 A quasi Monte Carlo variant of a multi level single linkage algorithm based on Sobol' sequences

A stochastic approach for global optimization, in its simplest form, consists only of random search and it is called Pure Random Search (PRS). In PRS an objective function $f(x)$ is evaluated at N randomly chosen points and the smallest value of $f(x)$ is taken as the global minimum. Advanced stochastic techniques use stochastic methods to search for local minima and then utilize deterministic methods to solve a local minimisation problem. Two phases are considered: global and local. In the global phase, the function is evaluated in a number of randomly sampled points from a uniform distribution over a unit hypercube H_n. In the local phase the sample points are used as starting points for a local minimization search. The efficiency of the multistage methods depends both on the performance of the global stochastic and the local minimization phases.

In the most basic form of the multistage approach a local search is applied to every sample point. Inevitably, some local minima would be found many times. Since the local search is the most CPU-time consuming stage, ideally it should start just once in every region of attraction. This is the idea behind various versions of the so-called clustering methods. Extensive reviews on this subject can be found in [7–9] and [10]. One of the most efficient clustering methods is a multi level single linkage (MLSL) algorithm developed by Rinnooy-Kan and Timmer in [8,9].

The efficiency of stochastic methods depends on the quality of sampled points. It has been recognized through theory and practice that uniformly distributed deterministic sequences provide more accurate results than purely random sequences. Low-discrepancy sequences (LDS) are designed specifically to place sample points as uniformly as possible. Unlike random numbers, successive low discrepancy points "know" about the position of their predecessors and fill the gaps left previously. Methods based on LDS are known as quasi Monte Carlo (QMC) methods. In the majority of applications, QMC methods have superior performance compared to that of MC methods. Improvement in time-to-accuracy using QMC methods can be as large as several orders of magnitude. It was shown in [5] that application of LDS can significantly increase the efficiency of MLSL methods.

Central to the QMC approach is the choice of LDS. Different principles were used for constructing LDS by Holton, Faure, Sobol', Niederreiter and others. Many practical studies have proven that Sobol' LDS in many aspects are superior to other LDS [11], [12]. A C++ program called SobolOpt which employs a QMC variant of MLSL based on Sobol' sequences [5] was used in the present study.

4 Computational results

We solved the KNP by using the stochastic solver SobolOpt within the framework of a general-purpose global optimization software *oo*OPS [4]. The solution yielded a result of $\alpha = 0.924126$ in 7m36s of CPU time on a 2.66 GHz Pentium IV CPU with 1GB RAM. This indicates that the solution of the KNP is 24 spheres, and not 25 (we would need $\alpha = 1$ for 25 spheres).

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