OPTIMIZATION OF SPHERE PACKING PROBLEMS

Tatiana Romanova [1] Petro Stetsyuk [2]

[1] A. Pidgorny Institute for Mechanical Engineering Problems of the National Academy of Sciences of Ukraine, Kharkiv, Ukraine

tarom27@yahoo.com

[2] V. Glushkov Institute of Cybernetics of the National Academy of Sciences of Ukraine, Kyiv, Ukraine

stetsyukp@gmail.com

GPCO 2022 – 8th German-Polish Conference on Optimization, September 27–30, 2022, Apolda, Germany

OUTLINE

1. **Motivation**
2. The Phi-Function Technique
3. Problem A. Packing Spheres into a Minimum-Radius Sphere with Distance and Balance Conditions
4. Problem B. Sparse Sphere Packing with Balance Condition

Space engineering

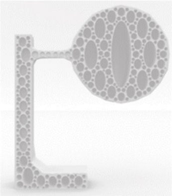
- Optimal placement of equipment in spacecraft (satellite) design

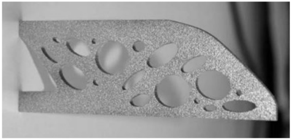
Additive manufacturing

- Cleaning $3D$ parts produced by $3D$ printing from particles of non-sintered powder by detonating gas mixtures in a deburring chamber (Thermal Energy Method)

Additive manufacturing

- Generating void structures for topological optimization of $3D$ parts





OUTLINE

Basic Placement Constraints in Packing Problems

$A \subset R^{\sigma}, B \subset R^{\sigma}, \Omega \subset R^{\sigma},\ \sigma = 2, 3$

- non-overlapping constraint: $intA \cap intB = \emptyset$
- containment constraint

$$A \subset \Omega \Leftrightarrow intA \cap \Omega^{*} = \emptyset,\ \Omega^{*} = R^{\sigma} \backslash int\Omega$$

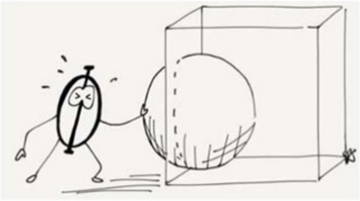
- distance constraint:

$$dist(A, B) \geq \rho$$

where $dist(A, B) = \min_{a \in A, b \in B} d(a, b)$, $d(a, b)$ stands for the Euclidean distance between two points $a, b \in R^{\sigma}$

Phi-functions

(a)



(b)

Figure: Phi-functions in their positive mood serve two purposes: keeping objects apart (a) and keeping objects into a target container (b)

The picture is produced by Diana Kallrath for chapter Yu.Stoyan & T. Romanova “Cutting & Packing beyond and within Mathematical Programming” in book Kallrath, J.: Business Optimisation Using Mathematical Programming, 2nd Edition, 2021, Springer, http://www.springer.com.

Phi-objects

A point set $A \subset R^{\sigma}, \sigma = 2, 3$ is referred to **phi-object** if

1) $A = cl(intA)$ (a canonically closed set).

2) A and $intA$ must have the same homotopy type.

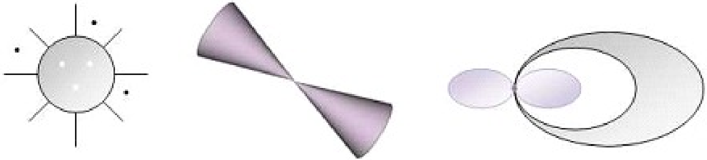
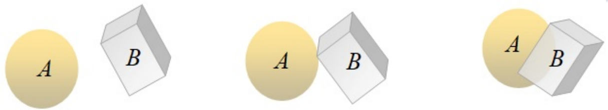


Figure: Invalid phi-objects

Chernov, N., Stoyan, Y., Romanova, T. (2010). Mathematical model and efficient algorithms for object packing problem. Comput. Geom.: Theory and Appl., 43(9), 535–553.

Phi-functions

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
$\Phi^{AB}(u_A, u_B) > 0$, if $A(u_A) \bigcap B(u_B) = \emptyset$,
$\Phi^{AB}(u_A, u_B) = 0$, if $intA(u_A) \bigcap intB(u_B) = \emptyset$ and $frA(u_A) \bigcap frB(u_B) \neq \emptyset$,
$\Phi^{AB}(u_A, u_B) < 0$, if $intA(u_A) \bigcap intB(u_B) \neq \emptyset$.



Non-overlapping constraint:

$$\Phi^{AB}(u_A, u_B) \geq 0 \Leftrightarrow intA(u_A) \bigcap intB(u_B) = \emptyset$$

Containment constraint: $\Phi^{A\Omega^*}(u_A, p) \geq 0 \Leftrightarrow A(u_A) \subseteq \Omega(p)$,

$\Omega^*(p) = R^\sigma \backslash int\Omega(p)$, for $\sigma = 2, 3$

Chernov, N., Stoyan, Y., Romanova, T. (2010). Mathematical model and efficient algorithms for object packing problem. Comput. Geom.: Theory and Appl., 43(9), 535–553.

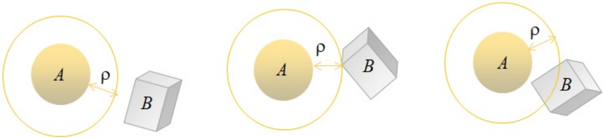
Adjusted Phi-function

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

$\overset{\frown}{\Phi}^{AB}(u_A, u_B) > 0$, if $dist(A(u_A), B(u_B)) > \rho$,

$\overset{\frown}{\Phi}^{AB}(u_A, u_B) = 0$, if $dist(A(u_A), B(u_B)) = \rho$,

$\overset{\frown}{\Phi}^{AB}(u_A, u_B) < 0$, if $dist(A(u_A), B(u_B)) < \rho$.



Distance constraint: $\overset{\frown}{\Phi}^{AB}(u_A, u_B) \geq 0 \Leftrightarrow dist(A(u_A), B(u_B)) \geq \rho$

Chernov, N., Stoyan, Y., Romanova, T. (2010). Mathematical model and efficient algorithms for object packing problem. Comput. Geom.: Theory and Appl., 43(9), 535–553.

Phi-functions

- In terms of phi-functions the packing problem can be formulated as a constrained optimization problem suitable to be solved by general methods of mathematical programming.
- The combined use of phi-functions and mathematical programming can improve the performance of packing algorithms.

OUTLINE

Problem A. Packing Spheres into a Minimum-Radius Sphere with Distance and Balance Conditions

Problem formulation

$S_i(v_i) = (\mathbf{x} \in \mathbb{R}^2 : \|\mathbf{x} - v_i\| \leq r_i),\ i = 1, \ldots, n$ – a family of spheres;
$r_i,\ i = 1, \ldots, n$ – a given radii of spheres;
$w_i,\ i = 1, \ldots, n$ – a given weights of spheres;
$v_i = (x_i, y_i),\ i = 1, \ldots, n$ – unknown centres of spheres;
$S(R) = (\mathbf{x} \in \mathbb{R}^2 : \|\mathbf{x}\| \leq R)$ – an external sphere (container);
R – unknown radius;
ρ_{ij} – a given minimal allowable distance between each pair of spheres $S_i(v_i)$ and $S_j(v_j)$, $1 \leq i < j \leq n$;
ρ_i – a given minimal allowable distance between a sphere $S_i(v_i)$ and the boundary of $S(R),\ i = 1, \ldots, n$.

Problem A. Packing Spheres into a Minimum-Radius Sphere with Distance and Balance Conditions

Problem formulation

Problem A. Pack the spheres $S_i(v_i)$, $i = 1, \dots, n$ in the minimum-radius container $S(R)$ considering the distance constraints, such that the gravity centre of the system of spheres $S_i(v_i)$, $i = 1, \dots, n$ is located at the origin (coincides with the gravity centre of $S(R)$).

Problem A. Packing Spheres into a Minimum-Radius Sphere with Distance and Balance Conditions

Mathematical model

$$R^* = \min_{R,x,y} R, \quad (1)$$

subject to

$$-(x_i^2 + y_i^2) + (R - r_i - \rho_i)^2 \geq 0, \; i = 1, \ldots, n, \quad (2)$$

$$(x_i - x_j)^2 + (y_i - y_j)^2 - (r_i + r_j + \rho_{ij})^2 \geq 0, \; 1 \leq i < j \leq n, \quad (3)$$

$$\sum_{i=1}^{n} w_i x_i = 0, \; \sum_{i=1}^{n} w_i y_i = 0, \quad (4)$$

$$R \geq R_{low}, \quad (5)$$

where

$$x = (x_1, x_2, ..., x_n), y = (y_1, y_2, ..., y_n),$$

$$R_{low} = \max_{i=1,...,n} r_i + \rho, \; \rho = \max\{\max_{i=1,...,n} \rho_i, \; 0.5 \cdot \max_{1 \leq i < j \leq n} \rho_{ij}\}$$

Solution Algorithm

The algorithm for finding the best local solution of the problem (1)-(5) is based on the multistart strategy and uses the Shor's r-algorithm.

The algorithm does not require feasible starting point for the problem (1)-(5).

P.I. Stetsyuk, 'Shor's r-Algorithms: Theory and practice. In: Optimization Methods and Applications: In Honor of the 80th Birthday of Ivan V. Sergienko. Butenko S., Pardalos P.M, Shylo V (Eds). Springer, pp. 495-520, 2017.

Solution Algorithm

The problem (1)-(5) can be transformed to the unconstrained minimization of a nonsmooth function

$$\min_{R,x,y}\{f(R,x,y) = R + \Phi_P(R,x,y)\}, \tag{6}$$

where penalty function $\Phi_P(r,x,y)$ has the form

$$\Phi_P(R,x,y) = P_1F_1(R,x,y) + P_2F_2(x,y) + P_3F_3(R), \tag{7}$$

$P = \{P_1, P_2, P_3\}$, P_k, $k = 1,2,3$ are positive penalty coefficients that allow adjusting violation of the placement constraints (2)-(5)

Solution Algorithm

$$F_1(R,x,y) = \sum_{i=1}^{n} \max\{0, x_i^2 + y_i^2 - (R - r_i - \rho_i)^2\} +$$

$$+\sum_{i=1}^{n}\sum_{j=i+1}^{n} \max\{0, -(x_i - x_j)^2 - (y_i - y_j)^2 + (r_i + r_j + \rho_{ij})^2\},$$

$$F_2(x,y) = \max\left\{\sum_{i=1}^{n} w_i x_i, -\sum_{i=1}^{n} w_i x_i\right\} + \max\left\{\sum_{i=1}^{n} w_i y_i, -\sum_{i=1}^{n} w_i y_i\right\}$$

$$F_3(R) = \max\{0, -R + R_{low}\}$$

Problem A. Packing Spheres into a Minimum-Radius Sphere with Distance and Balance Conditions

Computational results

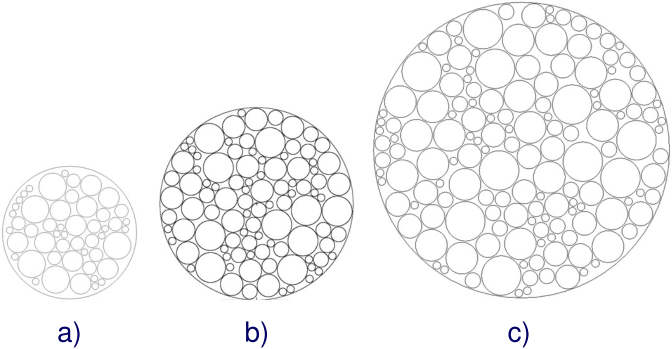


Figure: a) $n = 50$, $R^{*} = 182.6996$, $t = 1355$ sec; b) $n = 100$, $R^{*} = 257.35311$, $t = 6464$ sec, c) $n = 300$, $R^{*} = 520.5562$, $t = 24185$ sec

Romanova, T., Pankratov, O., Litvinchev, I., Stetsyuk, P., Lykhovyd, O., Marmolejo-Saucedo, J.A., Vasant, P. Balanced Circular Packing Problems with Distance Constraints. Computation, 2022, 10(7), 113

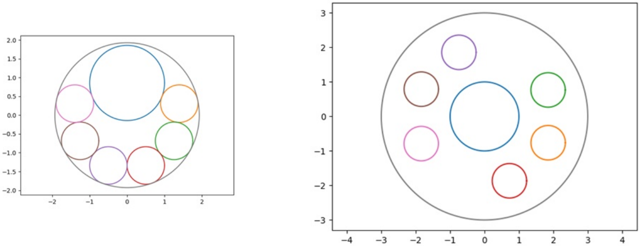
Computational results for small instances using BARON

The global extrema of the Problem A were found by solver BARON (Branch-And-Reduce Optimization Navigator) [1] using NEOS server (https://neos-server.org/neos/) and AMPL (A Mathematical Programming Language) [2].

[1] Sahinidis N.V., BARON 21.1.13: Global Optimization of Mixed-Integer Nonlinear Programs, User's manual, 2021.
[2] Fourer, R., Gay, D.M., Kernighan, B.W. AMPL: A Modeling Language for Mathematical Programming. Duxbury Press, Pacific Grove (2002).

Problem A. Packing Spheres into a Minimum-Radius Sphere with Distance and Balance Conditions

Computational results, using BARON



a) b)

Figure:

$\rho = 0$, $R^* = 1.92889$, $t =$ 22142 sec

Lower bound	Upper bound
1.92889	1.92889

$\rho = 0.5$, $R^* = 3$, $t =$ 27997 sec

Lower bound	Upper bound
2.2482	3.00000

Stetsyuk P., Romanova T., Scheithauer G. (2016) On the global minimum in a balanced circular packing problem. Optimization Letters. Volume 10, 347–1360.

OUTLINE

Problem formulation

Problem B. Place a family of non-overlapping spheres $S_i(v_i)$, $i = 1, ..., n$, into a fixed spherical container S maximizing minimal distance between all pairs of spheres as well as between each sphere and the boundary of the container subject to the gravity centre of the spheres $S_i(v_i)$, $i = 1, ..., n$, placed at the origin (centre of the container S).

Problem formulation

Let

$$\rho = \min\{\rho_{ij}, i > j = 1, ..., n, \rho_i, i = 1, ..., n\},$$

ρ_{ij} – the distance between spheres $S_i(v_i)$ and $S_j(v_j)$,
ρ_i – the distance between a sphere $S_i(v_i)$ and the boundary of S.

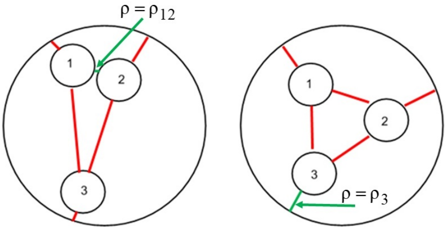


Figure: $\rho = \min\{\rho_{12}, \rho_{13}, \rho_{23}, \rho_1, \rho_2, \rho_3\}$

Mathematical model

$$\rho^* = \max_{\rho,x,y} \rho \tag{8}$$

subject to

$$-(x_i^2 + y_i^2) + (R - r_i - \rho)^2 \geq 0, \; i = 1, \ldots, n, \tag{9}$$

$$(x_i - x_j)^2 + (y_i - y_j)^2 - (r_i + r_j + \rho)^2 \geq 0, \; 1 \leq i < j \leq n, \tag{10}$$

$$\sum_{i=1}^{n} w_i x_i = 0, \quad \sum_{i=1}^{n} w_i y_i = 0, \tag{11}$$

$$0 \leq \rho \leq R - \max_{i=1,\ldots,n} r_i. \tag{12}$$

Mathematical model

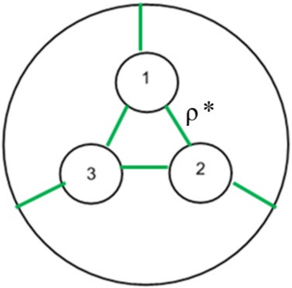


Figure: $\rho^* = \max\min\{\rho_{12}, \rho_{13}, \rho_{23}, \rho_1, \rho_2, \rho_3\}$, $\rho^* = \rho_{12} = \rho_{13} = \rho_{23} = \rho_1 = \rho_2 = \rho_3$

Solution Strategy

The following multistart strategy is applied to solve the problem (8)-(12).

Stage 1. Generate a number of feasible starting points based on the homothetic transformations of objects subject to balance condition.

Stage 2. Search for a local maximum of the problem (8)-(12) starting from each point obtained at Stage 1 using the decomposition algorithm. The algorithm reduces the problem (8)-(12) with $O(n^2)$ nonlinear non-overlapping constraints to a sequence of nonlinear programming subproblems with $O(n)$ nonlinear non-overlapping constraints.

Stage 3. Find the best local maximum obtained at Stage 2 and consider it as a solution to the problem (8)-(12) .

Solution Algorithm

Generating feasible starting points

Step 1. Form a set of randomly chosen points $v_i^0 = (x_i^0, y_i^0) \in S$ for $i = 1, ..., n$.

Step 2. Search for a local maximum of the problem

$$\max_{\lambda, v=(x,y)} \lambda$$

$$-(x_i^2 + y_i^2) + (R - \lambda r_i)^2 \geq 0, \; i = 1, \ldots, n,$$

$$(x_i - x_j)^2 + (y_i - y_j)^2 - \lambda^2 (r_i + r_j)^2 \geq 0, \; 1 \leq i < j \leq n,$$

$$\sum_{i=1}^{n} w_i x_i = 0, \; \sum_{i=1}^{n} w_i y_i = 0,$$

$$0 \leq \lambda \leq 1.$$

Step 3. If $\lambda^* < 1$ go to Step 1. Otherwise take v^* as a feasible starting point of the problem (8)-(12).

Solution Algorithm

Decomposition algorithm

For each fixed vector v^{k-1} (found by the *Feasible starting point algorithm*):

- set $\Delta = \sum_{i=1}^{n} r_i/n$ and form set

$$\Lambda_k = \{(x, y) \left| x_i^{k-1} - \Delta \le x_i \le x_i^{k-1} + \Delta, y_i^{k-1} - \Delta \le y_i \le y_i^{k-1} + \Delta, i = 1, ..., n\right\}$$

(allow moving each sphere S_i within the fixed Δ-square Ω_i^k)

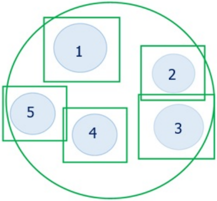


Figure: Constructing set Λ_k

Solution Algorithm

Decomposition algorithm

- form a subset W_k of the feasible set W of the problem (8)-(12) :
  - add $4n$ linear inequalities to (9)-(12);
  - eliminate from (10) non-overlapping inequalities for all

$$(i,j) \in \Sigma_k = \left\{(i,j) \in I_n \times I_n, i < j \,\middle|\, int\Omega_i^k \cap int\Omega_j^k = \emptyset\right\}.$$

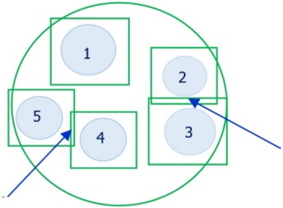


Figure: Constructing subset Σ_k

Solution Algorithm

Decomposition algorithm

- search for a local maximum of the k-th subproblem

$$\max_{\rho,x,y} \rho$$

$$-(x_i^2 + y_i^2) + (R - r_i - \rho)^2 \geq 0, \; i = 1, \ldots, n,$$

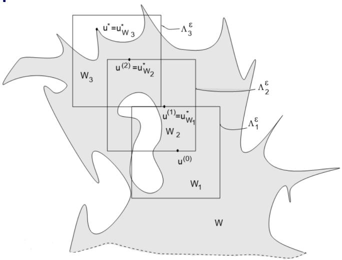
$$x_i^{k-1} - \varepsilon \leq x_i \leq x_i^{k-1} + \varepsilon,$$

$$y_i^{k-1} - \varepsilon \leq y_i \leq y_i^{k-1} + \varepsilon, \; i = 1, \ldots, n,$$

$$(x_i - x_j)^2 + (y_i - y_j)^2 - (r_i + r_j + \rho)^2 \geq 0, \; (i,j) \in \Sigma_k$$

$$\sum_{i=1}^{n} w_i x_i = 0, \; \sum_{i=1}^{n} w_i y_i = 0,$$

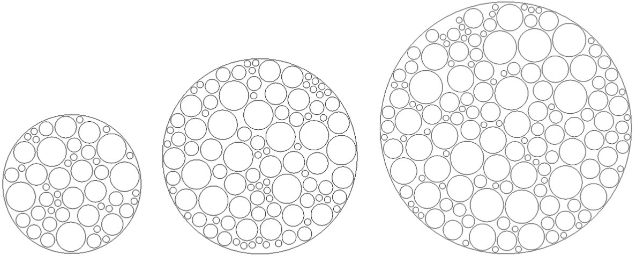
$$0 \leq \rho \leq R - \max_{i=1,\ldots,n} r_i.$$



If $(\rho^*, v^*) \in int\Lambda_k$ then a local maximum of the problem (8)-(12) is found, $v^* = (x^*, y^*)$.

T. Romanova, Y. Stoyan, A. Pankratov, I. Litvinchev, J.A. Marmolejo, 'Decomposition algorithm for irregular placement problems', In P. Vasant, I. Zelinka, & G. W. Weber (Eds.), Advances in Intelligent Systems and Computing: Volume 1072. Intelligent Computing and Optimization. ICO 2019, pp. 214-221, 2020.

Computational results using decomposition algorithm and IPOPT



a) b) c)

Figure: Local-optimal arrangement of spheres: a) $n = 50$, $\rho^* = 2.0551$, $t = 1201$ sec, b) $n = 100$, $\rho^* = 2.04864$, $t = 8090$ sec, c) $n = 150$, $\rho^* = 2.05183$, $t = 19571$ sec

Wachter, A., Biegler, L.T. On the implementation of an interior-point filter line-search algorithm for large-scale nonlinear programming, Mathematical Programming, 2006 , 106, 1, 25–57.

Computational results for small instances using BARON

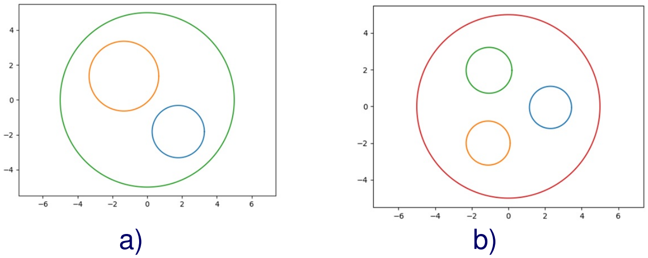


Figure:

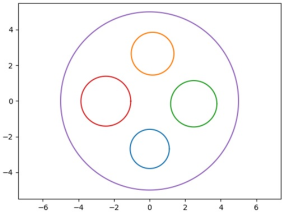
$n = 2, \ \rho^* = 0.954547, \ t = 1381$ sec

Lower bound	Upper bound
0.954547	0.954547

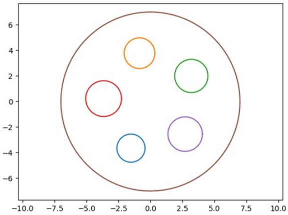
$n = 3, \ \rho^* = 1.51683, \ t = 89$ sec

Lower bound	Upper bound
1.51683	1.51683

Computational results for small instances using BARON



a)



b)

Figure:

$n = 4,\ \rho^* = 1.14188,\ t =$ 971 sec

Lower bound	Upper bound
1.14188	1.14188

$n = 5,\ \rho^* = 1.9262,\ t =$ 3999 sec

Lower bound	Upper bound
1.92620	1.92620

Future Plans

- A non-standard sphere packing problem with ratio and quasi-containment constraints arising in material science is studied.
- A maximal number of different non-overlapping spheres must be arranged in a container such that spheres are allowed to intersect the boundary of the container within prescribed deviations (quasi-containment). A certain ratio between the number of different types of spheres placed in the container must be maintained.

Acknowlegdements

The research is supported by the Volkswagen Foundation (#Az97775, #9C086)

Thank you for your kind attention!