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PACKING OF ELLIPSOIDS IN A CONVEX CONTAINER

We consider the problem of optimal packing of a given collection of unequal ellipsoids into an arbitrary convex container of minimal sizes. To describe non-overlapping, containment and distance constraints we derive phi-functions and quasi-phi-functions. We propose a relaxation approach related to constructing a phi-function for containment constraints to avoid equations of more than four degree. We formulate the packing problem in the form of a nonlinear programming problem and propose a solution method that allows us to search for local optimal packings. We provide computational results illustrated with figures.

Keywords: *packing, ellipsoids, convex container, non-overlapping, containment, quasi-phi-functions, nonlinear optimisation.*

Introduction

The optimal ellipsoid packing problem is NP-hard problem and has multiple applications in modern biology, medicine, mineral industries, molecular dynamics, nanotechnology, as well as in the chemical industry, power engineering etc. For example, the formation and growth of crystals, the structure of liquids, crystals and glasses, the flow and compression of granular materials, the thermodynamics of liquid to crystal transition and other.

The 3D Modeling software product family is a set of scientific tools for three dimensional modeling of granular structures and substances. It provides comprehensive visual and quantitative analysis of structural characteristics, such as spatial density, spatial porosity, spatial distribution, grain and pore structure.

Robotics: a robot arm and other elements in a scene are approximated by three-dimensional ellipsoids and it allows the authors [1] to explore the relation between the overlapping of ellipsoids and the overlapping of free-form objects.

A problem related to the chromosome organization in the human cell nucleus and that falls between ellipsoid packing and covering is considered in [2].

Related works

Many works have tackled the optimal ellipsoid packing problem.

In [3] is analysed the density of three-dimensional ellipsoid packings. Technique that considered in [4] allow to statistically explore the geometrical structure of random packings of spheroids. In [2] the problem consists in minimizing a measure of the total overlap of a given set of ellipsoids arranged within a given ellipsoidal container. In [5] consider the problem of packing ellipsoids within rectangular containers of minimum volume. The non-overlapping constraints are based on separating hyperplanes.

Nonlinear programming models are proposed and tackled by global optimisation methods. Instances with up to 100 ellipsoids.

Analytical description of placement constraints (non-overlapping, containment and distance constraints) for ellipsoids with continuous rotations to produce NonLinear Programming models (NLP-models) of ellipsoids' packing problems is of paramount importance.

Problem formulation

We consider here a packing problem in the following setting.

Let n be the number of ellipsoids to be packed. And let Ω be a given convex container of variable sizes p. The objective of the problem is to find ellipsoids

$$E_i(u_i),\ i \in I_n = \{1, 2, \ldots, n\},$$

such that

$$\operatorname{int} E_i \bigcap \operatorname{int} E_j = \varnothing,$$

for each j, $i \in I_n$ with $i \neq j, E_i \subset \Omega$ for each j, $i \in I_n$ and the volume of the container will be minimized.

Ellipsoid E is given by semi-axes a, b and c, $u = (v, \theta)$ is a variable vector of placement parameters, $v = (x, y, z)$ is a translation vector, $\theta = (\theta^1, \theta^2, \theta^3)$ is a vector of rotation parameters, where $\theta_i^1, \theta_i^2, \theta_i^3$ are Euler angles.

Within the research as a container Ω we consider a convex 3D region bounded by surfaces which described by infinitely differentiable functions, in particular, a sphere, a cylinder, a cuboid, an ellipsoid of variable sizes.

Tools of mathematical modeling

To describe non-overlapping and containment constraints we use quasi-phi-functions and phi-functions. To describe distance constraints we apply adjusted quasi-phi-functions and adjusted phi-functions. Let us consider clear definitions of a phi-function [6] and a quasi-phi-function [7].

Definition. A continuous and everywhere defined function $\Phi^{AB}(u_A, u_B)$ is called a phi-function for objects $A(u_A)$ and $B(u_B)$ if

$\Phi^{AB} < 0$, if $\operatorname{int} A(u_A) \bigcap \operatorname{int} B(u_B) \neq \varnothing$;

$\Phi^{AB} = 0$, if $\operatorname{int} A(u_A) \bigcap \operatorname{int} B(u_B) = \varnothing$ and $\operatorname{fr}A(u_A) \bigcap \operatorname{fr}B(u_B) \neq \varnothing$;

$\Phi^{AB} > 0$, if $A(u_A) \bigcap B(u_B) = \varnothing$.

Let ρ be a given minimal allowable distance between objects $A(u_A)$ and $B(u_B)$:

$$\operatorname{dist}(A, B) \geq \rho.$$

Definition. A continuous and everywhere defined function $\Phi'^{AB}(u_A, u_B, u')$ is called a quasi-phi-function for two objects $A(u_A)$ and $B(u_B)$ if

$$\max_{u' \in U} \Phi'^{AB}(u_A, u_B, u')$$

is a phi-function for the objects.

The general property of a quasi-phi-function is: if

$$\Phi'^{AB}(u_A, u_B, u') \geq 0$$

for some u', then

$$\operatorname{int} A(u_A) \bigcap \operatorname{int} B(u_B) = \varnothing.$$

A function defined by

$$\Phi'^{AB}(u_A, u_B, u') = \min\{\Phi^{AP}(u_A, u'), \Phi^{BP^*}(u_B, u')\}$$

is a quasi-phi-function for the pair of convex objects A and B.

$\Phi^{AP}(u_A, u')$ is a phi-function for $A(u_A)$ and a half-space $P(u')$ and $\Phi^{BP^*}(u_B, u_P)$ is a phi-function for $B(u_B)$ and

$$P^*(u') = R^3 \setminus \operatorname{int} P(u').$$

Nonoverlapping constraints

A function defined by

$$\Phi(u_1, u_2, u') = \min\{\chi(\theta_1, \theta_2, u'), \chi_1^+(u_1, u_2, u'), \chi_1^-(u_1, u_2, u'), \chi_2^+(u_1, u_2, u'), \chi_2^-(u_1, u_2, u')\}$$

is a quasi-phi-function for ellipsoids $E_1(u_1)$ and $E_2(u_2)$, where

$$u' = (t_1, g_1, t_2, g_2)$$

is a vector of parametric variables of ellipsoids,

$$\chi = -\left\langle N_1', N_2' \right\rangle = -\alpha_1'\alpha_2' - \beta_1'\beta_2' - \gamma_1'\gamma_2';$$

$$\chi_k^{\pm} = \alpha_1'(x_{2k}^{\pm} - x_1) + \beta_1'(y_{2k}^{\pm} - y_1) + \gamma_1'(z_{2k}^{\pm} - z_1) - 1;$$

$$(x_i', y_i', z_i') = v_i + M(\theta_i) \cdot (x_i^t, y_i^t, z_i^t), \quad i = 1, 2;$$

$$(x_{22}^{\pm}, y_{22}^{\pm}, z_{22}^{\pm}) = v_2 + M(\theta_2)(a_2 \cos t_2, b_2 \sin t_2, \sqrt{2a_2})^T;$$

$$\alpha_i = \frac{\cos t_i}{a_i};$$

$$\beta_i = \frac{\sin t_i \cos g_i}{b_i};$$

$$\gamma_i = \frac{\sin t_i \sin g_i}{b_i},$$

$$(\alpha_i', \beta_i', \gamma_i') = M(\theta_i)(\alpha_i, \beta_i, \gamma_i), \; i = 1, 2;$$

$(x_{2k}^+, y_{2k}^+, z_{2k}^+)$ is a vector of coordinates of point g_{2k}^+;

$(x_{2k}^-, y_{2k}^-, z_{2k}^-)$ is a vector of coordinates of point g_{2k}^-, $M(\theta)$ is a rotation matrix of the form

$$M(\theta) = \begin{pmatrix} \mu_{11} & \mu_{12} & \mu_{13} \\ \mu_{21} & \mu_{22} & \mu_{23} \\ \mu_{31} & \mu_{32} & \mu_{33} \end{pmatrix},$$

$$\mu_{11} = \cos\theta^1 \cos\theta^3 - \sin\theta^1 \cos\theta^2 \sin\theta^3;$$

$$\mu_{12} = -\cos\theta^1 \sin\theta^3 - \sin\theta^1 \cos\theta^2 \cos\theta^3;$$

$$\mu_{13} = \sin\theta^1 \sin\theta^2;$$

$$\mu_{21} = \sin\theta^1 \cos\theta^3 + \cos\theta^1 \cos\theta^2 \sin\theta^3;$$

$$\mu_{22} = -\sin\theta^1 \sin\theta^3 + \cos\theta^1 \cos\theta^2 \cos\theta^3;$$

$$\mu_{23} = -\cos\theta^1 \sin\theta^2;$$

$$\mu_{31} = \sin\theta^2 \sin\theta^3;$$

$$\mu_{32} = \sin\theta^2 \cos\theta^3;$$

$$\mu_{33} = \cos\theta^2.$$

In order to obtain the containment constraints of an ellipsoid in a region, a construction of the phi-function is required.

When constructing this function, essential difficulties arise that are associated with the appearance of equations of more than four degree. In this regard, we propose an approach related to constructing a phi-function for an object approximating the ellipsoid with a required accuracy.

At the first step, an approximation of the ellipsoid with the circumscribed polyhedron is constructed. Starting with, e.g., a parallelepiped we sequentially choose the vertex most distant to the ellipsoid. Then we find its projection to the ellipsoid.

In the projection point on the ellipsoid surface we construct the tangent plane and then section the polyhedron with this plane. We do so till required accuracy is achieved.

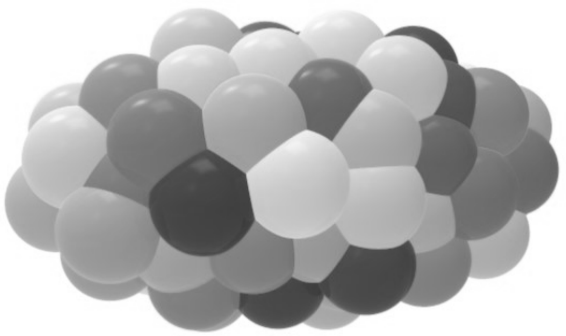
Projection may be found as a solution of an appropriate optimisation problem using IPOPT optimisation package.

Since the simplest form of phi-function is in case the included object is a sphere, an outer approximation of the obtained polyhedron with the spheres is applied using the method described in [8].

For spheroids me use another approximation approach, based on mathematical model of circular covering of arbitrary domain [9] and ellipse parameterization proposed in [10].

Within the research we assume that each ellipsoid $E_i(u_i)$ is approximated by a collection of spheres

$$E_i(u_i) \subset \hat{E}_i(u_i) = \bigcup_{k=1}^{n_i} S_{ik}(u_i) \text{ (Fig 1).}$$



a

b

Fig. 1. Covering of:
a – ellipsoid by identical spheres;
b – spheroid by spheres of dissimilar radii.

To describe the containment constraint

$$E_i \subset \Omega(p)$$

we use a phi-function for

$$\hat{E}_i(u_i)$$

and

$$\Omega^* = R^3 \setminus \operatorname{int}\Omega$$

that may be defined in the form

$$\Phi(u_i, p) = \\ = \min\left\{\Phi_1(u_i, p), ..., \Phi_{n_i}(u_i, p)\right\},$$

where $\Phi_k(u_i, p)$ is a phi-function for sphere S_{ik} and Ω^*.

Mathematical model

Mathematical model of the ellipsoid packing problem can be presented in the form

$$\min_{u \in W \subset R^\sigma} F(u), \quad (1)$$

where

$$W = \left\{ \begin{array}{c} u \in R^\sigma : \gamma_{ij}(u) \geq 0, \gamma_i(u) \geq 0, \\ i = \overline{1,n}, j = \overline{1,n}, j > i \end{array} \right\}; \quad (2)$$

$F(u)$ is the volume of the container Ω.

$u = (l, w, u_1, u_2, ..., u_n, \tau) \in R^\sigma$ is the vector of all variables

p denotes the variable metrical characteristics of the container Ω

$u_i = (x_i, y_i, \theta_i)$ is the vector of placement parameters for E_i, $i \in I_n$

τ is the vector of additional variables for quasi-phi-functions

γ_{ij} is a phi-function (quasi-phi-function) for E_i and E_j

$\gamma_i(u)$ is a phi-function for approximated ellipsoid E_i and the object Ω^*

Problem (1)-(2) is NP-hard nonlinear programming problem (exact, non-convex and continuous NLP-model).

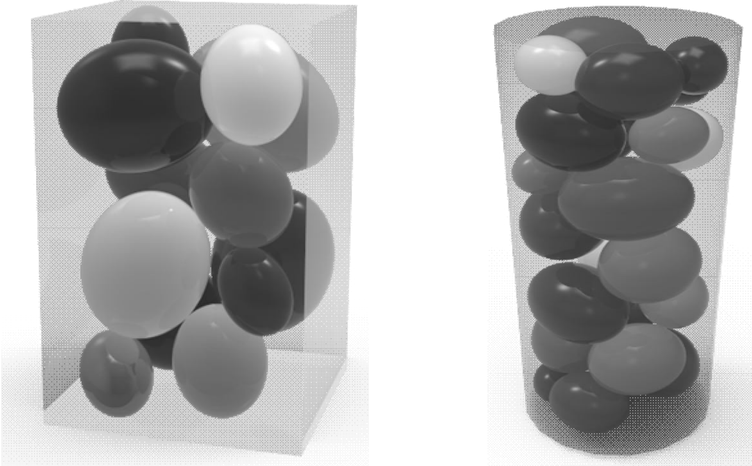
To search for a local minimum of problem (1)-(2) we employ a special local optimisation procedure described in [7].

Here we present a number of examples to demonstrate the efficiency of our methodology.

Conclusions

We developed here a continuous NLP-model of optimal packing of a given collection of unequal ellipsoids.

The use of quasi-phi-functions allows us to handle arbitrary ellipsoids which can be continuously rotated and translated, and relaxation approach allows us to formalize containment constraints for arbitrary convex container and avoid equations of more than four degree.



a b

Fig. 2. Instances of local optimal placement of ellipsoids in: a – cuboid; b – cylinder

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УПАКОВКА ЕЛІПСОЇДІВ У ВИПУКЛОМУ КОНТЕЙНЕРІ

Ю.Є. Панкратова, О.М. Хлуд, В.М. Пацук

Розглядається задача оптимальної упаковки заданого набору нерівних еліпсоїдів в довільному випуклому контейнері мінімальних розмірів. Для опису обмежень неперетину, належності та мінімально припустимих відстаней будуються phi-функції та квазі-phi-функції. Пропонується релаксаційний підхід, пов'язаний з побудовою phi-функції для обмеження належності, щоб уникнути рівнянь ступенів вище чотирьох. Формулюється задача упаковки у формі задачі нелінійного програмування та пропонується метод рішення, що дозволяє шукати локально-оптимальні упаковки. Надаються обчислювальні результати, ілюстровані рисунками.

Ключові слова: *упаковка, еліпсоїди, опуклі контейнери, обмеження неперетину, квазі-phi-функції, нелінійна оптимізація.*

УПАКОВКА ЕЛЛИПСОИДОВ В ВЫПУКЛОМ КОНТЕЙНЕРЕ

Ю.Е. Панкратова, О.М. Хлуд, В.Н. Пацук

Рассматривается задача оптимальной упаковки заданного набора неравных эллипсоидов в произвольном выпуклом контейнере минимальных размеров. Для описания ограничений непересечения, принадлежности и минимально допустимых расстояний строятся phi-функции и квази-phi-функции. Предлагается релаксационный подход для того, чтобы избежать появления уравнений степеней выше четырех при построении phi-функций для ограничений принадлежности. Формулируется задача упаковки в форме задачи нелинейного программирования и предлагается метод решения, позволяющий искать локально-оптимальные упаковки. Предоставляются вычислительные результаты, иллюстрированные рисунками.

Ключевые слова*: упаковка, эллипсоиды, выпуклые контейнеры, ограничения непересечения, квази-phi-функции, нелинейная оптимизация.*