Covering Solids By Spheres of Different Diameters

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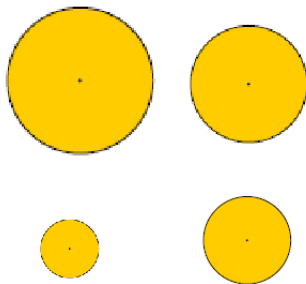
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Agenda

The Problem

(a) Solid to be covered.   (b) Available spheres sizes.
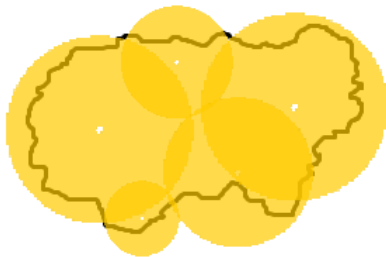
An Example

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 $\rho : N \to R$,

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:

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

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

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

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

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

[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.

The Covering Problem
A Formulation

Nonlinear nonconvex mixed-integer <u>infinite</u> 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
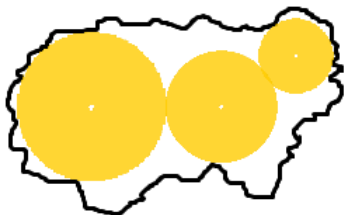- the spheres must be totally inside the container.

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

$$a_m x + b_m y + c_m z \geq d_m, \quad m = 1, \ldots, M,$$

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.

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[1] 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.

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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:

$$\max \quad \frac{4}{3}\pi \sum_{i=1}^{N} \sum_{k=1}^{K} r_k^3 w_{ik}$$

$$\text{s.a} \quad ||x^i - x^j||^2 \geq \Big(\sum_{k=1}^{K} r_k w_{ik} + \sum_{k=1}^{K} r_k w_{jk} \Big)^2, \quad \forall i \neq j$$

$$|a_m x_i + b_m y_i + c_m z_i - d_m|/\sqrt{a_m^2 + b_m^2 + c_m^2} \geq \sum_{k=1}^{K} r_k w_{ik}, \quad \forall i, m$$

$$a_m x_i + b_m y_i + c_m z_i - d_m \geq 0, \quad \forall i, \forall m$$

$$\sum_{k=1}^{K} w_{ik} \leq 1, \quad \forall i$$

$$w_{ik} \in \{0, 1\}, \quad \forall i, \forall k$$

Proposed Model

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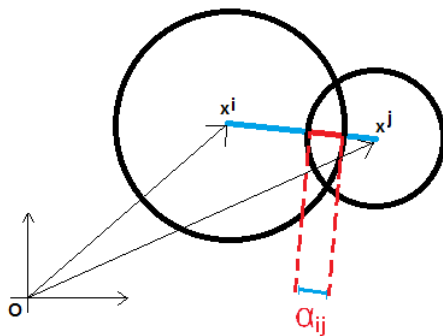
Proposed Model

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

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

Proposed Model

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

We could have

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

But to avoid the multiplication of variables, we will use

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

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The Covering Problem
Proposed Model

Proposed Model for the Covering Problem

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

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

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

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

The Covering Problem
Proposed Model

Proposed Model for the Covering Problem

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

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Proposed Model

Parameters Existence Theorem

There are

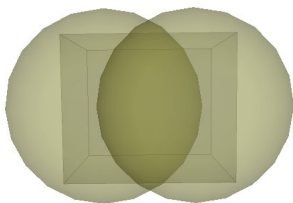$$\{\alpha_{ij} \geq 0\}_{1 \leq i < j \leq n}$$
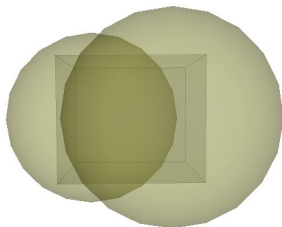
and

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

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.
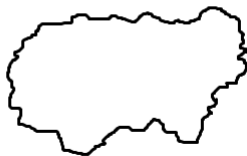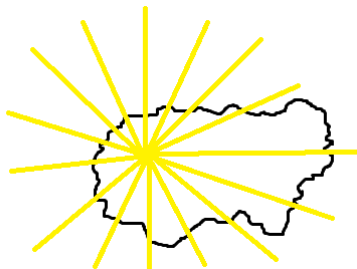
Motivation

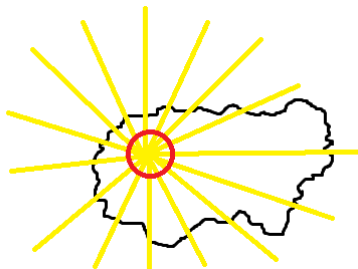- The *Gamma Knife* radiosurgery planning process.

Motivation

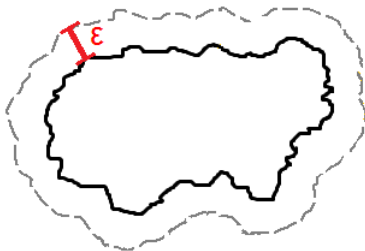- The *Gamma Knife* radiosurgery planning process.

Motivation

- The *Gamma Knife* radiosurgery planning process.

Security Region

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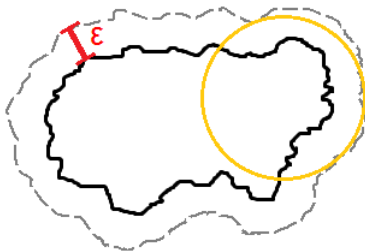
Security Region

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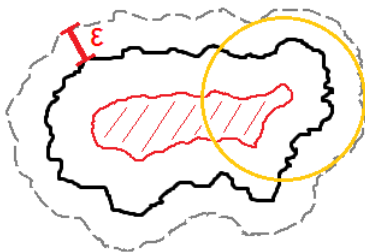# Security Region

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

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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Results

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

- COV: percentage of T's volume covered by the spheres;

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- 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.
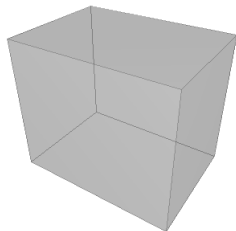
Results

For the parameters, we used

$$c_i = r_i^3$$

and

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

Couenne

	Couenne
Algorithm	sB&B
z^*	352
$|S|$	9
t_e	20h
t_t	9d
cov	68.12%
miscov	7.66%
overlap	9.03%
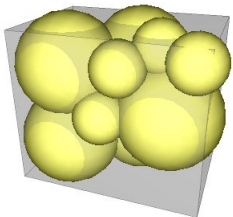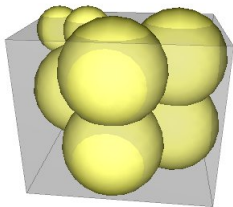
- $z*$: objective function value
- $|S|$: amount of spheres used
- t_e: time to find solution
- t_t: execution time till forced stop

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%

- t_t: total execution time
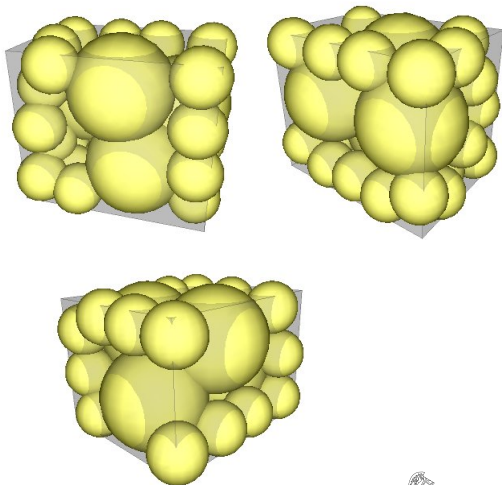
Xpress-SLP

- 30 spheres of radius 2mm

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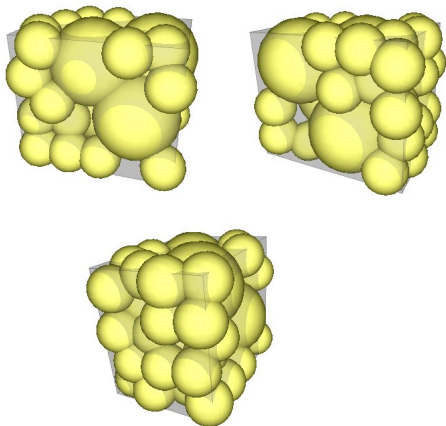
- t_t: total execution time

Heuristic

Hypothesis
Spheres of larger radius are more interesting in the solution.

Heuristic based on solving the following problem:

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

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

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 randomically;

- If the solver claims the problem is infeasible, reduce the last added sphere's radius.

Results from Ipopt

	Ipopt
Algorithm	Interior Points
z^*	514
$|S|$	29
t_t	17s
cov	91.40%
miscov	9.91%
overlap	16.13%
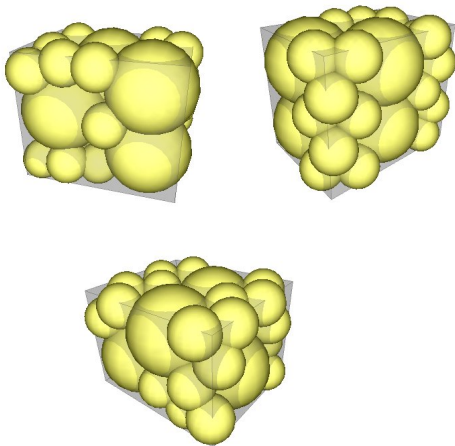
- t_t: total execution time

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 $[a, b]$;

- $a \leq w_1 < \cdots < w_L \leq b$;

- $\lambda_i \in \{0, 1\}, \quad \forall i \in \{1, \ldots, L\}$; e

- $\sum_{i=1}^{L} \lambda_i = 1$.

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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

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

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

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:

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

Discretization

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

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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%

- t_e: time the solution was found (and subsequent abortion)
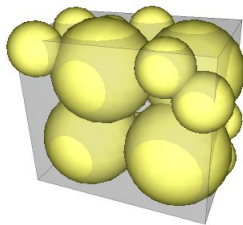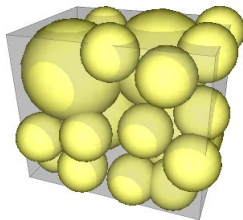
Comparison

	COUENNE	BONMIN	Xpress	Xpress	Ipopt
	sB&B	B-BB	SLP	$\delta = 0.2$	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

		Ipopt	
	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

- t: execution time
- β: overlap parameter
- ε: security region parameter

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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.

Graph Approach

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- $V = \{ (r, p) \mid r \in R, \ p \in P \}$;

- 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.

We aim to find the maximum clique in this graph.

Graph Approach

Maximum-weight clique model:

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

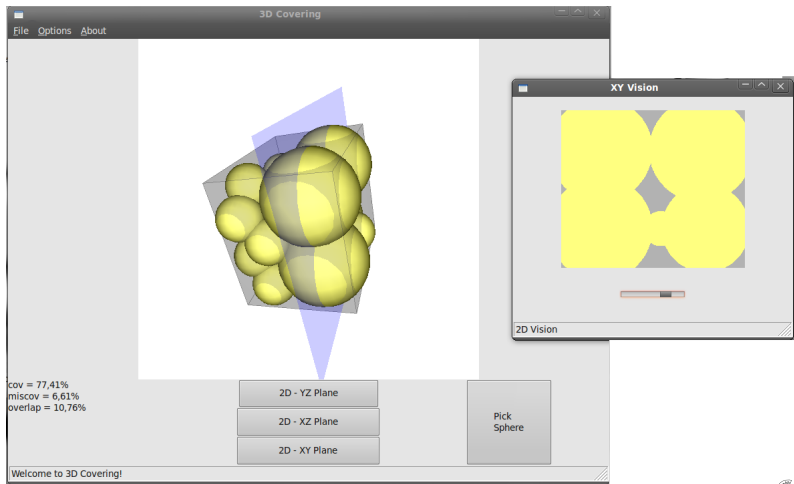$$s.t. \quad y_i + y_j \leq 1\,, \quad \forall (i,j) \notin E$$

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

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.

3D Program

Future Work

Working with the complement of the graph:

- Branch and Cut
    cuts: violated cliques

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

- Branch and Bound
    branching: violated cliques

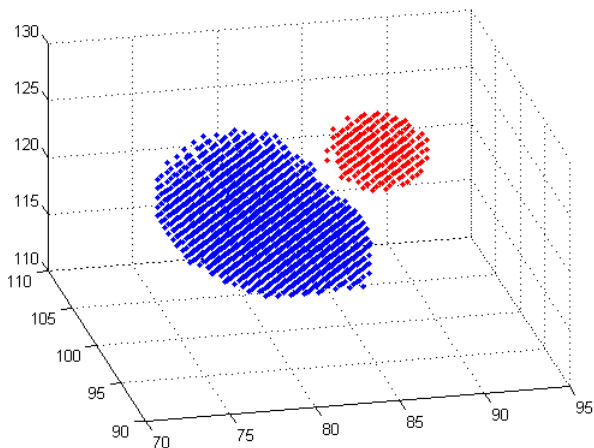# Future Work

- More realistic data
  .

Target volume
Organ at risk

References

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- [3] R. Quirino & A. F. Macambira & L. Cabral & R. Pinto. "The Discrete Ellipsoid Covering problem: a Discrete Geometric Programming Approach". *Discrete Applied Mathematics*, 2012.

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