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METHODOLOGY TO SOLVE MULTI-DIMENTIONAL SPHERE PACKING PROBLEMS

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This paper discusses the problem of optimally packing spheres of various dimensions into containers of arbitrary geometrical shapes. According to the international classification, this problem belongs to Sphere Packing Problems (SPPs). The problem is to pack a set of spheres (circles, hyperspheres) with given radii into a container with given metric characteristics. The aim of this work is to create an integrated methodology for solving SPPs. The basic formulations of the problem are presented: in the form of the knapsack problem (KP), open dimension problem (ODP), and their corresponding mathematical models. The solution strategy selection is influenced by the form of problem statement, dimension of the space where the spheres are to be packed, metric peculiarities of the spheres (equal or unequal), number of the spheres to be packed, geometric shape of the container, presence of technological restraints, and count time limit. The structural elements of the methodology are mathematical models, methods for constructing initial packings, and methods of local and global optimization. In developing the solution method, we construct the initial feasible packings by using both the random and lattice methods, using a greedy algorithm and solving an auxiliary nonlinear programming problem. As local optimization methods, we consider the modifications of the feasible direction method, interior point method, Lagrange multiplier method, and method of optimization in groups of variables. For global optimization, we use the method of enumerating the subsets of spheres of a given set and method of enumerating the extreme points of the feasible region, which are implemented by using the branch and bound algorithm, the modifications of the decremental neighborhood search method, method of smooth transition from one local minimum to another by increasing problem dimensionality and introducing additional variable metric characteristics, solution method implemented as a sequence of nonlinear programming problems of increasing dimensionality, and a multi-start method. Strategies for solving different SPP statements are proposed.

Keywords: *sphere, hypersphere, sphere packing, knapsack problem, open dimension problem, nonlinear optimization.*

Introduction

Problems of optimally packing geometric objects are the problems of geometric design [1]. According to the international classification, such problems belong to cutting and packing (C & P) problems [2]. One of the C & P problems is SPP of various dimensions (2D – circles, 3D – spheres, nD – hyperspheres). SPP is to pack spheres of a set with given radii in a given container. It is necessary either to obtain the maximum infill factor of the container, or find the minimum possible container size.

SPPs are widely used both in scientific and practical applications, for example, in the textile, clothing, automotive, aerospace and chemical industries [3], in nuclear power engineering for modeling processes in a nuclear reactor [4], in additive manufacturing to optimize the geometric shapes of parts and components [5] and in medicine for planning automated radiosurgical treatment [6]. Hypersphere packing is used for modeling the geometry of crystalline states [7]. Such problems also arise in the numerical evaluation of the integrals either on the surface of a sphere or inside it [8]. The main applications of SPPs are coding theory, digital communication, and information storage, for example, CDs, cellular phones and the Internet [8, 9].

Depending on the problem statement, there are two main classes of SPPs: KPs and ODPs [2]. KP is to pack spheres of a given set into a container of given fixed sizes with the maximum infill factor. In ODP, all the spheres of a given set must be packed into a container, with all its dimensions fixed except for one whose value must be minimized.

In [10–14], some researchers use SPP formulation in the form of KP. If it is necessary to go to solving ODP, a dichotomous search for the minimum container size is used, i.e. a sequence of KPs is solved. At the same time, in order to search for the initial points, rather efficient heuristic greedy algorithms (GAs) are used [10, 11, 13, 14].

In [15], SPP is formulated as ODP. As a minimum container size, the radius, length, height, perimeter, area, volume, and surface area are used. A nonlinear mathematical model with twice differentiable functions is proposed. This model allows a local minimum of the problem to be obtained. Initial sphere packings are randomly selected.

In [16, 17], in order to solve SPP formulated as KP, a mathematical model based on increasing problem dimensionality is used. It is assumed that the radii of the spheres temporarily become variable and the sum of volumes (areas in 2D) is maximized. The optimization process continues until the radii of the spheres reach their original values.

The idea of introducing additional variables was also used to solve ODP in order to pack unequal spheres [18, 19]. Additional variables improve the distribution of spheres in a container where there is unused space allowing the sphere radius to be increased. A transition is made from one local minimum point to another, with the best value of the objective function. When using such an algorithm, it is important to find the connection between the original and auxiliary problems with additional variables.

With a small number of spheres, we can use the methods of complete enumeration of the problem extreme points and theoretically get a global extremum. However, in practice, this is hampered by the complexity of solving systems of nonlinear equations [20].

With increasing the number of the spheres to be packed, the problem dimensionality increases proportionally and the number of constraints, nonlinearly. For large dimensionality, in order to solve the problem, we use either random sphere packings [21] or the approximate methods based on problem decomposition, for example, using the optimization method in groups of variables (OMGV) or GA [22, 23].

Thus, with different formulations of a packing problem, different approaches and methods for their solution are used. However, there is still no integrated methodology for solving such problems.

Therefore, the goal of this work is to create a methodology for solving problems of packing multidimensional spheres.

Mathematical models of the multidimensional sphere packing problem

It is obvious that, first of all, the solution strategy selection is influenced by the type of problem statement. Consider the statements of KPs and ODPs and their mathematical models in more detail.

KP is formulated as follows. Let there be a container $C \subset \mathbf{R}^d$ of a given geometric shape with fixed sizes and a set of spheres $S_i(u_i) \subset \mathbf{R}^d, i \in I_N = \{1,2,...,N\}$ with given radii, where u_i is the sphere translation vector, $S_i, i \in I_N$, $d \geq 2$ is the space dimension. The problem is to pack the spheres from the set $S_i(u_i), i \in I_N$ (all or part of them) without mutual overlapping in the container *C* with the maximum infill factor.

Suppose that there are K sizes of the spheres from the set $S_i(u_i), i \in I_N$ with the radii r_k, $k \in I_K = \{1,2,...,K\}$. Denote the number of the spheres with the radius r_k that can be packed inside the container *C* as n_k, $k \in I_K$, and generate a tuple $t = (n_1, n_2, ..., n_K)$. The tuple t must contain at least one nonzero element n_k, $k \in I_K$. Denote the set of all possible tuples *t* as *T*. The power of the set *T* is equal to

$$\prod_{k=1}^{K}(n_k + 1) .$$

Form a subset S^t of the spheres $S_j(u_j)$, $j \in J = \{1,2,...,n\}$ of the set $S_j(u_j)$, $j \in J = \{1,2,...,n\}$ in accordance with the tuple $t = (n_1, n_2, ..., n_K)$, where

$$n = \sum_{k=1}^{K} n_k .$$

The subset S^t, taking into account the translation, is denoted as $S^t(v) = \{E_j(v_j), j \in J\}$, where $v = (v_1, v_2, ..., v_n) \in \mathbf{R}^{dn}$ is the vector of packing parameters, $S_j(v_j),\ j \in J$, $v_j = (x_{1j}, x_{2j}, ..., x_{dj})$ is the translation vector of the sphere $S_j(v_j)$.

KP can be formulated as follows. Find a subset of spheres $S^t(v^*)$, $q \in I_Q$, which can be fully packed in the container C with the maximum infill factor

$$F^* = F(v^*, t^*) = \max_{t \in T} \sum_{j \in J} (r_j)^d \text{ given } (v,t) \in W \subset \mathbf{R}^{dn} \times T, \qquad (1)$$

$$W = \{(v,t) : \Phi_{ij}(v_i, v_j) \geq 0, i, j \in J, i > j, \Phi_i(v_i) \geq 0, i \in J\}, \qquad (2)$$

where $\Phi_i(v_i)$ is the Φ-function for $S_i \in S^t$ and the object $C^* = R^2 \setminus \operatorname{int} C$ [24, 25],

$$\Phi_{ij}(v_i, v_j) = \sum_{k=1}^{d} (x_{ki} - x_{kj})^2 - (r_i + r_j)^2 \geq 0 .$$

The solution to problem (1)–(2) can be reduced to the enumeration of the elements of the set T. A point $v \in W$ can be found for the elements and the search for this point can be performed by solving the following optimization nonlinear programming problem where the radii of the spheres are variable:

$$\kappa^* = \kappa(v^*, r^*) = \max \sum_{j \in J} r_j \text{ given } (v, r) \in M, \qquad (3)$$

where $r = (r_1, r_2, ..., r_n)$;

$$M = \{(v, r) \in \mathbf{R}^{(d+1)n} : \Phi_{ij}(v_i, v_j, r_i, r_j) \geq 0, i, j \in J, i < j \qquad (4)$$

$$\Phi_i(v_i, r_i) \geq 0, \; i \in J, \; r - r_i \geq 0, \; i \in J\},$$

$$\Phi_{ij}(v_i, v_j, r_i, r_j) = \sum_{k=1}^{n} \left(x_{ki} - x_{kj}\right)^2 - (r_i + r_j)^2 .$$

Problem (3)–(4) is multi-extremal. The objective function is linear, so the extrema are at the extreme points of the feasible region *M*. The function $\Phi_{ij}(v_i, v_j, r_i, r_j)$ is a quadratic form. The type of the function $\Phi_i(v_i, r_i)$ depends on the geometric shape of the container.

Now consider ODP. A set of spheres $S_i(u_i), i \in I_N$ must be packed in the container C with a minimum size (area, volume, or metric characteristic).

The mathematical model of ODP [16] can be represented as

$$\mu^* = \min f(\mu) \text{ given } Y = (u, \mu) \in \tilde{W} \subset \mathbf{R}^{dN+\lambda}, \qquad (5)$$

where μ is the variable metric characteristic (vector of variable metric characteristics); λ is the number of variable metric characteristics ($\lambda = 1$ for a linear characteristic, for example, length, height, etc., and $\lambda \geq 2$ if the container size is specified by several metric characteristics, for example, area, surface area, volume); $f(\mu)$ is the function that determines the variable size of the container C ($f(\mu) = \mu$ for $\lambda = 1$);

$$\tilde{W} = \{Y \in \mathbf{R}^{dN+\lambda} : \Phi_{ij}(u_i, u_j) \geq 0, 0 < i < j \in I_N, \Phi_i(u_i, \mu) \geq 0, i \in I_N\}; \qquad (6)$$

$$\Phi_{ij}(u_i, u_j) = \sum_{k=1}^{d} (x_{ki} - x_{kj})^2 - (r_i + r_j)^2.$$

Problem (5)–(6) is a multi-extremal nonlinear programming problem.

Problem Solving Methodology

The methodology for solving optimization sphere packing problems is based on the analysis of the problem statement, initial data and constraints. It includes the construction of mathematical models that cover SPPs, study of their features and development of strategies for solving the problem assigned. A structure, logical connections, proposed methods and means of solving the problem are studied.

The solution strategy selection is influenced by the following factors:

– type of problem statement (KP or ODP);

– dimensionality of the space in which the spheres ($d = 2$, $d = 3$ and $d \geq 4$) must be packed;
– metric features of the spheres (equal or unequal);
– number of the spheres to be packed;
– geometric shape of the container;
– presence of technological limitations;
– constraint on the count time.

Depending on the peculiarities of the problem statement and mathematical model, a strategy for solving the problem is proposed, with the methods for constructing admissible packings (initial points or approximate solutions), local optimization methods and global optimization methods being its structural elements.

It is proposed to use the following methods for constructing admissible packings: random, lattice, greedy algorithm, auxiliary nonlinear programming problem. The random method is to randomly select the coordinates of the centers of the spheres and check the admissibility of packing [16]. In the lattice method, the centers of the spheres coincide with the lattice nodes [16, 23, 26]. When using GA, which is a modification of OMGV, the problem is decomposed into subproblems [27]. The coordinates of one sphere are chosen as a group of variables, and the objective function can be chosen heuristically. In order to obtain an admissible packing, an auxiliary nonlinear programming problem or a sequence of such problems can also be used [26]. In some cases, it is advisable to use combinations of these methods [16, 26].

As methods of local optimization, depending on the peculiarities of the mathematical model and number of the spheres to be packed, modifications of the feasible direction method (FDM) [16, 23, 26], interior-point method (IPM) [18, 19, 28, 29], Lagrange multiplier method (LMM) [30], and optimization method in groups of variables (OMGV) [30] should be used. In all the methods, it is advisable to apply the strategy of an active set of constraints [31], due to which computational costs are significantly reduced.

FDM makes it possible to reduce the solution of a nonlinear programming problem to a sequence of linear programming problems. For SPPs, the specifics of the constraints are taken into account: some of them may be linear, the matrices of the first and second derivatives are highly sparse. Such peculiarities make it possible to apply special software packages [32, 33] and solve problems of a sufficiently large dimensionality (5000–10 000) variables. At the same time, such programs work more steadily for the spheres of smaller dimension $d \leq 3$.

IPM is designed for solving problems of nonlinear programming and works effectively for problems of medium dimensionality (up to 1000 variables).

LMM is used to search for a local extremum in combination with the steepest descent method and is based on the analysis of Lagrange multipliers of active constraints.

In the case of packing a large number of spheres (with the number of variables greater than 10 000), we should use OMGV, choosing from 1000 to 10 000 variables in a group. To obtain a quick result with a constraint on the count time, we can optimize the packing of each sphere locally and separately by selecting a group of variables d that define the coordinates of the sphere center. This packing method is also called the sequential addition method (SEM) [1, 22, 34].

Global optimization methods are presented by: the method of enumerating the sphere subsets of a set (MESS), method of enumerating the extreme points (MEEP) of the feasible region on the basis of the branch and bound algorithm [20]; modifications of the decremental neighbourhood search methods (DNSM) [35, 36]; method of smooth transition (STM) from one local minimum to another based on increasing the dimensionality of the problem by introducing additional variable metric characteristics [18, 19, 29], method of solving sequences of non-linear programming problems of increasing dimensionality (MSSP) [16, 26]. A combination of these methods can also be used. For all these methods, we apply a multi-start method (MMS), which allows us to expand the selection of possible packing options.

MESS is used to solve KPs. To obtain a solution, we enumerate various options for selecting a spherical subset of a given set, with the enumeration implemented in the form of a tree [37]. To reduce the number of the tree tops under consideration, cut-off rules are used with the help of which non-perspective tops are discarded based on the analysis of the lower and upper estimates of the objective function.

In MEEP, all the subsystems are solved from a system of constraints, i.e. all the surfaces describing the feasible region boundary are investigated. For this, the branch and bound algorithm is used. In the case of a linear objective function, a solution is found at one of the extreme points of the feasible region. If all the constraints in a problem are reverse convex (for example, the packing of hyper-spheres in a hyperparallelepiped), then the extreme point is determined by a system of equations whose number is equal to the number of the problem variables.

With the help of DNSM modifications, the objective function is optimized on the various permutations of spheres and solution tree based on the probabilistic properties of the objective function.

Now we will consider the basic statements and strategies for solving the problem.

KP. If a problem formulated in the form of KP is under consideration, then for each option selected, it is necessary to solve problem (3)–(4) with the help of FDM and IPM. With a small number of spheres and dimensionality of spheres $d \le 3$, a complete enumeration of the extreme points of the feasible region (using MEEP) is also possible. If the number of spheres is greater than 10, then either a truncated solution tree or MSSP is used. With a large number of spheres (more than 10 000 variables), various modifications of OMGV are used.

The method of obtaining the initial packing depends on the problem dimensionality, ratio between the sphere sizes and container, and type of the container. If the problem of packing equal spheres is to be solved, the size of the container is significantly larger than that of the spheres, and the problem dimensionality is no more than four, then a lattice method of constructing the initial packing is used. In other cases, either a random method or a special GA [26] is used, for example, in the step-by-step process of MSSP.

If the container has a complex geometric shape (for example, if there are a large number of prohibited zones), then, in order to obtain the initial point, an auxiliary nonlinear programming problem should be used, whose solution allows us to restore permissibility from any randomly selected point not belonging to the container [26].

The presence of technological constraints, for example, those on the minimum and maximum permissible distances, narrows the feasible region, and consequently the number of packing options. Usually, in this case, the lattice method of obtaining initial packings is not applied.

ODP. In order to solve problems with a variable container size, formulated as (5)–(6), the solution strategy also depends on the number of the spheres to be packed and problem dimensionality. Usually, in ODPs, the container with prohibited zones is not considered.

If the number of the spheres is not greater than 10, and the sphere dimensionality $d \le 3$, then MEEP is used, implemented as a modification of the branch and bound algorithm [20]. In order to solve systems of equations, the Newton method is used. In this case, a set of extreme points includes a set of local extrema and there is no need to apply a method of local optimization.

When increasing the number of spheres or space dimensionality, it is necessary to use methods of local optimization (FDM, DNSM), MST, and MPP, which work well for problems of medium dimensionality (10–300) spheres. For high dimensionality problems, only an FDM algorithm, consisting in solving a sequence of linear programming problems (5000–10 000 variables), is applicable as a method of local optimization. In order to obtain an approximate solution to the problem, it is necessary to apply OMGV. The same method can be used to obtain approximate solutions.

As a method of obtaining initial packings, the lattice method is used for identical spheres and GA, for different spheres.

It should be noted that KP can be solved as ODP, in which the container homothety coefficient is minimized. Such a transition is expedient in solving problems of packing unequal spheres. It allows using MST for solving KPs.

Conclusions

An integrated methodology for solving problems of packing multidimensional spheres is proposed. This methodology is a development of the theory of geometric design and can be used by specialists in this field to select a strategy for solving the problem. With the help of the methodology developed, it is possible to solve sphere packing problems formulated as both KPs and ODPs. The methodology is focused both on modern developments in the field of geometric design and use of powerful software packages for solving problems of linear and nonlinear programming.

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Методологія розв’язання задач розташування багатовимірних куль

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В статті розглядається задача оптимального розміщення куль різної розмірності в контейнерах довільних геометричних форм. Згідно з міжнародною класифікацією ця задача належить до класу SPP (Sphere Packing Problems). Вона полягає в розміщенні набору куль (кругів, гіперкуль) заданих радіусів у контейнері з заданими метричними характеристиками. Метою даної роботи є створення єдиної методології розв’язання задач SPP. Наведено основні постановки задачі: у вигляді задачі про рюкзак і задачі зі змінним розміром контейнера та відповідні математичні моделі. На вибір стратегії розв’язання впливають вид постановки задачі, розмірність простору, в якому розміщуються кулі, метричні особливості куль (рівні чи нерівні), кількість розміщуваних куль, геометрична форма контейнера, наявність технологічних обмежень, обмеження на час обчислень. Структурними елементами методології є математичні моделі, способи побудови початкових розміщень, методи локальної й *глобальної оптимізації. Під час розробки методу розв'язання використовується побудова допустимих розміщень випадковим, гратчастим способами, за допомогою жадібного алгоритму й шляхом розв'язання допоміжної задачі нелінійного програмування. Як методи локальної оптимізації розглядаються модифікації методу можливих напрямів, метод внутрішньої точки, метод множників Лагранжа та метод оптимізації за групами змінних. Для глобальної оптимізації використовуються метод перебору підмножин куль із заданого набору, метод перебору крайніх точок області допустимих розв'язків, реалізовані за допомогою алгоритму гілок і меж, модифікації методів околів, що звужуються, метод плавного переходу з одного локального мінімуму в інший на основі збільшення розмірності задачі шляхом уведення додаткових змінних метричних характеристик, метод розв'язання, реалізований у вигляді послідовності задач нелінійного програмування зростаючої розмірності, метод мультистарту. Запропоновано стратегії розв'язання задач SPP для різних її постановок.*

Ключові слова: *куля, гіперкуля, упаковка куль, задача про рюкзак, задача зі змінним розміром, нелінійна оптимізація.*

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