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PACKING NON-EQUAL HYPERSPHERES INTO A HYPERSPHERE OF MINIMAL RADIUS

The problem of packing different hyperspheres into a hypersphere of minimal radius is considered. All hypersphere radii are supposed to be variable. Solving the problem is reduced to solving a sequence of mathematical programming problems. A special way of construction of starting pointsis suggested. A smooth transition from one local minimum point to another providing a decrease of the objective value is realized using the jump algorithm is fulfilled. Then, solution results are improved due to reduction of the solution space dimension by step-by-step fixing radii of hyperspheres and rearrangements of hypersphere pairs. Non-linear mathematical programming problems are solved with the IPOPT (Interior Point Optimizer) solver and the concept of active inequalities. A number of numerical results are given.

Рассматривается задача упаковки разных гипершаров в гипершаре минимального радиуса. Считается, что радиусы всех гипершаров являются переменными. Решение задачи сводится к решению последовательности задач математического программирования. Используя jump-алгоритм, выполняется плавный переход от одной точки локального минимума к другой, в которой уменьшается значение целевой функции. В дальнейшем результаты решения улучшаются благодаря уменьшению размерности пространства решений за счет фиксации радиусов гипершаров и перестановки пар гипершаров. Приведено несколько численных примеров.

Розглядається задача упаковки різних гіперкуль у гіперкулю мінімального радіуса. Вважається, що радіуси всіх гіперкуль є змінними. Розв'язання задачі зводиться до розв'язання послідовності задач математичного програмування. Використовуючи jump-алгоритм, виконується плавний перехід від однієї точки локального мінімуму до іншої, в якій зменшується значення цільової функції. В подальшому результати розв'язання покращуються завдяки зменшенню розмірності простору розв'язків за рахунок фіксації радіусів гіперкуль та перестановки пар гіперкуль. Наведені декілька чисельних прикладів.

Key words: *hypersphere, packing, mathematical modeling, jump algorithm*

Introduction

Packing hard hyperspheres in two and three dimensions has application in studying properties of many materials, for example, simple fluids, colloids, glasses, and granular media [1]. In higher dimensions hard hyperspheres are used to investigate properties such as geometrical frustration and the geometry of the crystalline state [2]. Packing hyperspheres may be used in the numerical evaluation of integrals, either on the surface of a sphere or in its interior [3]. The problems arise in digital communications and storage, including compact disks, cell phones, and the Internet [3, 4].

Many studies of randomly packed hyperspheres in higher dimensions are performed using Monte Carlo Method for Molecular Dynamics simulations [2]. In order to reach higher packing fractions a compression algorithm [5] or a particle scaling algorithm [6] is used.

Skoge et al [1] present a study of disordered jammed hard-sphere packings in four-, five-, and six-dimensional Euclidean spaces. They use a collision-driven packing generation algorithm and obtain the first estimates for the packing fractions of the maximally random jammed states.

Morse et al [7] investigate granocentric model for polydisperse sphere packings polydisperse sphere packing in high dimensions.

A method of packing equal hyperspheres into a given hypersphere, based on increasing problem dimension is considered in [8]. In this paper, we adopt the jump algorithm (JA) developed for unequal circle packing [9] to solve the problem of packing unequal hypersphere into the hypersphere of minimal radius in space of dimension greater than 3. JA allows to transit from one local minimum point to another one so that a hypersphere radius decreases.

The paper considers the following problem.

Let there be hyperspheres

$$S_i = \left\{ (x_1, x_2, ..., x_n) \in \mathrm{R}^n : \sum_{k=1}^{n} (x_i - x_{ki})^2 - (\hat{r}_i)^2 \le 0 \right\}$$

where $v_i = (x_{1i}, x_{2i}, ..., x_{ni})$ is center coordinates, $\hat{r}_i$ is radius of S_i, $i \in I = \{1, 2, ..., N\}$, and a hypersphere S:

$$S(\rho) = \left\{ (x_1, x_2 ..., x_n) \in \mathrm{R}^n : \sum_{k=1}^{n} x_k^2 - \rho^2 \le 0 \right\}$$

of radius ρ where ρ is variable.

A hypersphere S_i translated by a vector v_i is denoted by $S_i(v_i)$. A vector $v = (v_1, v_2, \ldots, v_n) \in R^{nN}$ defines a location of S_i, $i \in I$, in the Euclidean n-dimensional space R^n

We without loss of generality suppose that

$$\hat{r}_1 \le \hat{r}_2 \le ... \le \hat{r}_N, \quad \hat{r}_1 < \hat{r}_N. \tag{1}$$

Problem. Find such a vector v ensuring a packing of hyperspheres $S_i(v_i)$, $i \in I$, without their mutual overlappings within the hypersphere $S(\rho)$ that radius would be minimal $\rho = \rho^*$.

1. A mathematical model and its characteristics

A mathematical model of the problem can be stated as

$$\rho^* = \min\rho, \text{ s.t. } Y = (v, \rho) \in W \subset R^\tau, \tag{2}$$

where $\tau = Nn + 1$,

$$W = \{Y \in \mathrm{R}^\tau : \Phi_{ij}(v_i, v_j) \ge 0, 0 < i < j \in I, \Phi_i(v_i, \rho) \ge 0, i \in I\}. \tag{3}$$

Inequality $\Phi_{ij}(v_i, v_j) = \sum_{k=1}^{n} (x_{ki} - x_{kj})^2 - (\hat{r}_i + \hat{r}_j)^2 \ge 0$ guarantees non-overlapping hyperspheres S_i and S_j and inequality $\Phi_i(v_i, \rho) = (\rho - \hat{r}_i)^2 - \sum_{k=1}^{n} (x_i - x_{ki})^2 \ge 0$ provides a placement of $S_i(v_i)$ within $S(\rho)$.

The mathematical model (2)–(3) possesses the same characteristics as that of the mathematical models considered in [9], i. e. local minima are reached at extreme points of W, the matrix of the inequality system in (3) is strongly sparse, the number of inequalities specifying W is $\eta \ge n(n-1)/2 + n$ and the problem stated is NP-hard. Thus, a global minimum of the problem can be in general reached theoretically only.

To tackle the problem (2)–(3) with advantage one needs to construct starting points belonging to the feasible region W, to compute local minima and to carry out a directed non-exhaustive search for local minima.

2. Generating starting points and searching for local minima

First of all, we suppose that radii r_i of hyperspheres S_i, $i \in I$ are variables and form a vector $r = (r_1, r_2, \ldots, r_n) \in R^n$ [8]. In this case $X = (v, r) \in R^{\tau + N - 1}$ is the vector of all variables. Thus, the inequalities in system (3) take the form

$$\Phi_{ij}(v_i, v_j, r_i, r_j) \ge 0, \qquad 0 < i < j \in I, \qquad \Phi_i(v_i, r_i, \rho) \ge 0, \qquad i \in I.$$

Let $\rho=\rho^0>0$ and $r_i=0$, $i\in I$. We give $v^{\#}$ in a random way so that $v_i^{\#}\in S(\rho^0)$, $i\in I$. Then $X^{\#}=(v^{\#},0)$.

In order to construct a point $(v,\rho^0)\in W$ on the ground of the point $(v^{\#},\rho^0)$ we solve the problem

$$\Psi(\widehat{r})=\max\Psi(r)=\max\sum_{i=1}^{N}r_i\text{, s.t. } X=(v,r)\in D\subset R^{\tau+N-1}, \tag{4}$$

where

$$D=\{X\in R^{\tau+N-1},\ \Phi_{ij}(v_i,v_j,r_i,r_j)\ge 0, 0<i<j\in I, \Phi_i(v_i,r_i,\rho^0)\ge 0,\\ \varphi_i(r_i)=\hat{r}_i-r_i\ge 0, r_i\ge 0, i\in I\}. \tag{5}$$

Whence, problem (4)–(5) ensures an increase of the hypersphere radii limited by their initial values due to inequalities $\varphi_i(r_i)\ge 0$, $i\in I$.

It follows from the construction of $X^{\#}$ that $X^{\#}\in D$. So taking starting point $X^{\#}$ we solve problem (4)–(5) and obtain a local maximal point $\widehat{X}=(\widehat{v},\widehat{r})$.

Note that in addition to the characteristics of problem (2)–(3), problem (4)–(5) possesses the properties.

1. Inequalities $\varphi_i(r_i)\ge 0$, $i\in I$, in (5) imply that if

$$\Psi(\widehat{r})=\sum_{i=1}^{N}\widehat{r}_i=\sum_{i=1}^{N}\hat{r}_i=b \tag{6}$$

then $\widehat{r}=\hat{r}$ and spheres S_i, $i\in I$, are packed into $S(\rho^0)$. This means that the point $\widehat{X}$ is a global maximal point of problem (4)–(5).

2. If $\Psi(\widehat{r})<b$, and $\widehat{X}$ is a global maximal point of problem (4)–(5), then spheres S_i, $i\in I$, can not be packed into $S(\rho^0)$.

3. Value ρ^0 can be always chosen such that the attainment of a global maximum is guaranteed.

Let $\Psi(\widehat{r})=b$. The point $(\widehat{v},\rho^0)$ is not in the general case a local minimal point of problem (2)–(3). So, taking starting point $(\widehat{v},\rho^0)$, we calculate a local minimal point $(\breve{v}^0,\breve{\rho}^0)$ of problem (2)–(3).

4. Transition from one local maximum to another one

Let $\widehat{X}=(\widehat{v},\widehat{r})$ be a local maximal point of the problem (4)–(5) and $\Psi(\widehat{r})=\sum_{i=1}^{N}\widehat{r}_i<b$, i.e. at least one of the inequalities $\hat{r}_i-\widehat{r}_i\ge 0$, $i\in I$, is not active. We consider the auxiliary problem by analogy with the 2D case [9]

$$\max V(r)=\sum_{i=1}^{N}r_i^n\text{, s.t. } X\in M\subset R^{\tau+N-1}, \tag{6}$$

$$M=\{X\in R^{\tau+N-1},\ \Phi_{ij}(v_i,v_j,r_i,r_j)\ge 0, 0<i<j\in I,\ \Phi_i(v_i,r_i,\rho^0)\ge 0,\\ \psi_{1i}(r_i)=r_{\max}-r_i\ge 0, \psi_{2i}(r_i)=-r_{\min}+r_i\ge 0, i\in I\}, \tag{7}$$

where $r_{\max}=\max\{\hat{r}_i, i\in I\}=\hat{r}_N$ and $r_{\min}=\min\{\hat{r}_i, i\in I\}=\hat{r}_1$. Note that the feasible region M differs from D in (4)–(5) by the inequalities $\psi_{1i}(r_i)\ge 0$, $\psi_{2i}(r_i)\ge 0$, $i\in I$, instead of $\varphi_i(r_i)=\hat{r}_i-r_i\ge 0$, $r_i\ge 0$ in (5). This means that radii $r_i\ge 0$, $i\in I$ take any values from the segment $[r_{\min},r_{\max}]$.

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It is proved [9] that there exists the steepest ascent vector Z^0 at the point $\widehat{X}$ for problem (7)–(8) that $\Psi(\widehat{X}+Z^0)>\Psi(\widehat{X})$.

Let $(\breve{v}^0,\breve{\rho}^0)$ be a local minimal point of problem (2)–(3). We compute

$$r_i^\lambda=\hat{r}_i-\left(\frac{1}{2}\right)^{\lambda+2}\hat{r}_i=\hat{r}_i\left(1-\left(\frac{1}{2}\right)^{\lambda+2}\right),\qquad i\in I,\lambda=0,1,....$$

and assume that sphere radii are equal to $r_i^\lambda,\ i\in I$. Then problem (2)–(3) takes the form

$$\breve{\rho}=\min\rho\ \text{ s.t. } Y=(v,\rho)\in W^\lambda\subset \mathrm{R}^{\tau+N-1} \tag{9}$$

where

$$W^\lambda=\{Y\in\mathrm{R}^{\tau+N-1}:\Phi_{ij}^\lambda(v_i,v_j)\ge 0,0<i<j\in I,\Phi_i^\lambda(v_i,\rho)\ge 0,i\in I\},$$

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

Since $r_i^\lambda<\hat{r}_i,\ i\in I,$ then the point $(\breve{v}^0,\breve{\rho}^0)\in W^\lambda$ and $(\breve{v}^0,\breve{\rho}^0)$ is not a local minimal point of problem (9). So, taking starting point $(\breve{v}^0,\breve{\rho}^0)$, we solve problem (9) and define a local minimal point $(\breve{\breve{v}}^0,\breve{\breve{\rho}}^0)$. Since $\sum_{i=1}^{n}r_i^\lambda<b$ (see (6)), then, tackling problem (4)–(5) for starting point $X^0=(\breve{\breve{v}}^0,r^\lambda)\in D$, we compute a local maximal point $\widehat{X}^\lambda=(\widehat{v}^\lambda,\widehat{r}^\lambda)$. Two cases are possible: $\Psi(\widehat{r}^\lambda)=b$ and $\Psi(\widehat{r}^\lambda)<b$.

If $\Psi(\widehat{r}^\lambda)=b$, then $\widehat{r}_i^\lambda=\hat{r}_i,\ i\in I,$ and hence $(\widehat{v}^\lambda,\breve{\breve{\rho}}^0)\in W$ (3). Since the solution spaces of problems (2)–(3) and (4)–(5) are different, then $(\widehat{v}^\lambda,\breve{\breve{\rho}}^0)$ in general is not a local minimal point of problem (2)–(3). So, taking starting point $(\widehat{v}^\lambda,\breve{\breve{\rho}}^0)$, we solve problem (2)–(3). As a result, a new local minimum point $(\breve{v}^1,\breve{\rho}^1)$ is computed. In the case a local minimal point $(\breve{\breve{v}}^1,\breve{\breve{\rho}}^1)$ of problem (9) for the starting point $(\breve{v}^1,\breve{\rho}^1)$ is defined again and so on until $\Psi(\widehat{r}^\lambda)<b$ becomes, i.e. we have $\sum_{i=1}^{n}\widehat{r}^\lambda<b$, $\widehat{X}^\lambda=(\widehat{v}^\lambda,\widehat{r}^\lambda)$ and $(\breve{v}^\lambda,\breve{\rho}^\lambda)\notin W$ after λ iterations.

In this situation ($\Psi(\widehat{r}^\lambda)<b$) we compute the steepest ascent vector Z^0 at the point $\widehat{X}^\lambda$ for problem (6)–(7), calculate points

$$X^\gamma=\widehat{X}+(1/2)^\gamma Z^0,\qquad \gamma\in\Gamma=\{0,1,2,...,q<\infty\} \tag{10}$$

define *m*, for which $X^\gamma\in M$. Then, making use of $X^m=(v^m,r^m)\in M$ we compose the ascending sequence according to (1)

$$r_{i_1}^m\le r_{i_2}^m\le ....\le r_{i_n}^m . \tag{11}$$

Since $V(r^m)>V(\hat{r})$ may occur, then, on the ground of sequence (11), we compute $r_{i_j}^{m0}=\min\{r_{i_j}^m,\hat{r}_j\},\quad j\in I.$ This ensures the inequality $V(r^{m0})\le V(\hat{r})$ where $r^{m0}=(r_1^{m0},r_2^{m0},...,r_n^{m0})$. Based on sequence (11), we construct two points: $\tilde{\tilde{X}}^m=(\tilde{v}^m,\tilde{\tilde{r}}^m)$ where $\tilde{v}_j^m=v_{i_j}^m,\ \tilde{\tilde{r}}_j^m=r_{i_j}^{m0},\ j\in I$, and a point $\widetilde{X}^m=(\tilde{v}^m,\tilde{r}^m)$ where $\tilde{v}_j^m=v_{i_j}^m,\ \tilde{r}_j^m=r_{i_j}^m,\ j\in I$.

If $V(\hat{r})>V(\tilde{\tilde{r}}^m)>V(\widehat{r}^\lambda)$, then the new steepest ascent vector Z^0 at the point $\widetilde{X}^m$ for problem (7)–(8) is calculated. Taking $\widehat{X}=\widetilde{X}^m$, we build a new point $X^m=\widehat{X}+(1/2)^m Z^0$ (see

(10)) and derive new points $\tilde{\tilde{X}}^m = (\breve{v}^m, \tilde{\tilde{r}}^m)$ and $\tilde{X}^m = (\tilde{v}^m, \tilde{r}^m)$ in accordance with sequence (11) and so on. The iterative process is continued until either $V(\tilde{\tilde{r}}^m) = V(\hat{r})$ or $V(\tilde{\tilde{r}}^m) \le V(\hat{r}^\lambda) < V(\hat{r})$ occurs.

If $V(\tilde{\tilde{r}}^m) = V(\hat{r})$, i.e. $\tilde{\tilde{r}}_i^m = \hat{r}_i$, $i \in I$, then taking starting point $(\breve{v}_i^m, \breve{\mu}^\lambda)$, we tackle problem (2)–(3) and calculate a new local minimal point $(\breve{v}^0, \breve{\rho}^0)$. The process is repeated until $V(\tilde{\tilde{r}}^m) \le V(\hat{r}^\lambda) < V(\hat{r})$ becomes and next, we go to Subsection 5.3.

Note that JA executes a smooth transition from one local maximum to another one of problem (4)–(5).

5. Decrease of the problem dimension and rearrangement of hypersphere pairs

Reduction of the solution space dimension is realized by means of sequencial fixing initial values of sphere radii without fixing their center coordinates in the same manner as in [9].

Rearrangements of pairs of spheres whose radii are slightly distinguished allow to improve the objective value of problem (2)–(3). An algorithm executing such rearrangements is described in [10].

In order to obtain a good approximation to a global minimum of problem (2)–(3) we repeat the step-by-step procedure consisting of the construction of a starting point and the search for a local minimum of problem (2)–(3) with JA ν times. As a result local minimum points (v^{*t}, ρ^{*t}), $t \in T = \{1,2,...,\nu \le 10\}$ are computed.

Then we single out a local minimal point (v^{*0}, ρ^{*0}) corresponding to $\rho^{*0} = \min\{\rho^{*t}, t \in T\}$. The point (v^{*0}, ρ^{*0}) is taken as an approximation to a global minimum of problem (2)–(3).

6. Numerical examples

We solve a number of instances for different number of hyperspheres in the Euclidean spaces of dimensions from 4 to 13.

The Interior Point Optimizer (IPOPT) exploiting information on Jacobians and Hessians [11], and the concept of ε-active inequalities [8,12] are used to solve non-linear programming problems.

The algorithms were coded in Delphi and performed using an AMD Athlon 64 X2 6000+ (3.1Ghz) processor.

The average runtimes (hours) for the instances are presented in Table 1. Rows of the table correspond to the space dimensions and columns correspond to the numbers of hyperspheres. Instances considered may be downloaded from the webpage: http://f-bit.ru/uploads/295485.zip.

Table 1. The averaged runtimes depending on the space dimension and the number of hyperspheres

Space dimension	Number of hyperspheres				
n	$N = 30$	$N = 40$	$N = 50$	$N = 60$	$N = 70$
4	0.5	2	4	10	18
5	0.7	3	6	16	24
6	1	5	9	20	36
7	2	8	15	30	36
8	3.5	12	30	–	–
9	6	18	39	–	–
10	10	24	48	–	–
11	14	30	–	–	–
12	18	37	–	–	–
13	24	48	–	–	–

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Conclusion

Algorithm JA which expoits the assumption that radii of all hyperspheres are variable is adopted for higher dimensional spaces. Smooth transitions between local maximal points proveding a growth of the objective values. The algorithm is especially effective if neighbor initial radii of hyperspheres are slightly distinguished.

A decrease of the problem dimension by means of sequential fixing sphere radius values and rearrangements of hypersphere pairs allow to improve results.

Numerical results are presented.

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