

The Problem of Covering Solids By Spheres of Different Radii

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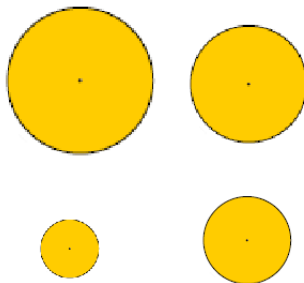
Agenda

- 1 The Covering Problem
- 2 The Packing Problem
- 3 Proposed Model
- 4 Heuristic
- 5 Discretization
- 6 Graph Approach

The Problem



(a) Solid to be covered.



(b) Available spheres sizes.

An Example

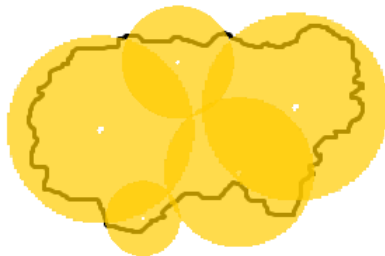


Figure : Example of a covering.

The Covering Problem

Definition

The Covering Problem

Given:

- a compact set $T \subset \mathbb{R}^3$,
- a finite set $R \subset \mathbb{R}_+$ of radii,
- a set N indexing the spheres and
- a function $\rho : N \rightarrow R$,

we have to find a set of spheres

$$\{ B(x(i), \rho(i)) \mid i \in N \}$$

of minimum cardinality and covering all the points in T .

The Covering Problem

A Formulation

In Liberti et al.¹, the authors formulated the problem as follows:

$$\|x^i - p\|^2 \leq u_i(p) \sum_{j \in U} w_{ij} r_j^2 + (1 - u_i(p)) M^2, \forall i \in N, \forall p \in T$$

$$\sum_{j \in U} w_{ij} = 1, \quad \forall i \in N$$

$$\sum_{i \in N} u_i(p) \geq 1, \quad \forall p \in T$$

$$\int_{p \in T} u_i(p) dp \geq \epsilon y_i, \quad \forall i \in N$$

$$\int_{p \in T} u_i(p) dp \leq \text{Vol}(T) y_i, \quad \forall i \in N$$

¹L. Liberti, N. Maculan & Y. Zhang. "Optimal configuration of gamma ray machine radiosurgery units: the sphere covering subproblem" *Optimization Letters*: Vol. 3, pp. 109-121, 2009.

The Covering Problem

A Formulation

Nonlinear nonconvex mixed-integer infinite programming problem:

$$\|x^i - p\|^2 \leq u_i(p) \sum_{j \in U} w_{ij} r_j^2 + (1 - u_i(p)) M^2, \forall i \in N, \forall p \in T$$

$$\sum_{j \in U} w_{ij} = 1, \quad \forall i \in N$$

$$\sum_{i \in N} u_i(p) \geq 1, \quad \forall p \in T$$

$$\int_{p \in T} u_i(p) dp \geq \epsilon y_i, \quad \forall i \in N$$

$$\int_{p \in T} u_i(p) dp \leq \text{Vol}(T) y_i, \quad \forall i \in N$$

The Packing Problem

Characteristics of the **packing** problem:

- Overlappings are not allowed; and
- the spheres must be totally inside the container.

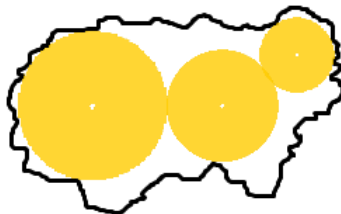


Figure : Example of a packing.

The Packing Problem

The goal is to maximize the density:

$$\text{density} = \frac{\sum_i \text{volume}(\text{object}_i)}{\text{volume}(\text{container})}.$$

Objective function:

$$\max \frac{\sum_i \frac{4}{3} \pi r_i^3 y_i}{\text{volume}(\text{container})}.$$

Removing the constants:

$$\max \sum_{i \in S} r_i^3 y_i.$$

The Packing Problem

A Formulation

For the problem of packing unequal spheres in a 3-dimensional polytope defined by

$$a_mx + b_my + c_mz \geq d_m, \quad m = 1, \dots, M,$$

A. Sutou and Y. Dai ¹ used the following variables in their model:

- (a) $x^i \in \mathbb{R}^3$ is the center of sphere i ; and
- (b) $w_{ik} \in \{0, 1\}$ is set to 1, if sphere i has radius r_k .

¹A. Sutou & Y. Dai. "Global Optimization Approach to Unequal Sphere Packing Problems in 3D". *Journal of Optimization Theory and Applications*. Vol. 114, No 3, pp. 671-694, 2002.

The Packing Problem

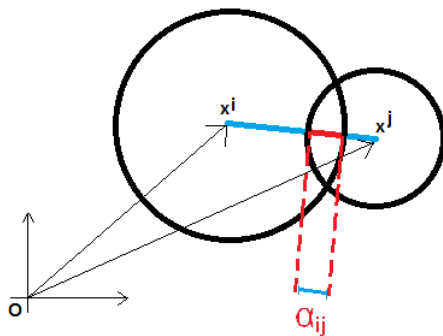
A Formulation

In Sutou et al., the authors formulated the problem of packing unequal spheres in a 3-dimensional polytope as follows:

$$\begin{aligned}
 \max \quad & \frac{4}{3}\pi \sum_{i=1}^N \sum_{k=1}^K r_k^3 w_{ik} \\
 \text{s.a.} \quad & \|x^i - x^j\|^2 \geq \left(\sum_{k=1}^K r_k w_{ik} + \sum_{k=1}^K r_k w_{jk} \right)^2, \quad \forall i \neq j \\
 & |a_m x_i + b_m y_i + c_m z_i - d_m| / \sqrt{a_m^2 + b_m^2 + c_m^2} \geq \sum_{k=1}^K r_k w_{ik}, \quad \forall i, m \\
 & a_m x_i + b_m y_i + c_m z_i - d_m \geq 0, \quad \forall i, \forall m \\
 & \sum_{k=1}^K w_{ik} \leq 1, \quad \forall i \\
 & w_{ik} \in \{0, 1\}, \quad \forall i, \forall k
 \end{aligned}$$

Proposed Model

We propose a model based essentially on the parameters α , which represent the maximum allowed overlap between each pair of spheres.



Proposed Model

So the constraints

$$||x^i - x^j||^2 \geq (r_i + r_j)^2$$

by introducing parameters α become

$$||x^i - x^j||^2 \geq (r_i + r_j - \alpha_{ij})^2.$$

But they should only constrain variables associated with spheres used in the packing.

Proposed Model

Let $y_i \in \{0, 1\}$ assume value 1 if sphere i is packed.

We could have

$$\|x^i - x^j\|^2 \geq (r_i + r_j - \alpha_{ij})^2 y_i y_j.$$

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We could have

$$||x^i - x^j||^2 \geq (r_i + r_j - \alpha_{ij})^2 y_i y_j.$$

But to avoid the multiplication of variables, we will use

$$||x^i - x^j||^2 \geq (r_i + r_j - \alpha_{ij})^2 (y_i + y_j - 1).$$

The Covering Problem

Proposed Model

Proposed Model for the Covering Problem

$$\max \sum_{i=1}^n c_i y_i$$

$$\|x^i - x^j\|^2 \geq (r_i + r_j - \alpha_{ij})^2 (y_i + y_j - 1), \quad \forall 1 \leq i < j \leq n$$

$$x^i \in T, \quad \forall i$$

$$y \in \{0, 1\}^n$$

The Covering Problem

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$$x^i \in T, \quad \forall i$$

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Proposed Model

Parameters Existence Theorem

There are

$$\{\alpha_{ij} \geq 0\}_{1 \leq i < j \leq n}$$

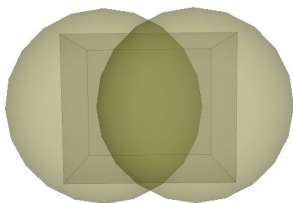
and

$$\{c_i \geq 0\}_{1 \leq i \leq n}$$

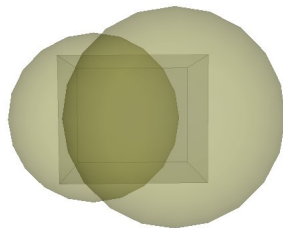
for which an optimal solution of the **proposed model** is also an optimal solution of the **covering problem**.

Small remark

Let $r < R$.



(a) Two spheres of radius r .



(b) One sphere of radius r and one sphere of radius R .

Figure : Two optimal solutions.

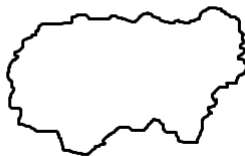
Motivation

- The *Gamma Knife* radiosurgery planning process.



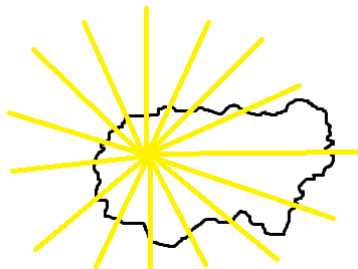
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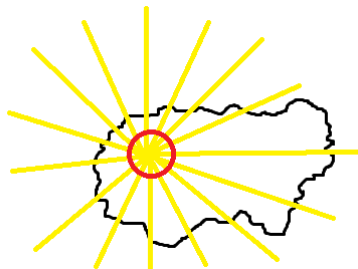
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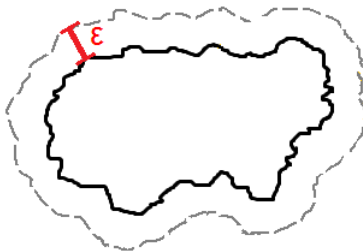
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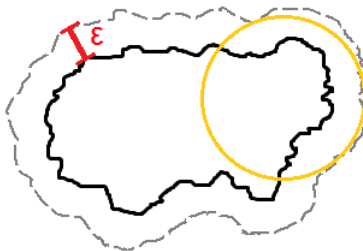
Security Region

To avoid a large volume of the spheres on the outside of the target volume, we define the **security region**.



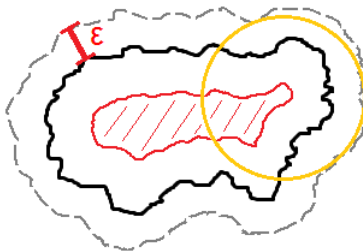
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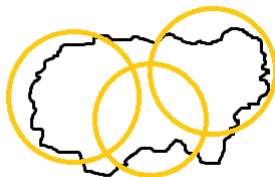
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Results

To present the results, let's define 3 parameters [3]:

- COV: percentage of T 's volume covered by the spheres;
- OVERLAP: percentage of T 's volume covered by more than one sphere;
- MISCOV: percentage of the total volume of the spheres outside T .



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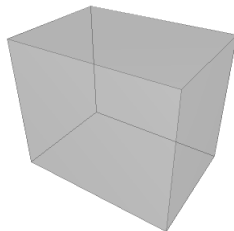
- COV: percentage of T 's volume covered by the spheres;
- OVERLAP: percentage of T 's volume covered by more than one sphere;
- **MISCOV**: percentage of the total volume of the spheres outside T .



Results

Data used in the tests:

- a parallelepiped with dimensions 14mm x 12mm x 10mm;
- $\epsilon = 1$ for the security region; and
- spheres of radius 4mm and 2mm.



Results

For the parameters, we used

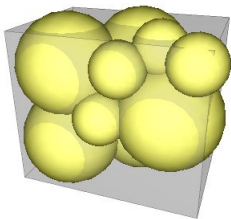
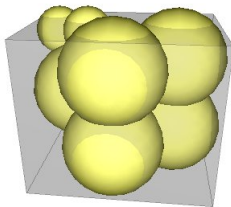
$$c_i = r_i^3$$

and

$$\alpha_{ij} = 0.5 \cdot \min\{r_i, r_j\}.$$

Couenne

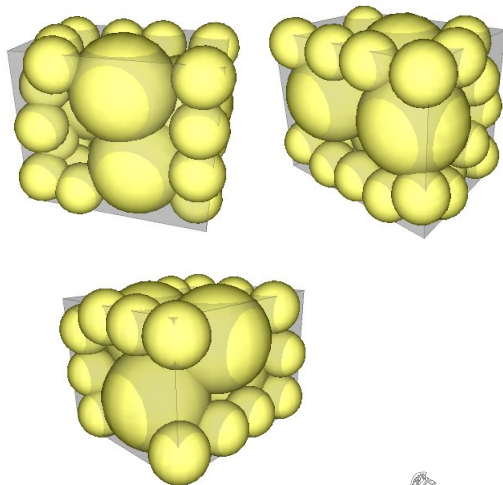
Algorithm	Couenne sB&B
z^*	352
$ S $	9
t_e	20h
t_t	9d
cov	68.12%
miscov	7.66%
overlap	9.03%



Bonmin

- 24 spheres of radius 2mm;
- Parameters c_i modified.

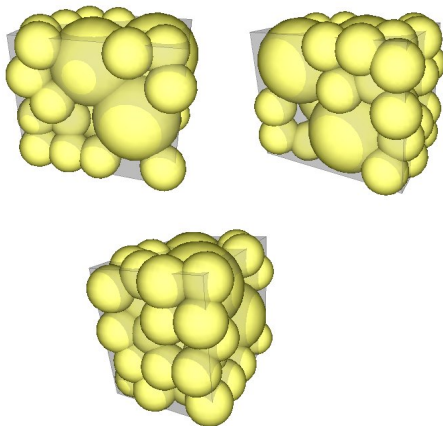
Algorithm	Bonmin B&B
z^*	448
$ S $	28
t_t	390s
cov	84.08%
miscov	9.66%
overlap	10.22%



Xpress-SLP

- 30 spheres of radius 2mm

Algorithm	Xpress-SLP SLP
z^*	496
$ S $	34
t_t	4s
cov	87.67%
miscov	10.58%
overlap	15.87%



Heuristic

Hypothesis

Spheres of larger radius are more interesting in the solution.

Heuristic based on solving the following problem:

$$\begin{aligned} \|x^i - x^j\|^2 &\geq (r_i + r_j - \alpha_{ij})^2, \quad \forall 1 \leq i < j \leq n \\ x^i &\in T, \quad \forall i \end{aligned}$$

It considers a fixed set of spheres.

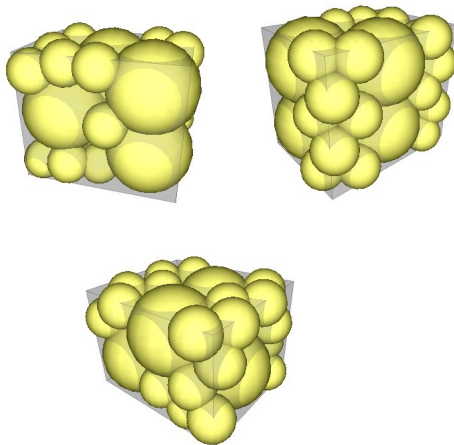
Heuristic

Idea:

- Start with a single sphere or only a few of them, all of the larger radius;
- If the solver returned a solution for this problem, use it as an initial solution for the next one, which has one more sphere available. For this sphere, its initial position will be generated randomly;
- If the solver claims the problem is infeasible, reduce the last added sphere's radius.

Results from Ipopt

Algorithm	Ipopt Interior Points
z^*	514
$ S $	29
t_e	17s
cov	91.40%
miscov	9.91%
overlap	16.13%



Discretization

Let x be a real variable assuming values in the interval $[a, b]$:

$$a \leq x \leq b .$$

Discretization:

$$x = w_1 \lambda_1 + \cdots + w_L \lambda_L ,$$

where

- L is the quantity of points used in the discretization of the interval $[a, b]$;
- $a \leq w_1 < \cdots < w_L \leq b$;
- $\lambda_i \in \{0, 1\}, \quad \forall i \in \{1, \dots, L\}$; e
- $\sum_{i=1}^L \lambda_i = 1$.

Discretization

In our model, we can apply this technique to the variables which represent the center of the spheres:

$$a_k^i \leq x_k^i \leq b_k^i .$$

Using the discretization we have just explained, we have:

$$x_k^i = w_{k,1}^i \lambda_{k,1}^i + \cdots + w_{k,L_k^i}^i \lambda_{k,L_k^i}^i ,$$

where

$$\sum_{i=1}^{L_k^i} \lambda_i = 1$$

$$\lambda_i \in \{0, 1\}, \quad \forall i \in \{1, \dots, L_k^i\}$$

Discretization

It will be used in the calculation of the term $\|x^i - x^j\|^2$, present in the constraints of the model:

$$\|x^i - x^j\|^2 = \sum_{k=1}^3 (x_k^i - x_k^j)^2 = (x_k^i)^2 + 2 x_k^i x_k^j + (x_k^j)^2$$

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The term in focus is rewritten as:

$$(x_k^i)^2 = (w_{k,1}^i)^2 \lambda_{k,1}^i + \dots + (w_{k,L_k^i}^i)^2 \lambda_{k,L_k^i}^i$$

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$$x_k^i x_k^j = \sum_{p=1}^{L_k^i} \sum_{q=1}^{L_k^j} w_{k,p}^i w_{k,q}^j \lambda_{k,p}^i \lambda_{k,q}^j$$

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Linearization

We can linearize the term $\lambda_{k,p}^i \lambda_{k,q}^i$ replacing it with the variables

$$z_{k,p,q}^{i,j} = \lambda_{k,p}^i \lambda_{k,q}^i$$

and adding the following constraints to the model:

$$z_{k,p,q}^{i,j} \leq \lambda_{k,p}^i$$

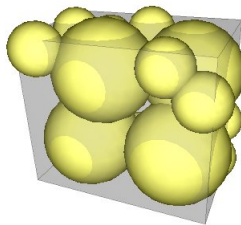
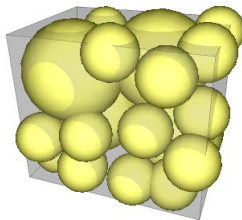
$$z_{k,p,q}^{i,j} \leq \lambda_{k,q}^i$$

$$z_{k,p,q}^{i,j} \geq \lambda_{k,p}^i + \lambda_{k,q}^i - 1$$

$$z_{k,p,q}^{i,j} \geq 0$$

Results

	Xpress
δ	0.2
z^*	376
$ S $	19
t_e	36h
cov	76.81%
miscov	7.27%
overlap	5.01%



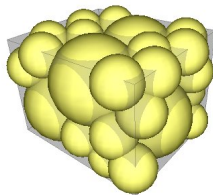
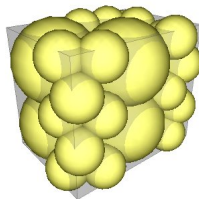
Comparison

	COUENNE sB&B	BONMIN B-BB	Xpress SLP	Xpress $\delta = 0.2$	Ipopt Heur
z^*	352	448	496	376	514
$ S $	9	28	34	19	29
t	20 h	390 s	4 s	36h	17 s
cov	68.12	84.08	87.67	76.81	91.40
miscov	7.66	9.66	10.58	7.27	9.91
overlap	9.03	10.22	15.87	5.01	16.13

Table : Comparing the best solution found by the tested methods.

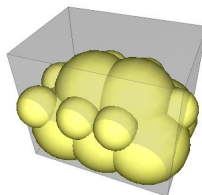
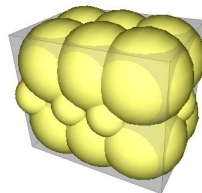
Parameters

		lpopt	
	Sol 1	Sol 2	Sol 3
z^*	514	960	1408
$ S $	29	22	36
t	17s	10s	112s
cov	91.40	97.25	100
miscov	9.91	13.45	35.26
overlap	16.13	60.21	80.65
β	0.5	1	1
ϵ	1	1	2



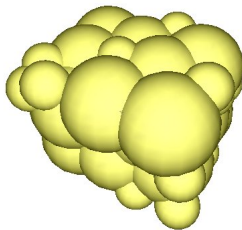
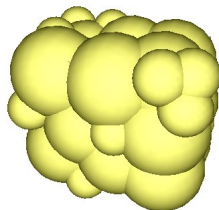
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Graph Approach

Let $G = (V, E)$ be the following graph:

- $V = \{ (r, p) \mid r \in R, p \in P \};$
- There is an arc $e \in E$ connecting vertices $i = (r_i, p_i)$ and $j = (r_j, p_j)$ if there is a feasible solution containing a sphere of radius r_i centered at point p_i and a sphere of radius r_j centered at point p_j .

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We aim to find the **maximum clique** in this graph.

Graph Approach

Maximum-weight clique model:

$$\max \sum_{i=1}^{|V|} c_i y_i$$

$$s.t. \quad y_i + y_j \leq 1, \quad \forall (i, j) \notin E$$

$$\mathbf{y} \in \{0, 1\}^{|V|}$$

Results

	$\delta = 1$	$\delta = 0.2$	$\delta = 2$	$\delta = 1$
	Discret	Discret	Graph	Graph
z^*	128	376	432	480
$ S $	9	19	54	60
t	10h	36h	2s	4s
cov	27.87	76.81	82.75	82.45
miscov	2.85	7.27	10.13	6.83
overlap	1.18	5.01	5.91	21.87

Table : Comparing the solutions obtained in the linearized model and in the graph approach.

Future Work

Working with the complement of the graph:

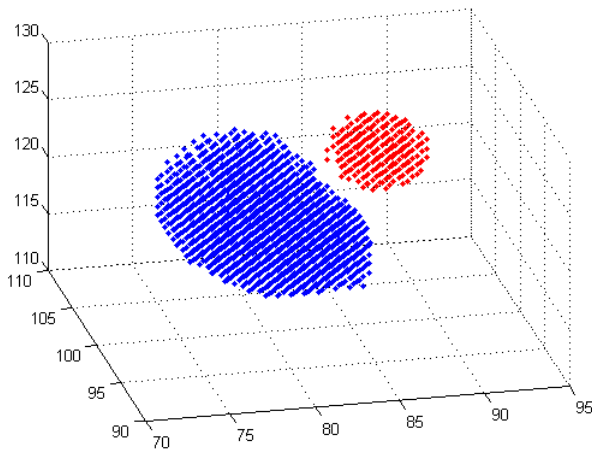
- Branch and Cut
cuts: violated cliques

$$y_1 + y_2 + y_3 + \dots \leq 1$$

- Branch and Bound
branching: violated cliques

Future Work

- More realistic data



References

- [1] L. Liberti, N. Maculan & Y. Zhang. “Optimal configuration of gamma ray machine radiosurgery units: the sphere covering subproblem”. *Optimization Letters*: Vol. 3, pp. 109-121, 2009.
- [2] A. Sutou & Y. Dai. “Global Optimization Approach to Unequal Sphere Packing Problems in 3D”. *Journal of Optimization Theory and Applications*: Vol. 114, No 3, pp. 671-694, 2002.
- [3] R. Quirino & A. F. Macambira & L. Cabral & R. Pinto. “The Discrete Ellipsoid Covering problem: a Discrete Geometric Programming Approach”. *Discrete Applied Mathematics*, 2012.