The Kissing Number Problem: New Results 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, 3 and very recently for 4 dimensions. 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.

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. Notationally, we indicate the Kissing Number Problem in D dimensions by KNP(D).

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 [Lee56]. The question for the 4-dimensional case was very recently settled by O. Musin of Moscow State University [Mus04], proving that the solution of KNP(4) is 24 spheres. In this paper, we propose a mathematical programming approach to solve KNP(D). The computational results are validated by the theoretical results.

The continuous nonconvex optimization model we shall propose is derived from those found in [MMMS96]. However, whereas that report carried the infamous sentence "the solution of the above programs remains an open question" in its conclusion, computational solutions of those programs are reported in this paper. The models were solved by using a general-purpose global optimization software [LTKP01] that includes a very efficient stochastic method [KS04].

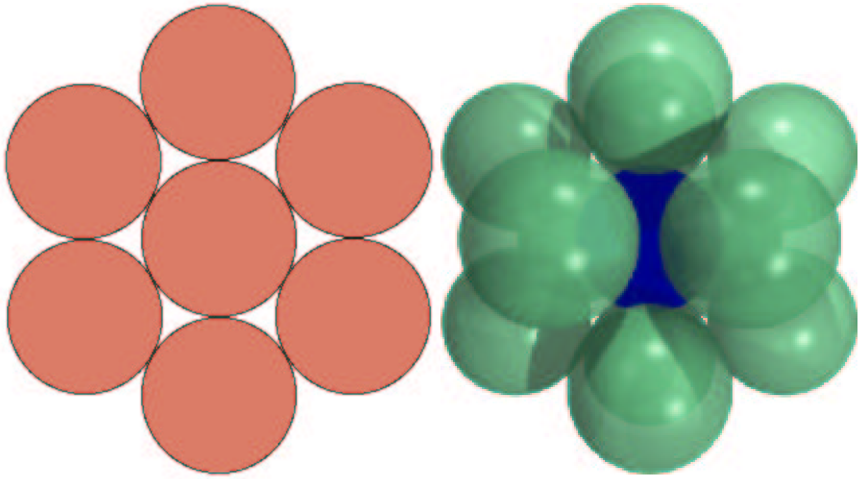

Figure 1: The problem in $\mathbb{R}^2$ (a) and $\mathbb{R}^3$ (b)

2 The model

The formulation we propose is a special case of a more general formulation found in [MMMS96]. Given parameters D (number of dimensions) and N (number of spheres), the variables $x^i = (x^i_1, \ldots, x^i_D)$, $1 \leq i \leq N$ determine the position of the center of the i-th sphere around the central one. We maximize a decision variable $\alpha \geq 0$ which represents the minimum pairwise sphere separation distance in the N-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 $\alpha \geq 1$, then there is enough space for N spheres; if the globally optimal α is strictly less than 1, it means that the N configuration has overlapping spheres, hence the kissing number is $N-1$. By solving this decision problem repeatedly for different values of N, we are able to quickly pinpoint the maximum N for which $\alpha > 1$.

The following formulation correctly models the problem:

$$\max \quad \alpha \tag{1}$$
$$\forall i \leq N \quad ||x^i||_2 = 2R \tag{2}$$
$$\forall i < j \leq N \quad ||x^i - x^j||_2 \geq 2R\alpha \tag{3}$$
$$\alpha \geq 0 \tag{4}$$
$$\forall i \leq N \quad x^i \in \mathbb{R}^D \tag{5}$$

Constraints (2) ensure that the centers of the N spheres all have distance $2R$ from the center of the central sphere (i.e., the N spheres kiss the central sphere). Constraints (3) makes the N spheres non-overlapping.

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 are 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 [Tu89, RKT87a, RKT87b] and [Sch02]. One of the most efficient clustering methods is a multi level single linkage (MLSL) algorithm developed by Rinnooy-Kan and Timmer in [RKT87a, RKT87b].

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 [KS04] 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 [PT95], [Sob98]. A global optimization solver called SobolOpt, which employs a QMC variant of MLSL based on Sobol' sequences [KS04], was used in the present study.

4 Computational results

We solved the KNP by using the quasi-stochastic solver SobolOpt within the framework of a general-purpose global optimization software $oo\mathcal{OPS}$ [LTKP01]. The SobolOpt solver needs to call a local NLP solver code in the local phase. In order to make sure that the local solution phase was numerically stable, we double-checked all our results with two local solvers: SNOPT [Gil99] and the E04VCF solver from the NAG library [Num84]. All tested instances gave the same results with both solver codes.

We validated the robustness of our approach by testing the KNP instances in two, three and four dimensions, where the optimal solutions are known (respectively, N=6, N=12 and N=24). SobolOpt correctly found the global optimum for these instances.

Table 1 reports our computational results, all obtained with a 2.66GHz Intel Pentium IV CPU with 1.5 GB RAM running Linux. In Table 1 we have solved the KNP for cases $D = 2, 3, 4$ (where the solution is known). In each cases, model and solution method were validated. In the table, n is the number of variables, the row marked α_K reports the known solutions to the KNP (obtained by geometrical proofs, see [CS93]), whilst the corresponding solutions found by SobolOpt are in the row marked with α_S. Each column corresponds to a different (N, D) pair. It is known that for the case $D = 2$ the solution is 6 circles, densely packed, with a value $\alpha_K = 1$. For $D = 3$, the vertices of a regular dodecahedron correspond to a value $\alpha_K = 1.1055727$ (this means that the spheres in the configuration $N = 12$ are not densely packed together, as $\alpha > 1$). For $D = 4$, the $N = 24$ spheres are densely packed together ($\alpha_K = 1$).

	$D = 2$		$D = 3$		$D = 4$	
	$N = 6$	$N = 7$	$N = 12$	$N = 13$	$N = 24$	$N = 25$
n	13	15	37	40	97	101
α_K	1	< 1	1.1055727	< 1	1	< 1
α_S	1.00002	0.75302	1.10558	0.91473	1	0.924646

Table 1: Computational results for the KNP problem in dimensions 2-4 (validation of method); n is the number of variables, α_K is the known result, α_S is the result found by SobolOpt.

5 Conclusion

In this paper we present a nonconvex mathematical programming model to solve the Kissing Number Problem in D dimensions. The solution of the problem has been carried out using the stochastic global optimization software SobolOpt, based on sampling the solution space using Sobol' sequences.

References

[CS93] J.H. Conway and N.J.A. Sloane, editors. *Sphere Packings, Lattices and Groups.* Springer-Verlag, Berlin, 1993.

[Gil99] P.E. Gill. *User's Guide for SNOPT 5.3.* Systems Optimization Laboratory, Department of EESOR, Stanford University, California, feb 1999.

[KS04] S. Kucherenko and Yu. Sytsko. Application of deterministic low-discrepancy sequences to nonlinear global optimization problems. *Computational Optimization and Applications (accepted for publication)*, 2004.

[Lee56] J. Leech. The problem of the thirteen spheres. *Mathematical Gazette*, 40:22–23, 1956.

[LTKP01] L. Liberti, P. Tsiakis, B. Keeping, and C.C. Pantelides. *ooOPS.* Centre for Process Systems Engineering, Chemical Engineering Department, Imperial College, London, UK, 1.24 edition, jan 2001.

[MMMS96] N. Maculan, P. Michelon, and J. MacGregor Smith. Bounds on the kissing numbers in $\mathbb{R}^n$: Mathematical programming formulations. *Technical Report, University of Massachussets, Amherst, USA*, 1996.

[Mus04] O. Musin. The kissing number in four dimensions. *Technical Report, Moscow State University*, 2004.

[Num84] Numerical Algorithms Group. *NAG Fortran Library Manual Mark 11.* 1984.

[PT95] S. Paskov and J.F. Traub. Faster evaluation of financial derivatives. *Journal of Portfolio Management*, 22(1):113–120, 1995.

[RKT87a] A.H.G. Rinnooy-Kan and G.T. Timmer. Stochastic global optimization methods; part i: Clustering methods. *Mathematical Programming*, 39:27–56, 1987.

[RKT87b] A.H.G. Rinnooy-Kan and G.T. Timmer. Stochastic global optimization methods; part ii: Multilevel methods. *Mathematical Programming*, 39:57–78, 1987.

[Sch02] F. Schoen. Two-phase methods for global optimization. 2:151–177, 2002.

[Sob98] I.M. Sobol'. On quasi-monte carlo integrations. *Mathematics and Computers in Simulation*, 47:103–112, 1998.

[Tu89] A. Törn and A. Žilinskas. *Global Optimization.* Springer-Verlag, Berlin, 1989.