Vietnam Journal of Mathematics **40**:2&3(2012) 345-354

Vietnam Journal of MATHEMATICS

A Model to the Ellipsoidal Filling Problem

Roberto Quirino do Nascimento[1], **Ana Flavia U. S. Macambira**[1], **Lucidio dos Anjos Formiga Cabral**[1] and **Nelson Maculan**[2]

[1] *Universidade Federal da Paraiba, Departamento de Informatica, 58.051-900 - Joao Pessoa, Paraiba, Brazil*

[2] *Universidade Federal do Rio de Janeiro, COPPE-Engenharia de Sistemas e Computação, Caixa Postal 68511, 21941-972 Rio de Janeiro, RJ, Brasil*

Dedicated to Professor Phan Quoc Khanh on the occasion of his 65th birthday

Received November 6, 2011
Revised April 16, 2012

Abstract. The ellipsoidal filling problem consists in covering an ellipsoid with spheres whose radii belong to a discrete set. The discrete nature of the radii of the spheres is one of the difficulties inherent to this problem when one tries to solve it and another dificulty is ensuring that every point of the ellipsoid is covered by at least one sphere. Despite these difficulties, a good reason to study this problem is its application in configuring Gamma ray machines, used in brain tumors treatments. This problem is a semi-infinite nonlinear discrete one and we present a weak version that uses the idea of the Facility Location Problem to determine a likely location for the center of the spheres in such a way that the ellipsoid must be filled by them.

2000 Mathematics Subject Classification. 90C11.

Key words. Discrete optimization, global optimization, Gamma Knife.

1. Introduction

The discrete problem of ellipsoidal filling has an application in configuring Gamma ray machines. These machines are used in stereotactic radiation therapy to brain tumors treatments. It delivers “shots” that are extremely precise, reaching the tumor area in a shape of spheres. Due to the use of multiple shots centered at the disease area, the healthy tissue receives minimal dose of radiation. On the other hand, the use of multiple shots can result in exposing the tumor to a higher dose of radiation which happens when the spheres are superimposed, and such action must not happen. All the tumor area should be covered homogeneously by the treatment. In order to achieve this goal we must define the number of shots that have to be done as well as its positions and dosages (see [1] and [3]). This task nowadays demands time and a lot of experience and knowledge from the person that is planning the treatment and it makes the treatment very expensive. By automating the treatments planning these costs may decrease and more people can access it.

We present in this work a new model for the discrete problem of ellipsoidal filling that uses the idea of the Facility Location Problem [4] to determine the probable positions for the centers of the spheres in such a way that each sphere is like a facility that attends parts of the ellipsoid. Given an ellipsoid with (x_0, y_0, z_0) as center coordinates and R_x, R_y, R_z as its radii and a set of radii of spheres, $r \in \{r_1, r_2, r_3..., r_M\}, r < \min\{R_x, R_y, R_z\}$, the problem is to fill the ellipsoid with spheres. There are two peculiarities that make this problem a discrete one: the radii of the spheres belong to the set above and the number of spheres that must be integer. For this reason, most of the existent approaches to solve this problem are based in discrete optimization techniques. We want to emphasize that our goal is to solve the ellipsoidal filling problem, which differs from the complete solution for the configuration of Gamma ray machines in the sense that it is not in our scope the determination of the dosage of each shot (see [1] and [3]).

In this work, the model proposed is mixed integer which differs from the integer models presented in [1]. This work also differs from [2] because the model is totally different and we do not use Geometric Programming to solve it.

The text is organized like that: in Section 2 we present in detail the Discret Ellipsoidal Filling Problem (DEFP) and the Weak Discret Ellipsoidal Filling Problem (WDEFP) and a theoretical basis to solve the first (DEFP) using the second one (WDEFP). Besides that, we present a model for the Discret Ellipsoidal Filling Problem (DEFP). In Section 3 the computational results are presented.

Terminology:
$c = (x_0, y_0, z_0)$ is the center of the ellipsoid;
$C(w, r)$ is the cube of center w and inscribed in the sphere of radius r;
$D(w, r)$ is the dodecahedron of center w and inscribed in the sphere of radius r;
$E(c, R)$ is the ellipsoid of center c and radii (R_x, R_y, R_z), where $R = \text{diag}(R_x, R_y, R_z)$;
γ is the level of intersection between two different spheres;
r_i is the radius of the i-sphere, $i = 1, \ldots, n$;
R is the matrix whose diagonal elements are the radii of the ellipsoid;
$\{R_x, R_y, R_z\}$ are the radii of the ellipsoid;
$S(w, r)$ is the sphere of center w and radius r;

θ is the ratio between the volume of a sphere and the volume of the inscribed cube or dodecahedron;
$\|v\|$ is the euclidean norm; $\sqrt{\sum_{i=1}^{n} v_i^2}$;
$\|v\|_\infty$ is the maximum norm; $\|v\|_\infty = \max\{|v_1|, \ldots, |v_n|\}$;
Vol(S) is the volume of solid S;
$w_i = (w_i^x, w_i^y, w_i^z)$ is the center of the ith-sphere;
$\aleph_0(C)$ is the cardinality of the set C;
$\overline{R} = \max\{R_x, R_y, R_z\}$.

2. The discrete ellipsoidal filling problem - DEFP

The goal of this section is to detail the DEFP. This problem consists in filling an ellipsoid with spheres. It is more specifically defined below:

Given $(R_x, R_y, R_z) \in \mathcal{R}^3_{++}, c \in \mathcal{R}^3, n \in N$, the ellipsoid of center c and radii (R_x, R_y, R_z) is defined by the following set:

$$E(c, R) = \left\{w \in \mathcal{R}^3; (w - c)^t R^{-2} (w - c) \leq 1\right\},$$

where $R = \text{diag}(R_x, R_y, R_z)$.

We can define DEFP as:

Definition 2.1. Given an ellipsoid $E(c, R)$ a **discrete ellipsoidal filling** (DEF) is a structure of the form:

$$Pell(E) = \{\mathbf{C}, \mathbf{r}\},$$

where $\mathbf{C} = \{w_1, w_2, \ldots, w_n\}$, $\mathbf{r} = \{r_i \in \{\mathrm{r}_1, \mathrm{r}_2, \ldots, \mathrm{r}_M\},\ i = 1, \ldots, n\}$, w_i and r_i satisfy the following conditions:

1. $w_i \in E(c, R)$ for all n;
2. if $w \in E(c, R)$ then $\|w - w_i\| \leq r_i$ for some $i = 1, \ldots, n$;
3. the number of spheres n must be as small as possible.

$\mathbf{C}$ and $\mathbf{r}$ are respectively the set of the centers of the spheres and the set of the discrete radii. If $\mathbf{r} = \{r \in [a, b]\}$ the filling is said to be continuous. The discrete ellipsoidal filling problem (DEFP) can be seen as determining a pair $P = \{\mathbf{C}, \mathbf{r}\}$.

The Definition 2.1 suggests that we treat the (DEFP) as a viability problem with semi infinite restrictions. To avoid this semi infinite characteristic, we propose a formulation named weak discrete ellipsoidal filling (WDEF), presented in Definition 2.2.

Definition 2.2. Given an ellipsoid $E(c, R)$ a **weak discrete ellipsoidal filling** (WDEF) is a structure of the form:

$$\underline{Pell}(E(c, R)) = \{\mathbf{C}, \mathbf{r}\},$$

where $\mathbf{C} = \{w_1, w_2, \dots, w_n\}$, $\mathbf{r} = \{r_i \in \{r_1, r_2, \dots, r_M\},\ i = 1, \dots, n\}$, w_i, r_i and r_j satisfy the following conditions:

1. $w_i \in E(c, R)$ for all n;
2. $\|w_i - w_j\| \geq \gamma(r_i + r_j)$ for all $i = 1, \dots, n,\ j = i+1, \dots, n,$ $r_i, r_j \in \{r_1, r_2, \dots, r_M\}$;
3. The number of spheres n must be as small as possible.

$\mathbf{C}$ and $\mathbf{r}$ are respectively the set of the centers of the spheres and the set of the discrete radii, the parameter γ is such that γr is the radius of the sphere that is inscribed in the cube ($\gamma = \frac{1}{\sqrt{3}}$) or in the dodecahedron $\left(\gamma = \frac{\sqrt{10(25+11\sqrt{5})}}{5\sqrt{3}(1+\sqrt{5})}\right)$ that is inscribed in $S(w, r)$. Mathematically we have $S(w, \gamma r) \subset C(w, r) \subset S(w, r)$.

Both of the above structures differ only with respect to item 2. In Definitions 2.1 and 2.2 at (WDEF) we relax the condition of total filling given by item 2 of Definition 2.1 and obtain a weaker condition that is given by item 2 of Definition 2.2 and aiming to solve the viability problem in Definition 2.1 we propose to solve a maximization problem whose constraints satisfy items 1, 2 and 3 of Definition 2.2 besides some aditional constraint that ensures the condition of total filling given by item 2 of Definition 2.1.

Here after, our work will be about finding a weak ellipsoidal filling for a given ellipsoid E_{seg} such that $E(c, R) \subset E_{seg}$ with $E_{seg} = E(c, R_{seg})$, whose radii of the spheres are as big as possible and impose the following condition:

Condition 2.3. If $S(w_i, r_i)$ is the i-sphere with center w_i and radius r_i then $S(w_i, r_i) \subset E_{seg}$.

E_{seg} will be called **security ellipsoid** and is defined as:

Definition 2.4. Given an ellipsoid $E(c, R)$ and $\epsilon > 0$ we define the security ellipsoid E_{seg} as:

$$E_{seg} = \left\{ w \in \mathcal{R}^3; (w-c)^t R_{seg}^{-2} (w-c) \leq 1 \right\},$$

where $R_{seg} = (1+\epsilon)\,\mathrm{diag}\,(R_x, R_y, R_z)$.

Condition 2.3 is not essential because it can be obtained in an indirect way as Proposition 2.5 shows.

Proposition 2.5. *Given* $\epsilon > 0, r > 0, c \in \mathcal{R}^3$ *and* $(R_x, R_y, R_z) \in \mathcal{R}^3_{++}$. *Let* $R_{\min} = \min\{R_x, R_y, R_z\}$, $r_{\max} = \max\{r_1, r_2, \dots, r_M\}$, $\widetilde{\epsilon} = (1 - \epsilon \frac{R_{\min}}{r_{\max}})$ *and* $R_{\widetilde{\epsilon}} = \mathrm{diag}(R_x - \widetilde{\epsilon} r, R_y - \widetilde{\epsilon} r, R_z - \widetilde{\epsilon} r)$. *If* $r \leq r_{\max} \leq R_{\min}$ *and* $w \in E(c, R_{\widetilde{\epsilon}})$ *then* $S(w, r) \subset E_{seg}$.

Proof. Given $p \in S(w, r)$,

$$(p-c)^t R_{seg}^{-2}(p-c) \leq \frac{\overline{R}+(1-\widetilde{\epsilon})r}{\overline{R}(1+\epsilon)} = \frac{\overline{R}+\epsilon r \frac{R_{\min}}{r_{\max}}}{\overline{R}(1+\epsilon)} \leq 1.$$

∎

Let $B_\infty[0,1] = \{v \in \mathcal{R}^3 | \, \|v\|_\infty = 1\}$ and $Z = \{x_1, x_2, \ldots, x_n\} \subset B_\infty[0,1]$. If

$$\|x_i - x_j\| \leq \frac{2(r-1)}{\overline{R}}$$

for some i, j, where r is the radius of the largest sphere contained in $E(c, R)$ then we have the following results.

Proposition 2.6. *If* $x \in B_\infty[0,1]$, *then*

$$w \in \partial E(0,R) = \left\{x \in \mathcal{R}^3 \mid x^t R^{-2} x = 1, \; R = \operatorname{diag}(R_x, R_y, R_z)\right\}.$$

Proof. $\dfrac{xR}{\|x\|} R^{-2} \dfrac{Rx}{\|x\|} = 1.$ ∎

Proposition 2.7. *If* $\|x_i - x_j\| \geq \dfrac{2(r-1)}{\overline{R}}$ *then* $\|w_i - w_j\| \leq 2(r-1)$.

Proof. $\|w_i - w_j\| = \left\| \dfrac{Rx_i}{\|x_i\|} - \dfrac{Rx_j}{\|x_j\|} \right\| \leq \overline{R} \left\| \dfrac{x_i}{\|x_i\|} - \dfrac{x_j}{\|x_j\|} \right\|.$
But

$$\left\| \frac{x_i}{\|x_i\|} - \frac{x_j}{\|x_j\|} \right\| \leq \frac{\overline{r}}{r} \|x_i - x_j\| \leq \|x_i - x_j\|,$$

where

$$\overline{r} = \|\overline{w}\| - r \text{ with } \overline{w}_i = x_i \text{ and } \overline{w}_j = \frac{x_j}{\|x_i\|} \text{ if } \|x_i\| \leq \|x_j\|$$

or

$$\overline{w}_i = \frac{x_i}{\|x_j\|} \text{ and } \overline{w_j} = x_j \text{ if } \|x_j\| \leq \|x_i\|.$$

As we have seen before, $\|x_i - x_j\| \leq \frac{2(r-1)}{\overline{R}}$ and therefore

$$\|w_i - w_j\| \leq \overline{R}\frac{2(r-1)}{\overline{R}} = 2(r-1).$$

∎

This proposition means that given two points inside the ellipsoid, there exists at least one that satisfies $\|w_i - w_j\| \leq 2(r-1)$.

Definition 2.8. For each $i = 1, \ldots, N$, where $N = \aleph_0(Z)$, $Z = \{x_1, x_2, \ldots, x_n\} \subset B_\infty[0,1]$, let

$$z_i = \{w_j; \|w_i - w_j\| \leq 2(r-1)\}, \; N_i = \aleph_0(z_i),$$

$$\overline{w}_i = \frac{1}{N_i}\left(\sum_{j=1}^{N_i} w_j^1,\ \sum_{j=1}^{N_i} w_j^2,\ \sum_{j=1}^{N_i} w_j^3\right)^t.$$

The points $\overline{w}_i$ are called barycentre of z_i or points of Weber of z_i.

Definition 2.9. Let $\overline{w}_i$ be the facility i, w_j be the location j,
$\delta_{ij} = 1$, if $\overline{w_i}$ attends w_j or $\delta_{ij} = 0$, otherwise;
$y_i = 1$, if $\overline{w}_i$ is a reference point for the center of the ith sphere or $y_i = 0$, otherwise;
$z_{ij} = 1$, if $S(x_i, r_i)$ and $S(x_j, r_j)$ intercept each other or $z_{ij} = 0$, otherwise.
The optimization problem associated to $\underline{Pell}(E(c, R))$ that uses the idea of the facility location problem is given by:

$$
\begin{aligned}
(\mathrm{P}_1) \qquad \text{Minimize} \quad & \sum_{i=1}^{N}\sum_{j=1}^{N} q_{ij}\delta_{ij} + \sum_{i=1}^{N} r_i + M\sum_{i=1}^{N} y_i \\
\text{subject to} \quad & \sum_{j=1}^{N} \delta_{ij} \le N y_i, && (1)\\
& \sum_{i=1}^{N} \delta_{ij} \ge 1, && (2)\\
& \|\overline{w}_i - x_i\| \le 1, && (3)\\
& \|x_i - x_j - (1 - z_{ij})(\overline{w}_i - \overline{w}_j)\| \le \gamma(r_i + r_j), && (4)\\
& \sum_{i=1}^{N} z_{ij} \le N y_i, && (5)\\
& \sum_{i=1}^{N} z_{ij} \ge 1, && (6)\\
& q_{ij}\delta_{ij} \le r_i, && (7)\\
& r_i \in \{2, 4, 7, 9\}.
\end{aligned}
$$

In the objective function, q_{ij} is the distance between the barycentre and the points at the border and M is a big constant. The first constraint (1) means that each barycentre is able to cover all border points. Constraint (2) assures that each border point will be covered by at least one barycentre. Constraint (3) allows the center of the spheres to have a certain mobility in relation to its barycentre. The center of the sphere can be located at maximum at the border of a sphere of radius 1, centered at the the barycentre. This distance is necessary to the further adjustement of the radii $\{2, 4, 7, 9\}$. Constraint (4) prevents the spheres to overlap. Constraint (5) allows one barycentre to intercept any other barycentre. Constraint (6) says that each sphere must intercept at least one other. Constraint (7) says that if one sphere has x_i as its centre so it has to cover all the points allocated to it. It is noteworthy that this model is convex.

The parameter γ has a fundamental importance in this model because it allows the spheres to have intersection without overlapping. In this work we consider two values for γ, namely:$\gamma_c = \frac{1}{\sqrt{3}}$ and $\gamma_d = \frac{\sqrt{10(25+11\sqrt{5})}}{5\sqrt{3}(1+\sqrt{5})}$.

The following set of constraints can be used to make the radii reach the desired values of $\{2, 4, 7, 9\}$.

$$r_i = 2\lambda_{i1} + 3\lambda_{i2}, \tag{8}$$

$$\lambda_{i1} - \lambda_{i2} \geq 1, \tag{9}$$

$$\lambda_{i1} - \lambda_{i2} \leq 2, \tag{10}$$

$$1 \leq \lambda_{i1} \leq 3, \tag{11}$$

$$0 \leq \lambda_{i2} \leq 1. \tag{12}$$

Proposition 2.10. *If the problem has an optimal solution in which the non linear constraints are inactive and λ_{i1} and λ_{i2}, $i = 1, \ldots, n$ are vertices of the set of constraints* (9)*,* (10)*,* (11) *and* (12)*, then the radii of the spheres belong to the set* $\{2, 4, 7, 9\}$.

Proof. The points (1, 0), (2, 0), (2, 1) and (3, 1) are the vertices of the polytope given by the set of constraints (9), (10), (11) and (12). When we put these values on equation (8), we get $\{2, 4, 7, 9\}$ as the only possible values to the radii of the spheres. ■

2.1. Evaluation of the level of filling in a weak discrete ellipsoidal filling (WDEF)

Here we try to evaluate if the (WDEF) can provide a good filling and give a simple condition to have $\underline{Pell}(E(c, R)) = Pell(E(c, R))$, that is, the weak discrete ellipsoidal filling equals the discrete ellipsoidal filling. Aiming at this purpose we build the results and definitions that are in this section.

Definition 2.11. Given $d > 0$, an ellipsoid $E(c, R)$ and $\underline{Pell}(E(c, R)) = (\mathbf{C},\mathbf{r})$ and a (WDEF) for $E(c, R)$ we define:

- A mesh for $E(c, R)$ is the intersection $E(c, R) \cap M(d)$, where

$$M(d) = \{w \in \mathcal{R}^3;\ w = c + (-R_x : d : R_x, -R_y : d : R_y, -R_z : d : R_z)\}.$$

  This means that the mesh is generated accordingly to each (R_x, R_y, R_z) of the ellipsoid and the distance d between its points will determine if there will be more or less points at the mesh.
- The level of filling of a (WDEF) $\underline{Pell}(E(c, R)) = (\mathbf{C},\mathbf{r})$ is defined by

$$IP(\underline{Pell}(E(c, R))) = \frac{\aleph_0(\underline{Pell}(E(c, R) \cap M(d)))}{\aleph_0(M(d))},$$

where $\underline{Pell}(E(c,R) \cap M(d)) = \{w \in M(d) \cap S(\tilde{w},\tilde{r})\}$ for some pair $(\tilde{w},\tilde{r}) \in$ (**C**,**r**).

- We say that a (WDEF) $\underline{Pell}(E(c,R)) =$ (**C**,**r**) of $(E(c,R))$ is total or perfect if $IP(\underline{Pell}(E(c,R))) = 1$.

Proposition 2.12 gives us a characterization between the ellipsoidal filling and the weak ellipsoidal filling.

Proposition 2.12. *Given $d > 0$, a mesh $M(d)$, a* (WDEF) $\underline{Pell}(E(c,R)) =$ (***C*,*r***) *for $E(c,R)$ and set $\underline{Pell_d}(E(c,R)) = (C, r_d)$, where $r_d(i) = r(i) - d\sqrt{3}, i = 1,\dots,n$, then*

$$\underline{Pell_d}(E(c,R)) = Pell_d(E(c,R)) \text{ if and only if } IP(\underline{Pell_d}(E(c,R))) = 1.$$

Proof. If $\underline{Pell_d}(E(c,R)) = Pell_d(E(c,R))$ then for all $v \in E(c,R), \exists S(w,r)$ such that $\|v-w\| \le r$. If it happens, particularly, the points that belong to the mesh are covered by at least one sphere, so we have

$$\frac{\aleph_0(\underline{Pell}(E(c,R) \cap M(d)))}{\aleph_0(M(d))} = \frac{\aleph_0(\underline{Pell}(E(c,R) \cap M(d)))}{\aleph_0(\underline{Pell}(E(c,R) \cap M(d)))} = 1.$$

Given $v \in E(c,R), \exists\, w \in M(d)$ so that $\|v-w\| \le d\sqrt{3}$. If $IP(\underline{Pell_d}(E(c,R))) = 1,\ \exists\, w_i \in \underline{Pell_d}(E(c,R))$ so that $\|w-w_i\| \le d(i) - d\sqrt{3}$. So we have

$$\|v-w_i\| \le \|v-w\| + \|w-w_i\| \le d\sqrt{3} + r_i - d\sqrt{3}.$$

So there exist $w_i \in c$ and $r_i \in R$ such that $\|v-w_i\| \le r_i$. ∎

3. Computational results

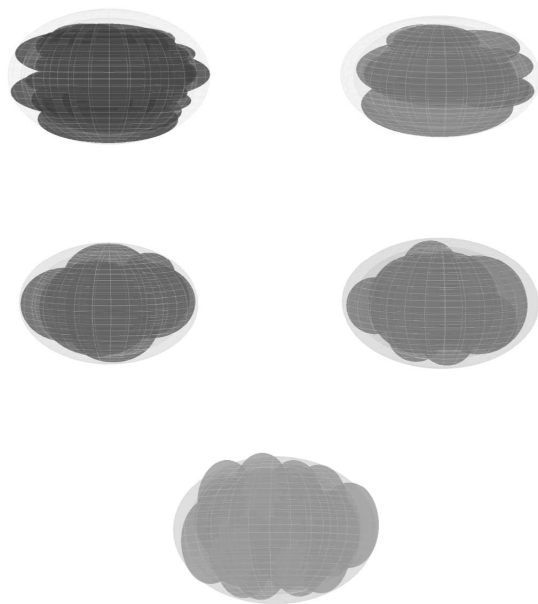
In this section we present computational results for our formulation. Although we have used the Global Optimization Toolbox of Matlab to solve the problem, only the function *fmincon* was necessary. According to the Matlab documentation, *fmincon* is a function that attempts to find a constrained minimum of a scalar function of several variables starting at an initial estimate. As the problem is convex, the solution given by *fmincon* is global, with no need of using other tools of the Global Optimization Toolbox of Matlab.

Further modifications are being made to improve the computational performance.

When the final result is avaiable, we put it in a fine mesh and calculate the percentage of grid points that are covered by at least one sphere. The table below shows some of the results of the computational experiments. The first column gives the number of the test. The second column gives the radii of the ellipsoid. The third, fourth and fifth columns give the number of spheres of radii 2, 4, 7 and 9. The last column gives the level of filling. The figures are in the order of the tests from the left to the right.

Table 1 Numerical results

Experiment	R	2	4	7	9	IP
1	(5, 8, 10)	9	9	1	1	99.61 %
2	(8, 10, 12)	-	4	3	2	97.30 %
3	(14, 12, 10)	-	1	5	2	95.32 %
4	(12, 10, 8)	-	5	2	2	98.41 %
5	(12, 8, 6)	11	17	-	1	97.47 %



Acknowledgements. This work was supported by Projeto Casadinho (UFPB-UFRJ)/CNPq. The authors want also to thank the referees for their comments on an earlier draft of this paper.

References

1. L. Liberti, N. Maculan and Y. Zhang, Optimal configuration of gamma ray machine radiosurgery units: the sphere covering subproblem, *Optim. Lett.* **3** (2009), 109–121.
2. R. Q. Nascimento, L. F. Cabral, A. R. U. S. Macambira and R. V. Pinto, The discrete ellipsoidal filling problem: a geometric discrete programming approach, submitted to publication in *Discrete Applied Math.*.

3. A. Sutou and Y. Dai, Global optimization approach to unequal sphere packing problems in 3D, *J. Optim. Theory Appl.* **114** (2002), 671–694.
4. Z. Drezner and H. W. Hamacher, *Facility Location: Applications and Theory*, Springer-Verlag, Berlin-Heidelberg, 2001.