Empacotamento de elipsoides

Rafael Durbano Lobato

Tese apresentada
ao
Instituto de Matemática e Estatística
da
Universidade de São Paulo
para
obtenção do título
de
Doutor em Ciências

Programa: Ciência da Computação
Orientador: Prof. Dr. Ernesto G. Birgin

Durante o desenvolvimento deste trabalho, o autor recebeu auxílio financeiro do CNPq (154103/2011-0) e da FAPESP (2012/23916-8)

São Paulo, novembro de 2015

Ellipsoid packing

Rafael Durbano Lobato

Thesis presented
to the
Institute of Mathematics and Statistics
of the
University of Sao Paulo
for the
obtention of the degree
of
Doctor of Science

Program: Computer Science
Advisor: Prof. Dr. Ernesto G. Birgin

During the development of this work, the author received financial aid from CNPq (154103/2011-0) and FAPESP (2012/23916-8)

São Paulo, November 2015

Empacotamento de elipsoides

Esta versão da tese contém as correções e alterações sugeridas pela Comissão Julgadora durante a defesa da versão original do trabalho, realizada em 6/11/2015. Uma cópia da versão original está disponível no Instituto de Matemática e Estatística da Universidade de São Paulo.

Comissão Julgadora:

- Prof. Dr. Ernesto Julián Goldberg Birgin (orientador) - IME-USP
- Prof^{a}. Dr^{a}. Yoshiko Wakabayashi - IME-USP
- Prof. Dr. José Mario Martínez Perez - UNICAMP
- Prof^{a}. Dr^{a}. Sandra Augusta Santos - UNICAMP
- Prof. Dr. Reinaldo Morabito Neto - UFSCar

Ellipsoid packing

This version of the thesis contains corrections and amendments suggested by the Examining Committee for the defense of the original version of the work held on 11.06.2015. A copy of the original version is available at the Institute of Mathematics and Statistics of the University of São Paulo.

Examining Committee:

- Prof. Dr. Ernesto Julián Goldberg Birgin (advisor) - IME-USP
- Prof. Dr. Yoshiko Wakabayashi - IME-USP
- Prof. Dr. José Mario Martínez Perez - UNICAMP
- Prof. Dr. Sandra Augusta Santos - UNICAMP
- Prof. Dr. Reinaldo Morabito Neto - UFSCar

Esta tese é dedicada
à memória do meu pai, Antonio Carlos,
e à minha mãe, Roseli.

This thesis is dedicated
to the memory of my dad, Antonio Carlos,
and to my mom, Roseli.

Agradecimentos

Agradeço ao Ernesto, por toda a sua atenção, motivação e dedicação em me orientar neste trabalho.

Agradeço aos professores Martínez, Reinaldo, Sandra, e Yoshiko pelas sugestões e comentários valiosos, que contribuíram para o aperfeiçoamento desta tese.

Agradeço aos meus amigos do IME pelas conversas, risadas, jogos e almoços.

Acima de tudo, agradeço à minha família, em especial ao meu pai, Antonio Carlos, e à minha mãe, Roseli, que sempre estiveram ao meu lado e me apoiaram. Serei eternamente grato por tudo o que fizeram por mim.

Acknowledgements

I would like to thank Ernesto for his attention, motivation and dedication in guiding me in this work.

I thank Professors Martínez, Reinaldo, Sandra, and Yoshiko for their valuable suggestions and comments, which have contributed to the improvement of this thesis.

Also I thank my friends and lab mates from IME for the talks, laughter, games and lunches.

Most of all, I thank my family, especially my father, Antonio Carlos, and my mother, Roseli, who have always been with me and supported me. I will be eternally grateful for everything they have done for me.

Resumo

LOBATO, R. D. **Empacotamento de elipsoides**. 2015. Tese (Doutorado) - Instituto de Matemática e Estatística, Universidade de São Paulo, São Paulo, 2015.

O problema de empacotamento de elipsoides consiste em arranjar uma dada coleção de elipsoides dentro de um determinado conjunto. Os elipsoides podem ser rotacionados e transladados e não podem se sobrepor. Um caso particular desse problema surge quando os elipsoides são bolas. O problema de empacotamento de bolas tem sido alvo de intensa pesquisa teórica e experimental. Em particular, muitos trabalhos têm abordado esse problema com ferramentas de otimização. O problema de empacotamento de elipsoides, por outro lado, começou a receber mais atenção apenas recentemente. Esse problema aparece em um grande número de aplicações práticas, como o projeto de materiais cerâmicos de alta densidade, na formação e crescimento de cristais, na estrutura de líquidos, cristais e vidros, no fluxo e compressão de materiais granulares e vidros, na termodinâmica e cinética da transição de líquido para cristal e em ciências biológicas, na organização de cromossomos no núcleo de células humanas. Neste trabalho, tratamos do problema de empacotamento de elipsoides dentro de conjuntos compactos do ponto de vista de otimização. Introduzimos modelos de programação não-linear contínuos e diferenciáveis e algoritmos para o empacotamento de elipsoides no espaço n-dimensional. Apresentamos dois modelos diferentes para a não-sobreposição de elipsoides. Como esses modelos têm números quadráticos de variáveis e restrições em função do número de elipsoides a serem empacotados, também propomos um modelo com variáveis implícitas que possui uma quantidade linear de variáveis e restrições. Também apresentamos modelos para a inclusão de elipsoides em semi-espaços e dentro de elipsoides. Através da aplicação de uma estratégia *multi-start* simples combinada com uma escolha inteligente de pontos iniciais e um resolvedor para otimização local de programas não-lineares, apresentamos experimentos numéricos que mostram as capacidades dos modelos propostos.

Palavras-chave: Empacotamento de elipsoides, programação não-linear, modelos matemáticos, algoritmos, experimentos computacionais.

Abstract

LOBATO, R. D. **Ellipsoid packing**. 2015. Doctoral Thesis - Institute of Mathematics and Statistics, University of São Paulo, São Paulo, 2015.

The problem of packing ellipsoids consists in arranging a given collection of ellipsoids within a particular set. The ellipsoids can be freely rotated and translated, and must not overlap each other. A particular case of this problem arises when the ellipsoids are balls. The problem of packing balls has been the subject of intense theoretical and empirical research. In particular, many works have tackled the problem with optimization tools. On the other hand, the problem of packing ellipsoids has received more attention only in the past few years. This problem appears in a large number of practical applications, such as the design of high-density ceramic materials, 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, in biological sciences, in the chromosome organization in human cell nuclei. In this work, we deal with the problem of packing ellipsoids within compact sets from an optimization perspective. We introduce continuous and differentiable nonlinear programming models and algorithms for packing ellipsoids in the n-dimensional space. We present two different models for the non-overlapping of ellipsoids. As these models have quadratic numbers of variables and constraints, we also propose an implicit variables models that has a linear number of variables and constraints. We also present models for the inclusion of ellipsoids within half-spaces and ellipsoids. By applying a simple multi-start strategy combined with a clever choice of starting guesses and a nonlinear programming local solver, we present illustrative numerical experiments that show the capabilities of the proposed models.

Keywords: Ellipsoid packing, nonlinear programming, mathematical models, algorithms, numerical experiments.

Contents

Nomenclature

$[A]_{:,j}$	The j-th column of matrix A.
$[A]_{i,:}$	The i-th row of matrix A.
I_n	The identity matrix of dimension n.
$\lambda_{\max}(A)$	The largest eigenvalue of matrix A.
$\lambda_{\min}(A)$	The least eigenvalue of matrix A.
$A^\top$	The transpose of matrix A.
∂S	The frontier of set S.
$\mathrm{int}(S)$	The interior of set S.
$\mathbb{R}$	The set of real number.
$\mathbb{R}^n$	The Euclidean space of dimension n.
$\mathbb{R}_+$	The set of nonnegative real numbers.
$\mathbb{R}_{++}$	The set of positive real numbers.
$\mathrm{ri}(S)$	The relative interior of set S.
I	The set $\{1, \dots, m\}$ of indices of ellipsoids.
m	The number of ellipsoids to be packed.
$[x]_i$	The i-th component of vector x.
$\|x\|_2$	The Euclidean norm of x.
$\frac{\partial f}{\partial x}$	The partial derivative of function f with respect to x.
$\frac{\mathrm{d}f}{\mathrm{d}x}$	The total derivative of function f with respect to x.

List of Figures

List of Tables

Chapter 1

Introduction

In a packing problem, we are given a collection of items (identical or non-identical sets) and a set called container. Each item can be translated and possibly rotated. The problem consists in arranging the items within the container and without overlap. In other words, each item must be included in the container and the items must not overlap each other, that is, the intersection of the interiors of any pair of items must be empty. The former type of restrictions is called containment constraints and the latter is called non-overlapping constraints. In the present work, the items to be packed are ellipsoids in $\mathbb{R}^n$ and the container can be either a polyhedron or an ellipsoid. A particular case of the ellipsoid packing problem arises when the items to be packed are balls. The problem of packing balls has been the subject of intense theoretical and empirical research. In particular, many works have tackled the problem with optimization tools. See, for example, [6, 9, 17, 18, 19, 22, 37, 53, 54, 55, 56] and the references therein. On the other hand, the problem of packing ellipsoids has received more attention only in the past few years. This problem appears in a large number of practical applications, such as the design of high-density ceramic materials, the formation and growth of crystals [21, 49], the structure of liquids, crystals and glasses [4], the flow and compression of granular materials [24, 34, 35], the thermodynamics of liquid to crystal transition [1, 20, 48], and, in biological sciences, in the chromosome organization in human cell nuclei [57].

The main problem when arranging the ellipsoids inside the container is to avoid the overlap between the ellipsoids. Consider the particular case where the ellipsoids are balls. In this case, there is a simple condition for two balls not to overlap. Suppose that one ball has radius r_i and is centered at c_i and that another ball has radius r_j ans is centered at c_j. A necessary and sufficient condition for these two balls not to overlap is that the distance between their centers must be at least the sum of their radius, that is $\|c_i - c_j\|_2 \geq r_i + r_j$. However, there is no known simple condition for avoiding the overlap of general ellipsoids. Conditions for a ball to be contained in a set can also be very simple depending on the set. For certain types of containers, these conditions can be written as a set of constraints applied to the center of the ball and involving a resized container. For example, the necessary and sufficient condition for a ball with radius r centered at c to be contained within a ball with radius R centered at the origin is $\|c\|_2 \leq R - r$, that is, the center c must belong to the ball with radius $R - r$ centered at the origin. Again, there is no known simple condition for ensuring that an ellipsoid be inside a ball.

In 1611, in an essay entitled "De Nive Sexangula" ("On the Six-Cornered Snowflake"), Johannes Kepler described an arrangement of identical balls and conjectured that no other arrangement could be tighter than that one [29]. This arrangement was an answer to the problem of stacking cannonballs on the ships' deck in the most efficient way. In this type of arrangement, the density (ratio of the volume occupied by the balls to the total volume) reached by identical balls arranged in the three-dimensional space is $\pi/\sqrt{18}$ (approximately 0.74048). This density is achieved, for example, when the balls are arranged according to the face-centered cubic lattice or the hexagonal close-packing. In 1998, nearly 400 years after Kepler formulated his conjecture, Thomas C. Hales managed to prove it with the help of computational methods. His proof was disclosed in a series of articles, the first one being published in 2005 [28].

Birgin *et al.* [7] consider the problem of packing circles within ellipses. Although the condition for a circle to be inside another circle is very simple, the condition for a circle to be inside an ellipse may not be. In order to develop conditions under which a circle is inside an ellipse, they have introduced a new ellipse-based system of coordinates. This system of coordinates is based on a reference ellipse and provides a closed-form expression to compute the distance of an arbitrary point to the frontier of the reference ellipse. Based on this system of coordinates, a continuous and differentiable nonlinear programming formulation for the problem of packing circle within an ellipse was proposed.

Donev *et al.* [23] analyse the density of three-dimensional ellipsoid packings. On the one hand, experiments with M&M's Milk Chocolate Candies (registered trademark of Mars, Inc.) are performed. Two varieties of the candies were used: mini and regular. Their shapes are very similar to oblate ellipsoids. The minis have semi-axis lengths 0.4625 ± 0.0055cm and 0.2465 ± 0.009cm, while the regular ones have semi-axis lengths 0.67 ± 0.01cm and 0.3465 ± 0.009cm. A 5-liter round flask was filled up with approximately 23,000 minis and 7,000 regular candies (separately). The density found in both experiments was about 0.685. On the other hand, a simulation technique that generalises the Lubachevsky-Stillinger sphere-packing algorithm [41] is proposed. Numerical experiments with 1,000 ellipsoids are presented. For ellipsoids with semi-axis lengths $a = \alpha^{-1}$, $b = 1$ and $c = \alpha$ with $\alpha \approx 1.3$, the density approaches 0.74. Since the main subject of the work is to analyse the density of "jammed disordered packings", the computer-aided simulations do not confine the ellipsoids to a compact container (but to a box with periodic boundary conditions) and optimization procedures are not employed.

Uhler and Wright [57] dealt with a problem related to the chromosome organization in the human cell nucleus. The problem is to arrange ellipsoids inside a container (with the shape of an ellipsoid) so as to minimize some measure of total overlap between ellipsoid pairs. The selected overlap measure was the sum of the lengths of the principal semi-axes of the largest ellipsoid that can be inscribed in the intersection of the ellipsoids. To solve this problem, they proposed a hard-to-solve bilevel programming model in which the lower-level problem is a semidefinite programming problem. The upper-level problem is to position and orient the ellipsoids in the container so as to minimize the maximum overlap between the ellipsoids; while the lower-level problem is a semidefinite program which aims at calculating the overlap measure.

Up to our knowledge, only five very recent works in the literature exploit mathematical programming formulations and optimization to deal with the problem of packing ellipses or ellipsoids within rectangular containers. These are the works by Galiev and Lisafina [26]

(2013), Kallrath and Rebennack [38] (2014), Kallrath [36] (2015), Stoyan *et al.* [52] (2015), and Pankratov *et al.* [47] (2015).

Galiev and Lisafina [26] considered the two-dimensional problem of packing the maximum possible number of identical ellipses within a given rectangle. They restricted the problem to the case where the ellipses are orthogonally oriented, that is, their axes are parallel to the axes of the rectangle. To simplify the problem, the centers of the ellipses are also required to belong to a given finite set of points as follows. Two finite sets of points lying in the container are constructed, so that the centers of the ellipses can only be placed on points that belong to one of these sets. If the center of an ellipse is placed on a point of the first set, then its major axis is parallel to the x-axis. On the other hand, if the center of an ellipse is placed on a point of the second set, then its major axis is parallel to the y-axis. These two sets are not required to be disjoint. Due to these assumptions, the authors were able to derive conditions under which two orthogonally oriented ellipses do not overlap and an integer linear programming model for the problem was presented. Binary variables were used to select the points where the centers of the ellipses should be placed and the objective was to maximize the sum of these variables subject to (linear) non-overlapping constraints. Galiev and Lisafina also presented a heuristic algorithm to deal with a possibly large number of variables. At each step of the algorithm, a few layers of ellipses is packed in a portion of the rectangle by solving the proposed integer model, taking into account previously packed ellipses. They have used CPLEX to solve the model and presented experiments with packings of less than seventy ellipses.

Kallrath and Rebennack [38] dealt with the two-dimensional problem of packing a fixed number of ellipses within a rectangle while minimizing the area of the container. The authors presented a non-convex nonlinear programming formulation for the problem. The non-overlapping constraints are based on separating lines. For each pair of ellipses, there is an associated line which forces the ellipses to lie on opposite half-planes determined by that line. To ensure that a certain ellipse be on one side of the separating line, the point on the boundary of that ellipse which is closest to the separating line is computed. Then, it is required that the distance between the center of the ellipse and the separating line be greater than or equal to the distance from the center of the ellipse to the line that is tangent to that point on the boundary. The authors derived closed-form solutions for those distances. To fit an ellipse inside the container, it is required that the least rectangle that contains the ellipse and have sides parallel to the sides of the container must be inside the container. This formulation has a quadratic number of variables and constraints on the number of ellipses to be packed. An equivalent non-convex quadratic model was also presented, which was more suitable considering the available optimization solvers. Kallrath and Rebennack also included three sets of symmetry breaking constraints. The first one requires that one of the ellipses must have its center in the first quadrant of the container. A second set of constraint imposes an order on the centers of identical ellipses with respect to the lower left corner of the container. The last set of constraints is responsible for moving the center of each ellipse towards the lower left corner of the container. The authors also presented a mixed-integer nonlinear programming extension of the proposed model. In this formulation, the container is partitioned into a rectangular grid so that the center of each ellipse is uniquely assigned to one of the cells of this grid. Binary variables are used to conduct this assignment. The number of binary variables introduced is equal to the number of ellipses times the number of cells in the grid. Lower and upper bounds on the area of the container are computed by packing circles instead of the ellipses. Lower bounds are obtained by packing circles whose radii are the length of the semi-minor axes of the ellipses and upper bounds are computed by packing circles whose radii are the length of the semi-major axes of the ellipses. The authors have developed two heuristic algorithms where the ellipses are gradually packed. Both of them keep the width of the container fixed while the length of the container is minimized. The first algorithm considers all possible sequences of the set of ellipses to be packed and, for each sequence, it works as follows. At each step, the centers and angles of previous packed ellipses are fixed, the next (up to) k ellipses of the sequence are selected to be packed and the length of the container is minimized. After this subset is packed, the centers and angles of all ellipses packed so far are unfixed and a global optimization solver is used to improve this solution. The procedure continues until all ellipses are packed. The second algorithm is similar. However, at each step, instead of fixing all previous ellipses packed, they are removed from the current subproblem except for the k right most ellipses. The analysis of the numerical experiments presented in [38] allow us to conclude that the state-of-the-art global optimization solvers BARON [51], LindoGlobal [39], and GloMIQO [45], available within the GAMS platform, were unable to find global solutions for instances with more than 4 ellipses (when restricted to a maximum of 5 hours of CPU time). For larger instances, the authors have used the heuristic methods and numerical experiments with up to 100 ellipses were presented.

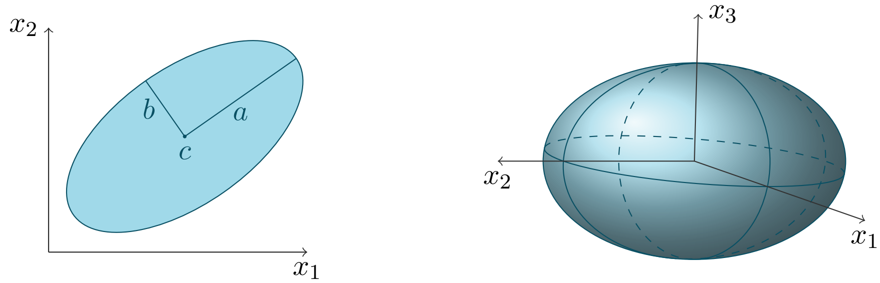
The methodology introduced in [38] for packing ellipses within rectangles of minimum area was extended by Kallrath [36] to tackle the problem of packing ellipsoids within rectangular containers of minimum volume. The non-overlapping constraints are based on separating hyperplanes. Nonlinear programming models were proposed and tackled by global optimization methods. Instances with up to 100 ellipsoids were considered, but, as well as in the two-dimensional case [38], state-of-the-art global optimization solvers available within GAMS were unable to find optimal solutions and only feasible points are reported.

The problem of placing a given set of ellipses within a rectangular container of minimal area was considered by Stoyan *et al.* [52]. Nonlinear programming models were proposed by considering "quasi-phi-functions" that are an extension of the phi-functions that were extensively used in the literature to model a large variety of packing problems (see, for example, [53, 54, 55, 56] and the references therein). Using *ad hoc* initial guesses, instances with up to 120 ellipses were tackled by a multi-start strategy combined with a local nonlinear programming solver. In [47], the methodology proposed in [52] is extended to deal with the problem of packing spheroids within a rectangular container of minimal volume and numerical experiments with up to 12 spheroids are presented.

1.1 The problem statement

An ellipsoid in $\mathbb{R}^n$ is a set of the form $\mathcal{E} = \{x \in \mathbb{R}^n \mid (x-c)^\top M^{-1}(x-c) \leq 1\}$, where $M \in \mathbb{R}^{n\times n}$ is a symmetric and positive definite matrix. Vector $c \in \mathbb{R}^n$ is the center of the ellipsoid. The eigenvectors of M^{-1} determine the principal axes of the ellipsoid and the eigenvalues of $M^{\frac{1}{2}}$ are the lengths of the semi-axes of the ellipsoid. If M is a positive multiple of the identity matrix, then the ellipsoid is a ball. More specifically, if $M = r^2 I_n$ for some $r > 0$, then the ellipsoid is a ball with radius r. An ellipsoid in a two-dimensional space is also called an ellipse.

Figure 1.1(a) shows an ellipse and Figure 1.1(b) illustrates an ellipsoid in a three-dimensional space.



(a) (b)

Figure 1.1: (a) An ellipse centered at c with semi-axes lengths a and b. (b) Illustration of an ellipsoid in a three-dimensional space.

Let $\mathcal{E} = \{x \in \mathbb{R}^n \mid (x-c)^\top M(x-c) \leq 1\}$, where $M \in \mathbb{R}^{n\times n}$. We denote by $\partial\mathcal{E}$ the frontier of $\mathcal{E}$, i.e., $\partial\mathcal{E} = \{x \in \mathbb{R}^n \mid (x-c)^\top M(x-c) = 1\}$. We denote by $\mathrm{int}(\mathcal{E})$ the interior of $\mathcal{E}$, i.e., $\mathrm{int}(\mathcal{E}) = \{x \in \mathbb{R}^n \mid (x-c)^\top M(x-c) < 1\}$. We say that two ellipsoids overlap if there exists a point in the interior of one of the ellipsoids that belongs to the other ellipsoid. We say that two ellipsoids touch each other if they do not overlap and there exists a point that belongs to the frontier of both ellipsoids.

In this work, we deal with the problem of packing ellipsoids in two- and three-dimensional spaces. We can state this problem as follows. Given ellipsoids $\bar{\mathcal{E}}_1, \dots, \bar{\mathcal{E}}_m$ in $\mathbb{R}^n$ and a set $\mathcal{C} \subset \mathbb{R}^n$, that we call a container from now on, we want to find ellipsoids $\mathcal{E}_1, \dots, \mathcal{E}_m$ such that

1. $\mathcal{E}_i$ is obtained by rotating and translating ellipsoid $\bar{\mathcal{E}}_i$ for all $i \in \{1, \dots, m\}$;
2. $\mathrm{int}(\mathcal{E}_i) \cap \mathrm{int}(\mathcal{E}_j) = \emptyset$ for all $i, j \in \{1, \dots, m\}$ with $i \neq j$;
3. $\mathcal{E}_i \subseteq \mathcal{C}$ for each $i \in \{1, \dots, m\}$.

The first constraint states that we can only rotate and translate the given ellipsoids. The second constraint says that the ellipsoids cannot overlap. The third constraint requires that each ellipsoid be inside the container. This is a feasibility problem whose variables are the center and angles of rotation of each ellipsoid. We also deal with optimization problems such as minimizing the volume of the container or packing the maximum possible number of ellipsoids into a given container.

It is easy to determine whether two balls overlap. If the distance between the centers of the balls is less than the sum of their radius then the balls overlap. Otherwise, they do not overlap. In the case of ellipsoids, however, there is no simple way to verify whether two ellipsoids overlap. For each $i \in \{1, 2\}$, consider the ellipsoid $\mathcal{E}_i = \{x \in \mathbb{R}^n \mid (x-c_i)^\top M_i^{-1}(x-c_i) \leq 1\}$. Ellipsoids $\mathcal{E}_1$ and $\mathcal{E}_2$ overlap if and only if there exists $x \in \mathbb{R}^n$ such that

$$(x-c_1)^\top M_1^{-1}(x-c_1) < 1 \quad \text{and} \quad (x-c_2)^\top M_2^{-1}(x-c_2) < 1.$$

In order to guarantee that ellipsoids $\mathcal{E}_1$ and $\mathcal{E}_2$ do not overlap, we will apply a linear transformation to both ellipsoids that converts the first ellipsoid into a ball $\mathcal{E}_{11}$ with radius r and the second ellipsoid into another ellipsoid $\mathcal{E}_{12}$. We will show that $\mathcal{E}_1$ and $\mathcal{E}_2$ overlap if and only if $\mathcal{E}_{11}$ and $\mathcal{E}_{12}$ overlap.

For $\mathcal{E}_{11}$ and $\mathcal{E}_{12}$ not to overlap, the distance between the center c_1' of $\mathcal{E}_{11}$ and the ellipsoid $\mathcal{E}_{12}$ must be greater than or equal to r. Nevertheless, there is no known formula for this distance and it may be necessary to solve an optimization problem in order to find it. Thus, to find this distance efficiently, we will propose a representation for the center of the ball $\mathcal{E}_{11}$ in terms of the ellipsoid $\mathcal{E}_{12}$ so that the distance between c_1' and $\mathcal{E}_{12}$ be easily obtained, without the need to solve an optimization problem.

1.2 Organization

This thesis is organized as follows. In Chapter 2, we derive two continuous and differentiable nonlinear programming models for the non-overlapping of ellipsoids. The first model, presented in Section 2.2.1, is based on a transformation presented in Section 2.1, which converts an ellipsoid into a ball. The second model is introduced in Section 2.2.2 and is based on separating hyperplanes. Next, in Section 2.3 we propose continuous and differentiable nonlinear programming models for the inclusion of an ellipsoid within an ellipsoid and within a half-space. Section 2.4 closes this chapter with some numerical experiments that show the capabilities of the introduced models.

Both non-overlapping models introduced in Chapter 2 have quadratic numbers of variables and constraints on the number of ellipsoids to be packed. In Chapter 3, we propose a nonlinear programming model that contains a linear number of variables and constraints. This model is a modification of the first non-overlapping model. The constraints are grouped into a linear number of constraints. Although these constraints are formed by a quadratic number of terms, a clever algorithm can be used to efficiently evaluate all constraints. The variables that are associated with every pair of ellipsoids become implicit variables, so that they have their values computed only when they are needed. This model is twice-differentiable but is not everywhere continuous on the domain. However, since it is discontinuous only on a zero measure subset of the domain, it can be solved in practice by using derivative-dependent methods as it is shown in Section 3.5.

Although the model proposed in Chapter 3 can be used to solve bigger problems than the first model, it also has its limitations and is not suitable for large-scale problems. In Chapter 4, we present a model and an algorithm for solving large-scale problems of packing the maximum number of ellipsoids within a fixed container. The model is based on the first non-overlapping model. By removing constraints that should never be active at a feasible solution and adding few constraints to replace them, we were able to keep the number of variables and constraints low, thus allowing the resolution of the larger problems.

In Chapter 5, we draw some conclusions and provide ideas for future work. Finally, in Appendix A, we show the first order derivatives of the transformation based non-overlapping model, and the first and second derivatives of the ball containment model. We also show how to compute the first and second order derivatives of the implicit variables model. As we will see in Chapter 3, the values of the implicit variables depend on the solution of an optimization problem so that the computation of the derivatives of the implicit variables is not a trivial task.

The computer implementation of the models and methods introduced in this thesis, as well as the reported solutions, are freely available for downloading at `http://www.ime.usp.br/~lobato/`.

Chapter 2

Nonlinear programming models

In this chapter, we present two continuous and differentiable nonlinear programming models for the non-overlapping of ellipsoids. The first model, introduced in Section 2.2.1, is based on a transformation described in Section 2.1. The second model is based on separating hyperplanes and is introduced in Section 2.2.2. Also, in Sections 2.3.1 and 2.3.2, we present continuous and differentiable nonlinear programming models for an ellipsoid to be contained in an ellipsoid and a half-space, respectively.

2.1 Transformations of ellipsoids

Consider a rotation matrix $Q \in \mathbb{R}^{n\times n}$ and the transformation $R : \mathbb{R}^n \to \mathbb{R}^n$ defined by $R(x) = Qx + c$, where $c \in \mathbb{R}^n$. In a two-dimensional space, we can represent a rotation matrix as

$$Q(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}, \tag{2.1}$$

which rotates a point counterclockwise through an angle θ. In a three-dimensional space, we can represent a rotation matrix as

$$Q(\psi,\theta,\phi) = \begin{pmatrix} \cos\theta\cos\psi & \sin\phi\sin\theta\cos\psi - \cos\phi\sin\psi & \sin\phi\sin\psi + \cos\phi\sin\theta\cos\psi \\ \cos\theta\sin\psi & \cos\phi\cos\psi + \sin\phi\sin\theta\sin\psi & \cos\phi\sin\theta\sin\psi - \sin\phi\cos\psi \\ -\sin\theta & \sin\phi\cos\theta & \cos\phi\cos\theta \end{pmatrix}, \tag{2.2}$$

which rotates a point through an angle ϕ about the x-axis, through an angle θ about the y-axis, and through an angle ψ about the z-axis. These rotations appear clockwise when the axis about which they occur points toward the observer. Consider the ellipsoid $\mathcal{E} = \{x \in \mathbb{R}^n \mid x^\top M^{-1}x \leq 1\}$, where M is a symmetric and positive definite matrix. After applying the transformation R

to the elements of $\mathcal{E}$ (that is centered at the origin), we obtain the set

$$\begin{aligned}\bar{\mathcal{E}} &= \{x \in \mathbb{R}^n \mid x = R(z), z \in \mathcal{E}\}\\ &= \{x \in \mathbb{R}^n \mid x = Qz + c, z \in \mathcal{E}\}\\ &= \{x \in \mathbb{R}^n \mid z = Q^\top(x - c), z \in \mathcal{E}\}\\ &= \{x \in \mathbb{R}^n \mid (x - c)^\top QM^{-1}Q^\top(x - c) \le 1\}.\end{aligned}$$

The set $\bar{\mathcal{E}}$ is an ellipsoid, since $QM^{-1}Q^\top$ is symmetric and positive definite. In fact, the transformation R is an isometry, since it is a rotation followed by a translation.

Now, consider the ellipsoids

$$\begin{aligned}\mathcal{E}_i &= \{x \in \mathbb{R}^n \mid (x - c_i)^\top Q_i P_i^{-1} Q_i^\top (x - c_i) \le 1\} \text{ and}\\ \mathcal{E}_j &= \{x \in \mathbb{R}^n \mid (x - c_j)^\top Q_j P_j^{-1} Q_j^\top (x - c_j) \le 1\},\end{aligned} \tag{2.3}$$

where P_i and P_j are positive definite diagonal matrices, and Q_i and Q_j are rotation matrices. Consider the linear transformation $T_i : \mathbb{R}^n \to \mathbb{R}^n$ defined by

$$T_i(x) = P_i^{-\frac{1}{2}} Q_i^\top x. \tag{2.4}$$

Let $\mathcal{E}_{ii}$ be the set obtained when the transformation T_i is applied to every element of $\mathcal{E}_i$, i.e.,

$$\begin{aligned}\mathcal{E}_{ii} &= \{x \in \mathbb{R}^n \mid x = T_i(z), z \in \mathcal{E}_i\}\\ &= \{x \in \mathbb{R}^n \mid x = P_i^{-\frac{1}{2}} Q_i^\top z, z \in \mathcal{E}_i\}\\ &= \{x \in \mathbb{R}^n \mid z = Q_i P_i^{\frac{1}{2}} x, z \in \mathcal{E}_i\}\\ &= \{x \in \mathbb{R}^n \mid (Q_i P_i^{\frac{1}{2}} x - c_i)^\top Q_i P_i^{-1} Q_i^\top (Q_i P_i^{\frac{1}{2}} x - c_i) \le 1\}\\ &= \{x \in \mathbb{R}^n \mid (x - P_i^{-\frac{1}{2}} Q_i^\top c_i)^\top (x - P_i^{-\frac{1}{2}} Q_i^\top c_i) \le 1\}.\end{aligned} \tag{2.5}$$

Note that $\mathcal{E}_{ii}$ is a ball with unitary radius centered at $P_i^{-\frac{1}{2}} Q_i^\top c_i$. By applying the transformation T_i to the elements of $\mathcal{E}_j$, we obtain the set

$$\begin{aligned}\mathcal{E}_{ij} &= \{x \in \mathbb{R}^n \mid x = T_i(z), z \in \mathcal{E}_j\}\\ &= \{x \in \mathbb{R}^n \mid x = P_i^{-\frac{1}{2}} Q_i^\top z, z \in \mathcal{E}_j\}\\ &= \{x \in \mathbb{R}^n \mid (Q_i P_i^{\frac{1}{2}} x - c_j)^\top Q_j P_j^{-1} Q_j^\top (Q_i P_i^{\frac{1}{2}} x - c_j) \le 1\}\\ &= \{x \in \mathbb{R}^n \mid (x - P_i^{-\frac{1}{2}} Q_i^\top c_j)^\top S_{ij} (x - P_i^{-\frac{1}{2}} Q_i^\top c_j) \le 1\},\end{aligned} \tag{2.6}$$

where

$$S_{ij} = P_i^{\frac{1}{2}} Q_i^\top Q_j P_j^{-1} Q_j^\top Q_i P_i^{\frac{1}{2}}. \tag{2.7}$$

Observe that S_{ij} can be written as $S_{ij} = V_{ij}^\top V_{ij}$, where $V_{ij} = P_j^{-\frac{1}{2}} Q_j^\top Q_i P_i^{\frac{1}{2}}$. Then, S_{ij} is symmetric. Moreover, since V_{ij} is nonsingular with $V_{ij}^{-1} = P_i^{-\frac{1}{2}} Q_i^\top Q_j P_j^{\frac{1}{2}}$, matrix S_{ij} is positive definite. Thus $\mathcal{E}_{ij}$ is an ellipsoid. Unlike transformation R, transformation T_i does not preserve the form of the ellipsoids. On the other hand, as shown in Lemma 2.1, the overlapping between the ellipsoids is preserved after transformation T_i is applied. In other words, the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ overlap if and only if ellipsoids $\mathcal{E}_{ii}$ and $\mathcal{E}_{ij}$ overlap.

Lemma 2.1 *Consider the ellipsoids $\mathcal{E}_i, \mathcal{E}_j, \mathcal{E}_{ii}$ and $\mathcal{E}_{ij}$ defined in (2.3), (2.5) and (2.6). Then, the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ overlap if and only if the ellipsoids $\mathcal{E}_{ii}$ and $\mathcal{E}_{ij}$ overlap.*

Proof: For any $x \in \mathbb{R}^n$, we have

$$\begin{aligned}(x-c_i)^\top Q_i P_i^{-1} Q_i^\top (x-c_i) &= (x-c_i)^\top Q_i P_i^{-\frac{1}{2}} P_i^{-\frac{1}{2}} Q_i^\top (x-c_i)\\ &= (x-c_i)^\top (P_i^{-\frac{1}{2}} Q_i^\top)^\top P_i^{-\frac{1}{2}} Q_i^\top (x-c_i)\\ &= (P_i^{-\frac{1}{2}} Q_i^\top x - P_i^{-\frac{1}{2}} Q_i^\top c_i)^\top (P_i^{-\frac{1}{2}} Q_i^\top x - P_i^{-\frac{1}{2}} Q_i^\top c_i)\\ &= (T_i(x) - P_i^{-\frac{1}{2}} Q_i^\top c_i)^\top (T_i(x) - P_i^{-\frac{1}{2}} Q_i^\top c_i).\end{aligned}$$

Then, $x \in \operatorname{int}(\mathcal{E}_i)$ if and only if $T_i(x) \in \operatorname{int}(\mathcal{E}_{ii})$. Moreover,

$$\begin{aligned}(x-c_j)^\top Q_j P_j^{-1} Q_j^\top (x-c_j) &= (x-c_j)^\top Q_i P_i^{-\frac{1}{2}} P_i^{\frac{1}{2}} Q_i^\top Q_j P_j^{-1} Q_j^\top Q_i P_i^{\frac{1}{2}} P_i^{-\frac{1}{2}} Q_i^\top (x-c_j)\\ &= (x-c_j)^\top Q_i P_i^{-\frac{1}{2}} S_{ij} P_i^{-\frac{1}{2}} Q_i^\top (x-c_j)\\ &= (x-c_j)^\top (P_i^{-\frac{1}{2}} Q_i^\top)^\top S_{ij} P_i^{-\frac{1}{2}} Q_i^\top (x-c_j)\\ &= (P_i^{-\frac{1}{2}} Q_i^\top x - P_i^{-\frac{1}{2}} Q_i^\top c_j)^\top S_{ij} (P_i^{-\frac{1}{2}} Q_i^\top x - P_i^{-\frac{1}{2}} Q_i^\top c_j)\\ &= (T_i(x) - P_i^{-\frac{1}{2}} Q_i^\top c_j)^\top S_{ij} (T_i(x) - P_i^{-\frac{1}{2}} Q_i^\top c_j).\end{aligned}$$

Therefore, $x \in \operatorname{int}(\mathcal{E}_j)$ if and only if $T_i(x) \in \operatorname{int}(\mathcal{E}_{ij})$. Hence, $\operatorname{int}(\mathcal{E}_i) \cap \operatorname{int}(\mathcal{E}_j) \neq \emptyset$ if and only if $\operatorname{int}(\mathcal{E}_{ii}) \cap \operatorname{int}(\mathcal{E}_{ij}) \neq \emptyset$. In other words, ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ overlap if and only if $\mathcal{E}_{ii}$ and $\mathcal{E}_{ij}$ overlap. $\square$

Figure 2.1 illustrates this transformation. Three ellipses are shown in Figure 2.1(a), where the ellipses $\mathcal{E}_1$ and $\mathcal{E}_2$ overlap. Figure 2.1(b) shows these ellipses after applying the transformation T_1, that turns the ellipse $\mathcal{E}_1$ into a unitary radius ball. Note that in Figure 2.1(b) only the ellipses $\mathcal{E}_{11}$ and $\mathcal{E}_{12}$ overlap.

To end this section, we present the following lemma, which will be used in later sections. In particular, this lemma will be applied together with transformation T_i defined in (2.4), which is invertible (namely, $T_i^{-1}(x) = Q_i P_i^{\frac{1}{2}} x$).

Lemma 2.2 *Let $T : \mathbb{R}^n \to \mathbb{R}^n$ be an invertible transformation. Let A and B be subsets of $\mathbb{R}^n$ and $A' = \{T(x) \mid x \in A\}$ and $B' = \{T(x) \mid x \in B\}$. Then, $A \subseteq B$ if and only if $A' \subseteq B'$.*

Proof: Suppose that $A \subseteq B$. Let $x \in A'$. Then, by the definition of A', we have $T^{-1}(x) \in A$. Thus, since $A \subseteq B$, we have $T^{-1}(x) \in B$. By the definition of B', we have $x = T(T^{-1}(x)) \in B'$. Therefore, $A' \subseteq B'$. Hence, $A' \subseteq B'$ if $A \subseteq B$. Analogously, we have $A \subseteq B$ if $A' \subseteq B'$. $\square$

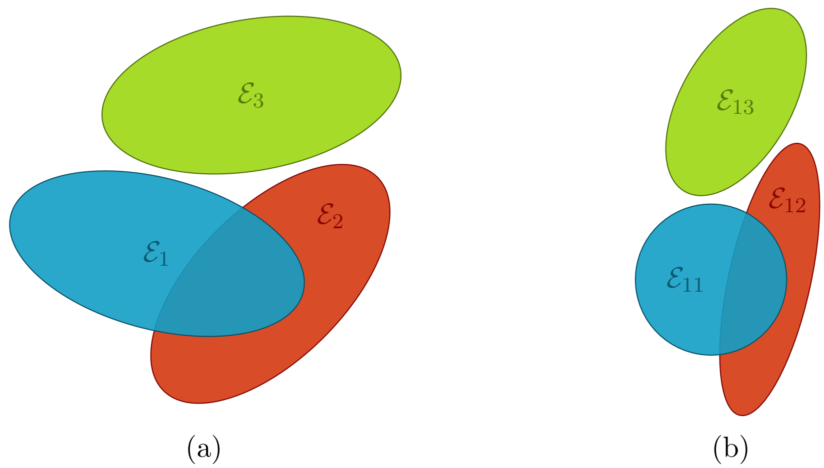


Figure 2.1: (a) Three ellipses and an overlapping between ellipses $\mathcal{E}_1$ and $\mathcal{E}_2$. Ellipse $\mathcal{E}_3$ does not overlap the other ellipses. (b) The transformation that converts $\mathcal{E}_1$ into a ball is applied to each ellipse.

2.2 Non-overlapping models

2.2.1 Transformation based model

Consider a ball $\mathcal{B}$ with radius $r > 0$ and an ellipsoid $\mathcal{E}$, both in $\mathbb{R}^n$. We know that $\mathcal{B}$ and $\mathcal{E}$ overlap if and only if the distance between the center of the ball $\mathcal{B}$ and the ellipsoid $\mathcal{E}$ is strictly less than r. Therefore, a necessary and sufficient condition for $\mathcal{B}$ and $\mathcal{E}$ not to overlap is that the distance between the center of the ball $\mathcal{B}$ and the ellipsoid $\mathcal{E}$ must be greater than or equal to r.

Now, consider the ellipsoids

$$\mathcal{E}_i = \{x \in \mathbb{R}^n \mid (x - c_i)^\top Q_i P_i^{-1} Q_i^\top (x - c_i) \leq 1\} \text{ and}$$
$$\mathcal{E}_j = \{x \in \mathbb{R}^n \mid (x - c_j)^\top Q_j P_j^{-1} Q_j^\top (x - c_j) \leq 1\},$$

where $c_i, c_j \in \mathbb{R}^n$, $Q_i, Q_j \in \mathbb{R}^{n\times n}$ are orthogonal matrices, and $P_i, P_j \in \mathbb{R}^{n\times n}$ are diagonal and positive definite matrices. As seen in Section 2.1, when transformation T_i defined in (2.4) is applied to both ellipsoids, we obtain the ball

$$\mathcal{E}_{ii} = \{x \in \mathbb{R}^n \mid (x - P_i^{-\frac{1}{2}} Q_i^\top c_i)^\top (x - P_i^{-\frac{1}{2}} Q_i^\top c_i) \leq 1\}$$

with unitary radius and the ellipsoid

$$\mathcal{E}_{ij} = \{x \in \mathbb{R}^n \mid (x - P_i^{-\frac{1}{2}} Q_i^\top c_j)^\top S_{ij} (x - P_i^{-\frac{1}{2}} Q_i^\top c_j) \leq 1\},$$

where

$$S_{ij} = P_i^{\frac{1}{2}} Q_i^\top Q_j P_j^{-1} Q_j^\top Q_i P_i^{\frac{1}{2}}.$$

In order to guarantee that $\mathcal{E}_{ii}$ and $\mathcal{E}_{ij}$ do not overlap, it is enough to require that the distance between the center c_{ii} of the ball $\mathcal{E}_{ii}$ and the ellipsoid $\mathcal{E}_{ij}$ be greater than or equal to one. Notice that, according to the discussion present in Section 2.1, this is a necessary and sufficient condition for the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ not to overlap. However, there is no known analytic expression for this distance. Thus, to find it, we can solve the problem of projecting c_{ii} onto $\mathcal{E}_{ij}$, that can be formulated as

$$\begin{array}{ll} \text{minimize} & \|x - c_{ii}\|_2^2 \\ \text{subject to} & x \in \mathcal{E}_{ij}. \end{array} \tag{2.8}$$

This is a convex quadratic programming problem whose optimal value is the squared distance between the center of the ball $\mathcal{E}_{ii}$ and the ellipsoid $\mathcal{E}_{ij}$. To find this distance more easily, we can represent the center of the ball $\mathcal{E}_{ii}$ as a function of ellipsoid $\mathcal{E}_{ij}$ in a convenient way detailed hereafter.

With a simple change of variables, we can rewrite problem (2.8) as the problem

$$\begin{array}{ll} \text{minimize} & \|x - (c_{ii} - P_i^{-\frac{1}{2}} Q_i^\top c_j)\|_2^2 \\ \text{subject to} & x^\top S_{ij} x \le 1. \end{array} \tag{2.9}$$

Let $\bar{\mathcal{E}}_{ij}$ be the ellipsoid determined by matrix S_{ij} and centered at the origin, i.e.,

$$\bar{\mathcal{E}}_{ij} = \{x \in \mathbb{R}^n \mid x^\top S_{ij} x \le 1\}.$$

Problem (2.9) is the problem of projecting the point $c_{ii} - P_i^{-\frac{1}{2}} Q_i^\top c_j$ onto ellipsoid $\bar{\mathcal{E}}_{ij}$. Suppose that $c_{ii} \notin \operatorname{int}(\mathcal{E}_{ij})$. Equivalently, we have $c_{ii} - P_i^{-\frac{1}{2}} Q_i^\top c_j \notin \operatorname{int}(\bar{\mathcal{E}}_{ij})$. Therefore, by Proposition 2.1 below, problem (2.9) has a unique solution $x_{ij} \in \mathbb{R}^n$. Moreover, its solution belongs to the frontier of ellipsoid $\bar{\mathcal{E}}_{ij}$, namely, $x_{ij}^\top S_{ij} x_{ij} = 1$, and there exists a unique $\mu_{ij} \in \mathbb{R}_+$ such that

$$c_{ii} - P_i^{-\frac{1}{2}} Q_i^\top c_j = x_{ij} + \mu_{ij} S_{ij} x_{ij}.$$

Thus, as long as $c_{ii} \notin \operatorname{int}(\mathcal{E}_{ij})$, c_{ii} is uniquely represented as a function of a point in the frontier of $\bar{\mathcal{E}}_{ij}$ and a non-negative scalar. In this case, the distance between the center c_{ii} of the ball $\mathcal{E}_{ii}$ and the ellipsoid $\mathcal{E}_{ij}$ is given by

$$\|x_{ij} - (c_{ii} - P_i^{-\frac{1}{2}} Q_i^\top c_j)\|_2 = \mu_{ij} \|S_{ij} x_{ij}\|_2.$$

On the other hand, by Proposition 2.2 below, any point of the form $y = x + \mu S_{ij} x$ with $x^\top S_{ij} x = 1$ and $\mu > 0$ is such that $y^\top S_{ij} y > 1$, i.e., it is a point that does not belong to the ellipsoid $\bar{\mathcal{E}}_{ij}$. If $\mu = 0$, then $y = x$ and, therefore, y is a point on the frontier of ellipsoid $\bar{\mathcal{E}}_{ij}$. Thus, any point of the form $y = x + \mu S_{ij} x$ such that $x^\top S_{ij} x = 1$ and $\mu \in \mathbb{R}_+$ does not belong to the interior of ellipsoid $\bar{\mathcal{E}}_{ij}$.

If c_{ii} lies in the interior of $\mathcal{E}_{ij}$, then the distance from c_{ii} to the ellipsoid $\mathcal{E}_{ij}$ is zero. So, for the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ not to overlap, c_{ii} must be outside the interior of $\mathcal{E}_{ij}$. Therefore, we can represent the center of the ball $\mathcal{E}_{ii}$ as a function of a point x_{ij} in the frontier of ellipsoid $\bar{\mathcal{E}}_{ij}$ and a nonnegative number μ_{ij} without loss of generality. Using this representation, the distance from the center of the ball $\mathcal{E}_{ii}$ to the ellipsoid $\mathcal{E}_{ij}$ is given by $\mu_{ij} \|S_{ij} x_{ij}\|_2$.

Proposition 2.1 *Let $\mathcal{E} = \{x \in \mathbb{R}^n \mid x^\top Mx \leq 1\}$, where $M \in \mathbb{R}^{n\times n}$ is a positive definite matrix. Thus, for each $y \in \mathbb{R}^n \setminus int(\mathcal{E})$, there exist unique $x^* \in \mathbb{R}^n$ and $\mu^* \in \mathbb{R}$ such that $y = x^* + \mu^* Mx^*$ and x^* is the projection of y onto $\mathcal{E}$. Moreover, $x^* \in \partial\mathcal{E}$ and $\mu^* \in \mathbb{R}_+$.*

Proof: Let $y \in \mathbb{R}^n$ be such that $y \notin \text{int}(\mathcal{E})$. The problem of projecting y onto the set $\mathcal{E}$ can be formulated as the problem

$$\begin{array}{ll} \text{minimize} & \|x-y\|_2^2 \\ \text{subject to} & x^\top Mx \leq 1. \end{array}$$

Since $\mathcal{E}$ is convex, this problem has a unique solution x^* (see, for example, Proposition 2.1.3 in [5]). The Lagrangian function associated with the above problem is

$$\mathcal{L}(x,\mu) = \|x-y\|_2^2 + \mu(x^\top Mx - 1),$$

whose gradient with respect to x is

$$\nabla_x \mathcal{L}(x,\mu) = 2(x-y) + 2\mu Mx.$$

Since the function that defines the inequality constraint is convex and the null vector strictly satisfies this constraint, this problem fulfills the Slater constraint qualification (see, for example, Proposition 3.3.9 in [5]). So, according to the Karush–Kuhn–Tucker first-order necessary conditions (see, for example, Proposition 3.3.1 in [5]), there exists a unique $\mu^* \in \mathbb{R}$ such that

$$\nabla_x \mathcal{L}(x^*,\mu^*) = 0 \tag{2.10}$$
$$\mu^*({x^*}^\top Mx^* - 1) = 0 \tag{2.11}$$
$$\mu^* \geq 0. \tag{2.12}$$

Therefore, by condition (2.10), we have that $y = x^* + \mu^* Mx^*$. If $y \in \partial\mathcal{E}$, then we must have $x^* = y$ and $\mu^* = 0$. On the other hand, if $y \notin \mathcal{E}$, then we must have $\mu^* \neq 0$. So, by condition (2.12), we must have $\mu^* > 0$. Consequently, condition (2.11) implies ${x^*}^\top Mx^* = 1$, i.e., $x^* \in \partial\mathcal{E}$. □

Proposition 2.2 *Let $\mathcal{E} = \{x \in \mathbb{R}^n \mid x^\top Mx \leq 1\}$, where $M \in \mathbb{R}^{n\times n}$ is a positive definite matrix. Thus, for each $x \in \partial\mathcal{E}$ and $\mu > 0$, we have $(x + \mu Mx)^\top M(x + \mu Mx) > 1$.*

Proof: Let $x \in \partial\mathcal{E}$ and $\mu > 0$. Thus, $x^\top Mx = 1$ and

$$\begin{aligned} (x+\mu Mx)^\top M(x+\mu Mx) &= x^\top Mx + 2\mu(Mx)^\top Mx + \mu^2(Mx)^\top M(Mx) \\ &= 1 + 2\mu\|Mx\|_2^2 + \mu^2(Mx)^\top M(Mx) \\ &> 1, \end{aligned}$$

where the inequality follows from the fact that $Mx \neq 0$ and M is positive definite. □

Based on this representation, we shall develop a model for the non-overlapping of ellipsoids in $\mathbb{R}^n$. Let $I = \{1,\ldots,m\}$ be the set of indices of the ellipsoids. For each $i \in I$, it is given a positive definite diagonal matrix $P_i^{\frac{1}{2}} \in \mathbb{R}^{n\times n}$ whose eigenvalues are the lengths of the semi-principal axes of ellipsoid i. In order to guarantee that all the m ellipsoids do not overlap each other, we ensure that ellipsoids i and j do not overlap for each $i, j \in I$ such that $i < j$.

For each $i \in I$, the decision variable $c_i \in \mathbb{R}^n$ will represent the center of ellipsoid i and $Q_i \in \mathbb{R}^{n\times n}$ will represent a rotation matrix for ellipsoid i. For each $i, j \in I$ such that $i < j$, the decision variable $c_{ij} \in \mathbb{R}^n$ will represent the center of ball $\mathcal{E}_{ii}$ as a function of ellipsoid $\mathcal{E}_{ij}$. But, since we must have $c_{i,i+1} = c_{i,k}$ for each $k \in \{i+2, \dots, m\}$, we can replace variable c_{ij} with variable c_{ii} for each $j > i$. Furthermore, for each $i, j \in I$ such that $i < j$, the decision variable $x_{ij} \in \mathbb{R}^n$ will represent a point in the frontier of ellipsoid $\bar{\mathcal{E}}_{ij}$ and $\mu_{ij} \in \mathbb{R}$ will be a nonnegative variable.

Let $i, j \in I$ be such that $i < j$. Since x_{ij} will be a point in the frontier of ellipsoid $\bar{\mathcal{E}}_{ij}$, we must have $x_{ij}^\top S_{ij} x_{ij} = 1$. Since μ_{ij} must be nonnegative, we must have the constraint $\mu_{ij} \geq 0$. Moreover, since the distance between the center of ball $\mathcal{E}_{ii}$ and the ellipsoid $\mathcal{E}_{ij}$ must be greater than or equal to one, we must have $\mu_{ij}\|S_{ij}x_{ij}\|_2 \geq 1$ or, equivalently, $\mu_{ij}^2\|S_{ij}x_{ij}\|_2^2 \geq 1$. According to the adopted representation, the center c_{ii} of the ball $\mathcal{E}_{ii}$ as a function of ellipsoid $\mathcal{E}_{ij}$ is given by

$$c_{ii} = x_{ij} + \mu_{ij} S_{ij} x_{ij} + P_i^{-\frac{1}{2}} Q_i^\top c_j.$$

Finally, for each $i \in I \setminus \{m\}$, the center of ball $\mathcal{E}_{ii}$ is $P_i^{-\frac{1}{2}} Q_i^\top c_i$. Thus, the center of ellipsoid i is given by $c_i = Q_i P_i^{\frac{1}{2}} c_{ii}$. So, we obtain the following model:

$$x_{ij}^\top S_{ij} x_{ij} = 1, \qquad \forall i, j \in I \text{ such that } i < j \tag{2.13}$$

$$\mu_{ij}^2 \|S_{ij} x_{ij}\|_2^2 \geq 1, \qquad \forall i, j \in I \text{ such that } i < j \tag{2.14}$$

$$\mu_{ij} \geq 0, \qquad \forall i, j \in I \text{ such that } i < j \tag{2.15}$$

$$c_{ii} = x_{ij} + \mu_{ij} S_{ij} x_{ij} + P_i^{-\frac{1}{2}} Q_i^\top c_j, \quad \forall i, j \in I \text{ such that } i < j \tag{2.16}$$

$$c_i = Q_i P_i^{\frac{1}{2}} c_{ii}, \qquad \forall i \in \{1, \dots, m-1\}. \tag{2.17}$$

This model has $\frac{1}{2}(m-1)(2n + m(n+3))$ constraints. The variables of this model are $x_{ij} \in \mathbb{R}^n$, $\mu_{ij} \in \mathbb{R}$ for each $i, j \in I$ such that $i < j$, and $Q_i \in \mathbb{R}^{n\times n}$, $c_{ii} \in \mathbb{R}^n$ and $c_i \in \mathbb{R}^n$ for $i \in I$. Thus, if the rotation matrices are represented as in (2.1) and (2.2), this model will have $\frac{1}{2}m(5+3m)$ variables in the two-dimensional case and $(6 + 2m(m+2))$ variables in the three-dimensional case.

2.2.1.1 Reducing the numbers of variables and constraints

The numbers of variables and constraints of the model (2.13)–(2.17) can be reduced by simply eliminating variables c_{ii} and constraints (2.17). The remaining constraints can also be somewhat simplified. Firstly, we present Proposition 2.3, which offers a strictly positive lower bound for the value of μ_{ij}. Lemma 2.3 is used in the proof of Proposition 2.3 and provides an upper bound on the norm of the vector $\|S_{ij}x_{ij}\|_2$ that depends only on the lengths of the semi-principal axes of ellipsoids i and j.

Lemma 2.3 *Let $x_{ij} \in \mathbb{R}^n$ and $S_{ij} = P_i^{\frac{1}{2}} Q_i^\top Q_j P_j^{-1} Q_j^\top Q_i P_i^{\frac{1}{2}} \in \mathbb{R}^{n\times n}$, where Q_i and Q_j are orthogonal matrices and P_i and P_j are positive definite diagonal matrices. Suppose that $x_{ij}^\top S_{ij} x_{ij} = 1$. Thus,*

$$\|S_{ij}x_{ij}\|_2 \leq \lambda_{\max}(P_i)\lambda_{\max}(P_j^{-1})\lambda_{\max}(P_j^{\frac{1}{2}})\lambda_{\max}(P_i^{-\frac{1}{2}}).$$

Proof: We have

$$\begin{aligned}
\|S_{ij}x_{ij}\|_2 &= \|P_i^{\frac{1}{2}} Q_i^\top Q_j P_j^{-1} Q_j^\top Q_i P_i^{\frac{1}{2}} x_{ij}\|_2 \\
&\leq \lambda_{\max}(P_i^{\frac{1}{2}})\|Q_i^\top Q_j P_j^{-1} Q_j^\top Q_i P_i^{\frac{1}{2}} x_{ij}\|_2 \\
&= \lambda_{\max}(P_i^{\frac{1}{2}})\|P_j^{-1} Q_j^\top Q_i P_i^{\frac{1}{2}} x_{ij}\|_2 \\
&\leq \lambda_{\max}(P_i^{\frac{1}{2}})\lambda_{\max}(P_j^{-1})\|Q_j^\top Q_i P_i^{\frac{1}{2}} x_{ij}\|_2 \\
&= \lambda_{\max}(P_i^{\frac{1}{2}})\lambda_{\max}(P_j^{-1})\|P_i^{\frac{1}{2}} x_{ij}\|_2 \\
&\leq \lambda_{\max}(P_i^{\frac{1}{2}})\lambda_{\max}(P_j^{-1})\lambda_{\max}(P_i^{\frac{1}{2}})\|x_{ij}\|_2 \\
&= \lambda_{\max}(P_i)\lambda_{\max}(P_j^{-1})\|x_{ij}\|_2,
\end{aligned}$$

where the second and third equalities hold since Q_i and Q_j are orthogonal matrices, and the inequalities and the last equality follow from the fact that $P_i^{\frac{1}{2}}$ and P_j^{-1} are positive definite diagonal matrices. Therefore,

$$\|S_{ij}x_{ij}\|_2 \leq \lambda_{\max}(P_i)\lambda_{\max}(P_j^{-1})\|x_{ij}\|_2. \tag{2.18}$$

Since $x_{ij}^\top S_{ij} x_{ij} = 1$, we have $\|x_{ij}\|_2 > 0$. Thus,

$$\lambda_{\min}(S_{ij}) \leq \frac{x_{ij}^\top S_{ij} x_{ij}}{\|x_{ij}\|_2^2} = \frac{1}{\|x_{ij}\|_2^2},$$

where the inequality follows from the Courant–Fischer Theorem (see, for example, Theorem 8.1.2 in [27]). Recalling from Section 2.1 that S_{ij} is positive definite, we have $\lambda_{\min}(S_{ij}) > 0$. Thus,

$$\|x_{ij}\|_2^2 \leq \frac{1}{\lambda_{\min}(S_{ij})}.$$

Moreover, we have

$$\begin{aligned}
\lambda_{\min}(S_{ij}) &= \lambda_{\min}(P_i^{\frac{1}{2}} Q_i^\top Q_j P_j^{-1} Q_j^\top Q_i P_i^{\frac{1}{2}}) \\
&\geq \lambda_{\min}(Q_i^\top Q_j P_j^{-1} Q_j^\top Q_i)\lambda_{\min}(P_i^{\frac{1}{2}} P_i^{\frac{1}{2}}) \\
&= \lambda_{\min}(Q_i^\top Q_j P_j^{-1} Q_j^\top Q_i)\lambda_{\min}(P_i) \\
&\geq \lambda_{\min}(P_j^{-1})\lambda_{\min}(Q_i^\top Q_j Q_j^\top Q_i)\lambda_{\min}(P_i) \\
&= \lambda_{\min}(P_j^{-1})\lambda_{\min}(P_i),
\end{aligned}$$

where the inequalities follow from Theorem 1.4 by Lu and Pearce [40] and the last equality holds since Q_i and Q_j are orthogonal matrices. Thus,

$$\|x_{ij}\|_2^2 \leq \frac{1}{\lambda_{\min}(P_j^{-1})\lambda_{\min}(P_i)} = \lambda_{\max}(P_j)\lambda_{\max}(P_i^{-1}),$$

where the equality holds since P_i and P_j are positive definite diagonal matrices. So,

$$\|x_{ij}\|_2 \leq \left(\lambda_{\max}(P_j)\lambda_{\max}(P_i^{-1})\right)^{\frac{1}{2}} = \left(\lambda_{\max}(P_j)\right)^{\frac{1}{2}}\left(\lambda_{\max}(P_i^{-1})\right)^{\frac{1}{2}} = \lambda_{\max}(P_j^{\frac{1}{2}})\lambda_{\max}(P_i^{-\frac{1}{2}}).$$

Therefore, from (2.18), we have

$$\|S_{ij}x_{ij}\|_2 \leq \lambda_{\max}(P_i)\lambda_{\max}(P_j^{-1})\lambda_{\max}(P_j^{\frac{1}{2}})\lambda_{\max}(P_i^{-\frac{1}{2}}).$$

□

Proposition 2.3 *Any solution to the system (2.13)–(2.17) is such that* $\mu_{ij} \geq \epsilon_{ij}$, *where*

$$\epsilon_{ij} = \lambda_{\min}(P_i^{-1})\lambda_{\min}(P_i^{\frac{1}{2}})\lambda_{\min}(P_j)\lambda_{\min}(P_j^{-\frac{1}{2}}) > 0,$$

for all $i < j$.

Proof: Consider a solution to the system (2.13)–(2.17). By constraints (2.13), we have $x_{ij}^\top S_{ij}x_{ij} = 1$ for each $i, j \in I$ such that $i < j$. Thus, by Lemma 2.3, we have

$$\|S_{ij}x_{ij}\|_2 \leq \lambda_{\max}(P_i)\lambda_{\max}(P_j^{-1})\lambda_{\max}(P_j^{\frac{1}{2}})\lambda_{\max}(P_i^{-\frac{1}{2}})$$

for all $i, j \in I$ such that $i < j$. By constraints (2.14) and (2.15), we must have $\|S_{ij}x_{ij}\|_2 > 0$ and $\mu_{ij} \geq \|S_{ij}x_{ij}\|_2^{-1}$ for all $i, j \in I$ such that $i < j$. Therefore, we can take

$$\begin{aligned}\epsilon_{ij} &= \left(\lambda_{\max}(P_i)\lambda_{\max}(P_j^{-1})\lambda_{\max}(P_j^{\frac{1}{2}})\lambda_{\max}(P_i^{-\frac{1}{2}})\right)^{-1} \\ &= \lambda_{\min}(P_i^{-1})\lambda_{\min}(P_i^{\frac{1}{2}})\lambda_{\min}(P_j)\lambda_{\min}(P_j^{-\frac{1}{2}})\end{aligned}$$

and the proposition holds. (Note that $\epsilon_{ij} > 0$ since P_i and P_j are positive definite matrices.) □

For each $i, j \in I$ such that $i < j$, the term $S_{ij}x_{ij}$ appears in constraints (2.13), (2.14), and (2.16). From constraints (2.16), we have

$$\mu_{ij}S_{ij}x_{ij} = c_{ii} - x_{ij} - P_i^{-\frac{1}{2}}Q_i^\top c_j, \quad \forall i, j \in I \text{ such that } i < j.$$

Thus, constraints (2.14) are equivalent to constraints

$$\|c_{ii} - x_{ij} - P_i^{-\frac{1}{2}}Q_i^\top c_j\|_2^2 \geq 1, \quad \forall i, j \in I \text{ such that } i < j. \tag{2.19}$$

Notice that any solution to the system (2.13)–(2.17) must strictly satisfy inequalities (2.15). In other words, any solution must be such that $\mu_{ij} > 0$ for all $i, j \in I$ such that $i < j$. This is a consequence of constraints (2.14). Hence, constraints (2.13) can be replaced by

$$x_{ij}^\top (c_{ii} - x_{ij} - P_i^{-\frac{1}{2}} Q_i^\top c_j) = \mu_{ij}, \quad \forall i, j \in I \text{ such that } i < j, \tag{2.20}$$

provided that $\mu_{ij} \neq 0$. By Proposition 2.3, there exist positive constants ϵ_{ij} such that constraints (2.13) and (2.15) are equivalent to constraints (2.20) and $\mu_{ij} \geq \epsilon_{ij}$ for all $i, j \in I$ such that $i < j$. By Proposition 2.3, we can take

$$\epsilon_{ij} = \lambda_{\min}(P_i^{-1}) \lambda_{\min}(P_i^{\frac{1}{2}}) \lambda_{\min}(P_j) \lambda_{\min}(P_j^{-\frac{1}{2}}), \tag{2.21}$$

where $\lambda_{\min}(M)$ denotes the least eigenvalue of matrix M. Therefore, we can replace constraints (2.13) and (2.14) with constraints (2.19), (2.20) and $\mu_{ij} \geq \epsilon_{ij}$, for all $i, j \in I$ such that $i < j$, and obtain an equivalent model.

Finally, for each $i \in I \setminus \{m\}$, we can replace c_{ii} with $P_i^{-\frac{1}{2}} Q_i^\top c_i$ in constraints (2.19) and (2.20). By doing so, we eliminate constraints (2.17) from the model and replace constraints (2.16), (2.19) and (2.20), respectively, with the following constraints:

$$\begin{aligned}
P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) &= x_{ij} + \mu_{ij} S_{ij} x_{ij}, && \forall i, j \in I \text{ such that } i < j \\
\| P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - x_{ij} \|_2^2 &\geq 1, && \forall i, j \in I \text{ such that } i < j \\
x_{ij}^\top \big(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - x_{ij} \big) &= \mu_{ij}, && \forall i, j \in I \text{ such that } i < j.
\end{aligned}$$

Hence, model (2.13)–(2.17) is equivalent to the following model:

$$x_{ij}^\top \big(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - x_{ij} \big) = \mu_{ij}, \quad \forall i, j \in I \text{ such that } i < j \tag{2.22}$$

$$\| P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - x_{ij} \|_2^2 \geq 1, \quad \forall i, j \in I \text{ such that } i < j \tag{2.23}$$

$$P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) = x_{ij} + \mu_{ij} S_{ij} x_{ij}, \quad \forall i, j \in I \text{ such that } i < j \tag{2.24}$$

$$\mu_{ij} \geq \epsilon_{ij}, \quad \forall i, j \in I \text{ such that } i < j. \tag{2.25}$$

The model (2.22)–(2.25) has $\frac{1}{2}m(m-1)(n+3)$ nonlinear constraints and $\frac{1}{2}m(m-1)$ bound-constraints. If the rotation matrices are represented as in (2.1) and (2.2), this model will have $\frac{3}{2}m(m+1)$ variables in the two-dimensional case and $2m(m+2)$ variables in the three-dimensional case.

2.2.1.2 Bounded domain for global optimization

Methods for global optimization rely heavily on bounds for the variables of the problem. In general, the tighter the lower bounds are, the better the performance of a global optimization method will be. We now derive some lower and upper bounds for the variables of model (2.22)–(2.25).

Due to symmetry, the angles of rotation of each ellipsoid can be restricted to the interval $[0, \pi]$. Lower and upper bounds on the center of each ellipsoid can be easily derived once the container is defined. For example, consider the case where the container is an n-dimensional cuboid centered at the origin whose edges have lengths $l_1, \ldots, l_n$. Since each ellipsoid must be inside the cuboid, so must their centers be. Therefore, we must have $|[c_i]_k| \leq l_k/2$ for each $k \in \{1, \ldots, n\}$ and for each $i \in I$. If the dimensions of the container are also variables of the problem, then bounds on the variables c_i can be derived from the bounds on the variables l_k. For each $k \in \{1, \ldots, n\}$, a valid upper bound for l_k could be

$$\sum_{i=1}^{m} \lambda_{\max}(P^{\frac{1}{2}}).$$

We now present some auxiliary results. Proposition 2.4 provides lower and upper bounds on the values of the variables x_{ij}. Lemma 2.4 is used in the proof of Proposition 2.4. Proposition 2.3 provides a positive lower bound for the value of μ_{ij}. So we derive an upper bound for the value of μ_{ij} in Proposition 2.5. Lemma 2.5 is used in the proof of Proposition 2.5.

Lemma 2.4 *Let $S_{ij} = P_i^{\frac{1}{2}} Q_i^\top Q_j P_j^{-1} Q_j^\top Q_i P_i^{\frac{1}{2}} \in \mathbb{R}^{n \times n}$, where Q_i and Q_j are $n \times n$ orthogonal matrices and P_i and P_j are $n \times n$ positive definite diagonal matrices. Then*

$$\lambda_{\min}(S_{ij}) \geq \lambda_{\min}(P_j^{-1})\lambda_{\min}(P_i) \text{ and } \lambda_{\max}(S_{ij}) \leq \lambda_{\max}(P_j^{-1})\lambda_{\max}(P_i).$$

Proof: We have

$$\begin{aligned}
\lambda_{\min}(S_{ij}) &= \lambda_{\min}(P_i^{\frac{1}{2}} Q_i^\top Q_j P_j^{-1} Q_j^\top Q_i P_i^{\frac{1}{2}}) \\
&\geq \lambda_{\min}(Q_i^\top Q_j P_j^{-1} Q_j^\top Q_i)\lambda_{\min}(P_i^{\frac{1}{2}} P_i^{\frac{1}{2}}) \\
&= \lambda_{\min}(Q_i^\top Q_j P_j^{-1} Q_j^\top Q_i)\lambda_{\min}(P_i) \\
&\geq \lambda_{\min}(P_j^{-1})\lambda_{\min}(Q_i^\top Q_j Q_j^\top Q_i)\lambda_{\min}(P_i) \\
&= \lambda_{\min}(P_j^{-1})\lambda_{\min}(P_i),
\end{aligned}$$

where the inequalities follow from Theorem 1.4 by Lu and Pearce [40] and the last equality holds since Q_i and Q_j are orthogonal matrices. Thus,

$$\lambda_{\min}(S_{ij}) \geq \lambda_{\min}(P_j^{-1})\lambda_{\min}(P_i).$$

Analogously, we conclude that

$$\lambda_{\max}(S_{ij}) \leq \lambda_{\max}(P_j^{-1})\lambda_{\max}(P_i).$$

$\square$

Proposition 2.4 *Let $x_{ij} \in \mathbb{R}^n$ and $S_{ij} = P_i^{\frac{1}{2}} Q_i^\top Q_j P_j^{-1} Q_j^\top Q_i P_i^{\frac{1}{2}} \in \mathbb{R}^{n \times n}$, where Q_i and Q_j are $n \times n$ orthogonal matrices and P_i and P_j are $n \times n$ positive definite diagonal matrices. Suppose that $x_{ij}^\top S_{ij} x_{ij} = 1$. Thus,*

$$\lambda_{\min}(P_j^{\frac{1}{2}})\lambda_{\min}(P_i^{-\frac{1}{2}}) \leq \|x_{ij}\|_2 \leq \lambda_{\max}(P_j^{\frac{1}{2}})\lambda_{\max}(P_i^{-\frac{1}{2}}).$$

Proof: Since $x_{ij}^\top S_{ij} x_{ij} = 1$, we have $\|x_{ij}\|_2 > 0$. Thus,

$$\lambda_{\min}(S_{ij}) \leq \frac{x_{ij}^\top S_{ij} x_{ij}}{\|x_{ij}\|_2^2} = \frac{1}{\|x_{ij}\|_2^2} \leq \lambda_{\max}(S_{ij}),$$

where the inequalities follow from the Courant–Fischer Theorem (see, for example, Theorem 8.1.2 in [27]). Recalling from Section 2.1 that S_{ij} is positive definite, we have $\lambda_{\min}(S_{ij}) > 0$ and $\lambda_{\max}(S_{ij}) > 0$. Thus,

$$\frac{1}{\lambda_{\max}(S_{ij})} \leq \|x_{ij}\|_2^2 \leq \frac{1}{\lambda_{\min}(S_{ij})}.$$

By Lemma 2.4, $\lambda_{\min}(S_{ij}) \geq \lambda_{\min}(P_j^{-1})\lambda_{\min}(P_i)$ and $\lambda_{\max}(S_{ij}) \leq \lambda_{\max}(P_j^{-1})\lambda_{\max}(P_i)$. Thus,

$$\|x_{ij}\|_2^2 \leq \frac{1}{\lambda_{\min}(P_j^{-1})\lambda_{\min}(P_i)} = \lambda_{\max}(P_j)\lambda_{\max}(P_i^{-1}),$$

and

$$\|x_{ij}\|_2^2 \geq \frac{1}{\lambda_{\max}(P_j^{-1})\lambda_{\max}(P_i)} = \lambda_{\min}(P_j)\lambda_{\min}(P_i^{-1}),$$

where the equalities hold since P_i and P_j are positive definite diagonal matrices. So,

$$\|x_{ij}\|_2 \leq \big(\lambda_{\max}(P_j)\lambda_{\max}(P_i^{-1})\big)^{\frac{1}{2}} = \big(\lambda_{\max}(P_j)\big)^{\frac{1}{2}}\big(\lambda_{\max}(P_i^{-1})\big)^{\frac{1}{2}} = \lambda_{\max}(P_j^{\frac{1}{2}})\lambda_{\max}(P_i^{-\frac{1}{2}})$$

and

$$\|x_{ij}\|_2 \geq \big(\lambda_{\min}(P_j)\lambda_{\min}(P_i^{-1})\big)^{\frac{1}{2}} = \big(\lambda_{\min}(P_j)\big)^{\frac{1}{2}}\big(\lambda_{\min}(P_i^{-1})\big)^{\frac{1}{2}} = \lambda_{\min}(P_j^{\frac{1}{2}})\lambda_{\min}(P_i^{-\frac{1}{2}}).$$

□

Lemma 2.5 *Let $x_{ij} \in \mathbb{R}^n$ and $S_{ij} = P_i^{\frac{1}{2}} Q_i^\top Q_j P_j^{-1} Q_j^\top Q_i P_i^{\frac{1}{2}} \in \mathbb{R}^{n\times n}$, where Q_i and Q_j are orthogonal matrices and P_i and P_j are positive definite diagonal matrices. Suppose that $x_{ij}^\top S_{ij} x_{ij} = 1$. Thus,*

$$\|S_{ij}x_{ij}\|_2 \geq \lambda_{\min}(P_i)\lambda_{\min}(P_j^{-1})\lambda_{\min}(P_j^{\frac{1}{2}})\lambda_{\min}(P_i^{-\frac{1}{2}}).$$

Proof: We have

$$\begin{aligned}
\|S_{ij}x_{ij}\|_2 &= \|P_i^{\frac{1}{2}} Q_i^\top Q_j P_j^{-1} Q_j^\top Q_i P_i^{\frac{1}{2}} x_{ij}\|_2 \\
&\geq \lambda_{\min}(P_i^{\frac{1}{2}})\|Q_i^\top Q_j P_j^{-1} Q_j^\top Q_i P_i^{\frac{1}{2}} x_{ij}\|_2 \\
&= \lambda_{\min}(P_i^{\frac{1}{2}})\|P_j^{-1} Q_j^\top Q_i P_i^{\frac{1}{2}} x_{ij}\|_2 \\
&\geq \lambda_{\min}(P_i^{\frac{1}{2}})\lambda_{\min}(P_j^{-1})\|Q_j^\top Q_i P_i^{\frac{1}{2}} x_{ij}\|_2 \\
&= \lambda_{\min}(P_i^{\frac{1}{2}})\lambda_{\min}(P_j^{-1})\|P_i^{\frac{1}{2}} x_{ij}\|_2 \\
&\geq \lambda_{\min}(P_i^{\frac{1}{2}})\lambda_{\min}(P_j^{-1})\lambda_{\min}(P_i^{\frac{1}{2}})\|x_{ij}\|_2 \\
&= \lambda_{\min}(P_i)\lambda_{\min}(P_j^{-1})\|x_{ij}\|_2,
\end{aligned}$$

where the second and third equalities hold since Q_i and Q_j are orthogonal matrices, and the inequalities and the last equality follows from the fact that $P_i^{\frac{1}{2}}$ and P_j^{-1} are positive definite diagonal matrices. Therefore,

$$\|S_{ij}x_{ij}\|_2 \geq \lambda_{\min}(P_i)\lambda_{\min}(P_j^{-1})\|x_{ij}\|_2.$$

By Proposition 2.4, $\|x_{ij}\|_2 \geq \lambda_{\min}(P_j^{\frac{1}{2}})\lambda_{\min}(P_i^{-\frac{1}{2}})$. Then,

$$\|S_{ij}x_{ij}\|_2 \geq \lambda_{\min}(P_i)\lambda_{\min}(P_j^{-1})\lambda_{\min}(P_j^{\frac{1}{2}})\lambda_{\min}(P_i^{-\frac{1}{2}}).$$

□

Proposition 2.5 *Any solution to the system (2.22)–(2.25) satisfies*

$$\mu_{ij} \leq \lambda_{\max}(P_i^{-\frac{3}{2}})\lambda_{\max}(P_j)\lambda_{\max}(P_j^{-\frac{1}{2}})\lambda_{\max}(P_i^{\frac{1}{2}})\left(2C + \lambda_{\max}(P_j^{\frac{1}{2}})\right)$$

for each $i, j \in I$ such that $i < j$, where C is an upper bound on the norm of the center of each ellipsoid.

Proof: Consider a solution to the system (2.22)–(2.25). Let $i, j \in I$ such that $i < j$. By (2.24), we have that

$$P_i^{-\frac{1}{2}}Q_i^\top(c_i - c_j) = x_{ij} + \mu_{ij}S_{ij}x_{ij}.$$

Thus,

$$\mu_{ij} = \|S_{ij}x_{ij}\|_2^{-1}\|P_i^{-\frac{1}{2}}Q_i^\top(c_i - c_j) - x_{ij}\|_2.$$

By Lemma 2.5, we have that

$$\begin{aligned}
\|S_{ij}x_{ij}\|_2^{-1} &\leq \left(\lambda_{\min}(P_i)\lambda_{\min}(P_j^{-1})\lambda_{\min}(P_j^{\frac{1}{2}})\lambda_{\min}(P_i^{-\frac{1}{2}})\right)^{-1} \\
&= \lambda_{\max}(P_i^{-1})\lambda_{\max}(P_j)\lambda_{\max}(P_j^{-\frac{1}{2}})\lambda_{\max}(P_i^{\frac{1}{2}}),
\end{aligned}$$

where the equality holds since P_i and P_j are positive definite matrices. Also, notice that

$$\begin{aligned}
\|P_i^{-\frac{1}{2}}Q_i^\top(c_i - c_j) - x_{ij}\|_2 &\leq \|P_i^{-\frac{1}{2}}Q_i^\top(c_i - c_j)\|_2 + \|x_{ij}\|_2 \\
&\leq \lambda_{\max}(P_i^{-\frac{1}{2}})\|Q_i^\top(c_i - c_j)\|_2 + \|x_{ij}\|_2 \\
&= \lambda_{\max}(P_i^{-\frac{1}{2}})\|c_i - c_j\|_2 + \|x_{ij}\|_2 \\
&\leq \lambda_{\max}(P_i^{-\frac{1}{2}})\left(\|c_i\|_2 + \|c_j\|_2\right) + \|x_{ij}\|_2 \\
&\leq \lambda_{\max}(P_i^{-\frac{1}{2}})\left(\|c_i\|_2 + \|c_j\|_2\right) + \lambda_{\max}(P_j^{\frac{1}{2}})\lambda_{\max}(P_i^{-\frac{1}{2}}) \\
&= \lambda_{\max}(P_i^{-\frac{1}{2}})\left(\|c_i\|_2 + \|c_j\|_2 + \lambda_{\max}(P_j^{\frac{1}{2}})\right),
\end{aligned}$$

where the first and third inequalities follow from the triangle inequality, the second inequality holds since $P_i^{-\frac{1}{2}}$ is diagonal and positive definite, the fourth inequality follows from Proposition 2.4, and the first equality holds since Q_i is orthogonal. Therefore,

$$\begin{aligned}\mu_{ij} &\leq \lambda_{\max}(P_i^{-1})\lambda_{\max}(P_j)\lambda_{\max}(P_j^{-\frac{1}{2}})\lambda_{\max}(P_i^{\frac{1}{2}})\lambda_{\max}(P_i^{-\frac{1}{2}})\left(\|c_i\|_2 + \|c_j\|_2 + \lambda_{\max}(P_j^{\frac{1}{2}})\right)\\ &= \lambda_{\max}(P_i^{-\frac{3}{2}})\lambda_{\max}(P_j)\lambda_{\max}(P_j^{-\frac{1}{2}})\lambda_{\max}(P_i^{\frac{1}{2}})\left(\|c_i\|_2 + \|c_j\|_2 + \lambda_{\max}(P_j^{\frac{1}{2}})\right).\end{aligned}$$

Considering that the norm of the center of each ellipsoid is bounded by C, we obtain

$$\mu_{ij} \leq \lambda_{\max}(P_i^{-\frac{3}{2}})\lambda_{\max}(P_j)\lambda_{\max}(P_j^{-\frac{1}{2}})\lambda_{\max}(P_i^{\frac{1}{2}})\left(2C + \lambda_{\max}(P_j^{\frac{1}{2}})\right).$$

□

2.2.2 Separating hyperplane based model

A hyperplane is a set of the form $\mathcal{H} = \{x \in \mathbb{R}^n \mid w^\top x = s\}$, where $w \in \mathbb{R}^n \setminus \{0\}$ and $s \in \mathbb{R}$. There are two half-spaces associated with hyperplane $\mathcal{H}$, namely, $\mathcal{H}^- = \{x \in \mathbb{R}^n \mid w^\top x \leq s\}$ and $\mathcal{H}^+ = \{x \in \mathbb{R}^n \mid w^\top x \geq s\}$. We say that a hyperplane $\mathcal{H}$ in $\mathbb{R}^n$ supports a subset $\mathcal{A}$ of $\mathbb{R}^n$ if $\mathcal{A}$ is contained in one of the half-spaces associated with $\mathcal{H}$ and there exists at least one element of $\mathcal{A}$ that belongs to the hyperplane $\mathcal{H}$. We denote the relative interior of set $\mathcal{A}$ by $\text{ri}(\mathcal{A})$.

Given non-empty subsets $\mathcal{A}$ and $\mathcal{B}$ of $\mathbb{R}^n$, we say that a hyperplane separates sets $\mathcal{A}$ and $\mathcal{B}$ if $\mathcal{A}$ is contained in one of the half-spaces associated with this hyperplane and $\mathcal{B}$ is contained in the other half-space associated with this hyperplane. If $\mathcal{A}$ and $\mathcal{B}$ are convex sets then, by Theorem 11.3 in [50], there exists a hyperplane that separates $\mathcal{A}$ and $\mathcal{B}$ if and only if $\text{ri}(\mathcal{A}) \cap \text{ri}(\mathcal{B}) = \emptyset$. Therefore, since the relative interior of an ellipsoid is the interior of this ellipsoid, there exists a hyperplane that separates ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ if and only if $\text{int}(\mathcal{E}_i) \cap \text{int}(\mathcal{E}_j) = \emptyset$. In this section, we propose a non-overlapping model based on separating hyperplanes.

Consider the ellipsoids

$$\begin{aligned}\mathcal{E}_i &= \{x \in \mathbb{R}^n \mid (x - c_i)^\top Q_i P_i^{-1} Q_i^\top (x - c_i) \leq 1\} \text{ and}\\ \mathcal{E}_j &= \{x \in \mathbb{R}^n \mid (x - c_j)^\top Q_j P_j^{-1} Q_j^\top (x - c_j) \leq 1\},\end{aligned}$$

where $c_i, c_j \in \mathbb{R}^n$, $Q_i, Q_j \in \mathbb{R}^{n\times n}$ are orthogonal matrices and $P_i, P_j \in \mathbb{R}^{n\times n}$ are positive definite and diagonal matrices. Let $M_i = Q_i P_i^{-1} Q_i^\top$ and $M_j = Q_j P_j^{-1} Q_j^\top$. For any $x \in \partial\mathcal{E}_i$, vector $M_i(x - c_i)$ defines a hyperplane that passes through the point x and supports the ellipsoid $\mathcal{E}_i$ (see Lemma 2.6 below). For the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ not to overlap, there must be a point $y \in \partial\mathcal{E}_j$ such that, for some $x \in \partial\mathcal{E}_i$, x can be expressed as the sum of y and a nonnegative multiple of $M_j(y - c_j)$ and the vector $M_j(y - c_j)$ must be a negative multiple of $M_i(x - c_i)$. Figure 2.2 illustrates this situation in $\mathbb{R}^2$. In this picture, we have $\tilde{x}_{ij} \in \partial\mathcal{E}_i$ and $\tilde{x}_{ji} \in \partial\mathcal{E}_j$. So, the vectors $M_i(\tilde{x}_{ij} - c_i)$ and $M_j(\tilde{x}_{ji} - c_j)$ determine hyperplanes that support the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ at the points $\tilde{x}_{ij}$ and $\tilde{x}_{ji}$, respectively.

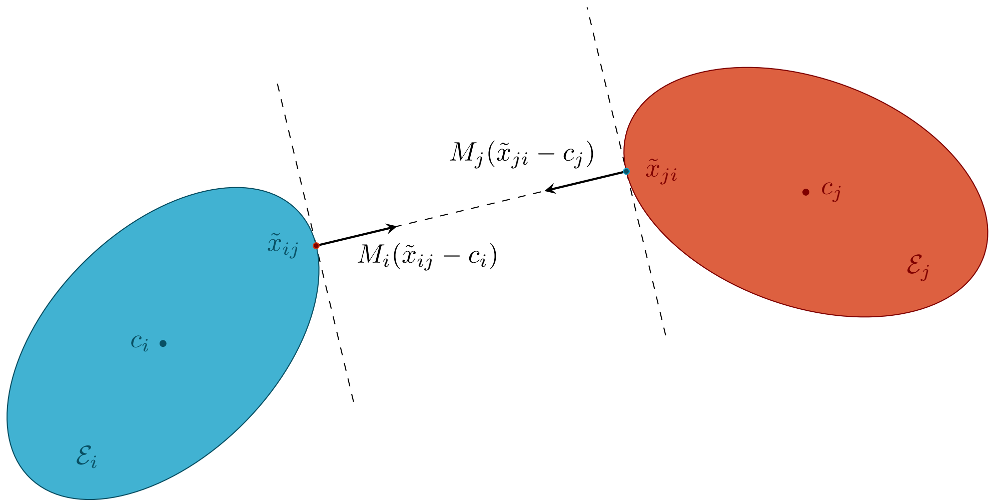


Figure 2.2: Separation of two ellipsoids by hyperplanes determined by the vectors $M_i(\tilde{x}_{ij} - c_i)$ and $M_j(\tilde{x}_{ji} - c_j)$, and the points $\tilde{x}_{ij}$ and $\tilde{x}_{ji}$.

We thus obtain the following model for the non-overlapping of ellipsoids, where the variables are $c_i \in \mathbb{R}^n$, the angles that form matrix $Q_i \in \mathbb{R}^{n\times n}$ for each $i \in I$, $\gamma_{ij}, \rho_{ij} \in \mathbb{R}$ for each $i, j \in I$ such that $i < j$, and $\tilde{x}_{ij} \in \mathbb{R}^n$ for each $i, j \in I$ such that $i \neq j$.

$$(\tilde{x}_{ij} - c_i)^\top M_i(\tilde{x}_{ij} - c_i) = 1 \qquad \forall i, j \in I \text{ such that } i < j \tag{2.26}$$
$$(\tilde{x}_{ji} - c_j)^\top M_j(\tilde{x}_{ji} - c_j) = 1 \qquad \forall i, j \in I \text{ such that } i < j \tag{2.27}$$
$$M_j(\tilde{x}_{ji} - c_j) = -\gamma_{ij} M_i(\tilde{x}_{ij} - c_i) \qquad \forall i, j \in I \text{ such that } i < j \tag{2.28}$$
$$\tilde{x}_{ij} = \tilde{x}_{ji} + \rho_{ij} M_j(\tilde{x}_{ji} - c_j) \qquad \forall i, j \in I \text{ such that } i < j \tag{2.29}$$
$$\rho_{ij} \geq 0 \qquad \forall i, j \in I \text{ such that } i < j \tag{2.30}$$
$$\gamma_{ij} \geq 0 \qquad \forall i, j \in I \text{ such that } i < j. \tag{2.31}$$

This model has $m(m-1)(n+1)$ nonlinear constraints and $m(m-1)$ bound-constraints. If the rotation matrices are represented as in (2.1) and (2.2) then this model will have $3m^2$ variables in the two-dimensional case and $4m^2 + 2m$ in the three-dimensional case.

By Propositions 2.6 and 2.7 below, constraints (2.26)–(2.31) indeed model the non-overlapping of ellipsoids. Lemma 2.6 is used in the proofs of Propositions 2.6 and 2.7.

Lemma 2.6 *Consider the ellipsoid $\mathcal{E} = \{x \in \mathbb{R}^n \mid (x - c)^\top M(x - c) \leq 1\}$, where $M \in \mathbb{R}^{n\times n}$ is positive definite. Let $x^* \in \partial\mathcal{E}$ and define $w = M(x^* - c)$ and $s = w^\top x^*$. Thus, $w^\top x \leq s$ for every $x \in \mathcal{E}$.*

Proof: Let $f : \mathbb{R}^n \to \mathbb{R}$ be the function defined by $f(x) = (x-c)^\top M(x-c)$. Since the Hessian of f (the matrix $2M$) is positive definite in every point of $\mathbb{R}^n$, we have that f is convex. Therefore, by the first-order condition of convexity, we have

$$f(x) \geq f(x^*) + \nabla f(x^*)^\top (x - x^*) \tag{2.32}$$

for all $x \in \mathcal{E}$. Since $w = \nabla f(x^*)/2$, $s = w^\top x^*$, $f(x^*) = 1$ and $f(x) \leq 1$ for all $x \in \mathcal{E}$, inequality (2.32) implies that $w^\top x \leq s$ for all $x \in \mathcal{E}$. □

Proposition 2.6 *Any solution to the system (2.26)–(2.31) is such that* $int(\mathcal{E}_i) \cap int(\mathcal{E}_j) = \emptyset$ *for all* $i, j \in I$ *such that* $i \neq j$.

Proof: Consider a solution to the system (2.26)–(2.31). Let $i, j \in I$ be such that $i < j$. Let $w_{ji} = M_j(\tilde{x}_{ji} - c_j)$ and $s_{ji} = w_{ji}^\top \tilde{x}_{ji}$ and consider the hyperplane $\mathcal{H}_{ji} = \{x \in \mathbb{R}^n \mid w_{ji}^\top x = s_{ji}\}$. We shall prove that $\mathcal{H}_{ji}$ separates ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$. By Lemma 2.6, we have $w_{ji}^\top x \leq s_{ji}$ for all $x \in \mathcal{E}_j$, i.e., $\mathcal{E}_j \subseteq \mathcal{H}_{ji}^-$. Point $\tilde{x}_{ij}$ belongs to half-space $\mathcal{H}_{ji}^+$ since

$$
\begin{aligned}
w_{ji}^\top \tilde{x}_{ij} &= w_{ji}^\top \left[\tilde{x}_{ji} + \rho_{ij} M_j(\tilde{x}_{ji} - c_j)\right] \\
&= w_{ji}^\top (\tilde{x}_{ji} + \rho_{ij} w_{ji}) \\
&= w_{ji}^\top \tilde{x}_{ji} + \rho_{ij} \|w_{ji}\|_2^2 \\
&= s_{ji} + \rho_{ij} \|w_{ji}\|_2^2 \\
&\geq s_{ji},
\end{aligned}
\tag{2.33}
$$

where the first equality follows from (2.29), the second equality follows from the definition of w_{ji}, the fourth equality follows from the definition of s_{ji} and the inequality holds since ρ_{ij} is nonnegative. Now, consider the hyperplane $\mathcal{H}_{ij} = \{x \in \mathbb{R}^n \mid w_{ij}^\top x = s_{ij}\}$, where $w_{ij} = M_i(\tilde{x}_{ij} - c_i)$ and $s_{ij} = w_{ij}^\top \tilde{x}_{ij}$. For all $x \in \mathcal{E}_i$, we have

$$
\begin{aligned}
w_{ji}^\top x &= -\gamma_{ij} w_{ij}^\top x \\
&\geq -\gamma_{ij} s_{ij} \\
&= -\gamma_{ij} w_{ij}^\top \tilde{x}_{ij} \\
&= w_{ji}^\top \tilde{x}_{ij} \\
&\geq s_{ji},
\end{aligned}
$$

where the first and third equalities follow from (2.28), the second equality follows from the definition of s_{ij}, the first inequality follows from Lemma 2.6 and the fact that γ_{ij} is nonnegative, and the last inequality follows from (2.33). Therefore, $x \in \mathcal{H}_{ji}^+$ for each $x \in \mathcal{E}_i$. Hence, we have $\mathcal{E}_j \subseteq \mathcal{H}_{ji}^-$ and $\mathcal{E}_i \subseteq \mathcal{H}_{ji}^+$, i.e., hyperplane $\mathcal{H}_{ji}$ separates ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$. In other words, ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ do not overlap. □

Proposition 2.7 *Let* $I = \{1, \ldots, m\}$. *For each* $i \in I$, *let* $\mathcal{E}_i = \{x \in \mathbb{R}^n \mid (x - c_i)^\top M_i(x - c_i) \leq 1\}$, *where* $c_i \in \mathbb{R}^n$ *and* $M \in \mathbb{R}^{n \times n}$ *is positive definite. If ellipsoids* $\mathcal{E}_1, \ldots, \mathcal{E}_m$ *do not overlap each other, then the system (2.26)–(2.31) has a solution.*

Proof: Let $i, j \in I$ be such that $i < j$. Suppose that $\mathcal{E}_i$ and $\mathcal{E}_j$ do not overlap. Let $x^* \in \mathcal{E}_i$ and $y^* \in \mathcal{E}_j$ be such that the distance between ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ is equal to $\|x^* - y^*\|_2$. Thus, (x^*, y^*) is an optimal solution to the problem

$$
\begin{aligned}
\text{minimize} \quad & \|x - y\|_2^2 \\
\text{subject to} \quad & (x - c_i)^\top M_i (x - c_i) \leq 1 \\
& (y - c_j)^\top M_j (y - c_j) \leq 1.
\end{aligned}
$$

Since both constraints of this problem are convex in $\mathbb{R}^{2n}$ and point (c_i, c_j) strictly satisfies both inequalities, this problem fulfills the Slater constraint qualification. Therefore, by Proposition 3.3.9 in [5], there exist Lagrange multipliers $\mu_i^* \in \mathbb{R}$ and $\mu_j^* \in \mathbb{R}$ such that

$$2(x^* - y^*) + 2\mu_i^* M_i(x^* - c_i) = 0 \tag{2.34}$$
$$2(y^* - x^*) + 2\mu_j^* M_j(y^* - c_j) = 0 \tag{2.35}$$
$$\mu_i^* \geq 0 \tag{2.36}$$
$$\mu_j^* \geq 0. \tag{2.37}$$

From (2.35), we have $x^* = y^* + \mu_j^* M_j(y^* - c_j)$. From (2.34) and (2.35), it follows that

$$\mu_j^* M_j(y^* - c_j) = -\mu_i^* M_i(x^* - c_i).$$

Since the ellipsoids do not overlap, we must have $x^* \in \partial\mathcal{E}_i$ and $y^* \in \partial\mathcal{E}_j$. Thus, since M_i and M_j are nonsingular, we have $M_i(x^* - c_i) \neq 0 \neq M_j(y^* - c_j)$. Therefore, $\mu_j^* \neq 0$ if $\mu_i^* \neq 0$, and $\mu_j^* = 0$ if $\mu_i^* = 0$.

Suppose that $\mu_i^* = 0$. Thus, equation (2.34) implies that $x^* = y^*$. Since $\mathrm{int}(\mathcal{E}_i) \cap \mathrm{int}(\mathcal{E}_j) = \emptyset$, there exists a hyperplane $\mathcal{H}$ that separates ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$. Since $x^* \in \partial\mathcal{E}_i$ and $x^* \in \partial\mathcal{E}_j$, point x^* must belong to the hyperplane $\mathcal{H}$. (Suppose that $x^* \notin \mathcal{H}$ and let $w \in \mathbb{R}^n$ and $s \in \mathbb{R}$ be such that $\mathcal{H} = \{x \in \mathbb{R}^n \mid w^\top x = s\}$. Since $x^* \notin \mathcal{H}$, we have either $w^\top x^* < s$ or $w^\top x^* > s$. Suppose, without loss of generality, that $w^\top x^* < s$. Thus, there exists a ball $\mathcal{B}$ with center in x^* and radius $r > 0$ such that $w^\top x < s$ for all $x \in \mathcal{B}$. Since $x^* \in \partial\mathcal{E}_i$, Theorem 6.1 in [50] implies that there exists $z_i \neq x^*$ such that $z_i \in \mathcal{B} \cap \mathrm{int}(\mathcal{E}_i)$. By the same reason, since $x^* \in \partial\mathcal{E}_j$, there exists $z_j \neq x^*$ such that $z_j \in \mathcal{B} \cap \mathrm{int}(\mathcal{E}_j)$. Therefore, $z_i \in \mathrm{int}(\mathcal{E}_i)$ and $z_j \in \mathrm{int}(\mathcal{E}_j)$ satisfies $w^\top z_i < s$ and $w^\top z_j < s$. But it contradicts the fact that $\mathcal{H}$ separates ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$.)

Since x^* belongs to the hyperplane $\mathcal{H}$ and $\mathcal{H}$ separates ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$, we have that $\mathcal{H}$ supports ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ in x^*. Let $\mathcal{H}_{ij} = \{x \in \mathbb{R}^n \mid w_{ij}^\top x = s_{ij}\}$, where $w_{ij} = M_i(x^* - c_i)$ and $s_{ij} = w_{ij}^\top x^*$. By Lemma 2.6, $\mathcal{H}_{ij}$ supports $\mathcal{E}_i$ in x^*. By Theorem 3.1 in [30], there exists only one hyperplane that supports $\mathcal{E}_i$ in x^*. Therefore, $\mathcal{H}_{ij} = \mathcal{H}$. Similarly, if we define $\mathcal{H}_{ji} = \{x \in \mathbb{R}^n \mid w_{ji}^\top x = s_{ji}\}$, where $w_{ji} = M_j(x^* - c_j)$ and $s_{ji} = w_{ji}^\top x^*$, we have that $\mathcal{H}_{ji} = \mathcal{H}$. Therefore, $\mathcal{H}_{ij} = \mathcal{H}_{ji}$. Hence, w_{ij} must be parallel to w_{ji}, i.e., there must exist $\gamma \in \mathbb{R} \setminus \{0\}$ such that $M_i(x^* - c_i) = \gamma M_j(x^* - c_j)$. Notice that $w_{ij}^\top c_i < s_{ij}$, since

$$-w_{ij}^\top c_i = -c_i^\top M_i(x^* - c_i) = (x^* - c_i - x^*)^\top M_i(x^* - c_i) = (x^* - c_i)^\top M_i(x^* - c_i) - s_{ij} = 1 - s_{ij}.$$

So, $c_i \notin \mathcal{H}$. Since $\mathcal{H}_{ji}$ separates ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$, Lemma 2.6 implies that $w_{ji}^\top c_i \geq s_{ji}$. Thus, since $c_i \notin \mathcal{H}$, we must have $w_{ji}^\top c_i > s_{ji}$. In order to derive a contradiction, suppose that γ is positive. Then,

$$w_{ij}^\top c_i < s_{ij} = w_{ij}^\top x^* = \gamma w_{ji}^\top x^* = \gamma s_{ji} < \gamma w_{ji}^\top c_i = w_{ij}^\top c_i,$$

which is a contradiction. Therefore, γ must be negative.

Hence, if we take $\tilde{x}_{ij} \doteq x^*$, $\tilde{x}_{ji} \doteq y^*$, $\rho_{ij} \doteq \mu_j^*$ and

$$\gamma_{ij} \doteq \begin{cases} -\frac{\mu_j^*}{\mu_i^*} & \text{if } \mu_i^* > 0 \\ -\frac{(x^* - c_j)^\top M_j M_i (x^* - c_i)}{\|M_j(x^* - c_j)\|_2^2} & \text{if } \mu_i^* = 0, \end{cases}$$

constraints (2.26)–(2.31) are satisfied. $\square$

By constraints (2.27)–(2.28), any solution to the system (2.26)–(2.31) must satisfy

$$-\gamma_{ij}(\tilde{x}_{ji} - c_j)^\top M_i(\tilde{x}_{ij} - c_i) = 1$$

for all $i < j$. Then, γ_{ij} cannot be zero. Hence, since $\gamma_{ij} \geq 0$ by constraints (2.31), we must have $\gamma_{ij} > 0$ for all $i < j$. The following lemma provides a positive lower bound on the value of γ_{ij}.

Lemma 2.7 *Any solution to the system (2.26)–(2.31) is such that $\gamma_{ij} \geq \lambda_{\min}(P_i)$ for all $i < j$.*

Proof: Consider a solution to the system (2.26)–(2.31). By constraints (2.27)–(2.28), we must have

$$-\gamma_{ij}(\tilde{x}_{ji} - c_j)^\top M_i(\tilde{x}_{ij} - c_i) = 1.$$

Thus,

$$\gamma_{ij} = -\left[(\tilde{x}_{ji} - c_j)^\top M_i(\tilde{x}_{ij} - c_i)\right]^{-1}.$$

Since M_i is positive definite, we have $(\tilde{x}_{ji} - c_j + \tilde{x}_{ij} - c_i)^\top M_i(\tilde{x}_{ji} - c_j + \tilde{x}_{ij} - c_i) \geq 0$. Then, since

$$\begin{aligned}(\tilde{x}_{ji} - c_j + \tilde{x}_{ij} - c_i)^\top M_i(\tilde{x}_{ji} - c_j + \tilde{x}_{ij} - c_i) = {} & (\tilde{x}_{ji} - c_j)^\top M_i(\tilde{x}_{ji} - c_j) \ + \\ & (\tilde{x}_{ij} - c_i)^\top M_i(\tilde{x}_{ij} - c_i) \ + \\ & 2(\tilde{x}_{ji} - c_j)^\top M_i(\tilde{x}_{ij} - c_i),\end{aligned}$$

we must have

$$\begin{aligned}-(\tilde{x}_{ji} - c_j)^\top M_i(\tilde{x}_{ij} - c_i) &\leq \frac{1}{2}\left[(\tilde{x}_{ji} - c_j)^\top M_i(\tilde{x}_{ji} - c_j) + (\tilde{x}_{ij} - c_i)^\top M_i(\tilde{x}_{ij} - c_i)\right] \\ &\leq \max\{(\tilde{x}_{ji} - c_j)^\top M_i(\tilde{x}_{ji} - c_j), (\tilde{x}_{ij} - c_i)^\top M_i(\tilde{x}_{ij} - c_i)\} \\ &\leq \lambda_{\max}(M_i) \\ &= \lambda_{\max}(Q_i P_i^{-1} Q_i^\top) \\ &= \lambda_{\max}(P_i^{-1}),\end{aligned}$$

where the last equality holds since Q_i is orthogonal. Hence,

$$\gamma_{ij} \geq \left[\lambda_{\max}(P_i^{-1})\right]^{-1} = \lambda_{\min}(P_i).$$

$\square$

According to Lemma 2.7, we can replace constraints (2.31) of the system (2.26)–(2.31) with constraints $\gamma_{ij} \geq \lambda_{\min}(P_i)$ for all $i < j$.

2.3 Containment models

2.3.1 Ellipsoid inside an ellipsoid

In this section, we present a model for the inclusion of an ellipsoid $\mathcal{E}_i$ inside an ellipsoid $\mathcal{C}$. Firstly, we apply a transformation to $\mathcal{E}_i$ that converts this ellipsoid into a ball $\mathcal{E}_{ii}$ with unitary radius and we apply the same transformation to $\mathcal{C}$, thus obtaining an ellipsoid $\mathcal{C}_i$. In this way, we have $\mathcal{E}_i \subseteq \mathcal{C}$ if and only if $\mathcal{E}_{ii} \subseteq \mathcal{C}_i$. In order to guarantee that $\mathcal{E}_{ii}$ be contained in $\mathcal{C}_i$, we require that the center c_{ii} of ball $\mathcal{E}_{ii}$ be in $\mathcal{C}_i$ and the distance between c_{ii} and the frontier of ellipsoid $\mathcal{C}_i$ be at least one. Since the computation of the distance between a point and the frontier of an ellipsoid demands the solution of a non-convex optimization problem, we will represent the center c_{ii} with respect to $\mathcal{C}_i$ in a similar manner to what was done in Section 2.2.1. In this representation, the distance between c_{ii} and the frontier of ellipsoid $\mathcal{C}_i$ is easily obtained.

To develop this model, we must first state some results. Next, we present Propositions 2.8 and 2.9 and Lemmas 2.8 and 2.9. Lemma 2.8 is used in the proof of Proposition 2.8 and Lemma 2.9 is used in the proof of Proposition 2.9. These lemmas consider particular cases of Propositions 2.8 and 2.9.

Lemma 2.8 *Consider the ellipsoid $\mathcal{E} = \{z \in \mathbb{R}^n \mid z^\top D z \le 1\}$, where $D \in \mathbb{R}^{n\times n}$ is a positive definite diagonal matrix. For each $y \in \mathcal{E}$, there exist $x \in \partial\mathcal{E}$ and $\alpha \in [-1/\lambda_{\max}(D), 0]$ such that $y = x + \alpha D x$.*

Proof: We shall prove the assertion by induction on the dimension of the ellipsoid. We will denote the i-th diagonal element of matrix D by d_i.

Consider the one-dimensional case, where $n = 1$. Then, $D = d_1 = \lambda_{\max}(D)$, $\mathcal{E} = \{z \in \mathbb{R} \mid d_1 z^2 \le 1\} = \{z \in \mathbb{R} \mid -1/\sqrt{d_1} \le z \le 1/\sqrt{d_1}\}$ and $\partial\mathcal{E} = \{-1/\sqrt{d_1}, 1/\sqrt{d_1}\}$. Let $y \in \mathcal{E}$. We will analyse the cases where $-1/\sqrt{d_1} \le y \le 0$ and $0 < y \le 1/\sqrt{d_1}$ separately. Suppose that $-1/\sqrt{d_1} \le y \le 0$. Take $x = -1/\sqrt{d_1}$ and consider the point $x + \alpha D x$ with

$$\alpha = \frac{y-x}{d_1 x} = -\frac{y + 1/\sqrt{d_1}}{\sqrt{d_1}}.$$

Then,

$$x + \alpha D x = x + \frac{y-x}{d_1 x} d_1 x = y.$$

Since $y \ge -1/\sqrt{d_1}$, we have $y + 1/\sqrt{d_1} \ge 0$. Thus, $\alpha \le 0$. In addition, since $y \le 0$, we have

$$\alpha = -\frac{y + 1/\sqrt{d_1}}{\sqrt{d_1}} \ge -\frac{1/\sqrt{d_1}}{\sqrt{d_1}} = -\frac{1}{d_1} = -\frac{1}{\lambda_{\max}(D)}.$$

Hence, $y = x + \alpha D x$ with $x \in \partial\mathcal{E}$ and $\alpha \in [-1/\lambda_{\max}(D), 0]$. The case where $0 < y \le 1/\sqrt{d_1}$ is analogous. Simply take $x = 1/\sqrt{d_1}$ and $\alpha = (y - x)/(d_1 x)$.

Consider $n > 1$ and suppose that the assertion is true for all ellipsoids lying in a dimension strictly less than n. Consider the ellipsoid $\mathcal{E} = \{z \in \mathbb{R}^n \mid z^\top D z \le 1\}$ and let $y \in \mathcal{E}$. Let

$\mathcal{I} = \{1, \dots, n\}$, $\mathcal{I}^+ = \{i \in \mathcal{I} \mid d_i = \lambda_{\max}(D)\}$ and $\mathcal{I}^- = \mathcal{I} \setminus \mathcal{I}^+$. Since D is diagonal, we must find $x \in \mathbb{R}^n$ and $\alpha \in \mathbb{R}$ such that

$$y_i = x_i + \alpha d_i x_i, \forall i \in \mathcal{I}, \tag{2.38}$$

$$x^\top D x = 1, \tag{2.39}$$

$$\alpha \in [-1/\lambda_{\max}(D), 0]. \tag{2.40}$$

For each $\alpha \in [-1/\lambda_{\max}(D), 0]$ and $i \in \mathcal{I}^-$, we have $1 + \alpha d_i \in (0, 1]$. Therefore, from (2.38), for all $i \in \mathcal{I}^-$ we must have

$$x_i = \frac{y_i}{1 + \alpha d_i}.$$

Now, we consider two cases: the first one where $y_i \neq 0$ for all $i \in \mathcal{I}^+$ and the second one where $y_j = 0$ for some $j \in \mathcal{I}^+$.

Case 1. Suppose that $y_i \neq 0$ for all $i \in \mathcal{I}^+$. In this case, we must have $\alpha > -1/\lambda_{\max}(D)$. Thus, from (2.38), we must have

$$x_i = \frac{y_i}{1 + \alpha d_i} \tag{2.41}$$

for all $i \in \mathcal{I}$. Then,

$$x^\top D x = \sum_{i=1}^{n} d_i x_i^2 = \sum_{i=1}^{n} d_i \frac{y_i^2}{(1 + \alpha d_i)^2} = \sum_{i \in \mathcal{I}^+} d_i \frac{y_i^2}{[1 + \alpha \lambda_{\max}(D)]^2} + \sum_{i \in \mathcal{I}^-} d_i \frac{y_i^2}{(1 + \alpha d_i)^2}.$$

Thus, for $\alpha > -1/\lambda_{\max}(D)$, we have $x^\top D x = 1$ if and only if

$$\sum_{i \in \mathcal{I}^+} d_i y_i^2 = [1 + \alpha \lambda_{\max}(D)]^2 \left[1 - \sum_{i \in \mathcal{I}^-} d_i \frac{y_i^2}{(1 + \alpha d_i)^2}\right].$$

Let $f : \mathbb{R} \to \mathbb{R}$ be the function defined by

$$f(t) = \sum_{i \in \mathcal{I}^+} d_i y_i^2 - [1 + t \lambda_{\max}(D)]^2 \left[1 - \sum_{i \in \mathcal{I}^-} d_i \frac{y_i^2}{(1 + t d_i)^2}\right].$$

We have

$$f(0) = \sum_{i \in \mathcal{I}^+} d_i y_i^2 - \left(1 - \sum_{i \in \mathcal{I}^-} d_i y_i^2\right) = \sum_{i \in \mathcal{I}} d_i y_i^2 - 1 = y^\top D y - 1 \leq 0,$$

where the inequality holds since $y \in \mathcal{E}$, i.e., $y^\top D y \leq 1$. We also have

$$f(-1/\lambda_{\max}(D)) = \sum_{i \in \mathcal{I}^+} d_i y_i^2 > 0.$$

Thus, since f is continuous in the interval $[-1/\lambda_{\max}(D), 0]$ and $f(0) \leq 0$ and $f(-1/\lambda_{\max}(D)) > 0$, by the Intermediate Value Theorem, there exist $t^* \in (-1/\lambda_{\max}(D), 0]$ such that $f(t^*) = 0$.

Therefore, by taking $\alpha = t^*$ and x as in (2.41), the system (2.38)–(2.40) is satisfied.

Case 2. Suppose that $y_j = 0$ for some $j \in \mathcal{I}^+$. We shall consider the cases where $|\mathcal{I}^+| = 1$ and $|\mathcal{I}^+| > 1$ individually.

Case 2.1. Suppose that $|\mathcal{I}^+| = 1$. Then, $\mathcal{I}^- = \mathcal{I} \setminus \{j\}$. Thus, from (2.38), we must have $x_i = y_i/(1+\alpha d_i)$ for all $i \in \mathcal{I} \setminus \{j\}$. Then, $x^\top D x = 1$ if and only if

$$\lambda_{\max}(D) x_j^2 = 1 - \sum_{i \in \mathcal{I}^-} d_i \frac{y_i^2}{(1+\alpha d_i)^2}.$$

Let $g : \mathbb{R} \to \mathbb{R}$ be the function defined by

$$g(t) = 1 - \sum_{i \in \mathcal{I}^-} d_i \frac{y_i^2}{(1+t d_i)^2}.$$

If $g(-1/\lambda_{\max}(D)) \geq 0$, then we can take $\alpha = -1/\lambda_{\max}(D)$, $x_i = y_i/(1+\alpha d_i)$ for all $i \in \mathcal{I} \setminus \{j\}$ and

$$x_j = \left[\frac{1}{\lambda_{\max}(D)} \left(1 - \sum_{i \in \mathcal{I}^-} d_i \frac{y_i^2}{(1+\alpha d_i)^2} \right) \right]^{\frac{1}{2}},$$

and therefore x and α form a solution to the system (2.38)–(2.40). Suppose that $g(-1/\lambda_{\max}(D)) < 0$. Since

$$g(0) = 1 - \sum_{i \in \mathcal{I}^-} d_i y_i^2 = 1 - y^\top D y \geq 0$$

and g is continuous in the interval $[-1/\lambda_{\max}(D), 0]$, by the Intermediate Value Theorem, there exists $t^* \in (-1/\lambda_{\max}(D), 0]$ such that $g(t^*) = 0$. Then, by taking $\alpha = t^*$, $x_j = 0$ and $x_i = y_i/(1+\alpha d_i)$ for all $i \in \mathcal{I} \setminus \{j\}$, we have a solution to the system (2.38)–(2.40).

Case 2.2. Suppose that $|\mathcal{I}^+| > 1$. Let $\tilde{y} \in \mathbb{R}^{n-1}$ be defined as

$$\tilde{y}_i = \begin{cases} y_i & \text{if } i < j, \\ y_{i+1} & \text{if } i \geq j. \end{cases}$$

Consider the diagonal matrix $\tilde{D} \in \mathbb{R}^{(n-1)\times(n-1)}$, where the i-th element of its diagonal is given by

$$\tilde{d}_i = \begin{cases} d_i & \text{if } i < j, \\ d_{i+1} & \text{if } i \geq j. \end{cases}$$

Then, since $|\mathcal{I}^+| > 1$, there exists $i \in \mathcal{I} \setminus \{j\}$ such that $d_i = \lambda_{\max}(D)$. Then, $\lambda_{\max}(\tilde{D}) = \lambda_{\max}(D)$. By construction, we have $\tilde{y}^\top \tilde{D} \tilde{y} = y^\top D y \leq 1$. Thus, by the induction hypothesis, there exist

$\tilde{\alpha} \in [-1/\lambda_{\max}(D), 0]$ and $\tilde{x} \in \mathbb{R}^{n-1}$ such that $\tilde{y} = \tilde{x} + \tilde{\alpha}\tilde{D}\tilde{x}$ and $\tilde{x}^\top \tilde{D}\tilde{x} = 1$. Therefore, if we define $\alpha = \tilde{\alpha}$ and $x \in \mathbb{R}^n$ by

$$x_i = \begin{cases} \tilde{x}_i & \text{if } i < j, \\ 0 & \text{if } i = j, \\ \tilde{x}_{i-1} & \text{if } i > j, \end{cases}$$

we have $y = x + \alpha Dx$, $x^\top Dx = 1$ and $\alpha \in [-1/\lambda_{\max}(D), 0]$. In other words, x and α form a solution to the system (2.38)–(2.40) and the proof is complete. $\square$

Proposition 2.8 *Consider the ellipsoid $\mathcal{E} = \{z \in \mathbb{R}^n \mid z^\top Sz \le 1\}$, where $S \in \mathbb{R}^{n\times n}$ is symmetric and positive definite. For each $y \in \mathcal{E}$, there exist $x \in \partial\mathcal{E}$ and $\alpha \in [-1/\lambda_{\max}(S), 0]$ such that $y = x + \alpha Sx$.*

Proof: Let $y \in \mathcal{E}$. Since S is symmetric, there exist an orthogonal matrix $Q \in \mathbb{R}^{n\times n}$ and a diagonal matrix $D \in \mathbb{R}^{n\times n}$ formed by the eigenvalues of S such that $S = QDQ^\top$ and $\lambda_{\max}(S) = \lambda_{\max}(D)$ (see, for example, Theorem 8.1.1 in [27]). Consider the ellipsoid $\mathcal{E}' = \{z \in \mathbb{R}^n \mid z^\top Dz \le 1\}$. Then, $y' = Q^\top y \in \mathcal{E}'$ and, by Lemma 2.8, there exist $x' \in \partial\mathcal{E}'$ and $\alpha' \in [-1/\lambda_{\max}(D), 0]$ such that $y' = x' + \alpha' Dx'$. By left multiplying by Q both sides of this equality, we obtain

$$\begin{aligned} y &= Qx' + \alpha' QDx' \\ &= Qx' + \alpha' QDQ^\top Qx' \\ &= Qx' + \alpha' SQx'. \end{aligned}$$

Since $x' \in \partial\mathcal{E}'$, we have $Qx' \in \partial\mathcal{E}$. Define $x = Qx'$ and $\alpha = \alpha'$. Therefore, $y = x + \alpha Sx$, with $x \in \partial\mathcal{E}$ and $\alpha \in [-1/\lambda_{\max}(S), 0]$. $\square$

Lemma 2.9 *Let $D \in \mathbb{R}^{n\times n}$ be a positive definite diagonal matrix. Consider the ellipsoid $\mathcal{E} = \{z \in \mathbb{R}^n \mid z^\top Dz \le 1\}$. Let $x \in \partial\mathcal{E}$ and $\alpha \in [-1/\lambda_{\max}(D), 0]$. Let $y = x + \alpha Dx$. Then, $y \in \mathcal{E}$ and the distance from y to the frontier of $\mathcal{E}$ is $\|y - x\|_2$.*

Proof: If $\alpha = 0$, then $y = x$ and, therefore, $y \in \mathcal{E}$ and $d(y, \partial\mathcal{E}) = d(x, \partial\mathcal{E}) = 0 = \|y - x\|_2$. Suppose that $\alpha < 0$. Consider the ball centered at y with radius $\|y - x\|_2$. We shall prove that this ball is contained in the ellipsoid $\mathcal{E}$. Let $z \in \mathbb{R}^n$ be a point belonging to this ball. Then,

$$\|z - y\|_2^2 \le \|y - x\|_2^2 = \alpha^2 \|Dx\|_2^2. \tag{2.42}$$

Since $y = x + \alpha Dx$, we have

$$\|z - y\|_2^2 = \|z - x - \alpha Dx\|_2^2 = \|z - x\|_2^2 - 2\alpha(z - x)^\top Dx + \alpha^2 \|Dx\|_2^2. \tag{2.43}$$

From (2.42) and (2.43), it follows that

$$\|z - x\|_2^2 - 2\alpha(z - x)^\top Dx \le 0.$$

Notice that

$$\begin{aligned}
\|z-x\|_2^2 - 2\alpha(z-x)^\top Dx &= (z-x)^\top(z-x-2\alpha Dx) \\
&= (z-x)^\top(z-x-\alpha Dx-\alpha Dx) \\
&= (z-x)^\top(z-y-\alpha Dx) \\
&= (z-x)^\top(z-y) - \alpha(z-x)^\top Dx \\
&= (z-x)^\top(z-y) - \alpha z^\top Dx + \alpha x^\top Dx \\
&= (z-x)^\top(z-y) - \alpha z^\top Dx + \alpha,
\end{aligned}$$

where the third equality holds since $y = x + \alpha Dx$ and the last equality holds since $x \in \partial\mathcal{E}$, i.e., $x^\top Dx = 1$. Thus,

$$(z-x)^\top(z-y) - \alpha z^\top Dx \le -\alpha.$$

By dividing both sides of this inequality by $-\alpha$ (that, by assumption, is positive), we obtain the following inequality:

$$\frac{1}{\alpha}(z-x)^\top(y-z) + z^\top Dx \le 1.$$

We have

$$\begin{aligned}
\frac{1}{\alpha}(z-x)^\top(y-z) + z^\top Dx &= \frac{1}{\alpha}(z-x)^\top(y-z) + z^\top D(x-z+z) \\
&= \frac{1}{\alpha}(z-x)^\top(y-z) - (z-x)^\top Dz + z^\top Dz \\
&= \frac{1}{\alpha}(z-x)^\top(y-z-\alpha Dz) + z^\top Dz \\
&= \frac{1}{\alpha}(z-x)^\top(x+\alpha Dx - z - \alpha Dz) + z^\top Dz \\
&= \frac{1}{\alpha}(z-x)^\top[x-z+\alpha D(x-z)] + z^\top Dz \\
&= -\frac{1}{\alpha}(x-z)^\top[x-z+\alpha D(x-z)] + z^\top Dz.
\end{aligned}$$

Therefore,

$$-\frac{1}{\alpha}(x-z)^\top[x-z+\alpha D(x-z)] + z^\top Dz \le 1.$$

Note that

$$-\frac{1}{\alpha}(x-z)^\top[x-z+\alpha D(x-z)] \ge 0,$$

since $-1/\alpha > 0$ and

$$\begin{aligned}
(x-z)^\top[x-z+\alpha D(x-z)] &= (x-z)^\top(x-z) + \alpha(x-z)^\top D(x-z) \\
&\ge \|x-z\|_2^2 + \alpha(x-z)^\top(\lambda_{\max}(D)I_n)(x-z) \\
&= \|x-z\|_2^2 + \alpha\lambda_{\max}(D)\|x-z\|_2^2 \\
&= [1+\alpha\lambda_{\max}(D)]\|x-z\|_2^2 \\
&\ge 0,
\end{aligned}$$

where the first inequality follows from the fact that D is a diagonal matrix and $\alpha < 0$, and the second inequality holds since $\alpha \geq -1/\lambda_{\max}(D)$. Consequently, we have $z^\top Dz \leq 1$, i.e., $z \in \mathcal{E}$. Thus, the ball centered at y with radius $\|y-x\|_2$ is contained in the ellipsoid $\mathcal{E}$. Therefore, $y \in \mathcal{E}$ and since x belongs to this ball and $x \in \partial\mathcal{E}$, we conclude that $d(y, \partial\mathcal{E}) = \|y - x\|_2$. (Suppose, in order to derive a contradiction, that $d(y, \partial\mathcal{E}) < \|y - x\|_2$. Then, there exists $v \in \partial\mathcal{E}$ such that $\|y - v\|_2 < \|y - x\|_2$. Then, v belongs to the interior of ball $\mathcal{B}(y, \|y - x\|_2)$ centered at y with radius $\|y - x\|_2$. Since $\mathcal{B}(y, \|y - x\|_2)$ is contained in $\mathcal{E}$, we have that v is also an interior point of $\mathcal{E}$, which is a contradiction. Thus, $d(y, \partial\mathcal{E}) = \|y - x\|_2$.) □

Proposition 2.9 *Consider the ellipsoid $\mathcal{E} = \{z \in \mathbb{R}^n \mid z^\top Sz \leq 1\}$, where $S \in \mathbb{R}^{n\times n}$ is a symmetric and positive definite matrix. Let $x \in \partial\mathcal{E}$ and $\alpha \in [-1/\lambda_{\max}(S), 0]$. Let $y = x + \alpha Sx$. Then, $y \in \mathcal{E}$ and the distance from y to the frontier of $\mathcal{E}$ is $\|y - x\|_2$.*

Proof: Since S is symmetric, there exist an orthogonal matrix $Q \in \mathbb{R}^{n\times n}$ and a diagonal matrix $D \in \mathbb{R}^{n\times n}$ formed by the eigenvalues of S such that $S = QDQ^\top$ and $\lambda_{\max}(S) = \lambda_{\max}(D)$ (see, for example, Theorem 8.1.1 in [27]). Consider the ellipsoid $\mathcal{E}' = \{z \in \mathbb{R}^n \mid z^\top Dz \leq 1\}$. Then, $Q^\top x \in \partial\mathcal{E}'$. Thus, by Lemma 2.9, $y' = Q^\top x + \alpha DQ^\top x$ is such that $y' \in \mathcal{E}'$ and the distance from y' to the frontier of $\mathcal{E}'$ is $\|y' - Q^\top x\|_2$. Since $y' \in \mathcal{E}'$, it follows that $Qy' \in \mathcal{E}$. Moreover,

$$Qy' = Q(Q^\top x + \alpha DQ^\top x) = x + \alpha QDQ^\top x = x + \alpha Sx = y.$$

Thus, $y = Qy'$ and, therefore, $y \in \mathcal{E}$. We also have

$$\begin{aligned} d(y', \partial\mathcal{E}') &= \min_{z\in\partial\mathcal{E}'} \|y' - z\|_2 \\ &= \min_{z\in\partial\mathcal{E}'} \|Q(y' - z)\|_2 \\ &= \min_{z\in\partial\mathcal{E}'} \|y - Qz\|_2 \\ &= \min_{w\in\partial\mathcal{E}} \|y - w\|_2 \\ &= d(y, \partial\mathcal{E}), \end{aligned}$$

where the second equality is valid since Q is orthogonal and the fourth equality holds since, for all $z \in \partial\mathcal{E}'$, we have $Qz \in \partial\mathcal{E}$ and, for all $w \in \partial\mathcal{E}$, we have $w = Q(Q^\top w)$ and $Q^\top w \in \partial\mathcal{E}'$. Thus, $d(y', \partial\mathcal{E}') = d(y, \partial\mathcal{E})$. Furthermore,

$$d(y', \partial\mathcal{E}') = \|y' - Q^\top x\|_2 = \|Q(y' - Q^\top x)\|_2 = \|Qy' - x\|_2 = \|y - x\|_2.$$

Hence, $y \in \mathcal{E}$ and $d(y, \partial\mathcal{E}) = \|y - x\|_2$. □

We are now able to develop the model. Consider the ellipsoid $\mathcal{C} = \{x \in \mathbb{R}^n \mid x^\top P^{-1}x \leq 1\}$, where P is a positive definite diagonal matrix. Consider also the ellipsoid $\mathcal{E}_i = \{x \in \mathbb{R}^n \mid (x - c_i)^\top Q_i P_i^{-1} Q_i^\top (x - c_i) \leq 1\}$, where $c_i \in \mathbb{R}^n$, $Q_i \in \mathbb{R}^{n\times n}$ is orthogonal and $P_i \in \mathbb{R}^{n\times n}$ is a positive definite diagonal matrix. By applying transformation T_i defined in (2.4) to ellipsoid $\mathcal{E}_i$, we obtain the ball

$$\mathcal{E}_{ii} = \{x \in \mathbb{R}^n \mid (x - P_i^{-\frac{1}{2}} Q_i^\top c_i)^\top (x - P_i^{-\frac{1}{2}} Q_i^\top c_i) \leq 1\}.$$

By applying the same transformation T_i to ellipsoid $\mathcal{C}$, we obtain the ellipsoid

$$\mathcal{C}_i = \{x \in \mathbb{R}^n \mid x^\top S_i x \leq 1\},$$

where

$$S_i = P_i^{\frac{1}{2}} Q_i^\top P^{-1} Q_i P_i^{\frac{1}{2}}. \tag{2.44}$$

Since T_i is an invertible transformation, we have $\mathcal{E}_i \subseteq \mathcal{C}$ if and only if $\mathcal{E}_{ii} \subseteq \mathcal{C}_i$ by Lemma 2.2. In order to guarantee that $\mathcal{E}_{ii} \subseteq \mathcal{C}_i$, we require that the center c_{ii} of ball $\mathcal{E}_{ii}$ be in $\mathcal{C}_i$ and that the distance between c_{ii} and the frontier of $\mathcal{C}_i$ be at least one. By Proposition 2.8, if $c_{ii} \in \mathcal{C}_i$ then there exist $\bar{x}_i \in \partial\mathcal{C}_i$ and $\alpha_i \in [-1/\lambda_{\max}(S_i), 0]$ such that

$$c_{ii} = \bar{x}_i + \alpha_i S_i \bar{x}_i. \tag{2.45}$$

Moreover, by Proposition 2.9, any point of the form (2.45) belongs to ellipsoid $\mathcal{C}_i$ and the distance between c_{ii} and $\partial\mathcal{C}_i$ is $\|c_{ii} - \bar{x}_i\|_2$. Thus, since $c_{ii} = P_i^{-\frac{1}{2}} Q_i^\top c_i$, we obtain the following model for the inclusion of ellipsoids into an ellipsoid.

$$\begin{aligned}
P_i^{-\frac{1}{2}} Q_i^\top c_i &= \bar{x}_i + \alpha_i S_i \bar{x}_i, && \forall i \in I && (2.46)\\
\bar{x}_i^\top S_i \bar{x}_i &= 1, && \forall i \in I && (2.47)\\
\|P_i^{-\frac{1}{2}} Q_i^\top c_i - \bar{x}_i\|_2^2 &\geq 1, && \forall i \in I && (2.48)\\
\alpha_i &\leq 0, && \forall i \in I && (2.49)\\
\alpha_i &\geq -1/\lambda_{\max}(S_i), && \forall i \in I. && (2.50)
\end{aligned}$$

2.3.1.1 Alternative model

Consider a solution to the system (2.46)–(2.50). Notice that the value of α_i must be strictly negative for each $i \in I$. Otherwise, if $\alpha_i = 0$ for some $i \in I$, constraint (2.46) implies that $c_{ii} = \bar{x}_i$ and, therefore, $\|c_{ii} - \bar{x}_i\|_2 = 0$, which violates constraint (2.48). Lemma 2.10 below provides a negative upper bound on the value of α_i.

Lemma 2.10 *Any solution to the system (2.46)–(2.50) is such that $\alpha_i \leq \epsilon_i$, where*

$$\epsilon_i = -\lambda_{\min}(P_i^{-1})\lambda_{\min}(P_i^{\frac{1}{2}})\lambda_{\min}(P)\lambda_{\min}(P^{-\frac{1}{2}}) < 0,$$

for each $i \in I$.

Proof: Consider a solution to the system (2.46)–(2.50). Let $i \in I$. By constraints (2.47), we have $\bar{x}_i^\top S_i \bar{x}_i = 1$. Then, by Lemma 2.3 (taking $x_{ij} \doteq \bar{x}_i$, $P_j \doteq P$ and $Q_j \doteq I_n$), we have

$$\|S_i \bar{x}_i\|_2 \leq \lambda_{\max}(P_i)\lambda_{\max}(P^{-1})\lambda_{\max}(P^{\frac{1}{2}})\lambda_{\max}(P_i^{-\frac{1}{2}}).$$

By constraints (2.48), we have $\alpha_i^2 \|S_i \bar{x}_i\|_2^2 \geq 1$. Thus, we must have $\|S_i \bar{x}_i\|_2 > 0$ and, therefore, $\alpha_i^2 \geq 1/\|S_i \bar{x}_i\|_2^2$. Consequently, since $\alpha_i \leq 0$ by constraints (2.49), we must have $\alpha_i \leq$

$-1/\|S_i\bar{x}_i\|_2$. Hence, α_i must satisfy

$$\begin{aligned}\alpha_i &\le -\Big(\lambda_{\max}(P_i)\lambda_{\max}(P^{-1})\lambda_{\max}(P^{\frac{1}{2}})\lambda_{\max}(P_i^{-\frac{1}{2}})\Big)^{-1}\\ &= -\lambda_{\min}(P_i^{-1})\lambda_{\min}(P_i^{\frac{1}{2}})\lambda_{\min}(P)\lambda_{\min}(P^{-\frac{1}{2}}).\end{aligned}$$

Then, we can take

$$\epsilon_i = -\lambda_{\min}(P_i^{-1})\lambda_{\min}(P_i^{\frac{1}{2}})\lambda_{\min}(P)\lambda_{\min}(P^{-\frac{1}{2}})$$

and the result follows. (Note that $\epsilon_i < 0$ since P_i and P are positive definite matrices.) $\square$

Based on this result, we can slightly modify model (2.46)–(2.50) and consider an alternative model. Constraints (2.46) imply

$$\bar{x}_i^\top P_i^{-\frac{1}{2}} Q_i^\top c_i = \bar{x}_i^\top \bar{x}_i + \alpha_i \bar{x}_i^\top S_i \bar{x}_i, \quad \forall i \in I.$$

Therefore, since α_i must be nonzero, we have that

$$\bar{x}_i^\top S_i \bar{x}_i = \frac{\bar{x}_i^\top (P_i^{-\frac{1}{2}} Q_i^\top c_i - \bar{x}_i)}{\alpha_i}, \quad \forall i \in I.$$

So, we can replace constraints (2.47) and (2.49), respectively, with constraints

$$\begin{aligned}&\alpha_i = \bar{x}_i^\top (P_i^{-\frac{1}{2}} Q_i^\top c_i - \bar{x}_i), && \forall i \in I\\ &\alpha_i \le \epsilon_i, && \forall i \in I,\end{aligned}$$

which are apparently simpler, and obtain an equivalent model.

2.3.1.2 Computing the largest eigenvalue of S_i

The i-th constraint in (2.50) depends on the largest eigenvalue of matrix S_i defined in (2.44). Thus, we must know how to compute it. Firstly, we consider the particular two-dimensional case. Next, we consider the problem in $\mathbb{R}^n$ where the container is a ball. Finally, we consider the general case in $\mathbb{R}^n$ where the container is an arbitrary ellipsoid (centered at the origin).

Let $i \in I$. Consider the two-dimensional problem and suppose that a_i and b_i are the eigenvalues of $P_i^{\frac{1}{2}}$, and a and b are the eigenvalues of $P^{\frac{1}{2}}$. In this case, if we represent the rotation matrix Q_i as in (2.1), the largest eigenvalue of S_i will be given by

$$\lambda_{\max}(S_i) = \frac{\delta_i + \sqrt{\beta_i}}{4a^2b^2},$$

where

$$\delta_i = (a^2+b^2)(a_i^2+b_i^2) - (a^2-b^2)(a_i^2-b_i^2)\cos(2\theta_i)$$

and

$$\beta_i = \delta_i^2 - (4aba_ib_i)^2.$$

Constraint $\alpha_i \geq -1/\lambda_{\max}(S_i)$ is therefore equivalent to constraint

$$\alpha_i \geq -\frac{4a^2b^2}{\delta_i + \sqrt{\beta_i}},$$

which in turn is equivalent to constraint

$$\alpha_i\sqrt{\beta_i} \geq -(4a^2b^2 + \alpha_i\delta_i). \tag{2.51}$$

By constraints (2.49), α_i must be nonpositive. Then, we must have $\alpha_i\sqrt{\beta_i} \leq 0$ and, therefore, $4a^2b^2 + \alpha_i\delta_i \geq 0$. In this way, constraint (2.51) is equivalent to constraints

$$\alpha_i^2\beta_i - (4a^2b^2 + \alpha_i\delta_i)^2 \geq 0 \tag{2.52}$$

$$4a^2b^2 + \alpha_i\delta_i \geq 0. \tag{2.53}$$

The function that defines constraint (2.51) is not everywhere differentiable in the domain of the variables of the model, whereas the functions that define constraints (2.52) and (2.53) are continuous and differentiable. So, for our purposes, the latter constraints are more suitable than the former one. This is because we are interested in solving the problem of packing ellipsoids in practice and, for this, we will use methods that make use of the derivatives of the functions that define the problem.

Now, consider the problem in $\mathbb{R}^n$ and suppose that the container is a ball with radius $r > 0$. In this case, we have $P = r^2I_n$ and thus

$$S_i = P_i^{\frac{1}{2}}Q_i^\top P^{-1}Q_iP_i^{\frac{1}{2}} = r^{-2}P_i^{\frac{1}{2}}Q_i^\top Q_iP_i^{\frac{1}{2}} = r^{-2}P_i.$$

Then, $\lambda_{\max}(S_i) = r^{-2}\lambda_{\max}(P_i)$ and the largest eigenvalue of P_i is simply the largest element of the diagonal of P_i.

Finally, consider the problem in $\mathbb{R}^n$ where the container is an ellipsoid centered at the origin. Since S_i is nonsingular, we have $\lambda_{\min}(S_i^{-1}) = 1/\lambda_{\max}(S_i)$. Then, the problem of computing the largest eigenvalue of matrix S_i is reduced to the problem of computing the least eigenvalue of matrix S_i^{-1}. Consider the system of equations

$$S_i^{-1}v_i = \lambda_iv_i \tag{2.54}$$

$$v_i^\top v_i = 1 \tag{2.55}$$

$$(S_i^{-1} - \lambda_iI_n) = B_i^\top B_i, \tag{2.56}$$

where the variables are $\lambda_i \in \mathbb{R}$, $v_i \in \mathbb{R}^n$ and $B_i \in \mathbb{R}^{n\times n}$. Equations (2.54) and (2.55) are satisfied if and only if v_i is an eigenvector of S_i^{-1} and λ_i is the eigenvalue associated with v_i. Equation (2.56) is satisfied if and only if matrix $S_i^{-1} - \lambda_iI_n$ is positive semidefinite. (A matrix A is positive semidefinite if and only if there exists a matrix B such that $A = B^\top B$. See, for example, page 566 in Meyer [44]). Since S_i^{-1} is positive definite, matrix $S_i^{-1} - \lambda_iI_n$ is positive semidefinite if and only if $\lambda_i \in [0, \lambda_{\min}(S_i^{-1})]$. Since equations (2.54) and (2.55) imply that λ_i is an eigenvalue of S_i^{-1}, equation (2.56) is satisfied if and only if $\lambda_i = \lambda_{\min}(S_i^{-1})$. Therefore, in the n-dimensional case, the i-th constraint in (2.50) of the model (2.46)–(2.50) must be replaced by constraints

$$\begin{aligned} \alpha_i &\geq -\lambda_i \\ S_i^{-1} v_i &= \lambda_i v_i \\ v_i^\top v_i &= 1 \\ (S_i^{-1} - \lambda_i I_n) &= B_i^\top B_i, \end{aligned} \tag{2.57}$$

and the variables λ_i, v_i and B_i are incorporated into the model. In this case, n constraints are removed from the model and $m(n^2+n+1)$ variables and $m(n^2+n+2)$ constraints are added to the model.

2.3.2 Ellipsoid inside a half-space

In this section, we propose a model to include an ellipsoid $\mathcal{E}_i$ into a half-space $\mathcal{H}$. A transformation is applied to the ellipsoid $\mathcal{E}_i$ which converts it into a ball $\mathcal{E}_{ii}$ and the same transformation is applied to the half-space $\mathcal{H}$, thus obtaining a half-space $\mathcal{H}_i$. Next, we model the inclusion of $\mathcal{E}_{ii}$ into $\mathcal{H}_i$ and observe that $\mathcal{E}_i$ is contained in $\mathcal{H}$ if and only if $\mathcal{E}_{ii}$ is contained in $\mathcal{H}_i$.

Consider the half-space $\mathcal{H} = \{x \in \mathbb{R}^n \mid w^\top x \leq s\}$, where $w \in \mathbb{R}^n \setminus \{0\}$ and $s \in \mathbb{R}$, and the ellipsoid $\mathcal{E}_i = \{x \in \mathbb{R}^n \mid (x-c_i)^\top Q_i P_i^{-1} Q_i^\top (x-c_i) \leq 1\}$, where $c_i \in \mathbb{R}^n$, $Q_i \in \mathbb{R}^{n \times n}$ is orthogonal and $P_i \in \mathbb{R}^{n \times n}$ is positive definite and diagonal. Let $\mathcal{H}_i$ be the set obtained when transformation T_i defined in (2.4) is applied to the half-space $\mathcal{H}$, i.e.,

$$\begin{aligned} \mathcal{H}_i &= \{x \in \mathbb{R}^n \mid x = T_i(z), z \in \mathcal{H}\} \\ &= \{x \in \mathbb{R}^n \mid x = P_i^{-\frac{1}{2}} Q_i^\top z, z \in \mathcal{H}\} \\ &= \{x \in \mathbb{R}^n \mid z = Q_i P_i^{\frac{1}{2}} x, z \in \mathcal{H}\} \\ &= \{x \in \mathbb{R}^n \mid w^\top Q_i P_i^{\frac{1}{2}} x \leq s\}. \end{aligned}$$

Since T_i is an invertible transformation, $\mathcal{E}_i \subseteq \mathcal{H}$ if and only if $\mathcal{E}_{ii} \subseteq \mathcal{H}_i$ by Lemma 2.2. Thus, in order to guarantee that ellipsoid $\mathcal{E}_i$ is contained in the half-space $\mathcal{H}$, we require that the ball $\mathcal{E}_{ii}$ be contained in the half-space $\mathcal{H}_i$, i.e., the center c_{ii} of ball $\mathcal{E}_{ii}$ must be in $\mathcal{H}_i$ and the distance from c_{ii} to the frontier of the half-space $\mathcal{H}_i$ must be at least one.

The frontier of the half-space $\mathcal{H}_i$ is the hyperplane $\partial\mathcal{H}_i = \{x \in \mathbb{R}^n \mid w^\top Q_i P_i^{\frac{1}{2}} x = s\}$. Thus, the distance $d(c_{ii}, \partial\mathcal{H}_i)$ from the point c_{ii} to the frontier of $\mathcal{H}_i$ is given by

$$d(c_{ii}, \partial\mathcal{H}_i) = \frac{|w^\top Q_i P_i^{\frac{1}{2}} c_{ii} - s|}{\|P_i^{\frac{1}{2}} Q_i^\top w\|_2}.$$

Therefore, the conditions

$$\frac{(w^\top Q_i P_i^{\frac{1}{2}} c_{ii} - s)^2}{\|P_i^{\frac{1}{2}} Q_i^\top w\|_2^2} \geq 1 \quad \text{and} \quad w^\top Q_i P_i^{\frac{1}{2}} c_{ii} \leq s \tag{2.58}$$

are satisfied if and only if $\mathcal{E}_i \subseteq \mathcal{H}$. Alternatively, since $c_{ii} = P_i^{-\frac{1}{2}} Q_i^\top c_i$, we have

$$w^\top Q_i P_i^{\frac{1}{2}} c_{ii} = w^\top Q_i P_i^{\frac{1}{2}} P_i^{-\frac{1}{2}} Q_i^\top c_i = w^\top c_i.$$

Hence, conditions (2.58) can also be written as

$$\frac{\left(w^\top c_i - s\right)^2}{\|P_i^{\frac{1}{2}} Q_i^\top w\|_2^2} \geq 1 \quad \text{and} \quad w^\top c_i \leq s. \tag{2.59}$$

2.4 Numerical experiments

In this section, we present a variety of numerical experiments that aim to illustrate the capabilities and limitations of the introduced models for packing ellipsoids. In a first set of experiments, we consider the problem tackled in [26] that consists in packing as many identical ellipses as possible within a given rectangle. In a second set of experiments, we deal with the problem approached in [38] that consists in, given a set of (not necessarily identical) ellipses, finding the rectangle with the smallest area within which the given set of ellipses can be packed. Finally, in a third set of experiments, we deal with the problem of packing three-dimensional ellipsoids within a ball or cuboid, trying to minimize the volume of the container.

All considered two-dimensional models were coded in AMPL [25] (Modeling Language for Mathematical Programming), while the three-dimensional models were coded in Fortran 90. The experiments were run on a 2.4GHz Intel Core2 Quad Q6600 machine with 4.0GB RAM memory and Ubuntu 12.10 (GNU/Linux 3.5.0-21-generic x86_64) operating system. As the nonlinear programming (NLP) solver, we have used Algencan [2, 13] version 3.0.0, which is available for downloading at the TANGO Project web page (`http://www.ime.usp.br/~egbirgin/tango/`). Algencan was compiled with GNU Fortran (GCC) 4.7.2 compiler with the `-O3` optimization directive enabled.

Algencan is an augmented Lagrangian method for nonlinear programming that solves the bound-constrained augmented Lagrangian subproblems using Gencan [3, 11, 12], an active-set method for bound-constrained minimization. Gencan adopts the leaving-face criterion described in [11], that employs spectral projected gradients defined in [15, 16]. For the internal-to-the-face minimization, Gencan uses an unconstrained algorithm that depends on the dimension of the problem and the availability of second-order derivatives. For small problems with available Hessians, a Newtonian trust-region approach is used (see [3]); while for medium- and large-sized problems with available Hessians a Newtonian line-search method that combines backtracking and extrapolation is used (this is the case of the two-dimensional problems presented in the current section that, since they were coded in AMPL, have second-order derivatives available). When second-order derivatives are not available, each step of Gencan computes the direction inside the face using a line-search truncated-Newton approach with incremental quotients to approximate the matrix-vector products and memoryless BFGS preconditioners (this is the case of the three-dimensional problems considered in the present section, that were coded in Fortran 90 and for which only first-order derivatives were coded).

Although Algencan is a local nonlinear programming solver, it was designed in such a way that global minimizers of subproblems are actively pursued, independently of the fulfillment of approximate stationarity conditions in the subproblems. In other words, Algencan's subproblem solvers try always to find the lowest possible function values, even when this is not necessary for obtaining approximate local minimizers. As a consequence, practical behavior of Algencan is usually well explained by the properties of their global-optimization counterparts [8]. The "preference for global minimizers" of Algencan has been discussed in [2]. This has also been observed in papers devoted to numerical experiments concerning Algencan and other solvers (see, for example, [33, 32] and the references therein). This does not mean at all that Algencan is able to find global minimizers. Moreover, in no case it would be able to prove that a global minimizer has been found. This simply means that, although unnecessary from the theoretical point of view, Algencan makes an effort to find good quality local minimizers.

2.4.1 Two-dimensional packing

2.4.1.1 Packing the maximum number of ellipses within a rectangle

Given positive numbers L, W, a, and b, the problem considered in this section consists in computing the maximum number m^* of identical ellipses with semi-axis lengths a and b that can be packed within a rectangle with length L and width W. To illustrate the capabilities of the introduced models, we have considered a very simple strategy for packing the maximum possible number of identical ellipses into a given rectangle. The algorithm iteratively packs an increasing amount of ellipses into the rectangle. At the m-th iteration, the algorithm tries to pack m ellipses. If it successfully packs the m ellipses inside the rectangle, then the iteration is over and the next one begins. If it cannot pack the m ellipses, a packing with $m^* = m - 1$ ellipses is returned and the algorithm terminates.

In order to pack m ellipses, a feasibility problem must be solved. This feasibility problem consists of the non-overlapping constraints (2.22)–(2.25) or, alternatively, the non-overlapping constraints (2.26)–(2.31), plus the fitting constraints that require the ellipses to be inside the rectangle. In (2.22)–(2.25) or (2.26)–(2.31), we have that $P_i \in \mathbb{R}^{2\times 2}$, for $i = 1, \ldots, m$, is the diagonal matrix with diagonal entries a^2 and b^2; while ϵ_{ij} $(i, j \in \{1, \ldots, m\}$ such that $i < j)$ is given by (2.21). The inclusion of an ellipse within the rectangle is obtained by requiring the ellipse to be contained in four half-spaces (each one associated with a particular side of the rectangle) as modeled in (2.59). Hence, considering that the rectangle with length L and width W is centered at the origin and has sides parallel to the Cartesian axes, the fitting constraints are given by

$$\left(w_\ell^\top c_i - s_\ell\right)^2 \geq \|P_i^{\frac{1}{2}} Q_i^\top w_\ell\|_2^2 \quad \text{and} \quad w_\ell^\top c_i \leq s_\ell \quad \text{for} \quad i \in \{1, \ldots, m\},\ \ell \in \{1, \ldots, 4\}, \tag{2.60}$$

where

$$w_1 = -w_2 = (1, 0)^\top, \quad w_3 = -w_4 = (0, 1)^\top, \quad s_1 = s_2 = \frac{L}{2} \quad \text{and} \quad s_3 = s_4 = \frac{W}{2}.$$

From now on, the feasibility problem with m ellipses and that uses the non-overlapping constraints (2.22)–(2.25) plus the fitting constraints (2.60) will be named $\mathcal{F}_1^m$; while the one that uses the non-overlapping constraints (2.26)–(2.31) plus the fitting constraints (2.60) will be named $\mathcal{F}_2^m$. The model $\mathcal{F}_1^m$ has $m(5m+11)/2$ constraints and $3m(m+1)/2$ variables; while the model $\mathcal{F}_2^m$ has $m(3m+5)$ constraints and $3m^2$ variables.

Since the feasibility problems $\mathcal{F}_1^m$ and $\mathcal{F}_2^m$ are non-convex and their numerical resolution can be a very hard task, we apply a multi-start strategy. We define a maximum number N_{att} of attempts to solve each problem launching the local NLP solver Algencan from different initial points. If the problem is successfully solved, a packing with m ellipses is found. In this case, m is incremented and the algorithm continues. Otherwise, if the maximum number of attempts has been reached, then the algorithm stops, suggesting that a packing with m ellipses is not possible, and a packing with $m^* = m - 1$ ellipses is returned.

The algorithm starts with $m = 1$ and increases m by one at each iteration. It is important to mention that most of the computational effort is spent when solving the problem with $m = m^*$ and trying to solve the problem with $m = m^*+1$. See, for example, [10, 14, 17] where exhaustive numerical experiments support this claim.

When trying to pack m ellipses, the first initial point is constructed as follows. First, $m-1$ ellipses are arranged as in the solution for the problem with $m-1$ ellipses and the m-th ellipse is randomly arranged in the rectangle (the center of the m-th ellipse is chosen uniformly at random inside the rectangle and its rotation angle is chosen uniformly at random in the interval $[0, \pi]$). For each subsequent attempt of packing m ellipses, the initial point is given by a small random perturbation (at most 15%) of the solution returned by the local NLP solver in the previous unsuccessful attempt. We have considered a maximum of $N_{\text{att}} = 100$ attempts to solve each subproblem for a fixed value of m. Also, we have considered a total CPU time limit of 5 hours to solve all subproblems for increasing values of m.

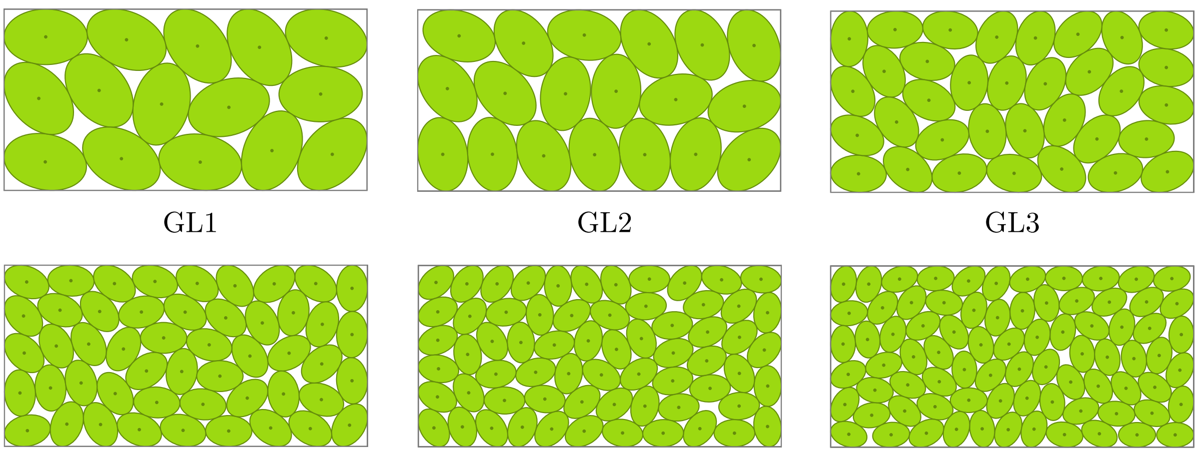
Table 2.1 shows the results obtained by applying the described strategy connected with models $\mathcal{F}_1$ and $\mathcal{F}_2$ to the six instances considered in [26], each one defined by a rectangle with length 6 and width 3 and identical ellipses with eccentricity 0.74536. In the table, the first column refers to the instance name and the second column shows the lengths of the semi-axes of the identical ellipses. The third column shows the number of ellipses packed by the method proposed in [26]. The fourth and fifth columns present, for models $\mathcal{F}_1$ and $\mathcal{F}_2$, respectively, the number of packed ellipses and the total CPU time spent (in seconds). As expected, the strategy of solving models $\mathcal{F}_1^m$ and $\mathcal{F}_2^m$ for increasing values of m was able to find better solutions than the ones found by the method proposed in [26], since our models do not impose constraints on the rotation angles of the ellipses (the method proposed in [26] considers only 90-degree rotations). It is worth noting that this set of experiments suggests that the usage of model $\mathcal{F}_1$ delivered solutions faster, even being able to deliver a better quality solution (within the considered CPU time limit of 5 hours and the maximum number of attempts) for instance GL6. Figures 2.3 and 2.4 show the graphical representation of the solutions found by considering the models $\mathcal{F}_1$ and $\mathcal{F}_2$, respectively.

2.4.1.2 Minimizing the area of the container

In this section, we first consider the problem of packing a given set of m (identical or non-identical) ellipses with semi-axis lengths a_i and b_i (for $i \in \{1, \dots, m\}$) within a rectangular container of minimum area. This problem can be modeled as the nonlinear programming problem that consists in minimizing the product of the variable length L and width W of

Instance	Semi-axis lengths	Sh. I. Galiev and M. S. Lisafina [26]	Model $\mathcal{F}_1$		Model $\mathcal{F}_2$	
		m^*	m^*	Time (s)	m^*	Time (s)
GL1	(0.68892,0.45928)	13	15	10.23	15	285.80
GL2	(0.61237,0.40825)	16	19	14.49	19	393.68
GL3	(0.45928,0.30619)	30	34	47.05	34	182.94
GL4	(0.38273,0.25515)	45	50	1025.24	50	1120.17
GL5	(0.33681,0.22454)	56	65	2122.40	65	2375.46
GL6	(0.30619,0.20412)	69	79	2131.65	78	7158.56

Table 2.1: Results obtained for the instances proposed in [26].



GL1 GL2 GL3

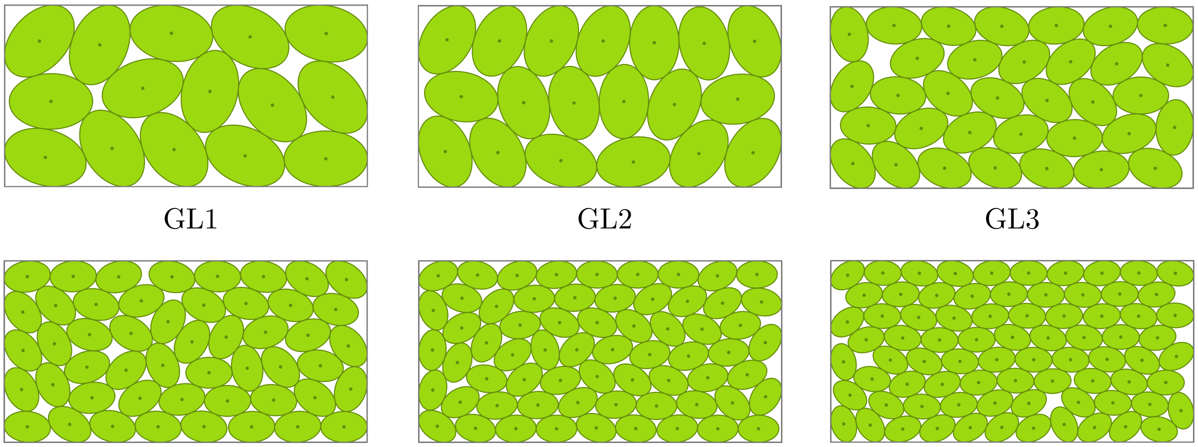
GL4 GL5 GL6

Figure 2.3: Solutions found by model $\mathcal{F}_1$ for the instances proposed in [26].

the rectangular container (centered at the origin and with their sides parallel to the Cartesian axes) subject to the non-overlapping constraints (2.22)–(2.25) plus the fitting constraints (2.60), where $P_i \in \mathbb{R}^{2\times 2}$ is the diagonal matrix with entries a_i^2 and b_i^2 for $i \in \{1, \ldots, m\}$ and ϵ_{ij} is given by (2.21) for $i, j \in \{1, \ldots, m\}$ such that $i < j$. This NLP problem will be named $\mathcal{M}$ from now on. The model $\mathcal{M}$ has $m(5m + 11)/2$ constraints and $3m(m + 1)/2 + 2$ variables.

Since problem $\mathcal{M}$ is a very hard non-convex nonlinear programming problem, we consider, once again, a multi-start strategy in order to obtain the best possible local solution using the NLP solver Algencan. The algorithm stops when either the number of attempts to solve the problem reaches $N_{\text{att}} = 1000$ or 5 hours of CPU time are spent.

For instances with identical ellipses with semi-axis lengths a and b, the initial point is given as follows. The centers of the ellipses are arranged in a regular lattice where the distance between consecutive points is $2 \max\{a, b\}$. The rotation angle of each ellipse is chosen uniformly at random in the interval $[0, \pi]$. The initial guess for the length and width of the container are



GL1 GL2 GL3

GL4 GL5 GL6

Figure 2.4: Solutions found by model $\mathcal{F}_2$ for the instances proposed in [26].

then chosen so that it contains all ellipses. In the case of instances with non-identical ellipses, the lattice is constructed so that the ellipses do not overlap when their centers are arranged in the lattice. Moreover, the order in which the ellipses are arranged in the lattice is random.

In a first set of experiments, we considered the three sets of instances introduced in [38] for the problem of packing a given set of identical or non-identical ellipses within a rectangular container of minimum area. The first set includes 15 instances with non-identical ellipses; the second set includes 14 instances with identical ellipses; and the third set includes 15 small instances with 3 non-identical ellipses with increasing eccentricity. Tables 2.2–2.4 show the results. The first column presents the names of the instances and the second column shows the number m of ellipses. The third column shows the area of the container found by the method proposed in [38]. A subset of the instances in Table 2.2 were also considered in [52]. Therefore, the third column in Table 2.2 also shows, when applicable, the area of the container found by the method proposed in [52]. The fourth column shows the area of the container found by our method. The area is rounded with 5 decimal places (results up to the machine precision can be found in `http://www.ime.usp.br/~lobato/`). The fifth column shows the number of attempts made to find the solution. The last column shows the average CPU time (in seconds) per local minimization. As it can be seen, our method was able to find solutions at least as good as the ones presented in [38]. Moreover, for 20 instances, our method found better solutions (marked with * in Tables 2.2 and 2.3) than the ones reported in [38]. In Table 2.2 it is also possible to see that, considering the 9 instances to which the methodology proposed in [52] was applied, our method found better quality solutions in 7 instances (TC05b, TC06, TC11, TC14, TC20, TC50, and TC100), same quality solution in one instance (TC05a), and a poorer quality solution in only one instance (TC30). Figures 2.5, 2.6, and 2.7 illustrate the solutions obtained for the instances with prefix TC, TS, and TE, respectively.

To end this section, we consider the problem of packing a given set of ellipses inside an ellipse with minimum area. This problem can be modeled as the problem of minimizing the

Instance	m	Areas reported in J. Kallrath and S. Rebennack [38] (left) and in Y. Stoyan *et al.* [52] (right)		Model $\mathcal{M}$		
				Area	# Local Minimizations	Avg. Time (s)
TC02a	2	18.00000		18.00000	1	0.03
TC02b	2	22.23152		22.23159	2	0.02
TC03a	3	21.38577		21.38577	2	0.04
TC03b	3	25.22467		25.22467	39	0.07
TC04a	4	23.18708		23.18708	2	0.11
TC04b	4	28.54159		28.54074*	74	0.07
TC05a	5	25.29557	24.55368	24.55368*	43	0.15
TC05b	5	31.28873	30.84870	30.64919*	20	0.14
TC06	6	25.27463	25.47173	25.08331*	19	0.54
TC11	11	57.24034	57.17830	55.91657*	348	5.27
TC14	14	24.67185	24.25099	24.17168*	75	5.73
TC20	20	67.83459	66.13647	65.70134*	45	19.28
TC30	30	103.45212	95.36535	95.61125*	272	58.27
TC50	50	166.91505	154.47049	152.69296*	42	278.71
TC100	100	322.64663	297.73798	297.70558*	2	2790.77

Table 2.2: Instances with non-identical ellipses considered in [38].

Instance	m	Area reported in J. Kallrath and S. Rebennack [38]	Model $\mathcal{M}$		
			Area	# Local Minimizations	Avg. Time (s)
TS02	2	16.00000	16.00000	1	0.06
TS03	3	23.53351	23.51416*	3	0.08
TS04	4	31.06838	31.06838	3	0.22
TS05	5	39.01646	39.01646	40	0.58
TS06	6	46.59133	46.06018*	5	1.50
TS07	7	54.13676	54.13676	40	4.04
TS08	8	61.26671	60.62435*	32	6.82
TS09	9	69.58409	68.39704*	43	10.67
TS10	10	76.49471	75.37894*	7	23.15
TS11	11	84.61446	83.22998*	155	28.33
TS12	12	91.67122	89.69699*	61	43.09
TS13	13	99.85158	97.84148*	230	54.41
TS14	14	106.78443	105.44099*	136	65.88
TS15	15	115.13250	111.26804*	8	91.15

Table 2.3: Instances with identical ellipses considered in [38].

product ab of the variable semi-axis lengths a and b of the elliptical container subject to the non-overlapping constraints (2.22)–(2.25) plus the fitting constraints (2.46)–(2.49) and (2.52)–(2.53). This model has $m(5m+1)/2$ constraints and $3m(m+3)/2+2$ variables. We have

Instance	m	Area reported in J. Kallrath and S. Rebennack [38]	Model $\mathcal{M}$		
			Area	# Local Minimizations	Avg. Time (s)
TE1.00	3	22.17171	22.17171	2	0.13
TE0.99	3	21.84169	21.84169	95	0.18
TE0.98	3	21.50833	21.50833	56	0.14
TE0.97	3	21.17669	21.17669	22	0.10
TE0.96	3	20.84672	20.84672	43	0.07
TE0.95	3	20.51837	20.51837	14	0.07
TE0.90	3	18.89960	18.89960	2	0.06
TE0.80	3	16.09992	16.09992	2	0.03
TE0.70	3	13.79909	13.79909	2	0.05
TE0.60	3	11.65005	11.65005	2	0.06
TE0.50	3	9.74384	9.74384	4	0.06
TE0.40	3	7.91654	7.91654	2	0.05
TE0.30	3	6.16566	6.16566	14	0.11
TE0.20	3	4.15789	4.15789	12	0.21
TE0.10	3	2.08193	2.08193	179	0.98

Table 2.4: Instances with three non-identical ellipses considered in [38].

considered only one instance where the ellipses to be packed have semi-axis lengths 2 and 1. Figure 2.8 illustrates the solution found by a single run of Algencan. This solution was found in 1h56m14s. The container has semi-axis lengths 19.136912 and 12.050124.

In all the experiments described in the present and the previous subsection, the local solver Algencan was run using its default parameters; while the optimality and feasibility tolerances $\varepsilon_{\text{feas}}$ and ε_{opt} (that are parameters that must be provided by the user) were both set to 10^{-8}. Those tolerances, related to the stopping criteria, are used to determine whether a solution to the optimization problem being solved has been found. See [13, pp. 116–117] for details. For the packing problems considered in the present work, independently of the stopping criterion satisfied by the optimizer, it is a relevant information the accuracy of the delivered solution in terms of (a) the fitting constraints and (b) the maximum overlapping between the ellipses being packed. Regarding the fitting constraints, once the multi-start process determines that a solution has been found with tolerances $\varepsilon_{\text{feas}} = \varepsilon_{\text{opt}} = 10^{-8}$, the optimization process is resumed with tighter tolerances in order to achieve a precision of the order of 10^{-14} in the sup-norm of the fitting constraints (2.60). Regarding the overlapping between the ellipses, in order to be able to deliver a measure that is independent of the model being solved, the approach introduced in [31] was considered. In particular, its C/C++ implementation (freely available at `https://github.com/chraibi/EEOver`) was used. The method is an exact method that is able to compute the intersection between ellipses and, for all the solutions reported here, overlapping between every pair of ellipses is always smaller than the machine precision 10^{-16}.

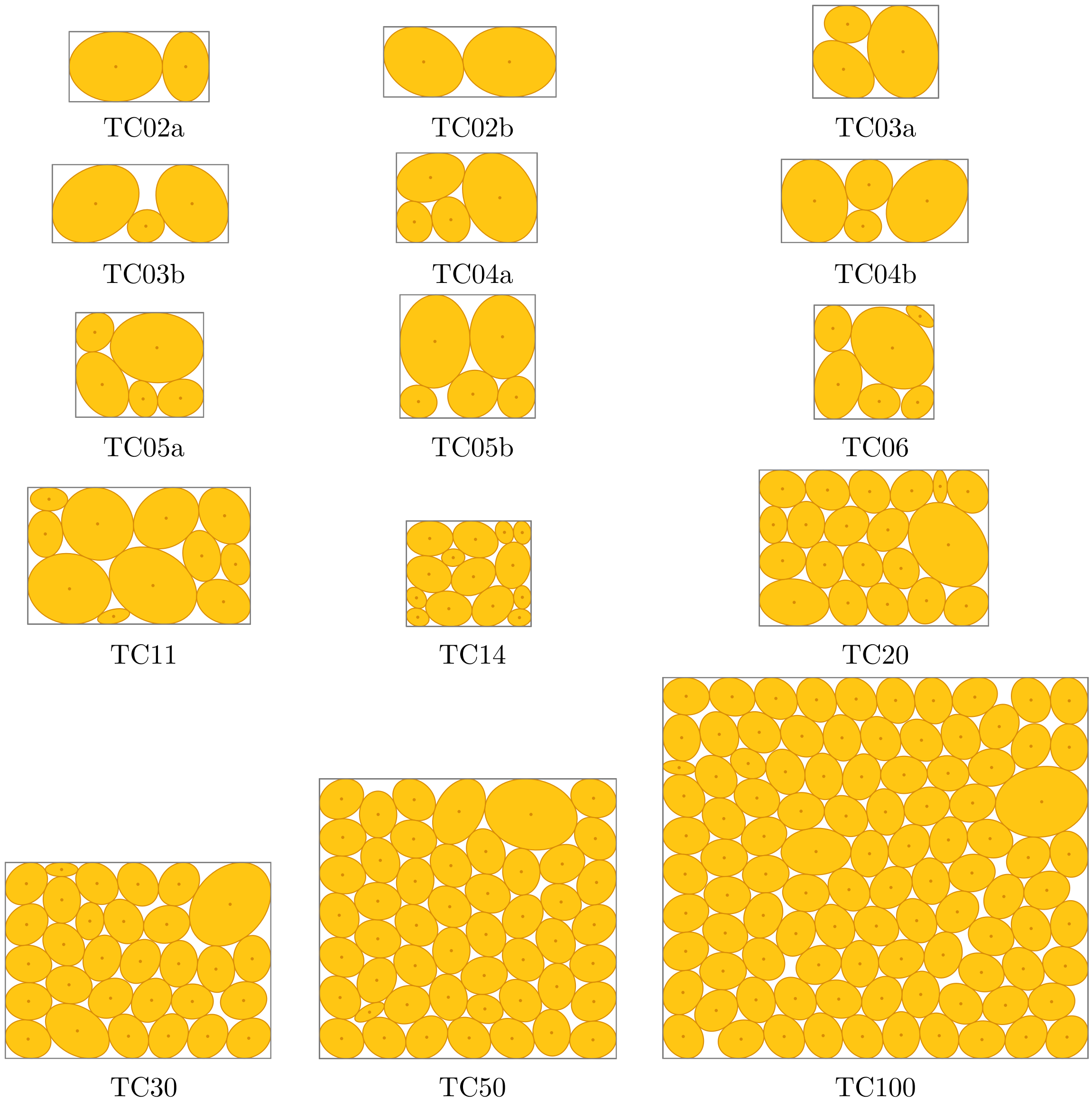


Figure 2.5: Illustrations of the solutions found for the instances with prefix TC.

2.4.2 Three-dimensional packing

In this section, we consider two problems of packing three-dimensional ellipsoids. The first problem is to pack a given set of m ellipsoids inside a ball with minimum volume. It can be modeled as the problem of minimizing the radius r of the ball subject to the non-overlapping constraints (2.22)–(2.25), where $P_i \in \mathbb{R}^{3\times3}$ is the diagonal matrix whose entries are the squared lengths of the semi-axes of the i-th ellipsoid for $i \in \{1, \ldots, m\}$ and ϵ_{ij} is given by (2.21) for $i, j \in \{1, \ldots, m\}$ such that $i < j$, plus the fitting constraints (2.46)–(2.50), where $S_i = r^{-2}P_i$ and

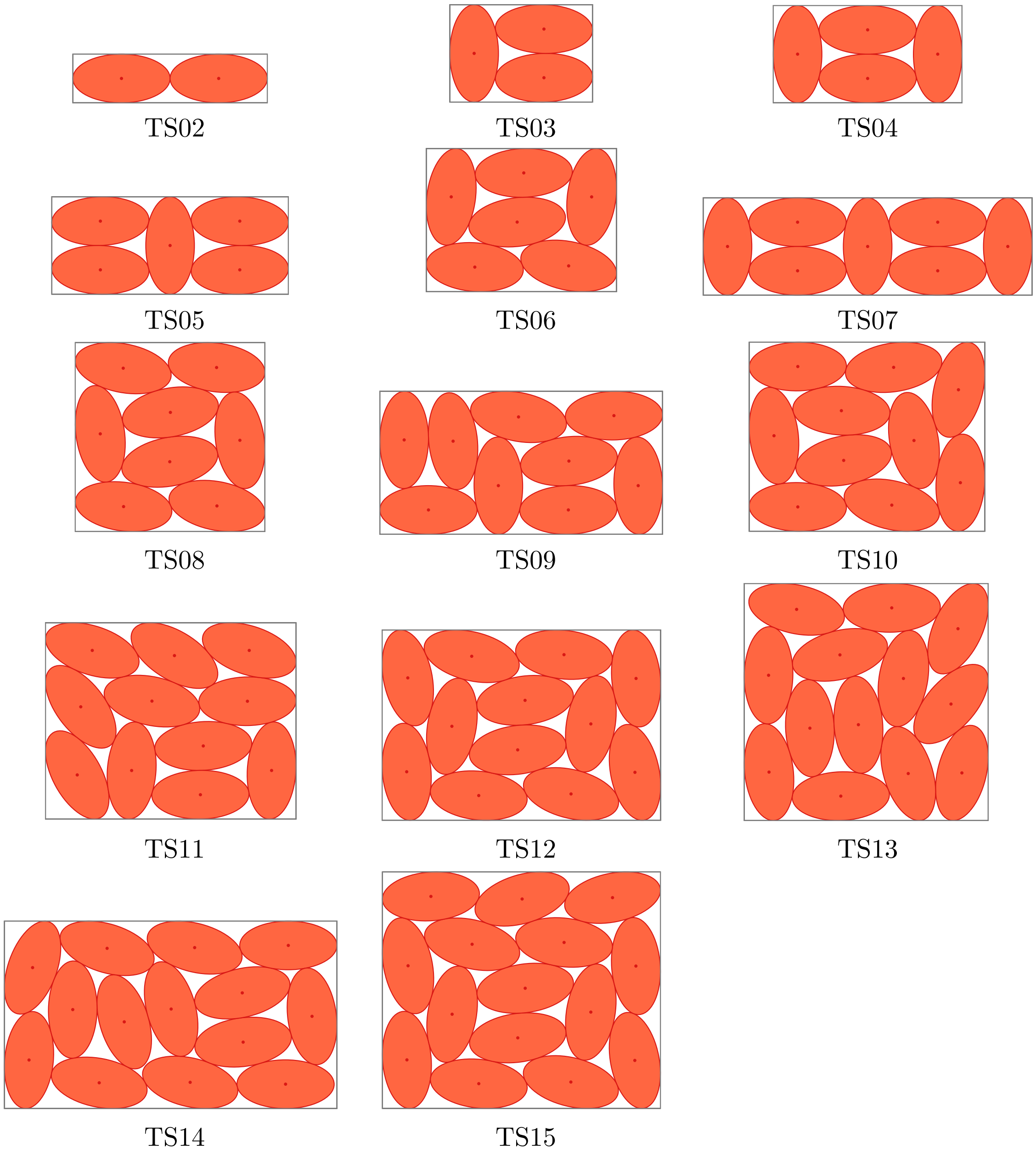


Figure 2.6: Illustrations of the solutions found for the instances with prefix TS.

$\lambda_{\max}(S_i) = r^{-2}\lambda_{\max}(P_i)$ for each $i \in \{1, \dots, m\}$. This problem has $3m^2+3m+1$ constraints and $2m^2+8m+1$ variables. The second problem is to pack a given set of m ellipsoids inside a cuboid with minimum volume. This problem can be modeled as the problem of minimizing the product of the variable length L, width W, and height H of the cuboid subject to the non-overlapping constraints (2.22)–(2.25) plus the fitting constraints. Assuming that the edges of the cuboid are

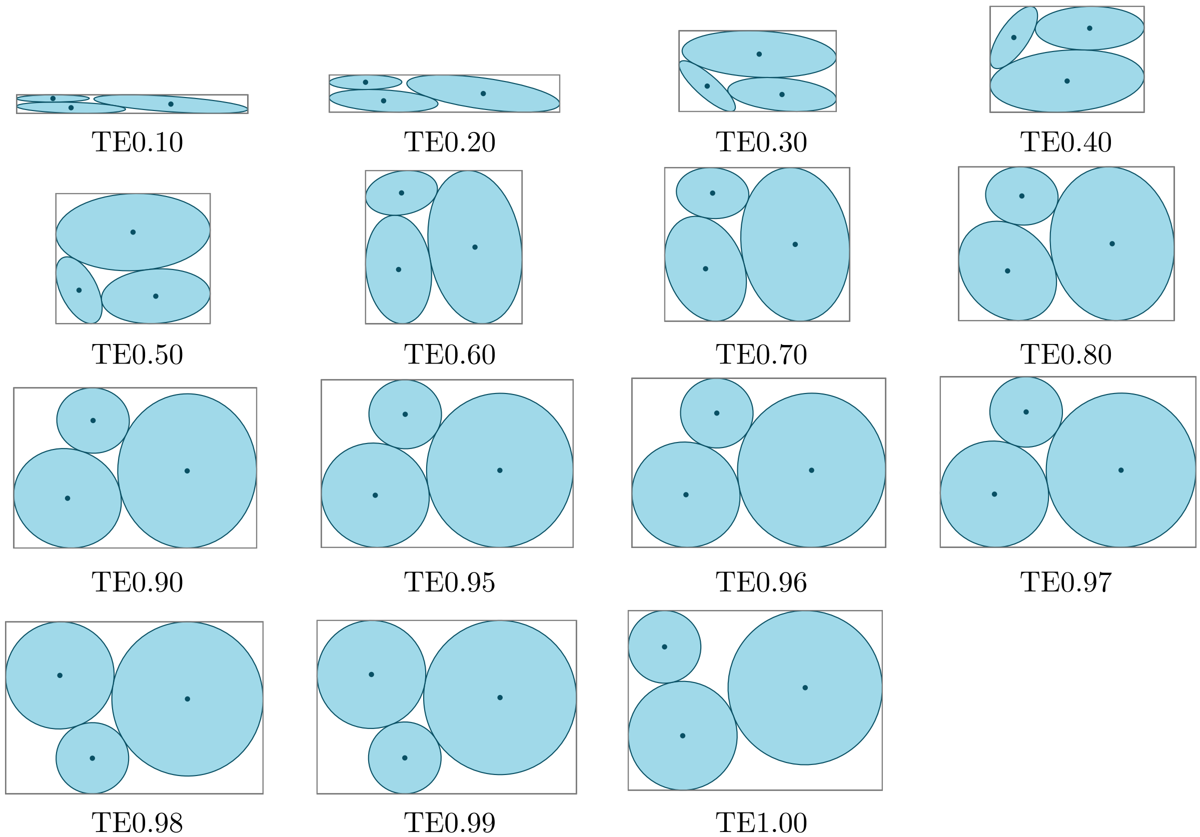


Figure 2.7: Illustrations of the solutions found for the instances with prefix TE.

parallel to the Cartesian axes, the fitting constraints are given by

$$\left(w_\ell^\top c_i - s_\ell\right)^2 \geq \|P_i^{\frac{1}{2}} Q_i^\top w_\ell\|_2^2 \quad \text{and} \quad w_\ell^\top c_i \leq s_\ell \quad \text{for} \quad i \in \{1,\dots,m\},\ \ell \in \{1,\dots,6\}, \tag{2.61}$$

where $w_1 = -w_2 = (1,0,0)^\top$, $w_3 = -w_4 = (0,1,0)^\top$, $w_5 = -w_6 = (0,0,1)^\top$, and

$$s_1 = s_2 = \frac{L}{2}, \quad s_3 = s_4 = \frac{W}{2}, \quad \text{and} \quad s_5 = s_6 = \frac{H}{2}.$$

This problem has $3m^2 + 9m$ constraints and $2m^2 + 4m + 3$ variables.

In our experiments, we have considered instances with $m \in \{10, 20, \dots, 100\}$ identical ellipsoids with semi-axis lengths $l_1 = 1$, $l_2 = 0.75$, and $l_3 = 0.5$. The initial solution we have used in our experiments is defined as follows. The ellipsoids are not rotated and their centers correspond to m points in the set $\{(\delta_1 l_1, \delta_2 l_2, \delta_3 l_3) \mid \delta_1, \delta_2, \delta_3 \in \mathbb{Z}\}$ that are closest to the origin. In this way, the ellipsoids do not overlap in the initial solution. The containers (ball and cuboid) in the initial solution are the smallest ones that contain the enclosing balls of each ellipsoid. Figure 2.9(a) illustrates the initial solution for the instance with $m = 50$. We have also

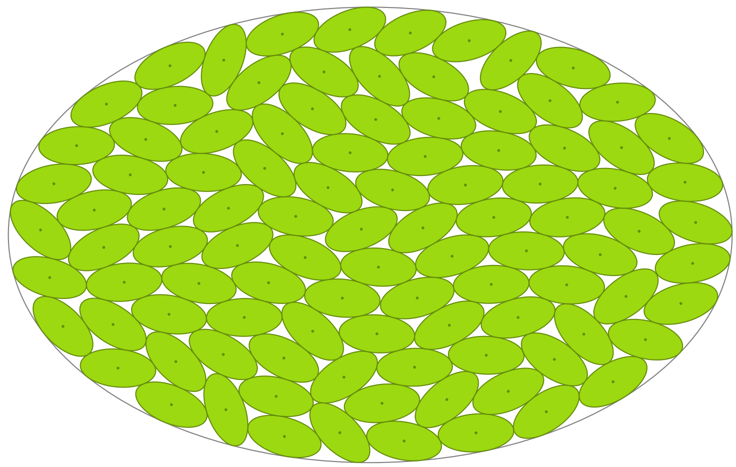
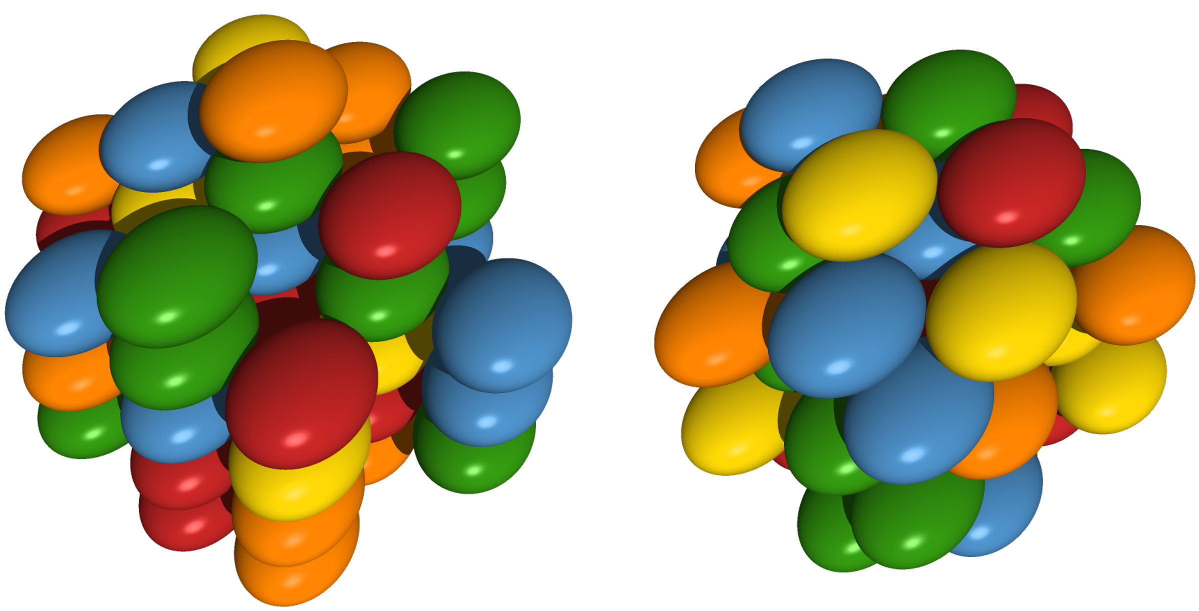


Figure 2.8: 100 ellipses with semi-axis lengths 2 and 1 inside a minimizing area ellipse with semi-axis lengths 19.136912 and 12.050124.

considered the initial solution where the centers of the ellipsoids belong to a generalisation of the hexagonal close-packing lattice for spheres. This initial solution is illustrated in Figure 2.9(b) for $m = 50$. These two types of initial solution produced similar results and we only show the results considering the first type.



(a) (b)

Figure 2.9: Initial solutions for $m = 50$.

Table 2.5 presents the results we have obtained for a single run of the local solver Algencan applied to each instance. In the table, the first column shows the number of ellipsoids. The second and third columns show the volume of the ball found and the CPU time, respectively. The fourth and fifth columns show the volume of the cuboid found and the CPU time, respectively. Figures 2.10 and 2.11 illustrate selected solutions for the problem of packing ellipsoids within a minimum volume ball and within a minimum volume cuboid, respectively.

m	Ball		Cuboid	
	Volume	Time	Volume	Time
10	23.80673	2s	28.59202	7s
20	48.58743	46s	53.44100	33s
30	75.40218	7m49s	77.76544	7m00s
40	101.58621	9m42s	101.44566	21m28s
50	122.76153	36m14s	127.20831	2h31m40s
60	145.26059	47m27s	152.05153	1h57m10s
70	171.22144	9h04m25s	175.10514	12h48m23s
80	192.62626	9h10m18s	198.85788	5h53m54s
90	214.63923	1d17h54m36s	223.17261	1d03h15m43s
100	242.49896	19h42m23s	245.27508	2d17h27m04s

Table 2.5: Results for the three-dimensional problem of minimizing the volume of the container (ball or cuboid) for an increasing number of ellipsoids $m \in \{10, 20, \ldots, 100\}$.

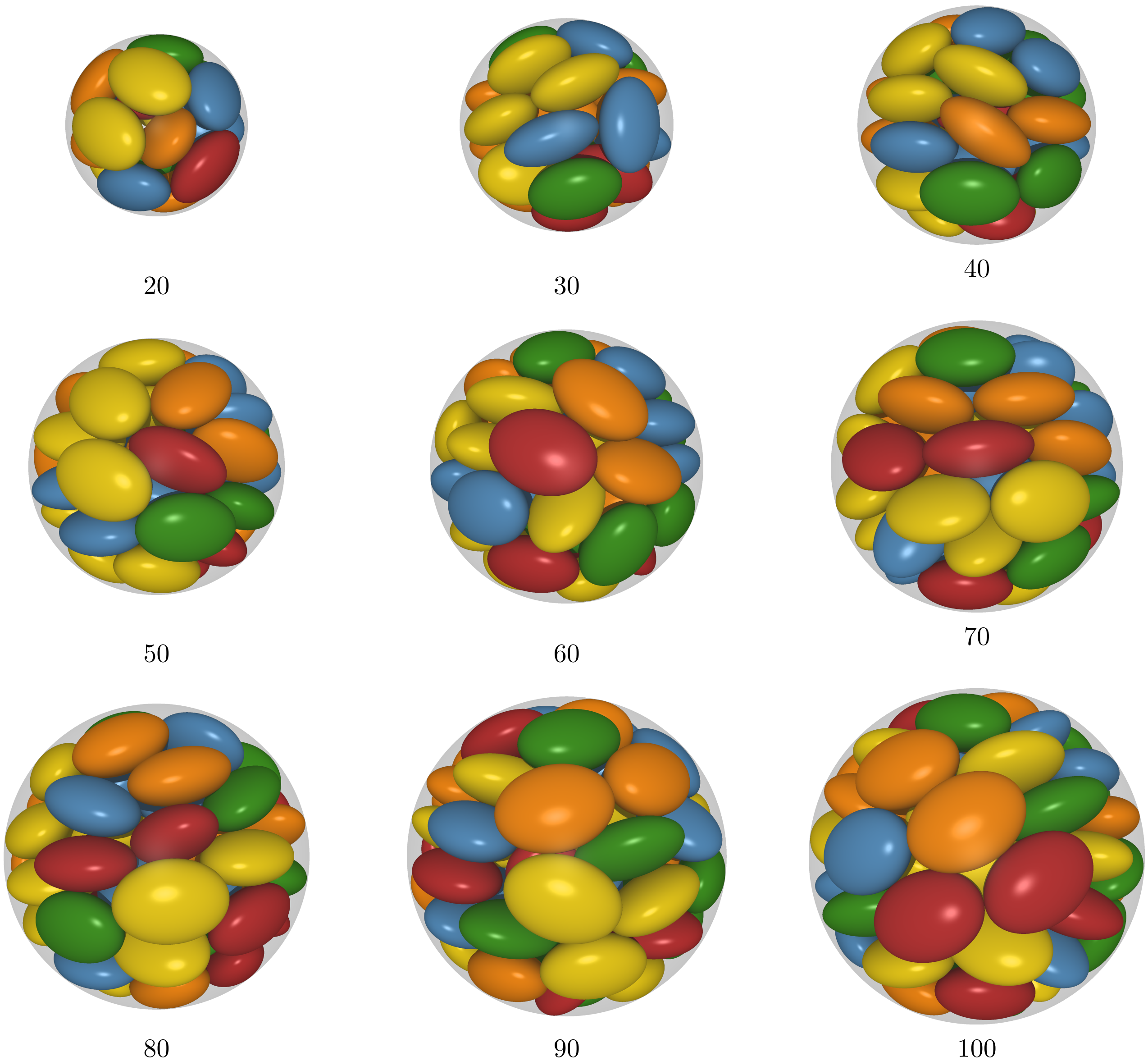


Figure 2.10: Illustration of the solutions obtained for the problem of packing ellipsoids within a ball of minimum volume.

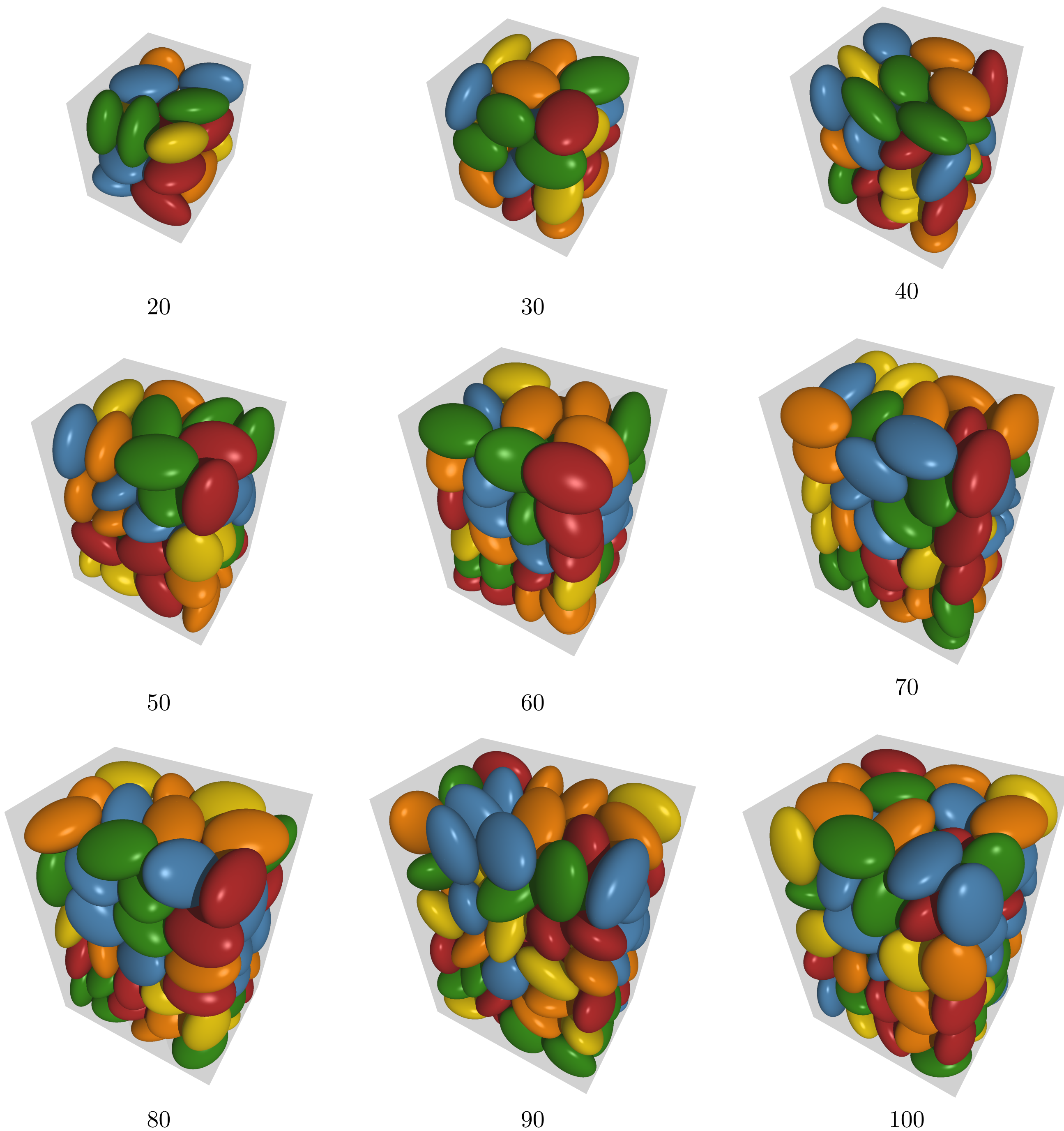


Figure 2.11: Illustration of the solutions obtained for the problem of packing ellipsoids within a cuboid of minimum volume.

Chapter 3

Model with implicit variables

The numbers of variables and constraints of the non-overlapping models presented in Sections 2.2.1 and 2.2.2 are quadratically proportional to the number of ellipsoids to be packed. Thus, when the number of ellipsoids is relatively high, these models become very hard to be numerically solved. In order to reduce the number of constraints, we will combine all constraints from the non-overlapping model (2.22)–(2.25) in one or more constraints. To reduce the number of variables, we will replace the variables x_{ij} and μ_{ij} from model (2.22)–(2.25) with functions that play the same roles as these variables.

3.1 Reduction of the number of constraints

Consider the non-overlapping model (2.22)–(2.25) presented in Section 2.2.1:

$$\begin{aligned}
x_{ij}^\top\big(P_i^{-\frac{1}{2}}Q_i^\top(c_i-c_j)-x_{ij}\big) &= \mu_{ij}, && \forall i,j\in I \text{ such that } i<j\\
\|P_i^{-\frac{1}{2}}Q_i^\top(c_i-c_j)-x_{ij}\|_2^2 &\geq 1, && \forall i,j\in I \text{ such that } i<j\\
P_i^{-\frac{1}{2}}Q_i^\top(c_i-c_j) &= x_{ij}+\mu_{ij}S_{ij}x_{ij}, && \forall i,j\in I \text{ such that } i<j\\
\mu_{ij} &\geq \epsilon_{ij}, && \forall i,j\in I \text{ such that } i<j.
\end{aligned}$$

By replacing each of the inequality constraints of this model with its squared infeasibility measure, we obtain the following model:

$$x_{ij}^\top\big(P_i^{-\frac{1}{2}}Q_i^\top(c_i-c_j)-x_{ij}\big)-\mu_{ij}=0, \quad \forall i,j\in I \text{ such that } i<j \tag{3.1}$$

$$\max\left\{0,1-\|P_i^{-\frac{1}{2}}Q_i^\top(c_i-c_j)-x_{ij}\|_2^2\right\}^2=0, \quad \forall i,j\in I \text{ such that } i<j \tag{3.2}$$

$$x_{ij}+\mu_{ij}S_{ij}x_{ij}-P_i^{-\frac{1}{2}}Q_i^\top(c_i-c_j)=0, \quad \forall i,j\in I \text{ such that } i<j \tag{3.3}$$

$$\max\big\{0,\epsilon_{ij}-\mu_{ij}\big\}^2=0, \quad \forall i,j\in I \text{ such that } i<j. \tag{3.4}$$

This model is equivalent to the model (2.22)–(2.25), in the sense that any solution to (3.1)–(3.4) is a solution to the model (2.22)–(2.25) and vice-versa.

For each $i, j \in I$ such that $i < j$, let the function $o_{ij} : \mathbb{R}^{3n+2q+1} \to \mathbb{R}_+$ be defined as

$$\begin{aligned} o_{ij}(c_i, c_j, \Omega_i, \Omega_j, x_{ij}, \mu_{ij}) = & \left(x_{ij}^\top \big(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - x_{ij}\big) - \mu_{ij} \right)^2 + \max\left\{0, \epsilon_{ij} - \mu_{ij}\right\}^2 \\ & + \|x_{ij} + \mu_{ij} S_{ij} x_{ij} - P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j)\|_2^2 + \max\left\{0, 1 - \|P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - x_{ij}\|_2^2\right\}^2 . \end{aligned} \tag{3.5}$$

Now, observe that the set of constraints (3.1)–(3.4) is equivalent to the constraints

$$o_{ij}(c_i, c_j, \Omega_i, \Omega_j, x_{ij}, \mu_{ij}) = 0, \quad \forall i, j \in I \text{ such that } i < j. \tag{3.6}$$

In order to obtain a model with a linear number of constraints, we can combine the constraints (3.6) in the following way

$$\sum_{j=i+1}^{m} o_{ij}(c_i, c_j, \Omega_i, \Omega_j, x_{ij}, \mu_{ij}) = 0, \quad \forall i \in I \setminus \{m\}, \tag{3.7}$$

or even combining them into a single constraint:

$$\sum_{i=1}^{m-1} \sum_{j=i+1}^{m} o_{ij}(c_i, c_j, \Omega_i, \Omega_j, x_{ij}, \mu_{ij}) = 0. \tag{3.8}$$

The constraints (3.7) (or the constraints (3.8)) are equivalent to the constraints (3.6). Therefore, we can replace the constraints (2.22)–(2.25) with constraints (3.7) (or constraint (3.8)) and obtain an equivalent model for the packing of ellipsoids.

Although this new model has a linear number of constraints that models the non-overlapping of ellipsoids, the total number of terms in the summations is quadratically proportional to the number of ellipsoids to be packed. Thus, the computational cost of evaluating the constraints (3.7) at a given point is practically the same as the cost of evaluating the constraints (2.22)–(2.25). In Section 3.3, we will see how to efficiently evaluate these constraints.

3.2 Reduction of the number of variables

Consider the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ with $i < j$ given by

$$\begin{aligned} \mathcal{E}_i &= \{x \in \mathbb{R}^n \mid (x - c_i)^\top Q_i P_i^{-1} Q_i^\top (x - c_i) \le 1\} \text{ and} \\ \mathcal{E}_j &= \{x \in \mathbb{R}^n \mid (x - c_j)^\top Q_j P_j^{-1} Q_j^\top (x - c_j) \le 1\}, \end{aligned}$$

where $c_i, c_j \in \mathbb{R}^n$, $Q_i, Q_j \in \mathbb{R}^{n\times n}$ are orthogonal matrices, and $P_i, P_j \in \mathbb{R}^{n\times n}$ are diagonal and positive definite matrices. Let $T_{ij} : \mathbb{R}^n \to \mathbb{R}^n$ be the linear transformation defined by

$$T_{ij}(x) = P_i^{-\frac{1}{2}} Q_i^\top (x - c_j). \tag{3.9}$$

Let $\mathcal{E}_i^{ij}$ and $\mathcal{E}_j^{ij}$ be the ellipsoids obtained when the transformation T_{ij} defined in (3.9) is applied to $\mathcal{E}_i$ and $\mathcal{E}_j$, respectively, i.e.,

$$\mathcal{E}_i^{ij} = \{x \in \mathbb{R}^n \mid [x - P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j)]^\top [x - P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j)] \le 1\}$$

and

$$\mathcal{E}_j^{ij} = \{x \in \mathbb{R}^n \mid x^\top S_{ij} x \le 1\},$$

where

$$S_{ij} = P_i^{\frac{1}{2}} Q_i^\top Q_j P_j^{-1} Q_j^\top Q_i P_i^{\frac{1}{2}}.$$

Thus, $\mathcal{E}_i^{ij}$ is a unitary radius ball centered at $y_{ij} \doteq P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j)$ and, since S_{ij} is positive definite, $\mathcal{E}_j^{ij}$ is an ellipsoid. By Lemma 3.1, we have that the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ overlap if and only if the ellipsoids $\mathcal{E}_i^{ij}$ and $\mathcal{E}_j^{ij}$ overlap. This lemma is similar to Lemma 2.1, but we present it here for completeness.

Lemma 3.1 *Consider the ellipsoids $\mathcal{E}_i, \mathcal{E}_j, \mathcal{E}_i^{ij}$ and $\mathcal{E}_j^{ij}$ defined above. Thus, the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ overlap if and only if the ellipsoids $\mathcal{E}_i^{ij}$ and $\mathcal{E}_j^{ij}$ overlap.*

Proof: For any $x \in \mathbb{R}^n$, we have

$$\begin{aligned}
(x - c_i)^\top Q_i P_i^{-1} Q_i^\top (x - c_i) &= (x - c_i)^\top Q_i P_i^{-\frac{1}{2}} P_i^{-\frac{1}{2}} Q_i^\top (x - c_i) \\
&= (x - c_i)^\top (P_i^{-\frac{1}{2}} Q_i^\top)^\top P_i^{-\frac{1}{2}} Q_i^\top (x - c_i) \\
&= [(x - c_j) - (c_i - c_j)]^\top (P_i^{-\frac{1}{2}} Q_i^\top)^\top P_i^{-\frac{1}{2}} Q_i^\top [(x - c_j) - (c_i - c_j)] \\
&= [P_i^{-\frac{1}{2}} Q_i^\top (x - c_j) - P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j)]^\top [P_i^{-\frac{1}{2}} Q_i^\top (x - c_j) - P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j)] \\
&= [T_{ij}(x) - P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j)]^\top [T_{ij}(x) - P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j)].
\end{aligned}$$

Therefore, we have that $x \in \operatorname{int}(\mathcal{E}_i)$ if and only if $T_{ij}(x) \in \operatorname{int}(\mathcal{E}_i^{ij})$. Furthermore,

$$\begin{aligned}
(x - c_j)^\top Q_j P_j^{-1} Q_j^\top (x - c_j) &= (x - c_j)^\top Q_i P_i^{-\frac{1}{2}} P_i^{\frac{1}{2}} Q_i^\top Q_j P_j^{-1} Q_j^\top Q_i P_i^{\frac{1}{2}} P_i^{-\frac{1}{2}} Q_i^\top (x - c_j) \\
&= (x - c_j)^\top Q_i P_i^{-\frac{1}{2}} S_{ij} P_i^{-\frac{1}{2}} Q_i^\top (x - c_j) \\
&= (x - c_j)^\top (P_i^{-\frac{1}{2}} Q_i^\top)^\top S_{ij} P_i^{-\frac{1}{2}} Q_i^\top (x - c_j) \\
&= [P_i^{-\frac{1}{2}} Q_i^\top (x - c_j)]^\top S_{ij} P_i^{-\frac{1}{2}} Q_i^\top (x - c_j) \\
&= T_{ij}(x)^\top S_{ij} T_{ij}(x).
\end{aligned}$$

Then, $x \in \operatorname{int}(\mathcal{E}_j)$ if and only if $T_{ij}(x) \in \operatorname{int}(\mathcal{E}_j^{ij})$. Hence, $\operatorname{int}(\mathcal{E}_i) \cap \operatorname{int}(\mathcal{E}_j) \neq \emptyset$ if and only if $\operatorname{int}(\mathcal{E}_i^{ij}) \cap \operatorname{int}(\mathcal{E}_j^{ij}) \neq \emptyset$. In other words, the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ overlap if and only if the ellipsoids $\mathcal{E}_i^{ij}$ and $\mathcal{E}_j^{ij}$ overlap. $\square$

Consider the constraint (3.7) and suppose that the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ do not overlap. In this case, we know that there are values for x_{ij} and μ_{ij} such that the term $o_{ij}(c_i, c_j, \Omega_i, \Omega_j, x_{ij}, \mu_{ij})$ as defined in (3.5) vanishes and, therefore, does not contribute to the summation in (3.7). We can just take x_{ij} as the projection of y_{ij} onto the ellipsoid $\mathcal{E}_j^{ij}$ and μ_{ij} as the nonnegative scalar that satisfies $y_{ij} = x_{ij} + \mu_{ij} S_{ij} x_{ij}$. The projection of y_{ij} onto the ellipsoid $\mathcal{E}_j^{ij}$ is the solution of the problem

$$\begin{array}{ll} \text{minimize} & \|x - y_{ij}\|_2^2 \\ \text{subject to} & x^\top S_{ij} x \leq 1. \end{array} \tag{3.10}$$

However, taking x_{ij} as the solution to the problem (3.10) does not lead to a good overlapping measure. If $y_{ij} \in \operatorname{int}(\mathcal{E}_j^{ij})$, then the solution to the problem (3.10) is y_{ij} and we must have $\mu_{ij} = 0$. Then, the term associated with the distance between y_{ij} and $\mathcal{E}_j^{ij}$ will be constant, as well as the term associated with the positivity of μ_{ij} in (3.7). Consider the following problem:

$$\begin{array}{ll} \text{minimize} & \|x - y_{ij}\|_2^2 \\ \text{subject to} & x^\top S_{ij} x = 1. \end{array} \tag{3.11}$$

If $y_{ij} \notin \operatorname{int}(\mathcal{E}_j^{ij})$, the problems (3.10) and (3.11) are equivalent and have a unique solution. Notice that the null vector is not a feasible solution to the problem (3.11). Thus, since the problem (3.11) has a single constraint and the matrix S_{ij} is positive definite, the gradient of the constraint is nonzero at every feasible point. Therefore, any solution to this problem satisfies the linear independence constraint qualification. This means that the Karush–Kuhn–Tucker optimality conditions of problem (3.11) (see, for example, the Proposition 3.3.1 in [5]) is satisfied by every solution to the problem (3.11). Thus, if x^* is a solution to this problem then there exists $\mu^* \in \mathbb{R}$ such that

$$x^* + \mu^* S_{ij} x^* - y_{ij} = 0. \tag{3.12}$$

If $y_{ij} \notin \operatorname{int}(\mathcal{E}_j^{ij})$ then, by Proposition 2.1, there exist a unique $x^* \in \partial\mathcal{E}_j^{ij}$ and a unique μ^* that satisfy (3.12). Moreover, $\mu^* \geq 0$. On the other hand, if $y_{ij} \in \operatorname{int}(\mathcal{E}_j^{ij})$ then the problem (3.11) may have more than one solution. But, by Proposition 3.1, the Lagrange multiplier associated with the constraint of this problem is the same for any solution and belongs to the interval $[-1/\lambda_{\max}(S_{ij}), 0]$.

Lemma 3.2 will be used in the proof of the Proposition 3.1, which shows that the Lagrange multiplier associated with the constraint of the problem (3.11) is the same for any solution to this problem. Lemma 3.2 is a particular case of Proposition 3.1.

Lemma 3.2 *Consider the ellipsoid $\mathcal{E} = \{z \in \mathbb{R}^n \mid z^\top D z \leq 1\}$, where $D \in \mathbb{R}^{n\times n}$ is diagonal and positive definite. Given $y \in \mathcal{E}$, there exists a unique $\alpha \in [-1/\lambda_{\max}(D), 0]$ and there exists $x \in \partial\mathcal{E}$ such that $y = x + \alpha D x$. Moreover, if $\alpha \in (-1/\lambda_{\max}(D), 0]$ then $x \in \partial\mathcal{E}$ is unique.*

Proof: Let $\mathcal{I} = \{1, \ldots, n\}$. For each $i \in \mathcal{I}$, denote the i-th diagonal element of matrix D by d_i. Consider the system

$$y_i = x_i + \alpha d_i x_i, \forall i \in I, \tag{3.13}$$

$$x^\top D x = 1, \tag{3.14}$$

$$\alpha \in [-1/\lambda_{\max}(D), 0]. \tag{3.15}$$

By Lemma 2.8, the system (3.13)–(3.15) has at least one solution. Suppose that (x^*, α^*) be a solution to this system and that $\alpha^* > -1/\lambda_{\max}(D)$. We shall prove that this is the only solution to this system. Notice that this is enough to prove the lemma.

Since $\alpha^* > -1/\lambda_{\max}(D)$, we have that

$$1 + \alpha^* d_i > 0, \forall i \in \mathcal{I}. \tag{3.16}$$

By (3.13), we have $y_i = (1 + \alpha^* d_i) x_i^*$ for each $i \in \mathcal{I}$. Then, (3.13) and (3.16) imply that, for each $i \in \mathcal{I}$, $x_i^* = 0$ if $y_i = 0$. However, since $x^* = 0$ does not satisfy (3.14), there must exist $i \in \mathcal{I}$ such that $y_i \neq 0$.

Since $1 + \alpha^* d_i > 0$ for each $i \in \mathcal{I}$, by (3.13) we have that

$$x_i^* = \frac{y_i}{1 + \alpha^* d_i}, \forall i \in \mathcal{I}. \tag{3.17}$$

In order to derive a contradiction, suppose that the system has a solution $(\bar{x}, \bar{\alpha}) \neq (x^*, \alpha^*)$. If $\bar{\alpha} = \alpha^*$, then $\bar{x} = x^*$ by (3.17). Thus, we must have $\bar{\alpha} \neq \alpha^*$. We shall divide the proof in the cases where $\bar{\alpha} > -1/\lambda_{\max}(D)$ and $\bar{\alpha} = -1/\lambda_{\max}(D)$.

Case 1. Suppose that $\bar{\alpha} > -1/\lambda_{\max}(D)$. Then, $1 + \bar{\alpha} d_i > 0$ for each $i \in \mathcal{I}$ and, therefore,

$$\bar{x}_i = \frac{y_i}{1 + \bar{\alpha} d_i}, \forall i \in \mathcal{I}.$$

By (3.14), we have that

$$1 = {x^*}^\top D x^* = \sum_{i=1}^n d_i (x_i^*)^2 = \sum_{i=1}^n d_i \frac{y_i^2}{(1 + \alpha^* d_i)^2}.$$

If $\bar{\alpha} < \alpha^*$, then $1 + \alpha^* d_i > 1 + \bar{\alpha} d_i > 0$ for each $i \in \mathcal{I}$ and

$$1 = \sum_{i=1}^n d_i \frac{y_i^2}{(1 + \alpha^* d_i)^2} < \sum_{i=1}^n d_i \frac{y_i^2}{(1 + \bar{\alpha} d_i)^2} = \sum_{i=1}^n d_i (\bar{x}_i)^2 = \bar{x}^\top D \bar{x}.$$

If $\bar{\alpha} > \alpha^*$, then $0 < 1 + \alpha^* d_i < 1 + \bar{\alpha} d_i$ for each $i \in \mathcal{I}$ and

$$1 = \sum_{i=1}^n d_i \frac{y_i^2}{(1 + \alpha^* d_i)^2} > \sum_{i=1}^n d_i \frac{y_i^2}{(1 + \bar{\alpha} d_i)^2} = \sum_{i=1}^n d_i (\bar{x}_i)^2 = \bar{x}^\top D \bar{x}.$$

In both cases we have that $\bar{x}^\top D \bar{x} \neq 1$ and, therefore, $(\bar{x}, \bar{\alpha})$ is not a solution to the system (3.13)–(3.15).

Case 2. Suppose that $\bar{\alpha} = -1/\lambda_{\max}(D)$. Let $\mathcal{I}^+ = \{ i \in \mathcal{I} \mid d_i = \lambda_{\max}(D) \}$ and $\mathcal{I}^- = \mathcal{I} \setminus \mathcal{I}^+$. By (3.13), we must have that $y_i = 0$ for each $i \in \mathcal{I}^+$, since $1 + \bar{\alpha} d_i = 0$ for each $i \in \mathcal{I}^+$. Thus, since $\alpha^* > -1/\lambda_{\max}(D)$, we must have that $x_i^* = 0$ for each $i \in \mathcal{I}^+$. Hence, since ${x^*}^\top D x^* = 1$, there exists $i \in \mathcal{I}^-$ such that $x_i^* \neq 0$ and, consequently, $y_i \neq 0$, since $y_i = (1 + \alpha^* d_i) x_i^*$. Since $1 + \bar{\alpha} d_i > 0$ for each $i \in \mathcal{I}^-$, by (3.13) we have that

$$\bar{x}_i = \frac{y_i}{1 + \bar{\alpha} d_i}, \forall i \in \mathcal{I}^-.$$

Therefore,

$$1 = x^{*\top} D x^* = \sum_{i \in \mathcal{I}} d_i (x_i^*)^2 = \sum_{i \in \mathcal{I}^-} d_i (x_i^*)^2 = \sum_{i \in \mathcal{I}^-} d_i \frac{y_i^2}{(1+\alpha^* d_i)^2} < \sum_{i \in \mathcal{I}^-} d_i \frac{y_i^2}{(1+\bar{\alpha} d_i)^2} = \sum_{i \in \mathcal{I}^-} d_i \bar{x}_i^2.$$

Thus,

$$\bar{x}^\top D \bar{x} = \sum_{i \in \mathcal{I}} d_i \bar{x}_i^2 \geq \sum_{i \in \mathcal{I}^-} d_i \bar{x}_i^2 > 1,$$

that is, $(\bar{x}, \bar{\alpha})$ is not a solution to the system (3.13)–(3.15).

Hence, (x^*, α^*) is the only solution to the system (3.13)–(3.15). □

Proposition 3.1 *Consider the ellipsoid $\mathcal{E} = \{z \in \mathbb{R}^n \mid z^\top S z \leq 1\}$, where $S \in \mathbb{R}^{n \times n}$ is a symmetric and definite positive matrix. Given $y \in \mathcal{E}$, there exists a unique $\alpha \in [-1/\lambda_{\max}(S), 0]$ and there exists $x \in \partial\mathcal{E}$ such that $y = x + \alpha S x$. Moreover, if $\alpha \in (-1/\lambda_{\max}(S), 0]$ then $x \in \partial\mathcal{E}$ is unique.*

Proof: By Proposition 2.8, there exist $x^* \in \partial\mathcal{E}$ and $\alpha^* \in [-1/\lambda_{\max}(S), 0]$ such that

$$y = x^* + \alpha^* S x^*. \tag{3.18}$$

Suppose that $\alpha^* \in (-1/\lambda_{\max}(S), 0]$. We shall prove that there do not exist $\bar{x} \in \partial\mathcal{E}$ and $\bar{\alpha} \in [-1/\lambda_{\max}(S), 0]$ such that $y = \bar{x} + \bar{\alpha} S \bar{x}$ and $(\bar{x}, \bar{\alpha}) \neq (x^*, \alpha^*)$. In order to derive a contradiction, suppose that there exist $\bar{x} \in \partial\mathcal{E}$ and $\bar{\alpha} \in [-1/\lambda_{\max}(S), 0]$ such that

$$y = \bar{x} + \bar{\alpha} S \bar{x} \tag{3.19}$$

and $(\bar{x}, \bar{\alpha}) \neq (x^*, \alpha^*)$.

Since S is symmetric, there exist an orthogonal matrix $Q \in \mathbb{R}^{n \times n}$ and a diagonal matrix $D \in \mathbb{R}^{n \times n}$ formed by the eigenvalues of S such that $S = QDQ^\top$ and $\lambda_{\max}(S) = \lambda_{\max}(D)$ (see, for example, Theorem 8.1.1 in [27]). Consider the ellipsoid $\mathcal{E}' = \{z \in \mathbb{R}^n \mid z^\top D z \leq 1\}$.

Then, $Q^\top y \in \mathcal{E}'$, $Q^\top x^* \in \partial\mathcal{E}'$, $Q^\top \bar{x} \in \partial\mathcal{E}'$. Moreover, since $\lambda_{\max}(S) = \lambda_{\max}(D)$, we have that $\alpha^* \in (-1/\lambda_{\max}(D), 0]$ and $\bar{\alpha} \in [-1/\lambda_{\max}(D), 0]$. By left multiplying both sides of equations (3.18) and (3.19) by Q, we obtain

$$Q^\top y = Q^\top x^* + \alpha^* D Q^\top x^* \tag{3.20}$$

and

$$Q^\top y = Q^\top \bar{x} + \bar{\alpha} D Q^\top \bar{x}. \tag{3.21}$$

By Lemma 3.2, if $\bar{\alpha} = \alpha^*$, we must have $Q^\top \bar{x} = Q^\top x^*$ and, consequently, $\bar{x} = x^*$, which contradicts the hypothesis that $(\bar{x}, \bar{\alpha}) \neq (x^*, \alpha^*)$. If $\bar{\alpha} \neq \alpha^*$, then (3.20) and (3.21) contradict Lemma 3.2.

Hence, if $\alpha^* \in (-1/\lambda_{\max}(S), 0]$, then the system

$$\begin{aligned} y &= x + \alpha S x, \\ x^\top S x &= 1, \\ \alpha &\in [-1/\lambda_{\max}(S), 0] \end{aligned}$$

has a unique solution. □

The equation (3.12) implies that

$$x^{*\top}(x^* + \mu^* S_{ij} x^* - y_{ij}) = 0.$$

Since $x^{*\top} S_{ij} x^* = 1$, this implies that

$$x^{*\top}(y_{ij} - x^*) - \mu^* = 0.$$

Therefore, since $y_{ij} = P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j)$, any solution x^* to the problem (3.11) together with the corresponding Lagrange multiplier μ^* satisfy

$$\begin{aligned} x^{*\top}\left(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - x^*\right) - \mu^* = 0 \\ x^* + \mu^* S_{ij} x^* - P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) = 0. \end{aligned}$$

Thus, if we take $\mathcal{X}_{ij}$ as a solution to the problem (3.11) and $\mathcal{U}_{ij}$ as the corresponding Lagrange multiplier, the constraints (3.7) become

$$\sum_{j=i+1}^{m} \max\left\{0, 1 - \|P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}_{ij}\|_2^2\right\}^2 + \max\left\{0, \epsilon_{ij} - \mathcal{U}_{ij}\right\}^2 = 0, \quad \forall i \in I \backslash \{m\}. \tag{3.22}$$

Thus, the variables x_{ij} and μ_{ij} cease to be part of the non-overlapping model. In (3.22), we define $\mathcal{X}_{ij}$ to be a function whose value is a solution to the problem (3.11) and $\mathcal{U}_{ij}$ is the function whose value is the Lagrange multiplier associated with the value of $\mathcal{X}_{ij}$.

3.3 Efficient evaluation of the constraints

The total number of terms presented in constraints (3.22) is $O(m^2)$. However, most of these terms do not need to be computed when the constraints are evaluated at a point that is almost feasible, that is, a point where most of the ellipsoids do not overlap each other. In a feasible solution, only a constant number of ellipsoids may touch a given ellipsoid. For example, suppose that the ellipsoids are identical balls. In the two-dimensional case, at most six balls can touch a given ball. In the three-dimensional case, this number is twelve. For identical ellipsoids, the number of ellipsoids that can touch a given one will depend on the eccentricities of these ellipsoids. Hence, in a (almost) feasible solution, only $O(m)$ terms need to be evaluated.

If the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ do not overlap, then the term associated with this pair of ellipsoids in the summation (3.22) is zero and need not be evaluated. A sufficient condition for the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ not to overlap is that their enclosing balls do not overlap. An enclosing ball of a set is a ball that contains that set. The minimal enclosing ball of $\mathcal{E}_i$ is the ball with radius $r_i = \lambda_{\max}(P_i^{\frac{1}{2}})$ centered at c_i. Therefore, if

$$\|c_i - c_j\|_2 \geq r_i + r_j$$

then the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ do not overlap. Let

$$R = \max_{i \in I} \{r_i\}.$$

Thus, every ellipsoid $\mathcal{E}_i$ is contained in a ball with radius R centered at c_i. Therefore, if

$$\|c_i - c_j\|_2 \geq 2R \tag{3.23}$$

then the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ do not overlap.

The method described here to identify the pairs of ellipsoids that do not meet the condition (3.23) has been used in other works, such as [18] and [43], to identify pairs of balls that may overlap. Let $l = 2R$ and consider a hypercube with edge length L that contains the container. This hypercube can be covered by $\lceil L/l \rceil^n$ hypercubes with edge lengths l whose interiors are mutually disjoint. We refer to each of these hypercubes with edge lengths l as a region. Two regions are adjacent if they share at least one vertex. Suppose that $\mathcal{E}_i$ and $\mathcal{E}_j$ have their centers in non-adjacent regions. In this case, since each region is a hypercube with edge length $2R$, we must have $\|c_i - c_j\|_2 \geq 2R$, that is, the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ do not overlap. Therefore, if two ellipsoids are in non-adjacent regions, they do not overlap. If two ellipsoids are in the same region or in adjacent regions, they may or may not overlap. Hence, considering all the terms that appear in the constraints (3.22), we can evaluate only those that are associated with ellipsoids that lie in the same region or in adjacent regions.

Each ellipsoid can be assigned to a region in constant time based on its center. The region of the ellipsoid $\mathcal{E}_i$ is defined as the tuple

$$(p([c_i]_1), \ldots, p([c_i]_n))$$

where

$$p(x) = \min\{\max\{1, \lfloor x/l \rfloor\}, N_{\text{reg}}\}$$

and $N_{\text{reg}} = \lceil L/l \rceil$. The method to determine which pairs of ellipsoids should be considered works as follows. First, an n-dimensional array with N_{reg} entries for each dimension is created. Each element of this array is associated with a region and stores a list with the indices of ellipsoids that belong to that region. This structure can be constructed in $O(m)$ time. Also, there is a list with the non-empty regions (regions that have at least one ellipsoid). This list is also constructed in $O(m)$ time. Then, for each non-empty region and for each ellipsoid $\mathcal{E}_i$ in that region, the term associated with the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ is computed for each ellipsoid $\mathcal{E}_j$ in that region and in adjacent regions. Considering the case where all the ellipsoids have approximately the same size, each region will contain only a constant number of ellipsoids in an almost feasible solution. In this case, this algorithm performs in $O(m)$ time.

3.4 Non-overlapping model

To make it clearer that x_{ij} and μ_{ij} are no longer variables of the model but functions of the centers and rotation angles of the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$, we shall rewrite (3.22) in the following way:

$$\begin{aligned}\sum_{j=i+1}^{m} \max\left\{0, 1 - \|P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)\|_2^2\right\}^2 + \\ \max\left\{0, \epsilon_{ij} - \mathcal{U}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)\right\}^2 = 0, \quad \forall i \in I \setminus \{m\}.\end{aligned} \tag{3.24}$$

The value of $\mathcal{X}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)$ is therefore a solution to the problem

$$\begin{array}{ll} \text{minimize} & \|x - y_{ij}\|_2^2 \\ \text{subject to} & x^\top S_{ij} x = 1 \end{array} \tag{3.25}$$

and $\mathcal{U}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)$ is the Lagrange multiplier associated with this solution.

This new non-overlapping model has $m - 1$ constraints given by (3.24) and its variables are the centers of the ellipsoids ($c_i \in \mathbb{R}^n$ for each $i \in \{1, \ldots, m\}$) and the rotation angles of the ellipsoids ($\Omega_i \in \mathbb{R}^q$ for each $i \in \{1, \ldots, m\}$). Therefore, this model has a linear number of variables and a linear number of constraints on the number of ellipsoids to be packed. The following lemma shows that the constraint (3.24) is indeed a non-overlapping model.

Lemma 3.3 *The function that defines the constraint (3.24) vanishes if and only if the ellipsoids do not overlap.*

Proof: Firstly, notice that the function is nonnegative at every point. Let $i, j \in \{1, \ldots, m\}$ be such that $i < j$. Suppose that the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ do not overlap. Thus, we have that the ellipsoids $\mathcal{E}_i^{ij}$ and $\mathcal{E}_j^{ij}$ do not overlap either. So, the distance from the center y_{ij} of the unitary radius ball $\mathcal{E}_i^{ij}$ to the ellipsoid $\mathcal{E}_j^{ij}$ is at least one. Since in this case $y_{ij} \notin \mathcal{E}_j^{ij}$, we have that $\mathcal{X}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)$ is the projection of y_{ij} onto the ellipsoid $\mathcal{E}_j^{ij}$. Therefore, recalling that $y_{ij} = P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j)$, we have

$$\|P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)\|_2 \geq 1.$$

Consequently, we have that

$$\max\left\{0, 1 - \|P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)\|_2^2\right\}^2 = 0.$$

Since $\mathcal{X}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)$ is the solution to the problem (3.11) and $\mathcal{U}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)$ is the Lagrange multiplier associated with this solution and satisfies (3.12), we have that $\mathcal{U}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j) \geq 0$ by Proposition 2.1. By Proposition 2.3, we have that $\mathcal{U}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j) \geq \epsilon_{ij}$. Therefore,

$$\max\left\{0, \epsilon_{ij} - \mathcal{U}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)\right\}^2 = 0.$$

Hence, if the ellipsoids do not overlap, the function that defines the constraint (3.24) takes the zero value.

Suppose that there exist two ellipsoids that overlap. Let $i, j \in \{1, \dots, m\}$ such that $i < j$ be the indices of those ellipsoids. Let y_{ij} be the center of the ball $\mathcal{E}_i^{ij}$, that is, $y_{ij} = P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j)$. Let us consider two cases. Suppose that $y_{ij} \notin \text{int}(\mathcal{E}_j^{ij})$. In this case, $\mathcal{X}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)$ is the projection of y_{ij} onto ellipsoid $\mathcal{E}_j^{ij}$. Since $\mathcal{E}_i$ and $\mathcal{E}_j$ overlap, we have that the ellipsoids $\mathcal{E}_i^{ij}$ and $\mathcal{E}_j^{ij}$ also overlap. Thus,

$$\|y_{ij} - \mathcal{X}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)\|_2 < 1.$$

Therefore,

$$\max\left\{0, 1 - \|P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)\|_2^2\right\}^2 > 0.$$

Now, suppose that $y_{ij} \in \text{int}(\mathcal{E}_j^{ij})$. Since $y_{ij} \in \text{int}(\mathcal{E}_j^{ij})$ and $\mathcal{X}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j) \in \partial \mathcal{E}_j^{ij}$, by (3.12) and by Proposition 2.2, we must have $\mathcal{U}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j) \leq 0$. Moreover, since $y_{ij} \neq \mathcal{X}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)$, we must have $\mathcal{U}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j) \neq 0$. Consequently, $\mathcal{U}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j) < 0$. Then,

$$\max\left\{0, \epsilon_{ij} - \mathcal{U}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)\right\}^2 > 0.$$

Therefore, if the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ overlap, the term in the summation in (3.24) corresponding to the indices i and j is positive. Hence, since each term in this summation is nonnegative, we have that the function takes a positive value if the ellipsoids overlap. □

The overlapping measure of two ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ is given by

$$\begin{aligned} f_{ij}(\mathcal{E}_i, \mathcal{E}_j) = \; & \max\left\{0, 1 - \|P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)\|_2^2\right\}^2 + \\ & \max\left\{0, \epsilon_{ij} - \mathcal{U}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)\right\}^2. \end{aligned} \tag{3.26}$$

This measure does not depend on the size of the ellipsoids as shown in the Lemma 3.4.

Definition 3.1 *Consider the set $\mathcal{E} \subseteq \mathbb{R}^n$. For each $\nu \in \mathbb{R}_{++}$, we define $\nu\mathcal{E} = \{\nu x \mid x \in \mathcal{E}\}$.*

Lemma 3.4 *The function defined in (3.26) is invariant with respect to the scaling of the ellipsoids. That is, $f_{ij}(\mathcal{E}_i, \mathcal{E}_j) = f_{ij}(\nu\mathcal{E}_i, \nu\mathcal{E}_j)$ for each $\nu \in \mathbb{R}_{++}$.*

Proof: Consider the ellipsoids $\mathcal{E}_i = \{x \in \mathbb{R}^n \mid (x - c_i)^\top Q_i P_i^{-1} Q_i^\top (x - c_i) \leq 1\}$ and $\mathcal{E}_j = \{x \in \mathbb{R}^n \mid (x - c_j)^\top Q_j P_j^{-1} Q_j^\top (x - c_j) \leq 1\}$. Let $\nu \in \mathbb{R}_{++}$. We have that

$$\begin{aligned} \nu\mathcal{E}_i &= \{\nu x \in \mathbb{R}^n \mid x \in \mathcal{E}_i\} \\ &= \{x \in \mathbb{R}^n \mid \nu^{-1} x \in \mathcal{E}_i\} \\ &= \left\{x \in \mathbb{R}^n \mid (\nu^{-1} x - c_i)^\top Q_i P_i^{-1} Q_i^\top (\nu^{-1} x - c_i) \leq 1\right\} \\ &= \left\{x \in \mathbb{R}^n \mid (x - \nu c_i)^\top Q_i (\nu^2 P_i)^{-1} Q_i^\top (x - \nu c_i) \leq 1\right\}. \end{aligned}$$

Analogously, we have that

$$\nu\mathcal{E}_j = \left\{ x \in \mathbb{R}^n \mid (x - \nu c_j)^\top Q_j (\nu^2 P_j)^{-1} Q_j^\top (x - \nu c_j) \leq 1 \right\}.$$

Notice that the constant ϵ_{ij} given by Proposition 2.3 for the pair of ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ is the same for the pair of ellipsoids $\nu\mathcal{E}_i$ and $\nu\mathcal{E}_j$, since

$$\begin{aligned}
\epsilon_{ij} &= \lambda_{\min}(P_i^{-1})\lambda_{\min}(P_i^{\frac{1}{2}})\lambda_{\min}(P_j)\lambda_{\min}(P_j^{-\frac{1}{2}}) \\
&= (\nu^{-2}\nu\nu^2\nu^{-1})\lambda_{\min}(P_i^{-1})\lambda_{\min}(P_i^{\frac{1}{2}})\lambda_{\min}(P_j)\lambda_{\min}(P_j^{-\frac{1}{2}}) \\
&= \nu^{-2}\lambda_{\min}(P_i^{-1})\nu\lambda_{\min}(P_i^{\frac{1}{2}})\nu^2\lambda_{\min}(P_j)\nu^{-1}\lambda_{\min}(P_j^{-\frac{1}{2}}) \\
&= \lambda_{\min}((\nu^2 P_i)^{-1})\lambda_{\min}((\nu^2 P_i)^{\frac{1}{2}})\lambda_{\min}(\nu^2 P_j)\lambda_{\min}((\nu^2 P_j)^{-\frac{1}{2}}).
\end{aligned}$$

Thus, we have that

$$\begin{aligned}
f_{ij}(\nu\mathcal{E}_i, \nu\mathcal{E}_j) = \; & \max\left\{0, 1 - \|(\nu^2 P_i)^{-\frac{1}{2}} Q_i^\top (\nu c_i - \nu c_j) - \mathcal{X}(\nu c_i, \nu c_j, \Omega_i, \Omega_j; \nu^2 P_i, \nu^2 P_j)\|_2^2 \right\}^2 + \\
& \max\left\{0, \epsilon_{ij} - \mathcal{U}(\nu c_i, \nu c_j, \Omega_i, \Omega_j; \nu^2 P_i, \nu^2 P_j)\right\}^2.
\end{aligned}$$

Let $(\nu\mathcal{E}_i)^{ij}$ be the set obtained by applying the transformation T_{ij} to the ellipsoid $\nu\mathcal{E}_i$, that is,

$$\begin{aligned}
(\nu\mathcal{E}_i)^{ij} &= \{x \in \mathbb{R}^n \mid x = T_{ij}(z), z \in \nu\mathcal{E}_i\} \\
&= \{x \in \mathbb{R}^n \mid x = (\nu^2 P_i)^{-\frac{1}{2}} Q_i^\top (z - \nu c_j), z \in \nu\mathcal{E}_i\} \\
&= \{x \in \mathbb{R}^n \mid z = Q_i (\nu^2 P_i)^{\frac{1}{2}} x + \nu c_j, z \in \nu\mathcal{E}_i\} \\
&= \{x \in \mathbb{R}^n \mid (Q_i(\nu^2 P_i)^{\frac{1}{2}} x + \nu c_j - \nu c_i)^\top Q_i (\nu^2 P_i)^{-1} Q_i^\top (Q_i (\nu^2 P_i)^{\frac{1}{2}} x + \nu c_j - \nu c_i) \leq 1\} \\
&= \{x \in \mathbb{R}^n \mid (\nu Q_i P_i^{\frac{1}{2}} x + \nu c_j - \nu c_i)^\top Q_i (\nu^2 P_i)^{-1} Q_i^\top (\nu Q_i P_i^{\frac{1}{2}} x + \nu c_j - \nu c_i) \leq 1\} \\
&= \{x \in \mathbb{R}^n \mid \nu[Q_i P_i^{\frac{1}{2}} x - (c_i - c_j)]^\top Q_i \nu^{-2} P_i^{-1} Q_i^\top \nu [Q_i P_i^{\frac{1}{2}} x - (c_i - c_j)] \leq 1\} \\
&= \{x \in \mathbb{R}^n \mid [Q_i P_i^{\frac{1}{2}} x - (c_i - c_j)]^\top Q_i P_i^{-1} Q_i^\top [Q_i P_i^{\frac{1}{2}} x - (c_i - c_j)] \leq 1\} \\
&= \{x \in \mathbb{R}^n \mid [x - P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j)]^\top P_i^{-\frac{1}{2}} Q_i^\top Q_i P_i^{-1} Q_i^\top Q_i P_i^{\frac{1}{2}} [x - P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j)] \leq 1\} \\
&= \{x \in \mathbb{R}^n \mid [x - P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j)]^\top [x - P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j)] \leq 1\} \\
&= \mathcal{E}_i^{ij}.
\end{aligned}$$

Thus, $(\nu\mathcal{E}_i)^{ij} = \mathcal{E}_i^{ij}$. Similarly, we obtain $(\nu\mathcal{E}_j)^{ij} = \mathcal{E}_j^{ij}$. Therefore, since $\mathcal{X}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)$ is a projection of the center of $\mathcal{E}_i^{ij}$ onto the frontier of $\mathcal{E}_j^{ij}$ and $\mathcal{X}(\nu c_i, \nu c_j, \Omega_i, \Omega_j; \nu^2 P_i, \nu^2 P_j)$ is a projection of the center of $(\nu\mathcal{E}_i)^{ij}$ onto the frontier of $(\nu\mathcal{E}_j)^{ij}$, $(\nu\mathcal{E}_i)^{ij} = \mathcal{E}_i^{ij}$ and $(\nu\mathcal{E}_j)^{ij} = \mathcal{E}_j^{ij}$ imply that

$$\mathcal{U}(\nu c_i, \nu c_j, \Omega_i, \Omega_j; \nu^2 P_i, \nu^2 P_j) = \mathcal{U}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)$$

by Proposition 3.2, and it is possible to take

$$\mathcal{X}(\nu c_i, \nu c_j, \Omega_i, \Omega_j; \nu^2 P_i, \nu^2 P_j) = \mathcal{X}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j).$$

Consequently,

$$\begin{aligned} f_{ij}(\nu\mathcal{E}_i, \nu\mathcal{E}_j) =\ & \max\left\{0, 1 - \|(\nu^2 P_i)^{-\frac{1}{2}} Q_i^\top(\nu c_i - \nu c_j) - \mathcal{X}(\nu c_i, \nu c_j, \Omega_i, \Omega_j; \nu^2 P_i, \nu^2 P_j)\|_2^2\right\}^2 + \\ & \max\left\{0, \epsilon_{ij} - \mathcal{U}(\nu c_i, \nu c_j, \Omega_i, \Omega_j; \nu^2 P_i, \nu^2 P_j)\right\}^2 \\ =\ & \max\left\{0, 1 - \|P_i^{-\frac{1}{2}} Q_i^\top(c_i - c_j) - \mathcal{X}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)\|_2^2\right\}^2 + \\ & \max\left\{0, \epsilon_{ij} - \mathcal{U}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)\right\}^2 \\ =\ & f_{ij}(\mathcal{E}_i, \mathcal{E}_j). \end{aligned}$$

□

We have defined $\mathcal{X}$ to be the function whose value is a solution to the problem (3.25) and $\mathcal{U}$ to be the function whose value is the Lagrange multiplier associated with that solution. Therefore, when solving the problem (3.25) in practice, it is important that the solver always returns the same solution when the same instance of the problem is solved multiple times. Let $y_{ij} \in \mathbb{R}^n$ and $S_{ij} \in \mathbb{R}^{n\times n}$ be a positive definite matrix. By Proposition 3.2, any solution to the problem (3.25) is associated with the same Lagrange multiplier. Therefore, no matter what optimal solution to the problem (3.25) is returned by the solver, $\mathcal{U}$ will behave like a function. However, this may not be the case for $\mathcal{X}$ and it will depend on the solver. If $y_{ij} \notin \operatorname{int}(\mathcal{E}_j^{ij})$ then the problem (3.25) has a unique solution. On the other hand, if $y_{ij} \in \operatorname{int}(\mathcal{E}_j^{ij})$ then the problem (3.25) may have multiple optimal solutions. In this case, the solver could return different solutions for the same problem in different executions. Figure 3.1 illustrates some cases where this problem has more than one solution. This picture shows an ellipse with semi-axis lengths a and b with $a > b$. The projection of the point y^1 onto the frontier of the ellipse is unique: the point x^1. However, for any point y^2 in the set $\{y \in \mathbb{R}^2 \mid b^2/a - a < y_1 < a - b^2/a, y_2 = 0\}$, there are two projections: $\bar{x}^2$ and $\underline{x}^2$. If the ellipse is a circle, that is, $a = b$, then every point in the frontier of the circle is a projection of the center of the circle onto the frontier. This undesirable behaviour can be avoided by using a deterministic algorithm for solving the problem (3.25). Also, $\mathcal{X}$ and $\mathcal{U}$ should be continuous and differentiable. These conditions, however, may not be easy to satisfy. Consider the example illustrated in Figure 3.2. In this picture, the points y^1 and y^2 are arbitrarily close. The point y^1 lies above the horizontal axis; while the point y^2 lies below the horizontal axis. Notice that the projection x^1 of y^1 onto the frontier of the ellipse is far from x^2, which is the projection of y^2 onto the frontier of the ellipse. The set of points c_i^{ij} where the problem (3.25) has multiple optimal solutions has zero measure so that it does not appear to be an issue in practice.

3.4.1 Evaluation of the overlapping measure

In order to evaluate the constraint (3.24) at a given point, we need to find the values of $\mathcal{X}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)$ and $\mathcal{U}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)$. As we have seen, if the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$

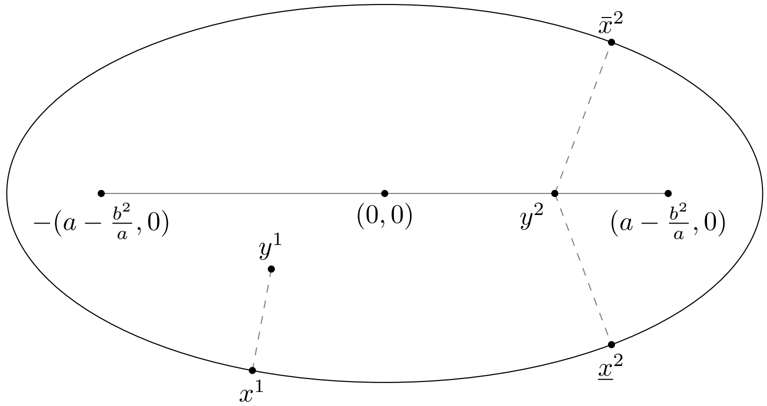


Figure 3.1: Projections of the points y^1 and y^2 onto the frontier of the ellipse.

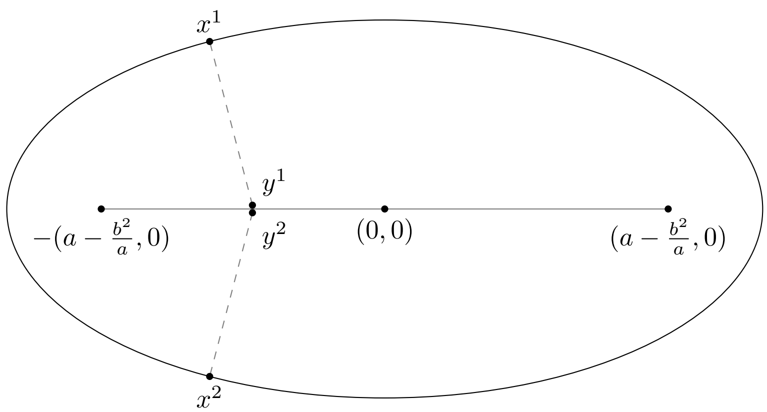


Figure 3.2: The points y^1 and y^2 can be arbitrarily close, but their projections x^1 and x^2 may be far from each other.

do not overlap, then the term associated with this pair of ellipsoids in the summation in (3.24) is zero. Thus, if we know that the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ do not overlap, then we do not need to evaluate the functions $\mathcal{X}$ and $\mathcal{U}$.

Suppose that we do not know whether the ellipsoids $\mathcal{E}_i$ and $\mathcal{E}_j$ overlap. In this case, we need to compute the values of $\mathcal{X}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)$ and $\mathcal{U}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)$. For this, we need to solve the problem

$$\begin{array}{ll} \text{minimize} & \frac{1}{2}\|x - y_{ij}\|_2^2 \\ \text{subject to} & x^\top S_{ij} x = 1, \end{array}$$

where $y_{ij} = P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j)$. By performing the change of variable $w = S_{ij}^{\frac{1}{2}} x$, this problem is equivalent to the problem

$$\begin{array}{ll} \text{minimize} & \frac{1}{2} w^\top S_{ij}^{-1} w - y_{ij}^\top S_{ij}^{-\frac{1}{2}} w \\ \text{subject to} & w^\top w = 1. \end{array} \tag{3.27}$$

The objective function of the problem (3.27) is a convex quadratic function and the feasible set is the frontier of the unitary radius ball centered at the origin. This problem can be solved by an algorithm proposed in [42]. Martínez [42] dealt with the problem of minimizing a quadratic function over the frontier of a ball, that is, a problem of the following form:

$$\begin{array}{ll} \text{minimize} & \frac{1}{2} w^\top G w + g^\top w \\ \text{subject to} & w^\top w = \Delta, \end{array} \tag{3.28}$$

where $G \in \mathbb{R}^{n \times n}$ is symmetric, $g \in \mathbb{R}^n$, and $\Delta \in \mathbb{R}_{++}$. In our case, we have $G = S_{ij}^{-1}$, $g = -y_{ij}^\top S_{ij}^{-\frac{1}{2}}$, and $\Delta = 1$.

3.5 Numerical experiments

In this section, we present some experiments to show that the non-overlapping model with implicit variables can be used to solve larger instances than the ones solved by the transformation based model presented in Section 2.2.1. Since the model introduced in this chapter can be solved faster, it opens the possibility for the use of a multi-start strategy to obtain better quality solutions. This strategy could not be applied with the original transformation based model for medium-sized instances due to the excessive amount of time spent to solve a single problem (a single local minimization of the problem of packing 100 three-dimensional ellipsoids within a minimum volume ball took 19h42m23s, as reported in Section 2.4.2, for example). The model with implicit variables, however, is not suitable for small-sized instances of problems, because of the overhead of evaluating the constraints (as described in Section 3.3) and solving the subproblems to compute the values of $\mathcal{X}_{ij}$ and $\mathcal{U}_{ij}$ (as seen in Section 3.4.1). For small-sized instances, the original transformation based model should be preferred. We have implemented both the two-dimensional and the three-dimensional non-overlapping models with implicit variables in Fortran 2003, as well as the optimization procedure. To solve the nonlinear programming problems, we used Algencan [2, 13] version 3.0.0. The models, the optimization procedure and Algencan were compiled with the GNU Fortran compiler (GCC) 4.7.2 with the

-O3 option enabled. The experiments were run on an Intel 2.4GHz Intel® Core™ i7-3770 with 16GB of RAM memory and Debian GNU/Linux 7.8 (Linux version 3.2.0-4-amd64) operating system.

3.5.1 Two-dimensional packing

In this section, we consider the problem of packing ellipses within a minimum area rectangle. We consider the instances with prefix TC, introduced by Kallrath and Rebennack [38], that were used in the experiments presented in Section 2.4.1.2. We considered the same multi-start strategy described in Section 2.4.1.2 and that uses the nonlinear programming solver Algencan. The algorithm stops when either the number of attempts to solve the problem reaches 1000 or 5 hours of CPU time are spent. The results are shown in Table 3.1. The first and second columns show the name of the instances and the number of ellipses, respectively. The next three columns show the results for the model $\mathcal{M}$ presented in Section 2.4.1.2; while the last three columns show the results for the model developed in this chapter. They show the area of the container, the number of local minimizations required to find the reported solution and the average time per local minimization. In the two-dimensional experiments presented Section 2.4.1, we checked the overlapping between every pair of ellipses in each solution. For this, we used the method introduced in [31] to compute the intersection area between the ellipses. We did the same for all the solutions reported here. The overlapping between every pair of ellipses is also always smaller than the machine precision 10^{-16}.

Instance	m	Model $\mathcal{M}$			Implicit variables model		
		Area	# Local Minimizations	Avg. Time (s)	Area	# Local Minimizations	Avg. Time (s)
TC02a	2	18.00000	1	0.03	18.00000	70	0.03
TC02b	2	22.23159	2	0.02	22.23146	777	0.04
TC03a	3	21.38577	2	0.04	21.38560	487	0.08
TC03b	3	25.22467	39	0.07	25.22444	733	0.09
TC04a	4	23.18708	2	0.11	23.18696	803	0.13
TC04b	4	28.54074	74	0.07	29.27856	851	0.12
TC05a	5	24.55368	43	0.15	24.55353	418	0.22
TC05b	5	30.64919	20	0.14	30.64913	337	0.23
TC06	6	25.08331	19	0.54	25.08320	640	0.43
TC11	11	55.91657	348	5.27	55.94734	220	1.01
TC14	14	24.17168	75	5.73	24.17342	500	2.87
TC20	20	65.70134	45	19.28	65.94474	353	4.31
TC30	30	95.61125	272	58.27	95.40195	919	9.58
TC50	50	152.69296	42	278.71	153.88090	215	33.83
TC100	100	297.70558	2	2790.77	297.14123	21	129.56

Table 3.1: Instances with non-identical ellipses considered in [38].

We also considered the problem of packing 500 identical ellipses with semi-axis lengths 2 and 1 within a minimum area rectangle. To solve this problem, we applied a multi-start strategy as follows. In the initial solution of the first iteration, the ellipses are not rotated and their centers are arranged in a generalisation of the hexagonal lattice for circles. For each of the subsequent iterations, the initial solution is given by a random perturbation of the previous solution. The centers and rotation angles of the ellipses are perturbed by at most 1%. We have imposed a time limit of 5 hours. Within this time interval, the best solution was found at the eighteenth iteration. The average time spent at each iteration was 16m40s. The area of the container is approximately 3533.65429, so the arrangement presents a density of approximately 0.88904. Figure 3.3 illustrates this solution.

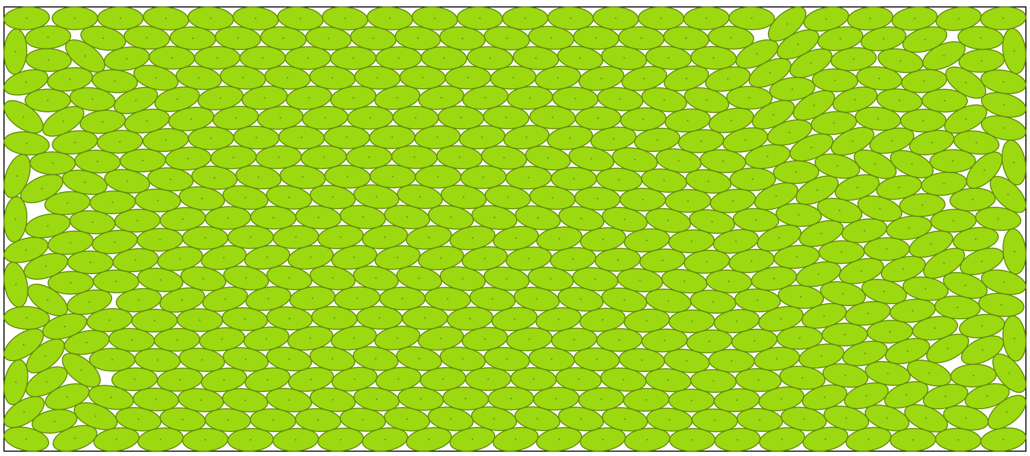


Figure 3.3: 500 ellipses with semi-axis lengths 2 and 1 inside a minimizing area rectangle with side lengths approximately 90.08609 and 39.22530.

3.5.2 Three-dimensional packing

In this section, we consider the problems of packing ellipsoids within a minimum volume ball and within a minimum volume cuboid. We have used some of the instances presented in Section 2.4.2, formed by $m \in \{50, \dots, 100\}$ identical ellipsoids with semi-axis lengths 1, 0.75, and 0.5. We have implemented a simple multi-start strategy. In the first iteration, the initial solution is the one used in the experiments presented in Section 2.4.2. For each of the subsequent iterations, the initial solution is given by a random perturbation of the last feasible solution found. The centers and rotation angles of the ellipsoids were perturbed by at most 10%. Tables 3.2 and 3.3 show a comparison between the transformation based non-overlapping model and the model with implicit variables. In Table 3.2 we have the results for the problem of packing ellipsoids within a minimum volume ball; while in Table 3.3 we present the results for the problem of packing ellipsoids within a minimum volume cuboid. The first column shows the number of ellipsoids. The second, third, and fourth columns are associated with the original transformation based non-overlapping model. The second column shows the volume of the container, the third column shows the density of the solution, and the fourth column shows the time spent to find the solution in a single local minimization. These results were presented in Section 2.4.2. The last four columns correspond to the model with implicit variables introduced in this chapter. The fifth column shows the volume of the container and the sixth column shows the density of the solution. The seventh column shows the number of local minimizations (multi-start iterations) required to find the best solution found and the last column shows the average time in seconds per local minimization. We have imposed a time limit of 5 hours for each instance. We can observe that the time spent in a single local minimization of the model with implicit variables is much smaller than the time spent in the original transformation based non-overlapping model. For example, a single local minimization of the problem of minimizing the volume of the ball took 19h42m23s for the original transformation based model, while for the model with implicit variables it took only 13m15s. The solutions for all instances were improved, except for the instance with $m = 100$ ellipsoids and minimization of the volume of the cuboid.

m	Transformation based model			Implicit variables model			
	Volume	Density	Time	Volume	Density	# Local Minimizations	Avg. Time
50	122.76153	0.63978	36m14s	120.04091	0.65428	26	4m01s
60	145.26059	0.64882	47m27s	143.45858	0.65697	38	5m26s
70	171.22144	0.64218	9h04m25s	166.81615	0.65914	15	8m49s
80	192.62626	0.65237	9h10m18s	189.94112	0.66159	34	8m51s
90	214.63923	0.65865	1d17h54m36s	212.94280	0.66390	26	11m31s
100	242.49896	0.64775	19h42m23s	237.81017	0.66053	23	13m15s

Table 3.2: Comparison between the transformation based model and the model with implicit variables for the problem of packing three-dimensional ellipsoids within a minimum volume ball.

m	Transformation based model			Implicit variables model			
	Volume	Density	Time	Volume	Density	# Local Minimizations	Avg. Time
50	127.20831	0.61741	2h31m40s	126.49258	0.62090	79	3m21s
60	152.05153	0.61984	1h57m10s	150.50514	0.62621	50	3m42s
70	175.10514	0.62794	12h48m23s	174.53424	0.63000	79	2m56s
80	198.85788	0.63193	5h53m54s	197.60740	0.63593	52	5m40s
90	223.17261	0.63346	1d03h15m43s	221.44723	0.63840	71	4m09s
100	245.27508	0.64042	2d17h27m04s	247.36635	0.63501	46	6m47s

Table 3.3: Comparison between the transformation based model and the model with implicit variables for the problem of packing three-dimensional ellipsoids within a minimum volume cuboid.

To end this section, we show the result of an experiment involving 500 identical ellipsoids with semi-axis lengths 1, 0.75, and 0.5. The problem is to minimize the volume of the ball. The solution illustrated in Figure 3.4 has a ball with radius approximately 6.53685, so this solution has a density of approximately 0.67126. It was found after 59 multi-start iterations, each iteration having spent 47m22s on average.

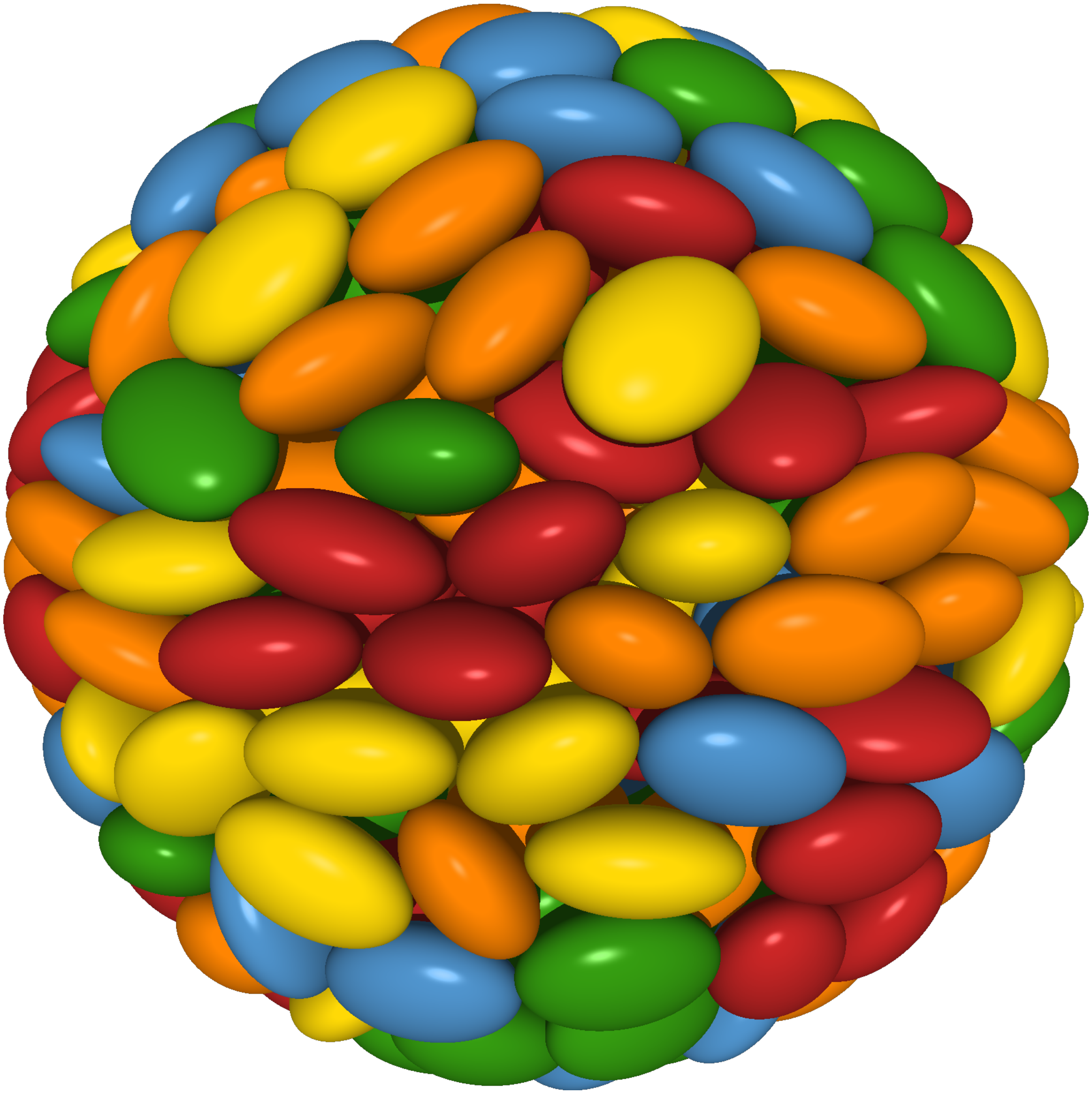


Figure 3.4: 500 three-dimensional ellipsoids with semi-axis lengths 1, 0.75, and 0.5 within a ball of radius approximately 6.53685.

Chapter 4

Large-scale packing problems

In Chapter 2, we proposed two non-overlapping models. Those models have quadratic numbers of variables and constraints, which make their use impractical from a computational point of view when the number of ellipsoids to be packed is large. To overcome this shortcoming, we proposed a model with a linear number of variables and constraints in Chapter 3. As we saw in Section 3.5, the implicit variables model can be used to solve larger problems. However, this model also has limitations on the number of ellipsoids to be packed. In this chapter, we deal with the problem of packing the largest possible number of ellipsoids inside a given container and present a different approach to solve large-scale problems.

In Section 4.1, we present a simple and general algorithm to solve this problem. In Section 4.2, we propose some strategies that can be used to compose the general algorithm. To deal with the case where the number of ellipsoids to be packed is large, we present what we call the isolation constraints in Section 4.3. These are additional constraints to the model to prevent large groups of ellipsoids from overlapping and thus reducing the total number of constraints of the model. Finally, we present some numerical experiments in Section 4.4.

4.1 Model algorithm

Briefly, the algorithm to pack ellipsoids inside a given container is as follows. At each iteration, a certain number of ellipsoids are packed within the container. Once these ellipsoids are packed, they are fixed in their positions (their centers and rotations are fixed). Then, a new group of ellipsoids is packed, so that they do not overlap each other and do not overlap the ellipsoids already fixed.

At the k-th iteration of the algorithm, let $\mathcal{N}_k$ be the set of indices of the new ellipsoids and let $\mathcal{F}_k$ be the set formed by the indices of the ellipsoids already packed and fixed in their positions. In order to pack the new ellipsoids, we must ensure that (i) they are arranged inside the container, (ii) do not overlap each other, and do not overlap the ellipsoids already fixed.

So, assuming the container is a ball of radius r and considering the models presented in Sections 2.2.1 and 2.3.1, at the k-th iteration of the algorithm, we must find a solution to the model

$$
\begin{aligned}
x_{ij}^\top\big(P_i^{-\frac{1}{2}}Q_i^\top(c_i-c_j)-x_{ij}\big) &= \mu_{ij}, && \forall i\in\mathcal{N}_k\cup\mathcal{F}_k, j\in\mathcal{N}_k \text{ such that } i<j\\
\|P_i^{-\frac{1}{2}}Q_i^\top(c_i-c_j)-x_{ij}\|_2^2 &\geq 1, && \forall i\in\mathcal{N}_k\cup\mathcal{F}_k, j\in\mathcal{N}_k \text{ such that } i<j\\
P_i^{-\frac{1}{2}}Q_i^\top(c_i-c_j) &= x_{ij}+\mu_{ij}S_{ij}x_{ij}, && \forall i\in\mathcal{N}_k\cup\mathcal{F}_k, j\in\mathcal{N}_k \text{ such that } i<j\\
\mu_{ij} &\geq \epsilon_{ij}, && \forall i\in\mathcal{N}_k\cup\mathcal{F}_k, j\in\mathcal{N}_k \text{ such that } i<j\\
P_i^{-\frac{1}{2}}Q_i^\top c_i &= \bar{x}_i+\frac{\alpha_i}{r^2}P_i\bar{x}_i, && \forall i\in\mathcal{N}_k\\
\frac{1}{r^2}\bar{x}_i^\top P_i\bar{x}_i &= 1, && \forall i\in\mathcal{N}_k\\
\|P_i^{-\frac{1}{2}}Q_i^\top c_i-\bar{x}_i\|_2^2 &\geq 1, && \forall i\in\mathcal{N}_k\\
\alpha_i &\leq \epsilon_i, && \forall i\in\mathcal{N}_k\\
\alpha_i &\geq -r^2/\lambda_{\max}(P_i), && \forall i\in\mathcal{N}_k.
\end{aligned}
$$

The variables of this model are $c_i, \bar{x}_i \in \mathbb{R}^n$, $Q_i \in \mathbb{R}^{n\times n}$ and $\alpha_i \in \mathbb{R}$ for each $i \in \mathcal{N}_k$, and $x_{ij} \in \mathbb{R}^n$ and $\mu_{ij} \in \mathbb{R}$ for each $i \in \mathcal{N}_k \cup \mathcal{F}_k$ and $j \in \mathcal{N}_k$ such that $i < j$. Notice that c_i and Q_i are constants for each $i \in \mathcal{F}_k$, since the ellipsoids in $\mathcal{F}_k$ have already been fixed.

4.2 Packing strategy

The algorithm described in the last section requires the new ellipsoids to be inside the container, not to overlap each other and not to overlap the ellipsoids already packed. However, it does not specify how the new ellipsoids should be packed. Since the goal is to pack as many ellipsoids as possible, the ellipsoids should stay tightly grouped within the container. An attempt to achieve this result is to minimize, in some sense, the height of the ellipsoid to be packed. The idea is that the new ellipsoids become in contact with other ellipsoids already packed, so that the ellipsoids are well packed inside the container. We define two types of heights for an ellipsoid. The upper height of an ellipsoid $\mathcal{E}$ is defined as $\max\{x_n \mid x \in \mathcal{E}\}$ and the lower height of an ellipsoid is defined as $\min\{x_n \mid x \in \mathcal{E}\}$. The computations of heights, however, are not easy. Since the goal is to minimize these heights, we need a simple way to model them. One way of doing this is to model the upper and lower heights of an ellipsoid by supporting hyperplanes. The idea is to consider hyperplanes that support the ellipsoid precisely at the points that realize the upper and lower heights.

Consider the half-space $\mathcal{S} = \{x \in \mathbb{R}^n \mid w^\top x \leq s\}$, where $w \in \mathbb{R}^n$ and $s \in \mathbb{R}$, and the ellipsoid $\mathcal{E}_i = \{x \in \mathbb{R}^n \mid (x-c_i)^\top Q_i P_i^{-1} Q_i^\top (x-c_i) \leq 1\}$, where $c_i \in \mathbb{R}^n$, $Q_i \in \mathbb{R}^{n\times n}$ is orthogonal and $P_i \in \mathbb{R}^{n\times n}$ is diagonal and positive definite. We saw in Section 2.3.2 that, in order to ensure that the ellipsoid be contained in the half-space $\mathcal{S}$, we can simply require the center of the ellipsoid to belong to that half-space and the distance between the center of the ball $\mathcal{E}_{ii}$ and the frontier of the half-space $\mathcal{S}_i$, obtained by transformation T_i defined in (2.4), be at least one. To ensure that $\partial\mathcal{S}$ supports the ellipsoid $\mathcal{E}_i$, we can just change the minimum distance condition and require it to be exactly one. Therefore, the conditions

$$\frac{\left(w^\top c_i - s\right)^2}{\|P_i^{\frac{1}{2}} Q_i^\top w\|_2^2} = 1 \quad \text{and} \quad w^\top c_i \le s \tag{4.1}$$

guarantee that the hyperplane $\partial\mathcal{S}$ supports the ellipsoid $\mathcal{E}_i$. Moreover, if we take $w = e_n$, the n-th standard basis vector, then $\partial\mathcal{S}$ will support the ellipsoid $\mathcal{E}_i$ at the point $\arg\max\left\{x_n \mid x \in \mathcal{E}_i\right\}$, and we will necessarily have $s = \max\left\{x_n \mid x \in \mathcal{E}_i\right\}$. If we take $w = -e_n$, then $\partial\mathcal{S}$ will support the ellipsoid $\mathcal{E}_i$ at the point $\arg\min\left\{x_n \mid x \in \mathcal{E}_i\right\}$, and we will have $s = -\min\left\{x_n \mid x \in \mathcal{E}_i\right\}$.

In order to minimize the upper height of the ellipsoid, we can then add the constraints (4.1) to the packing model, with $w = e_n$, and add the variable s, whose value should be minimized. Similarly, to minimize the lower height of the ellipsoid, we add the constraints (4.1) with $w = -e_n$ and minimize the value of $-s$.

As we will see in Section 4.4, experiments in the three-dimensional space show that the packed ellipsoid tends to have its semi-major axis parallel to the upper plane when its upper height is minimized (the ellipsoid is "standing"). But when the lower height is minimized, the tendency is that the semi-minor axis remains parallel to the upper plane (the ellipsoid is "lying"). To avoid this kind of behavior, which can result in poor quality solutions, we can consider the minimization of a convex combination of lower and upper heights. In this case, we add the following constraints to the model

$$\frac{\left(w^\top c_i - s_{\text{sup}}\right)^2}{\|P_i^{\frac{1}{2}} Q_i^\top w\|_2^2} = 1, \quad w^\top c_i \le s_{\text{sup}}, \quad \frac{\left(-w^\top c_i - s_{\text{inf}}\right)^2}{\|P_i^{\frac{1}{2}} Q_i^\top w\|_2^2} = 1 \quad \text{and} \quad -w^\top c_i \le s_{\text{inf}},$$

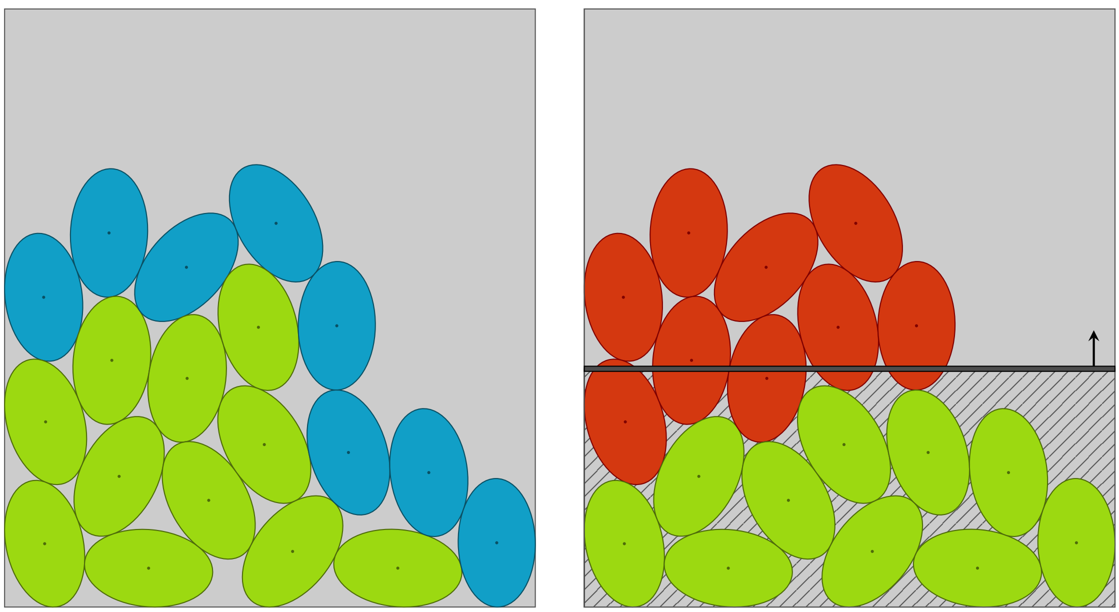
where $w = e_n$, and we minimize the value of $\xi s_{\text{sup}} - (1-\xi)s_{\text{inf}}$ for some constant $\xi \in [0,1]$. For $\xi = 1$, we have the minimization of the upper height of the ellipsoid being packed. For $\xi = 0$, we have the minimization of the lower height of the ellipsoid. For $\xi = \frac{1}{2}$, we have the minimization of $[c_i]_n$, the n-th component of the center of the ellipsoid.

4.3 The isolation constraints

In addition to ensuring that the new ellipsoids (to be packed) do not overlap each other, we have to make sure that these ellipsoids do not overlap the ellipsoids previously packed. Thus, the number of pairs of ellipsoids whose overlapping should be avoided grows as the number of previously packed ellipsoids increases. This makes the number of variables and constraints of each subproblem also increase, making each subproblem more and more difficult to be solved.

On the other hand, assuming that a sufficiently large number of ellipsoids has been packed, it is expected that there is no possibility for the new ellipsoids to be in contact with most of the fixed ellipsoids, since the latter should be surrounded by several other ellipsoids. Let $\mathcal{N}$ be the set of the new ellipsoids and $\mathcal{F}$ be the set formed by the ellipsoids already packed and that cannot touch the new ellipsoids in a feasible solution. By adding constraints to ensure that the ellipsoids in $\mathcal{N}$ are sufficiently distant from the ellipsoids in $\mathcal{F}$, we can remove the non-overlapping constraints between these two groups of ellipsoids. For this change in the model to have the desired effect (making the subproblems simpler), it is clear that the new constraints should be "easier" than the original non-overlapping constraints. By easy constraints we mean constraints that are smaller in number, defined by simpler functions and/or involve a small number of variables. We will call these new constraints the isolation constraints. We say that an ellipsoid is isolated if it is possible to easily infer that the isolation constraints ensure that the new ellipsoids not overlap the ellipsoid in question.

We present Figure 4.1 to illustrate the isolation of ellipsoids. Consider the packing of ellipses inside a rectangle. In Figure 4.1(a), it is shown some ellipses already packed inside the rectangle. Now consider the problem of packing a new ellipse. Due to the non-overlapping constraints, this new ellipse could touch only the blue ellipses. The set $\mathcal{F}$ is formed by the green ellipses in Figure 4.1(a). Now, consider the isolation constraint that requires the new ellipse to lie above the line illustrated in Figure 4.1(b). Thus, the green ellipses are isolated and the original non-overlapping constraints associated with these ellipses can be removed.



(a) (b)

Figure 4.1: Illustration of the isolation constraints. (a) Ellipses already packed and fixed in their positions. (b) The isolation constraint requires the new ellipse to be packed to lie above the highlighted line. Only the red ellipses are considered in the non-overlapping model.

Because of the simplicity of the isolation constraints, these constraints may isolate ellipsoids that could touch the new ellipsoids in a feasible solution (as it is the case for some green ellipses in Figure 4.1(b)). Anyway, it is important to point out that the isolation constraints ensure that the new ellipsoids do not overlap the isolated ellipsoids. Even if the isolation constraints are not able to isolate all ellipsoids of $\mathcal{F}$, the expectation is that most of these ellipsoids are isolated and the subproblems become to have very low numbers of constraints and variables.

4.4 Numerical experiments

In our numerical experiments, we considered the problem of packing the maximum number of three-dimensional ellipsoids within balls and cubes. We considered the non-overlapping model presented in Section 2.2.1. We implemented, in Fortran 90, the non-overlapping model (2.22)–(2.25), the model (2.46)–(2.50) for the inclusion of an ellipsoid in a ball, and the model described in Section 2.3.2 for the inclusion of an ellipsoid in a cube. We also implemented in Fortran 90 the optimization procedure described in Section 4. To solve the nonlinear programming problems, we used Algencan [2, 13] version 2.5.0. The models, the optimization procedure and Algencan were compiled with the GNU Fortran compiler (GCC) 4.7.2 with the `-O3` option enabled. The tests were run on an Intel 2.4GHz Intel® Core™ i7-3770 with 16GB of RAM memory and Linux operating system.

In our experiments, we considered three types of isolation constraints. The first one constrains the new ellipsoids to remain within a certain cylinder of infinite height. The second one requires the new ellipsoids to lie inside a box of infinite height. Actually, these constraints require the (x, y) coordinates of the centers of the new ellipsoids to lie within a circle and a box, respectively. The third type of isolation constraint requires the new ellipsoids to lie above a certain plane parallel to the plane x-y. The latter type of isolation constraint will be used together with one of the first two isolation constraints.

The isolation constraints depend on some parameters. The first type of isolation constraint depends on the choice of a value for the radius of the base of the cylinder. For the second kind of isolation constraint, we must choose the lengths of the sides of the base of the box. As for the third type, we need to decide at which point the plane must pass through. Ideally, the presence of isolation constraints should not affect the quality of the solution. Thus, we need to determine what would be good parameters for those constraints.

To assess the influence of these parameters on the quality of the solution, we considered the packing of ellipsoids with semi-axis lengths 0.67, 0.67 and 0.3465 withing a cube with side length 10. The ellipsoids are packed one by one ($\mathcal{N}_k = 1$ for each iteration k), minimizing the average of the upper and lower heights, according to the procedure described in Section 4. In the first experiment, we considered the isolation constraints given by a cylinder and a plane. Let a be the greatest length of a semi-axis among the ellipsoids already packed and the new ellipsoid. (In our case we have $a = 0.67$.) For the cylinder base radius, we take the values $2a$, $3a$, and $4a$. The initial position of the new ellipsoid to be packed is defined as follows. First, we choose the (x, y) coordinates of the center c of the cylinder uniformly random over the base of the cube. Let us denote by a_i the length of the semi-major axis of the i-th ellipsoid. Let j be the index of the new ellipsoid to be packed. As the new ellipsoid must have its center within the cylinder, any ellipsoid i such that

$$\|[c_i]_{1:2} - [c]_{1:2}\|_2 \geq r + a_i + a_j \tag{4.2}$$

will have no chance to overlap the ellipsoid j. Thus, the ellipsoid i can be removed from the non-overlapping model. For the ellipsoids whose condition (4.2) is not met, the non-overlapping constraints remain in the model. Let h be the maximum upper height among the packed ellipsoids whose condition (4.2) is not satisfied. (If there is no such ellipsoid, we take $h = -\infty$).

The height of the plane will be defined with respect to h. We consider the values $h-3a$, $h-4a$, and $h-5a$ for the plane height, i.e., the new ellipsoid should belong to the half-space

$$\mathcal{H} = \left\{ x \in \mathbb{R}^3 \mid w^\top x \geq s \right\},$$

where $w = (0,0,1)^\top$ and s takes some value in the set $\{h-3a, h-4a, h-5a\}$. Now, we are ready to set the starting position of the new ellipsoid. The (x, y) coordinates of the center of the new ellipsoid will be equal to the coordinates of the center of the cylinder, and the z coordinate will be equal to $h+2a$. The initial rotation angles are chosen uniformly randomly in the interval $[-\pi, \pi]$. Once the initial point has been set, we solve the problem defined by the non-overlapping and containment models using Algencan. If Algencan does not find a solution to the problem, we define a new cylinder and a new plane according to the method described earlier and try to solve the problem again. For each ellipsoid to be packed, we try to solve the problem of packing it up to 100 times. If this number of attempts is reached and the ellipsoid has not been packed, the optimization procedure is completed and the solution with the ellipsoids previously packed is returned.

In Table 4.1, we show the results we have obtained. N refers to the maximum number of packed ellipsoids, the next column shows the time elapsed until the N-th ellipsoid is packed, column A_c shows the amount of times the cylinder constraint was active at the solution, and column A_p shows the number of times that the plane constraint was active at the solution.

		Plane height											
		$h-3a$				$h-4a$				$h-5a$			
		N	Time	A_c	A_p	N	Time	A_c	A_p	N	Time	A_c	A_p
Cylinder radius	$2a$	844	23m31s	153	56	843	32m52s	169	17	858	51m43s	145	0
	$3a$	855	36m40s	15	59	870	1h7m45s	24	11	869	1h32m43s	23	0
	$4a$	839	45m32s	3	100	877	1h41m53s	3	12	879	2h38m40s	0	1

Table 4.1: Results obtained considering the isolation constraints defined by a cylinder and a plane, and minimizing the average of the upper and lower heights of the ellipsoid.

We can observe that as the radius of the cylinder increases and the plane height decreases, the quality of the solution is improved. The combination that produced the best result was considering the cylinder radius equal to $4a$ and the plane height equal to $h-5a$. For these parameters, we found that the isolation constraints have had little influence on the quality of the solution found, given that the plane constraint was active at a single solution and the cylinder constraint was never active.

In Table 4.2, we show the results obtained considering the box constraint instead of the cylinder constraint. In order to compare the cylinder and the box constraints, we considered square boxes with the same areas as the areas of the cylinder considered in the previous experiment. In this table, A_c refers to the number of times that the box constraint was active at a solution.

Only in two cases the solution obtained was better than the one obtained considering the cylinder constraint (namely, in the case where box side length was equal to $3a\sqrt{\pi}$ and the plane height equal to $h-3a$ and equal to $h-5a$). The best solution presented in Table 4.2 has 873 ellipsoids packed, whereas the best solution presented in Table 4.1 has 879 ellipsoids packed.

	Plane height												
	$h-3a$				$h-4a$				$h-5a$				
Box side length	N	Time	A_c	A_p	N	Time	A_c	A_p	N	Tempo	A_c	A_p	
$2a\sqrt{\pi}$	757	21m14s	221	120	833	36m8s	237	29	856	54m18s	185	2	
$3a\sqrt{\pi}$	860	37m6s	40	61	863	1h18m45s	51	20	873	1h26m12s	46	1	
$4a\sqrt{\pi}$	804	39m57s	14	130	869	1h39m8s	9	19	872	2h21m30s	15	4	

Table 4.2: Results obtained considering isolation constraints given by a box and a plane, and minimizing the average of the upper and lower heights of the ellipsoid.

In a third experiment, we evaluated the minimization of the heights of the ellipsoid to be packed. We considered two types of isolation constraints: one given by a cylinder with radius $4a$ and another one given by a box with side length $4a\sqrt{\pi}$. Both of them were employed together with a plane constraint with height $h-5a$, as described earlier. In Table 4.3, we present the results. We can observe that the quality of the solutions is much lower than those found in previous experiments in which the average of the upper and lower heights were minimized.

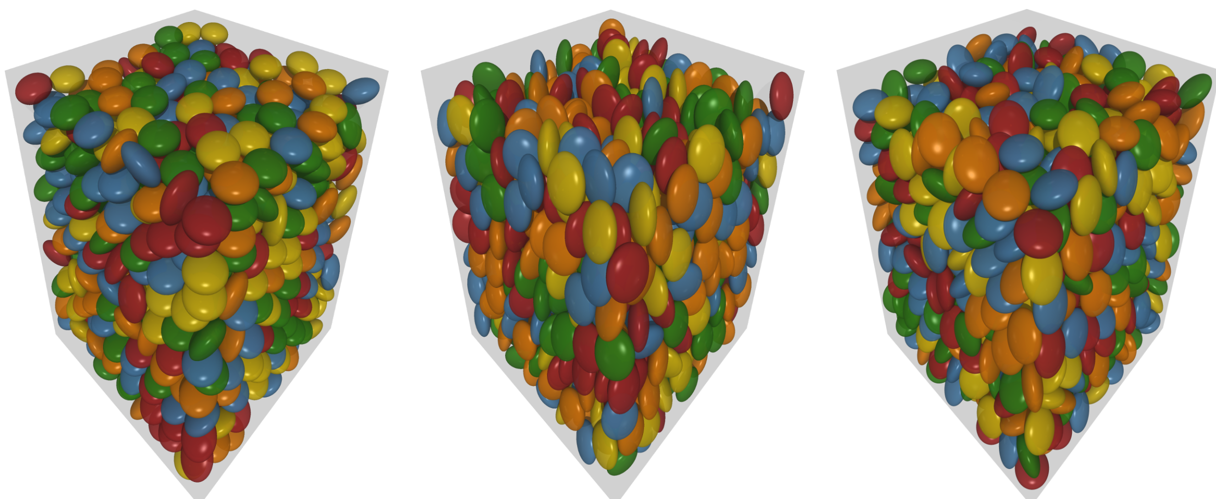
Minimization of the upper height				Minimization of the lower height			
Box and plane		Cylinder and plane		Box and plane		Cylinder and plane	
N	Time	N	Time	N	Time	N	Time
830	1h4m30s	833	59m0s	835	1h52m45s	828	1h40m37s

Table 4.3: Comparison between the minimization of the upper and lower heights of the ellipsoid being packed. The relative height of the plane is $-5a$, the length of the side of the box is $4a\sqrt{\pi}$, and the cylinder radius is $4a$.

In Figure 4.2, we show the graphical representations of the solutions obtained considering the isolation constraints given by by a cylinder with radius $4a$ and a plane with height $h-5a$. Figure 4.2(a) represents the solution obtained by minimizing the upper height of the ellipsoid to be packed. In this case, 833 were were packed. We can notice that the semi-minor axis of the ellipsoids tends to be almost perpendicular to the base of the cube (the ellipsoids are almost "lying"). In the Figure 4.2(b) we have the solution with 828 ellipsoids obtained by minimizing the lower height of the ellipsoid. We observe in this case another trend: the ellipsoids have their semi-major axes nearly perpendicular to base of the cube (the ellipsoids are almost "standing"). Figure 4.2(c) shows the solution with 879 ellipsoids found by minimizing the average of the upper and lower heights (which is the minimization of the third component of the center of the ellipsoid). Contrary to what occurred in the first two cases, we cannot notice any positioning trend of the ellipsoids. They are positioned in a more varied way (they are "messier"), which should have contributed in getting a higher quality solution.

Figure 4.3 shows the packing of 14541 ellipsoids with semi-axis lengths $(0.67, 0.67, 0.3465)$ within a cube with side length 25 using isolation constraints given by a cylinder with radius $4a$ and a plane with height $h-5a$. This solution was found in 5d5h46m3s.

Figure 4.4 shows the packing of 7649 ellipsoids with semi-axis lengths $(0.67, 0.67, 0.3465)$ within a ball of radius 12.75 using isolation constraints given by a cylinder with radius $4a$ and a plane with height $h-4a$. This solution was found in 4d8h54m7s.



(a) (b) (c)

Figure 4.2: Packing of ellipsoids with semi-axis lengths $(0.67, 0.67, 0.3465)$ within a cube with side length 10 using isolation constraints given by a cylinder with radius $4a$ and a plane with height $h - 5a$. (a) 833 ellipsoids obtained by minimizing the upper height of the ellipsoids. (b) 828 ellipsoids obtained by minimizing the lower height. (c) 879 ellipsoids obtained by minimizing the average of the lower and upper heights.

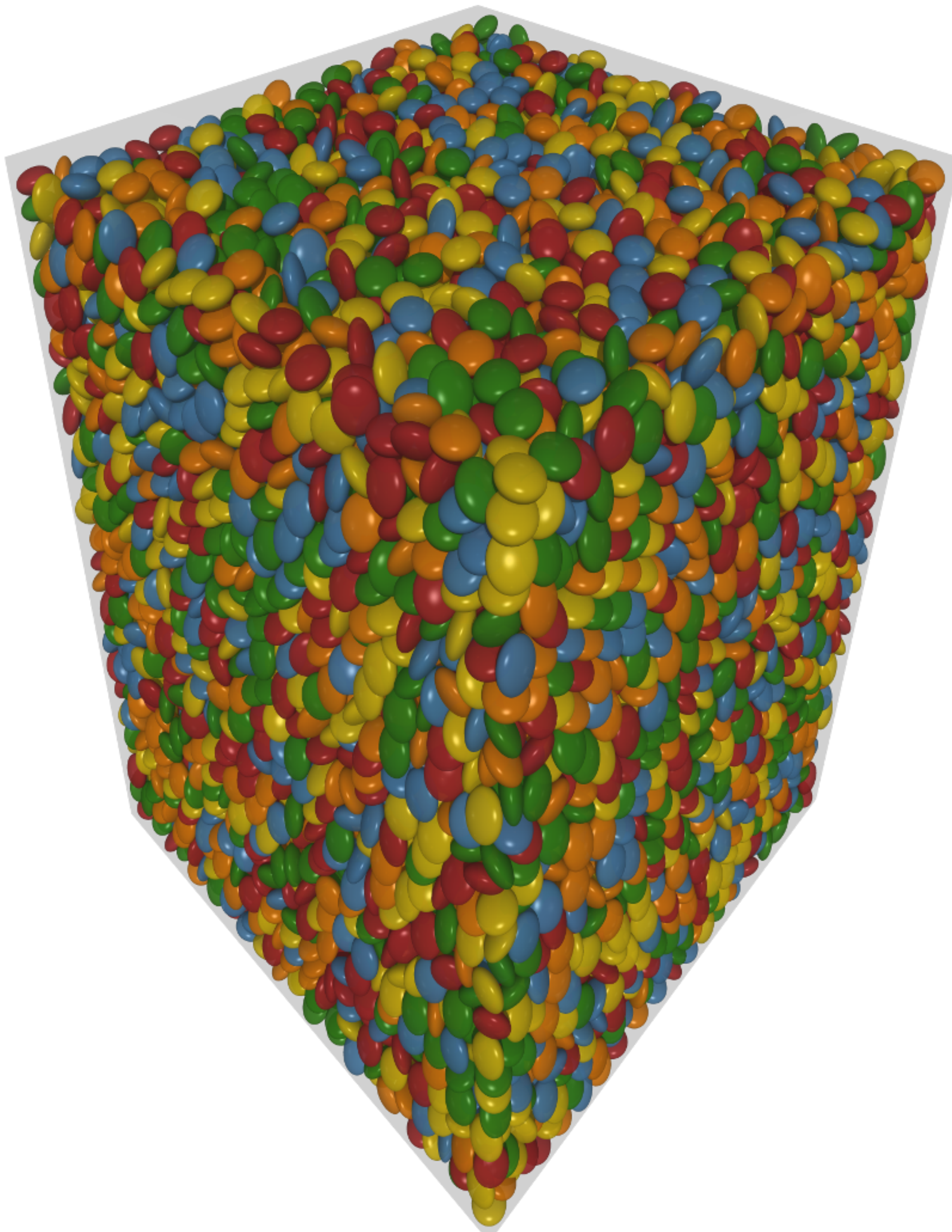


Figure 4.3: Packing of 14541 ellipsoids with semi-axis lengths $(0.67, 0.67, 0.3465)$ within a cube with side length 25 using isolation constraints given by a cylinder with radius $4a$ and a plane with height $h - 5a$.

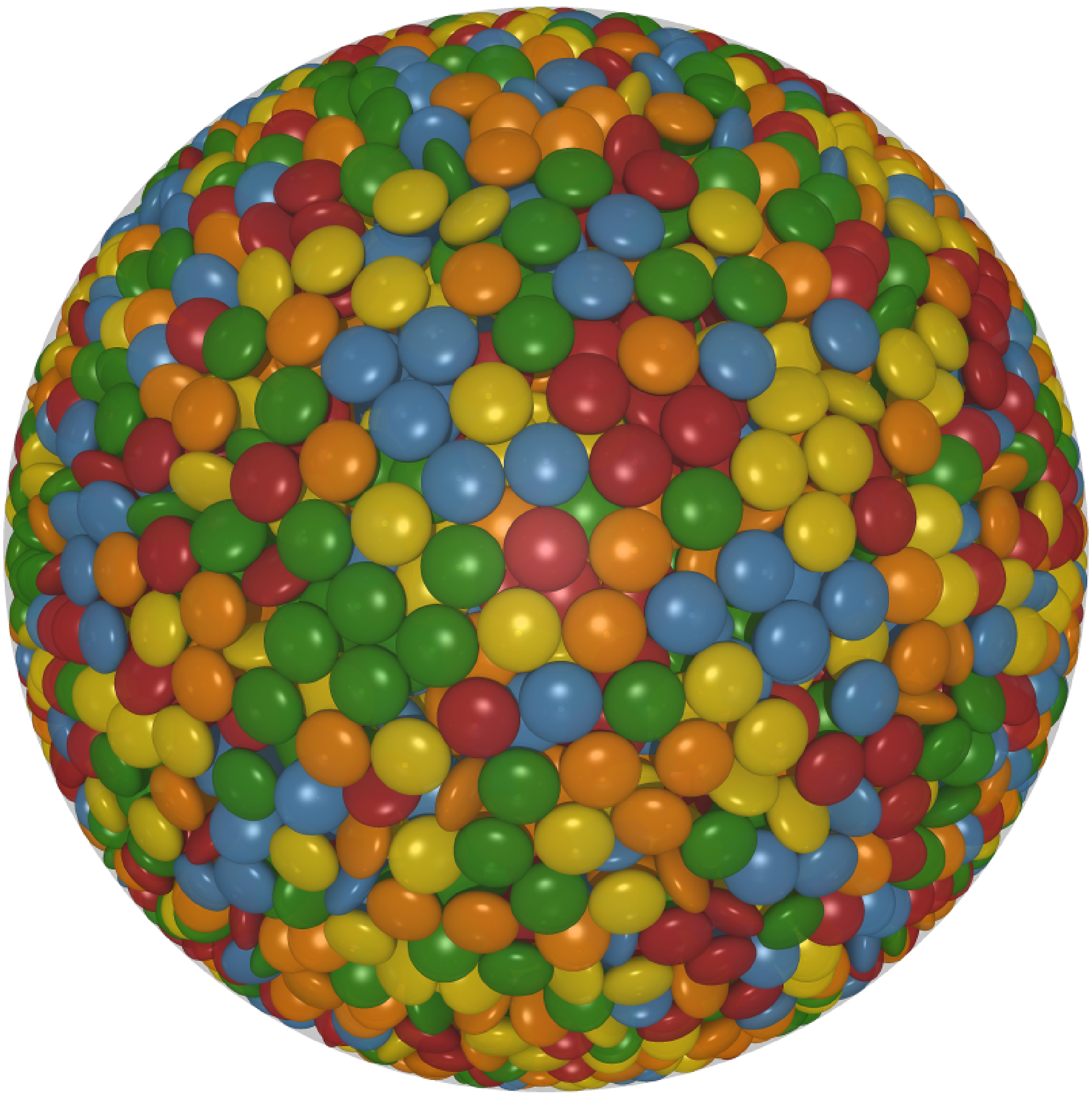


Figure 4.4: Packing of 7649 ellipsoids with semi-axis lengths $(0.67, 0.67, 0.3465)$ within a ball of radius 12.75 using isolation constraints given by a cylinder with radius $4a$ and a plane with height $h - 4a$.

Chapter 5

Conclusions

In this work, we dealt with the problem of packing ellipsoids within compact sets. We introduced two continuous and differentiable nonlinear programming models for the non-overlapping between ellipsoids. Also, we proposed continuous and differentiable nonlinear programming models for the inclusion of ellipsoids within half-spaces and ellipsoids. We performed some numerical experiments that showed the capabilities of the models. In particular, we were able to find better solutions to instances from the literature than other approaches.

Since the two non-overlapping models introduced in Chapter 2 have quadratic numbers of variables and constraints on the number of ellipsoids to be packed, the use of those models for solving problems with a relatively large number of ellipsoids become a prohibitive computational task. In order to alleviate this shortcoming, we proposed an implicit variables model that contains a linear number of variables and constraints. This model is based on the first non-overlapping model. First, to reduce the number of constraints, we replaced the constraints of the first model by their respective squared infeasibility measure. Then, we grouped those constraints to obtain a model with a linear number of constraints. Since each of the new constraints have a quadratic number of terms, we used a clever algorithm to be able to evaluate all constraints in linear time. Regarding the variables associated with pairs of ellipsoids, we replaced them by functions that were evaluated only when the ellipsoids were sufficiently close to each other. In this way, we were able to reduce the number of variables of the model. Numerical experiments showed that the implicit variables model was able to deal with problems with a larger number of ellipsoids.

Although the implicit variables model has a linear number of variables and constraints, its use is still not practical from the computational perspective when the number of ellipsoids is too large. In order to solve large-scale problems of packing the maximum number of ellipsoids within a given container, we proposed what we called the isolation constraints. Considering the algorithm that gradually packs the ellipsoids while minimizing their heights, the new ellipsoids would not be able to touch ellipsoids that were packed many iterations before. Therefore, the non-overlapping constraints between those ellipsoids could be removed and replaced by simpler ones that kept them sufficiently distant from each other.

We also plan to work on the ellipsoid contact number problem. The contact number problem consists in finding the largest number of congruent copies of a given convex body that

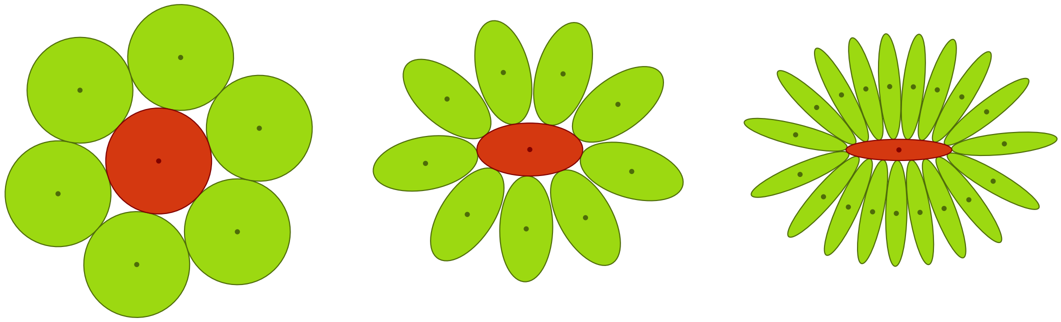


Figure 5.1: The contact number problem for ellipses with aspect ratios 1:1, 1:0.5, and 1:0.2, respectively.

do not overlap and that touch a given copy of this body. This problem is also known as the kissing number problem. In the most famous contact number problem, the convex body is a ball. For this problem, the contact number is only known for the dimensions 1, 2, 3, 4, 8 and 24 [46]. By using the non-overlapping model that we introduced in Section 2.2.1, we were able to model the ellipsoid contact number problem. Figure 5.1 shows the better solutions we obtained in the two-dimensional space for ellipses with semi-axis aspect ratios 1:1, 1:0.5, and 1:0.2. In comparison to the ball contact number problem, the ellipsoid contact number problem presents an additional difficulty which is the fact that the ellipsoids can be rotated. In the future, we intend to investigate this problem in more detail.

Appendix A

Derivatives

We shall present the derivatives of the functions that define some models introduced in this thesis. In Section A.1, we present the derivatives of the transformation based non-overlapping model introduced in Section 2.2.1. The derivatives of the functions that model the containment of an ellipsoid inside an ellipsoid, proposed in Section 2.3.1, is presented in Section A.2. Finally, in Section A.3, we show how to compute the derivatives of the implicit variables model presented in Chapter 3.

A.1 Derivatives of the transformation based non-overlapping model

In this section, we present the derivatives of the functions that define the model (2.22)–(2.25). Let $A \in \mathbb{R}^{n\times m}$. We will denote by $\frac{\partial A}{\partial v}$ the matrix in $\mathbb{R}^{n\times m}$ whose entry in row k and column l is the partial derivative with respect to v of the element in row k and column l of the matrix A. For each $i \in I$, we will denote by $\mathcal{O}_i$ the set of rotation angles associated with the ellipsoid i. Thus, in the two-dimensional case, we have $\mathcal{O}_i = \{\theta_i\}$, and in the three-dimensional case we have $\mathcal{O}_i = \{\theta_i, \psi_i, \phi_i\}$. We re-present the model (2.22)–(2.25) here:

$$x_{ij}^\top\big(P_i^{-\frac{1}{2}}Q_i^\top(c_i - c_j) - x_{ij}\big) = \mu_{ij}, \qquad \forall i,j \in I \text{ such that } i<j \tag{A.1}$$

$$\|P_i^{-\frac{1}{2}}Q_i^\top(c_i - c_j) - x_{ij}\|_2^2 \geq 1, \qquad \forall i,j \in I \text{ such that } i<j \tag{A.2}$$

$$P_i^{-\frac{1}{2}}Q_i^\top(c_i - c_j) = x_{ij} + \mu_{ij}S_{ij}x_{ij}, \quad \forall i,j \in I \text{ such that } i<j \tag{A.3}$$

$$\mu_{ij} \geq \epsilon_{ij}, \qquad \forall i,j \in I \text{ such that } i<j. \tag{A.4}$$

A.1.1 Derivatives of (A.1)

Let f_{ij} be the function defined by

$$f_{ij} \equiv f(c_i, c_j, x_{ij}, \mu_{ij}, \Omega_i) = x_{ij}^\top\left(P_i^{-\frac{1}{2}}Q_i^\top(c_i - c_j) - x_{ij}\right) - \mu_{ij}.$$

We have

$$\frac{\partial f_{ij}}{\partial c_i} = Q_i P_i^{-\frac{1}{2}} x_{ij}, \ \frac{\partial f_{ij}}{\partial c_j} = -\frac{\partial f_{ij}}{\partial c_i}, \ \frac{\partial f_{ij}}{\partial x_{ij}} = P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - 2x_{ij} \ \text{ e } \ \frac{\partial f_{ij}}{\partial \mu_{ij}} = -1.$$

For each $\omega \in \mathcal{O}_i$, we have

$$\frac{\partial f_{ij}}{\partial \omega} = x_{ij}^\top P_i^{-\frac{1}{2}} \frac{\partial Q_i}{\partial \omega}^\top (c_i - c_j),$$

where $\frac{\partial Q_i}{\partial \omega}$ is the component-wise derivative of matrix Q_i with respect to ω.

A.1.2 Derivatives of (A.2)

Let g_{ij} be the function defined by

$$g_{ij} \equiv g(c_i, c_j, x_{ij}, \Omega_i) = 1 - \|P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - x_{ij}\|_2^2$$

We have

$$\frac{\partial g_{ij}}{\partial c_i} = -2Q_i P_i^{-\frac{1}{2}} \left(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - x_{ij} \right), \ \frac{\partial g_{ij}}{\partial c_j} = -\frac{\partial g_{ij}}{\partial c_i} \ \text{ e } \ \frac{\partial g_{ij}}{\partial x_{ij}} = 2(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - x_{ij}).$$

For each $\omega \in \mathcal{O}_i$, we have

$$\frac{\partial g_{ij}}{\partial \omega} = -2 \left(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - x_{ij} \right)^\top P_i^{-\frac{1}{2}} \frac{\partial Q_i}{\partial \omega}^\top (c_i - c_j).$$

A.1.3 Derivatives of (A.3)

Let h_{ij} be the function defined by

$$h_{ij} \equiv h(c_i, c_j, x_{ij}, \mu_{ij}, \Omega_i, \Omega_j) = P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - x_{ij} - \mu_{ij} S_{ij} x_{ij}.$$

We have

$$\frac{\partial h_{ij}}{\partial c_i} = P_i^{-\frac{1}{2}} Q_i^\top, \ \frac{\partial h_{ij}}{\partial c_j} = -\frac{\partial h_{ij}}{\partial c_i}, \ \frac{\partial h_{ij}}{\partial x_{ij}} = -\mu_{ij} S_{ij} \ \text{ e } \ \frac{\partial h_{ij}}{\partial \mu_{ij}} = -S_{ij} x_{ij}.$$

Let $V_{ij} = P_j^{-\frac{1}{2}} Q_j^\top Q_i P_i^{\frac{1}{2}}$. Then, $S_{ij} = V_{ij}^\top V_{ij}$. Thus, for each $\omega \in \mathcal{O}_i$, we have

$$\frac{\partial V_{ij}}{\partial \omega} = P_j^{-\frac{1}{2}} Q_j^\top \frac{\partial Q_i}{\partial \omega} P_i^{\frac{1}{2}}$$

and

$$\frac{\partial h_{ij}}{\partial \omega} = P_i^{-\frac{1}{2}} \frac{\partial Q_i}{\partial \omega}^\top (c_i - c_j) - \mu_{ij} \left[\left(\frac{\partial V_{ij}}{\partial \omega} \right)^\top V_{ij} + V_{ij}^\top \left(\frac{\partial V_{ij}}{\partial \omega} \right) \right] x_{ij}.$$

For each $\omega \in \mathcal{O}_j$, we have

$$\frac{\partial V_{ij}}{\partial \omega} = P_j^{-\frac{1}{2}} \frac{\partial Q_j}{\partial \omega}^\top Q_i P_i^{\frac{1}{2}}$$

and

$$\frac{\partial h_{ij}}{\partial \omega} = -\mu_{ij} \left[\left(\frac{\partial V_{ij}}{\partial \omega} \right)^\top V_{ij} + V_{ij}^\top \left(\frac{\partial V_{ij}}{\partial \omega} \right) \right] x_{ij}.$$

A.2 Derivatives of the ellipsoid containment model

A.2.1 First order derivatives

We shall consider only the case where the container is a ball of radius r. In this case, we have $S_i = r^{-2}P_i$ for each $i \in I$. For each $i \in I$, let

$$
\begin{aligned}
f_i(c_i, \Omega_i, \bar{x}_i, \alpha_i, r) &= P_i^{-\frac{1}{2}} Q_i^\top c_i - \bar{x}_i - \alpha_i S_i \bar{x}_i, \\
g_i(c_i, \Omega_i, \bar{x}_i, \alpha_i, r) &= \bar{x}_i^\top S_i \bar{x}_i - 1, \\
h_i(c_i, \Omega_i, \bar{x}_i, \alpha_i, r) &= 1 - \|P_i^{-\frac{1}{2}} Q_i^\top c_i - \bar{x}_i\|_2^2.
\end{aligned}
$$

A.2.1.1 Derivatives of f_i

We have

$$
\frac{\partial f_i}{\partial c_i} = P_i^{-\frac{1}{2}} Q_i^\top, \ \frac{\partial f_i}{\partial \alpha_i} = -r^{-2} P_i \bar{x}_i, \ \frac{\partial f_i}{\partial r} = 2r^{-3} \alpha_i P_i \bar{x}_i, \ \frac{\partial f_i}{\partial \bar{x}_i} = -I_n - r^{-2} \alpha_i P_i
$$

and, for each $\omega \in \mathcal{O}_i$, we have

$$
\frac{\partial f_i}{\partial \omega} = P_i^{-\frac{1}{2}} \frac{\partial Q_i}{\partial \omega}^\top c_i.
$$

A.2.1.2 Derivatives of g_i

We have

$$
\frac{\partial g_i}{\partial r} = -2r^{-3} \bar{x}_i^\top P_i \bar{x}_i, \ \frac{\partial g_i}{\partial \bar{x}_i} = 2r^{-2} P_i \bar{x}_i.
$$

A.2.1.3 Derivatives of h_i

We have

$$
\frac{\partial h_i}{\partial c_i} = -2Q_i P_i^{-\frac{1}{2}} (P_i^{-\frac{1}{2}} Q_i^\top c_i - \bar{x}_i), \ \frac{\partial h_i}{\partial \bar{x}_i} = 2(P_i^{-\frac{1}{2}} Q_i^\top c_i - \bar{x}_i)
$$

and, for each $\omega \in \mathcal{O}_i$, we have

$$
\frac{\partial h_i}{\partial \omega} = -2c_i^\top \frac{\partial Q_i}{\partial \omega} P_i^{-\frac{1}{2}} (P_i^{-\frac{1}{2}} Q_i^\top c_i - \bar{x}_i).
$$

A.2.2 Second order derivatives

A.2.2.1 Derivatives of f_i

We have

$$
\frac{\partial^2 f_i}{\partial \alpha_i \partial \bar{x}_i} = -r^{-2} P_i, \ \frac{\partial^2 f_i}{\partial \alpha_i \partial r} = 2r^{-3} P_i \bar{x}_i, \ \frac{\partial^2 f_i}{\partial r^2} = -6r^{-4} \alpha_i P_i \bar{x}_i, \ \frac{\partial^2 f_i}{\partial r \partial \bar{x}_i} = 2r^{-3} \alpha_i P_i,
$$

and, for each $\omega, \sigma \in \mathcal{O}_i$, we have

$$\frac{\partial^2 f_i}{\partial \omega \partial c_i} = P_i^{-\frac{1}{2}} \frac{\partial Q_i}{\partial \omega}^\top, \ \frac{\partial^2 f_i}{\partial \sigma \partial \omega} = P_i^{-\frac{1}{2}} \frac{\partial^2 Q_i}{\partial \sigma \partial \omega}^\top.$$

A.2.2.2 Derivatives of g_i

We have

$$\frac{\partial^2 g_i}{\partial r^2} = 6r^{-4} \bar{x}_i^\top P_i \bar{x}_i, \ \frac{\partial^2 g_i}{\partial r \partial \bar{x}_i} = -4r^{-3} P_i \bar{x}_i, \ \frac{\partial^2 g_i}{\partial \bar{x}_i^2} = 2r^{-2} P_i.$$

A.2.2.3 Derivatives of h_i

We have

$$\frac{\partial^2 h_i}{\partial c_i^2} = -2 Q_i P_i^{-1} Q_i^\top, \ \frac{\partial^2 h_i}{\partial c_i \partial \bar{x}_i} = 2 P_i^{-\frac{1}{2}} Q_i^\top, \ \frac{\partial^2 h_i}{\partial \bar{x}_i^2} = -2 I_n,$$

and, for each $\omega \in \mathcal{O}_i$, we have

$$\frac{\partial^2 h_i}{\partial \omega \partial c_i} = -2 \left(\frac{\partial Q_i}{\partial \omega} P_i^{-1} Q_i^\top + Q_i P_i^{-1} \frac{\partial Q_i}{\partial \omega}^\top \right) c_i, \ \frac{\partial^2 h_i}{\partial \omega \partial \bar{x}_i} = 2 P_i^{-\frac{1}{2}} \frac{\partial Q_i}{\partial \omega}^\top c_i.$$

Moreover, for each $\omega, \sigma \in \mathcal{O}_i$, we have

$$\frac{\partial^2 h_i}{\partial \sigma \partial \omega} = -2 \left[c_i^\top \left(\frac{\partial^2 Q_i}{\partial \sigma \partial \omega} P_i^{-1} Q_i^\top + \frac{\partial Q_i}{\partial \omega} P_i^{-1} \frac{\partial Q_i}{\partial \sigma}^\top \right) c_i - c_i^\top \frac{\partial^2 Q_i}{\partial \sigma \partial \omega} P_i^{-\frac{1}{2}} \bar{x}_i \right].$$

A.3 Derivatives of the implicit variables model

The computation of the derivatives of the function defined in (3.24) is nontrivial. That is because this function depends on the functions $\mathcal{X}$ and $\mathcal{U}$ whose values are given by the solution of an optimization problem. In Section A.3.1, we show how to compute the first order derivatives of the function defined in (3.24) and, in Section A.3.2, we show how to compute the second order derivatives.

A.3.1 First order derivatives

Firstly, we will show the derivatives of the terms that compose the function defined in (3.24) in terms of the derivatives of the functions $\mathcal{X}$ and $\mathcal{U}$. Next, we will show how to compute the derivatives of the functions $\mathcal{X}$ and $\mathcal{U}$. The symbol $\mathbf{0}_{m,n}$ will be used to denote the $m \times n$ null matrix. Also, we will denote $\mathcal{X}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)$ by $\mathcal{X}_{ij}$ and $\mathcal{U}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)$ by $\mathcal{U}_{ij}$.

We have

$$\begin{aligned} \frac{\partial y_{ij}}{\partial c_i} &= \ \ P_i^{-\frac{1}{2}} Q_i^\top \\ \frac{\partial y_{ij}}{\partial c_j} &= -P_i^{-\frac{1}{2}} Q_i^\top \end{aligned}$$

and, for each $\omega_i \in \mathcal{O}_i$, we have

$$\frac{\partial y_{ij}}{\partial \omega_i} = P_i^{-\frac{1}{2}} \frac{\partial Q_i}{\partial \omega_i}^\top (c_i - c_j),$$

where $\frac{\partial Q_i}{\partial \omega_i} \in \mathbb{R}^{n \times n}$ is the matrix whose (l, k) entry has the value $\frac{\partial [Q_i]_{lk}}{\partial \omega_i}$.

Let $V_{ij} = P_j^{-\frac{1}{2}} Q_j^\top Q_i P_i^{\frac{1}{2}}$. Then, $S_{ij} = V_{ij}^\top V_{ij}$. Thus, for each $\omega_i \in \mathcal{O}_i$, we have

$$\frac{\partial V_{ij}}{\partial \omega_i} = P_j^{-\frac{1}{2}} Q_j^\top \frac{\partial Q_i}{\partial \omega_i} P_i^{\frac{1}{2}}$$

and, for each $\omega_j \in \mathcal{O}_j$, we have

$$\frac{\partial V_{ij}}{\partial \omega_j} = P_j^{-\frac{1}{2}} \frac{\partial Q_j}{\partial \omega_j}^\top Q_i P_i^{\frac{1}{2}},$$

where $\frac{\partial Q_j}{\partial \omega_j} \in \mathbb{R}^{n \times n}$ is the matrix defined in an analogous manner to $\frac{\partial Q_i}{\partial \omega_i}$.

For each $\omega \in \mathcal{O}_i \cup \mathcal{O}_j$, we have

$$\frac{\partial \mathcal{U}_{ij} S_{ij} \mathcal{X}_{ij}}{\partial \omega} = \frac{\partial \mathcal{U}_{ij}}{\partial \omega} S_{ij} \mathcal{X}_{ij} + \mathcal{U}_{ij} \left[\left(\frac{\partial V_{ij}}{\partial \omega}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \omega} \right) \mathcal{X}_{ij} + S_{ij} \frac{\partial \mathcal{X}_{ij}}{\partial \omega} \right] \Bigg\},$$

where $\frac{\partial \mathcal{X}_{ij}}{\partial \omega} \in \mathbb{R}^n$ is the vector whose l-th component has the value $\frac{\partial [\mathcal{X}_{ij}]_l}{\partial \omega}$.

Consider the functions f_{ij} and g_{ij} defined by

$$f_{ij}(c_i, c_j, \Omega_i, \Omega_j) = \max\left\{1 - \bar{f}_{ij}(c_i, c_j, \Omega_i, \Omega_j), 0\right\}^2 \tag{A.5}$$

$$g_{ij}(c_i, c_j, \Omega_i, \Omega_j) = \max\left\{\epsilon_{ij} - \mathcal{U}_{ij}, 0\right\}^2 \tag{A.6}$$

where

$$\bar{f}_{ij}(c_i, c_j, \Omega_i, \Omega_j) = \|P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}_{ij}\|_2^2.$$

Next, we compute the derivatives of these functions with respect to the variables of the non-overlapping model.

A.3.1.1 First order derivatives of (A.5)

If $\bar{f}_{ij}(c_i, c_j, \Omega_i, \Omega_j) \geq 1$ then

$$\frac{\partial f_{ij}}{\partial [c_i]_k} = \frac{\partial f_{ij}}{\partial [c_j]_k} = \frac{\partial f_{ij}}{\partial \omega} = 0$$

for each $k \in \{1, \ldots, n\}$ and for each $\omega \in \mathcal{O}_i \cup \mathcal{O}_j$. Otherwise, we have

$$\frac{\partial f_{ij}}{\partial c_i} = -4\left[1 - \bar{f}_{ij}(c_i, c_j, \Omega_i, \Omega_j)\right] \left(Q_i P_i^{-\frac{1}{2}} - \frac{\partial \mathcal{X}_{ij}}{\partial c_i} \right) \left(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}_{ij} \right)$$

$$\frac{\partial f_{ij}}{\partial c_j} = -4\left[1 - \bar{f}_{ij}(c_i, c_j, \Omega_i, \Omega_j)\right] \left(-Q_i P_i^{-\frac{1}{2}} - \frac{\partial \mathcal{X}_{ij}}{\partial c_j} \right) \left(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}_{ij} \right)$$

where $\frac{\partial \mathcal{X}_{ij}}{\partial c_i}$ is the matrix in $\mathbb{R}^{n\times n}$ whose (l,k) entry has the value $\frac{\partial [\mathcal{X}_{ij}]_k}{\partial [c_i]_l}$. Analogously, we define the matrix $\frac{\partial \mathcal{X}_{ij}}{\partial c_j}$. For each $\omega_i \in \mathcal{O}_i$, we have

$$\frac{\partial f_{ij}}{\partial \omega_i} = -4\left[1 - \bar{f}_{ij}(c_i, c_j, \Omega_i, \Omega_j)\right] \left(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}_{ij}\right)^\top \left(P_i^{-\frac{1}{2}} \frac{\partial Q_i}{\partial \omega_i}^\top (c_i - c_j) - \frac{\partial \mathcal{X}_{ij}}{\partial \omega_i}\right).$$

For each $\omega_j \in \mathcal{O}_j$, we have

$$\frac{\partial f_{ij}}{\partial \omega_j} = -4\left[1 - \bar{f}_{ij}(c_i, c_j, \Omega_i, \Omega_j)\right] \left(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}_{ij}\right)^\top \left(-\frac{\partial \mathcal{X}_{ij}}{\partial \omega_j}\right).$$

A.3.1.2 First order derivatives of (A.6)

If $\mathcal{U}_{ij} \geq \epsilon_{ij}$ then

$$\frac{\partial g_{ij}}{\partial [c_i]_k} = \frac{\partial g_{ij}}{\partial [c_j]_k} = \frac{\partial g_{ij}}{\partial \omega} = 0$$

for each $k \in \{1, \dots, n\}$ and for each $\omega \in \mathcal{O}_i \cup \mathcal{O}_j$. Otherwise, we have

$$\begin{aligned} \frac{\partial g_{ij}}{\partial c_i} &= -2(\epsilon_{ij} - \mathcal{U}_{ij}) \frac{\partial \mathcal{U}_{ij}}{\partial c_i} \\ \frac{\partial g_{ij}}{\partial c_j} &= -2(\epsilon_{ij} - \mathcal{U}_{ij}) \frac{\partial \mathcal{U}_{ij}}{\partial c_j} \end{aligned}$$

and, for each $\omega \in \mathcal{O}_i \cup \mathcal{O}_j$, we have

$$\frac{\partial g_{ij}}{\partial \omega} = -2(\epsilon_{ij} - \mathcal{U}_{ij}) \frac{\partial \mathcal{U}_{ij}}{\partial \omega}.$$

A.3.1.3 First order derivatives of $\mathcal{X}$ and $\mathcal{U}$

Let $i, j \in \{1, \dots, m\}$ such that $i < j$. We have that $\mathcal{X}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)$ is a solution to the problem

$$\begin{array}{ll} \text{minimize} & \frac{1}{2}\|x - y_{ij}\|_2^2 \\ \text{subject to} & x^\top S_{ij} x = 1, \end{array} \tag{A.7}$$

where $y_{ij} = P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j)$, and $\mathcal{U}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)$ is the corresponding Lagrange multiplier. To simplify the notation, we will denote by $\mathcal{X}_{ij}$ the value $\mathcal{X}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)$ and by $\mathcal{U}_{ij}$ the value $\mathcal{U}(c_i, c_j, \Omega_i, \Omega_j; P_i, P_j)$. According to the Karush–Kuhn–Tucker first-order necessary conditions for problem (A.7), we have

$$\begin{aligned} \mathcal{X}_{ij} + \mathcal{U}_{ij} S_{ij} \mathcal{X}_{ij} - y_{ij} &= 0 \\ \mathcal{X}_{ij}^\top S_{ij} \mathcal{X}_{ij} - 1 &= 0. \end{aligned}$$

Thus, by defining the function $F : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^q \times \mathbb{R}^q \to \mathbb{R}^{n+1}$ as

$$F(c_i, c_j, \Omega_i, \Omega_j) = \left[\begin{array}{c} \mathcal{X}_{ij} + \mathcal{U}_{ij} S_{ij} \mathcal{X}_{ij} - y_{ij} \\ \frac{1}{2}\left({\mathcal{X}_{ij}}^\top S_{ij} \mathcal{X}_{ij} - 1 \right) \end{array} \right], \tag{A.8}$$

we have that $F(c_i, c_j, \Omega_i, \Omega_j) = 0$ for all $c_i, c_j \in \mathbb{R}^n$ and for all $\Omega_i, \Omega_j \in \mathbb{R}^q$. That is, F is an identically zero function. Therefore, we have that the derivative of function F is also an identically zero function. Hence, for each variable v of the function F and for each component $\ell \in \{1, \dots, n+1\}$ of F, we have

$$\frac{\mathrm{d}F_\ell}{\mathrm{d}v} = \frac{\partial F_\ell}{\partial v}\frac{\mathrm{d}v}{\mathrm{d}v} + \frac{\partial F_\ell}{\partial \mathcal{U}_{ij}}\frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v} + \sum_{k=1}^{n} \frac{\partial F_\ell}{\partial [\mathcal{X}_{ij}]_k}\frac{\mathrm{d}[\mathcal{X}_{ij}]_k}{\mathrm{d}v} = 0. \tag{A.9}$$

Once the values of $\mathcal{X}_{ij}$ and $\mathcal{U}_{ij}$ are known, we have, for each $\ell \in \{1, \dots, n+1\}$, analytical expressions for $\frac{\partial F_\ell}{\partial v}$, $\frac{\partial F_\ell}{\partial \mathcal{U}_{ij}}$, and $\frac{\partial F_\ell}{\partial [\mathcal{X}_{ij}]_k}$ for each $k \in \{1, \dots, n\}$. On the other hand, the values of $\frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v}$ and $\frac{\mathrm{d}[\mathcal{X}_{ij}]_k}{\mathrm{d}v}$ for each $k \in \{1, \dots, n\}$ are unknown, but can be computed by solving the linear system provided by (A.9):

$$\begin{bmatrix} \frac{\partial F_1}{\partial [\mathcal{X}_{ij}]_1} & \cdots & \frac{\partial F_1}{\partial [\mathcal{X}_{ij}]_n} & \frac{\partial F_1}{\partial \mathcal{U}_{ij}} \\ \frac{\partial F_2}{\partial [\mathcal{X}_{ij}]_1} & \cdots & \frac{\partial F_2}{\partial [\mathcal{X}_{ij}]_n} & \frac{\partial F_2}{\partial \mathcal{U}_{ij}} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial F_{n+1}}{\partial [\mathcal{X}_{ij}]_1} & \cdots & \frac{\partial F_{n+1}}{\partial [\mathcal{X}_{ij}]_n} & \frac{\partial F_{n+1}}{\partial \mathcal{U}_{ij}} \end{bmatrix} \begin{bmatrix} \frac{\mathrm{d}[\mathcal{X}_{ij}]_1}{\mathrm{d}v} \\ \vdots \\ \frac{\mathrm{d}[\mathcal{X}_{ij}]_n}{\mathrm{d}v} \\ \frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v} \end{bmatrix} = - \begin{bmatrix} \frac{\partial F_1}{\partial v} \\ \frac{\partial F_2}{\partial v} \\ \vdots \\ \frac{\partial F_{n+1}}{\partial v} \end{bmatrix}.$$

Then, for each $i, j \in \{1, \dots, m\}$ such that $i < j$, we need to solve $2(n+q)$ linear systems with $n+1$ equations and $n+1$ variables (one linear system for each variable among c_i, c_j, Ω_i and Ω_j).

Once i and j are fixed, observe that the $2(n+q)$ linear systems have the same coefficient matrix. The only difference between these systems are their right-hand sides. Thus, in order to solve these linear systems, we can factorize the coefficient matrix only once and then, for each right-hand side, solve the linear system with the coefficient matrix already factorized.

A.3.1.4 First order partial derivatives of F

We shall present the first order partial derivatives of the function F. For each $\omega_i \in \mathcal{O}_i$, we have

$$\frac{\partial F}{\partial \omega_i} = \left[\begin{array}{c} \mathcal{U}_{ij}\left({\frac{\partial V_{ij}}{\partial \omega_i}}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \omega_i} \right) \mathcal{X}_{ij} - P_i^{-\frac{1}{2}} {\frac{\partial Q_i}{\partial \omega_i}}^\top (c_i - c_j) \\ \left(V_{ij}\mathcal{X}_{ij} \right)^\top \frac{\partial V_{ij}}{\partial \omega_i} \mathcal{X}_{ij} \end{array} \right].$$

For each $\omega_j \in \mathcal{O}_j$, we have

$$\frac{\partial F}{\partial \omega_j} = \left[\begin{array}{c} \mathcal{U}_{ij}\left({\frac{\partial V_{ij}}{\partial \omega_j}}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \omega_j} \right) \mathcal{X}_{ij} \\ \left(V_{ij}\mathcal{X}_{ij} \right)^\top \frac{\partial V_{ij}}{\partial \omega_j} \mathcal{X}_{ij} \end{array} \right].$$

With respect to the center of the ellipsoids, we have

$$\frac{\partial F}{\partial c_i} = \begin{bmatrix} -P_i^{-\frac{1}{2}} Q_i^\top \\ \mathbf{0}_{1,n} \end{bmatrix}$$

and

$$\frac{\partial F}{\partial c_j} = \begin{bmatrix} P_i^{-\frac{1}{2}} Q_i^\top \\ \mathbf{0}_{1,n} \end{bmatrix}.$$

With respect to the implicit variables, we have

$$\frac{\partial F}{\partial \mathcal{U}_{ij}} = \begin{bmatrix} S_{ij}\mathcal{X}_{ij} \\ 0 \end{bmatrix}$$

and

$$\frac{\partial F}{\partial \mathcal{X}_{ij}} = \begin{bmatrix} I_n + \mathcal{U}_{ij} S_{ij} \\ \left(S_{ij}\mathcal{X}_{ij}\right)^\top \end{bmatrix}.$$

A.3.2 Second order derivatives

In Sections A.3.2.1 and A.3.2.2, we present the second order derivatives of the functions f_{ij} and g_{ij}, respectively. These derivatives depend on the (first and second order) derivatives of the functions $\mathcal{X}_{ij}$ and $\mathcal{U}_{ij}$. As the first order derivatives of $\mathcal{X}_{ij}$ and $\mathcal{U}_{ij}$, the second order derivatives of these functions do not have an analytical expression. So, in Section A.3.2.3, we will show how to compute them.

A.3.2.1 Second order derivatives of (A.5)

If $\bar{f}_{ij}(c_i, c_j, \Omega_i, \Omega_j) \geq 1$ then

$$\frac{\partial^2 f_{ij}}{\partial [c_i]_k \partial c_i} = \frac{\partial^2 f_{ij}}{\partial [c_j]_k \partial c_i} = \frac{\partial^2 f_{ij}}{\partial \sigma \partial c_i} = \frac{\partial^2 f_{ij}}{\partial \sigma \partial c_j} = \mathbf{0}_{n,1}$$

for each $k \in \{1, \dots, n\}$ and for each $\sigma \in \mathcal{O}_i \cup \mathcal{O}_j$ and

$$\frac{\partial^2 f_{ij}}{\partial \sigma \partial \omega} = 0$$

for each $\sigma, \omega \in \mathcal{O}_i \cup \mathcal{O}_j$. Otherwise, for each $k \in \{1, \dots, n\}$, we have

$$\begin{aligned} \frac{\partial^2 f_{ij}}{\partial [c_i]_k \partial c_i} = {} & -4 \Bigg\{ -\frac{\partial \bar{f}_{ij}}{\partial [c_i]_k} \left(Q_i P_i^{-\frac{1}{2}} - \frac{\partial \mathcal{X}_{ij}}{\partial c_i} \right) \left(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}_{ij} \right) + \\ & \left[1 - \bar{f}_{ij}(c_i, c_j, \Omega_i, \Omega_j)\right] \Bigg[-\frac{\partial^2 \mathcal{X}_{ij}}{\partial [c_i]_k \partial c_i} \left(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}_{ij} \right) + \\ & \left(Q_i P_i^{-\frac{1}{2}} - \frac{\partial \mathcal{X}_{ij}}{\partial c_i} \right) \left(\left[P_i^{-\frac{1}{2}} Q_i^\top \right]_{:,k} - \frac{\partial \mathcal{X}_{ij}}{\partial [c_i]_k} \right) \Bigg] \Bigg\} \end{aligned}$$

$$\frac{\partial^2 f_{ij}}{\partial[c_j]_k \partial c_i} = -4\Bigg\{ -\frac{\partial \bar{f}_{ij}}{\partial[c_j]_k}\left(Q_i P_i^{-\frac{1}{2}} - \frac{\partial \mathcal{X}_{ij}}{\partial c_i}\right)\left(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}_{ij}\right) +$$
$$\left[1 - \bar{f}_{ij}(c_i, c_j, \Omega_i, \Omega_j)\right]\Bigg[-\frac{\partial^2 \mathcal{X}_{ij}}{\partial[c_j]_k \partial c_i}\left(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}_{ij}\right) +$$
$$\left(Q_i P_i^{-\frac{1}{2}} - \frac{\partial \mathcal{X}_{ij}}{\partial c_i}\right)\left(-\left[P_i^{-\frac{1}{2}} Q_i^\top\right]_{:,k} - \frac{\partial \mathcal{X}_{ij}}{\partial[c_j]_k}\right)\Bigg]\Bigg\}$$

$$\frac{\partial^2 f_{ij}}{\partial[c_j]_k \partial c_j} = -4\Bigg\{ -\frac{\partial \bar{f}_{ij}}{\partial[c_j]_k}\left(-Q_i P_i^{-\frac{1}{2}} - \frac{\partial \mathcal{X}_{ij}}{\partial c_j}\right)\left(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}_{ij}\right) +$$
$$\left[1 - \bar{f}_{ij}(c_i, c_j, \Omega_i, \Omega_j)\right]\Bigg[-\frac{\partial^2 \mathcal{X}_{ij}}{\partial[c_j]_k \partial c_j}\left(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}_{ij}\right) +$$
$$\left(-Q_i P_i^{-\frac{1}{2}} - \frac{\partial \mathcal{X}_{ij}}{\partial c_j}\right)\left(-\left[P_i^{-\frac{1}{2}} Q_i^\top\right]_{:,k} - \frac{\partial \mathcal{X}_{ij}}{\partial[c_j]_k}\right)\Bigg]\Bigg\}$$

For each $\sigma \in \mathcal{O}_i \cup \mathcal{O}_j$, we have

$$\frac{\partial^2 f_{ij}}{\partial \sigma \partial c_i} = -4\Bigg\{ -\frac{\partial \bar{f}_{ij}}{\partial \sigma}(c_i, c_j, \Omega_i, \Omega_j)\left(Q_i P_i^{-\frac{1}{2}} - \frac{\partial \mathcal{X}_{ij}}{\partial c_i}\right)\left(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}_{ij}\right) +$$
$$\left[1 - \bar{f}_{ij}(c_i, c_j, \Omega_i, \Omega_j)\right]\Bigg[\left(\frac{\partial Q_i}{\partial \sigma} P_i^{-\frac{1}{2}} - \frac{\partial^2 \mathcal{X}_{ij}}{\partial \sigma \partial c_i}\right)\left(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}_{ij}\right) +$$
$$\left(Q_i P_i^{-\frac{1}{2}} - \frac{\partial \mathcal{X}_{ij}}{\partial c_i}\right)\left(P_i^{-\frac{1}{2}} \frac{\partial Q_i}{\partial \sigma}^\top (c_i - c_j) - \frac{\partial \mathcal{X}_{ij}}{\partial \sigma}\right)\Bigg]\Bigg\}$$

$$\frac{\partial^2 f_{ij}}{\partial \sigma \partial c_j} = -4\Bigg\{ -\frac{\partial \bar{f}_{ij}}{\partial \sigma}(c_i, c_j, \Omega_i, \Omega_j)\left(-Q_i P_i^{-\frac{1}{2}} - \frac{\partial \mathcal{X}_{ij}}{\partial c_j}\right)\left(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}_{ij}\right) +$$
$$\left[1 - \bar{f}_{ij}(c_i, c_j, \Omega_i, \Omega_j)\right]\Bigg[\left(-\frac{\partial Q_i}{\partial \sigma} P_i^{-\frac{1}{2}} - \frac{\partial^2 \mathcal{X}_{ij}}{\partial \sigma \partial c_j}\right)\left(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}_{ij}\right) +$$
$$\left(-Q_i P_i^{-\frac{1}{2}} - \frac{\partial \mathcal{X}_{ij}}{\partial c_j}\right)\left(P_i^{-\frac{1}{2}} \frac{\partial Q_i}{\partial \sigma}^\top (c_i - c_j) - \frac{\partial \mathcal{X}_{ij}}{\partial \sigma}\right)\Bigg]\Bigg\}$$

where

$$\frac{\partial \bar{f}_{ij}}{\partial \sigma}(c_i, c_j, \Omega_i, \Omega_j) = 2\left(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}_{ij}\right)^\top \left(P_i^{-\frac{1}{2}} \frac{\partial Q_i}{\partial \sigma}^\top (c_i - c_j) - \frac{\partial \mathcal{X}_{ij}}{\partial \sigma}\right).$$

For each $\sigma, \omega \in \mathcal{O}_i \cup \mathcal{O}_j$, we have

$$\frac{\partial^2 f_{ij}}{\partial\sigma\partial\omega} = -4\Bigg\{ -\frac{\partial \bar{f}_{ij}}{\partial\sigma}(c_i, c_j, \Omega_i, \Omega_j)\left(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}_{ij}\right)^\top \left(P_i^{-\frac{1}{2}} \frac{\partial Q_i}{\partial\omega}^\top (c_i - c_j) - \frac{\partial \mathcal{X}_{ij}}{\partial\omega}\right) + \left[1 - \bar{f}_{ij}(c_i, c_j, \Omega_i, \Omega_j)\right]\Bigg[\left(P_i^{-\frac{1}{2}} \frac{\partial Q_i}{\partial\sigma}^\top (c_i - c_j) - \frac{\partial \mathcal{X}_{ij}}{\partial\sigma}\right)^\top \left(P_i^{-\frac{1}{2}} \frac{\partial Q_i}{\partial\omega}^\top (c_i - c_j) - \frac{\partial \mathcal{X}_{ij}}{\partial\omega}\right) + \left(P_i^{-\frac{1}{2}} Q_i^\top (c_i - c_j) - \mathcal{X}_{ij}\right)^\top \left(P_i^{-\frac{1}{2}} \frac{\partial^2 Q_i}{\partial\sigma\partial\omega}^\top (c_i - c_j) - \frac{\partial^2 \mathcal{X}_{ij}}{\partial\sigma\partial\omega}\right)\Bigg]\Bigg\}.$$

A.3.2.2 Second order derivatives of (A.6)

If $\mathcal{U}_{ij} \geq \epsilon_{ij}$ then

$$\frac{\partial^2 g_{ij}}{\partial[c_i]_k \partial c_i} = \frac{\partial^2 g_{ij}}{\partial[c_j]_k \partial c_i} = \frac{\partial^2 g_{ij}}{\partial\omega\partial c_i} = \frac{\partial^2 g_{ij}}{\partial\omega\partial c_j} = \mathbf{0}_{n,1}$$

for each $k \in \{1, \ldots, n\}$ and for each $\omega \in \mathcal{O}_i \cup \mathcal{O}_j$. Otherwise, for each $k \in \{1, \ldots, n\}$, we have

$$\begin{aligned}
\frac{\partial^2 g_{ij}}{\partial[c_i]_k \partial c_i} &= -2\left((\epsilon_{ij} - \mathcal{U}_{ij})\frac{\partial^2 \mathcal{U}_{ij}}{\partial[c_i]_k \partial c_i} - \frac{\partial \mathcal{U}_{ij}}{\partial[c_i]_k}\frac{\partial \mathcal{U}_{ij}}{\partial c_i}\right) \\
\frac{\partial^2 g_{ij}}{\partial[c_j]_k \partial c_i} &= -2\left((\epsilon_{ij} - \mathcal{U}_{ij})\frac{\partial^2 \mathcal{U}_{ij}}{\partial[c_j]_k \partial c_i} - \frac{\partial \mathcal{U}_{ij}}{\partial[c_j]_k}\frac{\partial \mathcal{U}_{ij}}{\partial c_i}\right)
\end{aligned}$$

and, for each $\omega \in \mathcal{O}_i \cup \mathcal{O}_j$, we have

$$\begin{aligned}
\frac{\partial^2 g_{ij}}{\partial\omega\partial c_i} &= -2\left((\epsilon_{ij} - \mathcal{U}_{ij})\frac{\partial^2 \mathcal{U}_{ij}}{\partial\omega\partial c_i} - \frac{\partial \mathcal{U}_{ij}}{\partial\omega}\frac{\partial \mathcal{U}_{ij}}{\partial c_i}\right) \\
\frac{\partial^2 g_{ij}}{\partial\omega\partial c_j} &= -2\left((\epsilon_{ij} - \mathcal{U}_{ij})\frac{\partial^2 \mathcal{U}_{ij}}{\partial\omega\partial c_j} - \frac{\partial \mathcal{U}_{ij}}{\partial\omega}\frac{\partial \mathcal{U}_{ij}}{\partial c_j}\right).
\end{aligned}$$

Moreover, for each $\omega, \sigma \in \mathcal{O}_i \cup \mathcal{O}_j$, we have

$$\frac{\partial^2 g_{ij}}{\partial\sigma\partial\omega} = -2\left((\epsilon_{ij} - \mathcal{U}_{ij})\frac{\partial^2 \mathcal{U}_{ij}}{\partial\sigma\partial\omega} - \frac{\partial \mathcal{U}_{ij}}{\partial\sigma}\frac{\partial \mathcal{U}_{ij}}{\partial\omega}\right).$$

A.3.2.3 Second order derivatives of $\mathcal{X}$ and $\mathcal{U}$

For each variable v of the function F defined in (A.8) and for each component ℓ of F, we define the function G_ℓ^v as the total derivative of the function F_ℓ with respect to v:

$$G_\ell^v(c_i, c_j, \Omega_i, \Omega_j) = \frac{\mathrm{d}F_\ell}{\mathrm{d}v}(c_i, c_j, \Omega_i, \Omega_j).$$

Since the function F is identically zero, its derivative is also identically zero. Then, for each variable u of the function G_ℓ^v, we have

$$\frac{\mathrm{d}G_\ell^v}{\mathrm{d}u} = \frac{\partial G_\ell^v}{\partial u}\frac{\mathrm{d}u}{\mathrm{d}u} + \frac{\partial G_\ell^v}{\partial \mathcal{U}_{ij}}\frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}u} + \sum_{k=1}^{n} \frac{\partial G_\ell^v}{\partial [\mathcal{X}_{ij}]_k}\frac{\mathrm{d}[\mathcal{X}_{ij}]_k}{\mathrm{d}u} = 0. \tag{A.10}$$

Next, we present the partial derivatives of the function G_ℓ^v, that appear in the expression (A.10). The partial derivative of G_ℓ^v with respect to the variable u is given by

$$\frac{\partial G_\ell^v}{\partial u} = \frac{\partial^2 F_\ell}{\partial u \partial v} + \frac{\partial^2 F_\ell}{\partial u \partial \mathcal{U}_{ij}}\frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v} + \frac{\partial F_\ell}{\partial \mathcal{U}_{ij}}\frac{\partial}{\partial u}\left(\frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v}\right) + \sum_{k=1}^{n}\frac{\partial^2 F_\ell}{\partial u \partial [\mathcal{X}_{ij}]_k}\frac{\mathrm{d}[\mathcal{X}_{ij}]_k}{\mathrm{d}v} + \sum_{k=1}^{n}\frac{\partial F_\ell}{\partial [\mathcal{X}_{ij}]_k}\frac{\partial}{\partial u}\left(\frac{\mathrm{d}[\mathcal{X}_{ij}]_k}{\mathrm{d}v}\right).$$

The partial derivative of G_ℓ^v with respect to $\mathcal{U}_{ij}$ is given by

$$\begin{aligned}
\frac{\partial G_\ell^v}{\partial \mathcal{U}_{ij}} &= \frac{\partial^2 F_\ell}{\partial \mathcal{U}_{ij} \partial v} + \frac{\partial^2 F_\ell}{\partial \mathcal{U}_{ij} \partial \mathcal{U}_{ij}}\frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v} + \frac{\partial F_\ell}{\partial \mathcal{U}_{ij}}\frac{\partial}{\partial \mathcal{U}_{ij}}\left(\frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v}\right) + \\
&\quad \sum_{k=1}^{n}\frac{\partial^2 F_\ell}{\partial \mathcal{U}_{ij} \partial [\mathcal{X}_{ij}]_k}\frac{\mathrm{d}[\mathcal{X}_{ij}]_k}{\mathrm{d}v} + \sum_{k=1}^{n}\frac{\partial F_\ell}{\partial [\mathcal{X}_{ij}]_k}\frac{\partial}{\partial \mathcal{U}_{ij}}\left(\frac{\mathrm{d}[\mathcal{X}_{ij}]_k}{\mathrm{d}v}\right) \\
&= \frac{\partial^2 F_\ell}{\partial \mathcal{U}_{ij} \partial v} + \sum_{k=1}^{n}\frac{\partial^2 F_\ell}{\partial \mathcal{U}_{ij} \partial [\mathcal{X}_{ij}]_k}\frac{\mathrm{d}[\mathcal{X}_{ij}]_k}{\mathrm{d}v}.
\end{aligned}$$

Finally, the partial derivative of G_ℓ^v with respect to $\mathcal{X}_{ij}$ is given by

$$\begin{aligned}
\frac{\partial G_\ell^v}{\partial [\mathcal{X}_{ij}]_t} &= \frac{\partial^2 F_\ell}{\partial [\mathcal{X}_{ij}]_t \partial v} + \frac{\partial^2 F_\ell}{\partial [\mathcal{X}_{ij}]_t \partial \mathcal{U}_{ij}}\frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v} + \frac{\partial F_\ell}{\partial \mathcal{U}_{ij}}\frac{\partial}{\partial [\mathcal{X}_{ij}]_t}\left(\frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v}\right) + \\
&\quad \sum_{k=1}^{n}\frac{\partial^2 F_\ell}{\partial [\mathcal{X}_{ij}]_t \partial [\mathcal{X}_{ij}]_k}\frac{\mathrm{d}[\mathcal{X}_{ij}]_k}{\mathrm{d}v} + \sum_{k=1}^{n}\frac{\partial F_\ell}{\partial [\mathcal{X}_{ij}]_k}\frac{\partial}{\partial [\mathcal{X}_{ij}]_t}\left(\frac{\mathrm{d}[\mathcal{X}_{ij}]_k}{\mathrm{d}v}\right) \\
&= \frac{\partial^2 F_\ell}{\partial [\mathcal{X}_{ij}]_t \partial v} + \frac{\partial^2 F_\ell}{\partial [\mathcal{X}_{ij}]_t \partial \mathcal{U}_{ij}}\frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v} + \sum_{k=1}^{n}\frac{\partial^2 F_\ell}{\partial [\mathcal{X}_{ij}]_t \partial [\mathcal{X}_{ij}]_k}\frac{\mathrm{d}[\mathcal{X}_{ij}]_k}{\mathrm{d}v}.
\end{aligned}$$

The simplifications in the expressions of the derivatives of G_ℓ^v with respect to $\mathcal{U}_{ij}$ and $\mathcal{X}_{ij}$ come from the removal of null elements.

Considering that the values of the first order derivatives of the function F are known, the equation (A.10) provides the following linear system

$$\begin{bmatrix}
\frac{\partial F_1}{\partial [\mathcal{X}_{ij}]_1} & \cdots & \frac{\partial F_1}{\partial [\mathcal{X}_{ij}]_n} & \frac{\partial F_1}{\partial \mathcal{U}_{ij}} \\
\frac{\partial F_2}{\partial [\mathcal{X}_{ij}]_1} & \cdots & \frac{\partial F_2}{\partial [\mathcal{X}_{ij}]_n} & \frac{\partial F_2}{\partial \mathcal{U}_{ij}} \\
\vdots & \vdots & \vdots & \vdots \\
\frac{\partial F_{n+1}}{\partial [\mathcal{X}_{ij}]_1} & \cdots & \frac{\partial F_{n+1}}{\partial [\mathcal{X}_{ij}]_n} & \frac{\partial F_{n+1}}{\partial \mathcal{U}_{ij}}
\end{bmatrix}
\begin{bmatrix}
\frac{\partial}{\partial u}\left(\frac{\mathrm{d}[\mathcal{X}_{ij}]_1}{\mathrm{d}v}\right) \\
\vdots \\
\frac{\partial}{\partial u}\left(\frac{\mathrm{d}[\mathcal{X}_{ij}]_n}{\mathrm{d}v}\right) \\
\frac{\partial}{\partial u}\left(\frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v}\right)
\end{bmatrix}
= -
\begin{bmatrix}
b_1^{u,v} \\
b_2^{u,v} \\
\vdots \\
b_{n+1}^{u,v}
\end{bmatrix}$$

for each variable u and for each variable v of the function F. The components of the right-hand side of this system are given by

$$b_\ell^{u,v} = \frac{\partial^2 F_\ell}{\partial u \partial v} + \frac{\partial^2 F_\ell}{\partial u \partial \mathcal{U}_{ij}} \frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v} + \sum_{k=1}^{n} \frac{\partial^2 F_\ell}{\partial u \partial [\mathcal{X}_{ij}]_k} \frac{\mathrm{d}[\mathcal{X}_{ij}]_k}{\mathrm{d}v} + \frac{\partial G_\ell^v}{\partial \mathcal{U}_{ij}} \frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}u} + \sum_{k=1}^{n} \frac{\partial G_\ell^v}{\partial [\mathcal{X}_{ij}]_k} \frac{\mathrm{d}[\mathcal{X}_{ij}]_k}{\mathrm{d}u}$$

for each $\ell \in \{1, \ldots, n+1\}$. Notice that the coefficient matrix of this linear system does not depend on the variables u and v. Therefore, for each $i, j \in \{1, \ldots, m\}$ such that $i < j$, we have $(n+q)(2(n+q)+1)$ linear systems (one for each pair of variables u and v of the function F) with $n+1$ variables each one, and all of them have the same coefficient matrix.

A.3.2.4 Second order partial derivatives of F

We now present the second order partial derivatives of the function F. For each $k \in \{1, \ldots, n\}$, we have

$$\frac{\partial^2 F}{\partial [c_i]_k \partial c_i} = \frac{\partial^2 F}{\partial [c_j]_k \partial c_j} = \frac{\partial^2 F}{\partial [c_i]_k \partial c_j} = \mathbf{0}_{4,n}$$

and, for each $\omega_j \in \mathcal{O}_j$, we have

$$\frac{\partial^2 F}{\partial \omega_j \partial c_i} = \frac{\partial^2 F}{\partial \omega_j \partial c_j} = \mathbf{0}_{4,n}.$$

For each $\omega_i \in \mathcal{O}_i$, we have

$$\frac{\partial^2 F}{\partial \omega_i \partial c_i} = \begin{bmatrix} -P_i^{-\frac{1}{2}} \frac{\partial Q_i}{\partial \omega_i}^\top \\ \mathbf{0}_{1,n} \end{bmatrix}$$

and

$$\frac{\partial^2 F}{\partial \omega_i \partial c_j} = \begin{bmatrix} P_i^{-\frac{1}{2}} \frac{\partial Q_i}{\partial \omega_i}^\top \\ \mathbf{0}_{1,n} \end{bmatrix}.$$

For each $\omega, \sigma \in \mathcal{O}_i \cup \mathcal{O}_j$, we have

$$\frac{\partial^2 F}{\partial \sigma \partial \omega} = \begin{bmatrix} \mathcal{U}_{ij} \left(\frac{\partial^2 V_{ij}}{\partial \sigma \partial \omega}^\top V_{ij} + \frac{\partial V_{ij}}{\partial \omega}^\top \frac{\partial V_{ij}}{\partial \sigma} + \frac{\partial V_{ij}}{\partial \sigma}^\top \frac{\partial V_{ij}}{\partial \omega} + V_{ij}^\top \frac{\partial^2 V_{ij}}{\partial \sigma \partial \omega} \right) \mathcal{X}_{ij} - P_i^{-\frac{1}{2}} \frac{\partial^2 Q_i}{\partial \sigma \partial \omega}^\top (c_i - c_j) \\ \left[\left(\frac{\partial V_{ij}}{\partial \sigma} \mathcal{X}_{ij} \right)^\top \frac{\partial V_{ij}}{\partial \omega} + \left(V_{ij} \mathcal{X}_{ij} \right)^\top \frac{\partial^2 V_{ij}}{\partial \sigma \partial \omega} \right] \mathcal{X}_{ij} \end{bmatrix}.$$

With respect to the implicit variables, we have

$$\frac{\partial^2 F}{\partial \mathcal{U}_{ij} \partial \mathcal{X}_{ij}} = \begin{bmatrix} S_{ij} \\ \mathbf{0}_{1,n} \end{bmatrix},$$

$$\frac{\partial^2 F}{\partial \mathcal{U}_{ij} \partial \mathcal{U}_{ij}} = \mathbf{0}_{4,1},$$

$$\frac{\partial^2 F}{\partial c_i \partial \mathcal{U}_{ij}} = \frac{\partial^2 F}{\partial c_j \partial \mathcal{U}_{ij}} = \frac{\partial^2 F}{\partial [c_i]_k \partial \mathcal{X}_{ij}} = \frac{\partial^2 F}{\partial [c_j]_k \partial \mathcal{X}_{ij}} = \mathbf{0}_{4,n},$$
$$\frac{\partial^2 F}{\partial [\mathcal{X}_{ij}]_k \partial \mathcal{X}_{ij}} = \begin{bmatrix} \mathbf{0}_{n,n} \\ \left([S_{ij}]_{:,k} \right)^\top \end{bmatrix}$$

for each $k \in \{1, \ldots, n\}$ and, for each $\omega \in \mathcal{O}_i \cup \mathcal{O}_j$, we have

$$\frac{\partial^2 F}{\partial \omega \partial \mathcal{U}_{ij}} = \begin{bmatrix} \left(\frac{\partial V_{ij}}{\partial \omega}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \omega} \right) \mathcal{X}_{ij} \\ 0 \end{bmatrix}$$

and

$$\frac{\partial^2 F}{\partial \omega \partial \mathcal{X}_{ij}} = \begin{bmatrix} \mathcal{U}_{ij} \left(\frac{\partial V_{ij}}{\partial \omega}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \omega} \right) \\ \left(\left(\frac{\partial V_{ij}}{\partial \omega}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \omega} \right) \mathcal{X}_{ij} \right)^\top \end{bmatrix}.$$

A.3.2.5 Right-hand side of the linear system

Let $u, v \in \left\{ [c_i]_{k_1}, [c_j]_{k_2} \right\}$ for some $k_1 \in \{1, \ldots, n\}$ and for some $k_2 \in \{1, \ldots, n\}$. We have

$$b^{u,v} = \begin{bmatrix} S_{ij} \left(\frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}u} \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}v} + \frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v} \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}u} \right) \\ \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}v}^\top S_{ij} \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}u} \end{bmatrix}.$$

Let $u = \omega \in \mathcal{O}_i$ and $v = [c_i]_k$ for some $k \in \{1, \ldots, n\}$. We have

$$b^{u,v} = \begin{bmatrix} -P_i^{-\frac{1}{2}} \frac{\partial Q_i}{\partial \omega}^\top \\ \mathbf{0}_{1,n} \end{bmatrix}_{:,k} + \frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v} \begin{bmatrix} \left(\frac{\partial V_{ij}}{\partial \omega}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \omega} \right) \mathcal{X}_{ij} \\ 0 \end{bmatrix} + \begin{bmatrix} \mathcal{U}_{ij} \left(\frac{\partial V_{ij}}{\partial \omega}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \omega} \right) \\ \mathcal{X}_{ij}^\top \left(\frac{\partial V_{ij}}{\partial \omega}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \omega} \right) \end{bmatrix} \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}v} +$$
$$\begin{bmatrix} S_{ij} \left(\frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}u} \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}v} + \frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v} \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}u} \right) \\ 0 \end{bmatrix} + \begin{bmatrix} \mathbf{0}_{n,1} \\ \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}v}^\top S_{ij} \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}u} \end{bmatrix}.$$

Let $u = \omega \in \mathcal{O}_i$ and $v = [c_j]_k$ for some $k \in \{1, \ldots, n\}$. We have

$$b^{u,v} = \begin{bmatrix} P_i^{-\frac{1}{2}} \frac{\partial Q_i}{\partial \omega}^\top \\ \mathbf{0}_{1,n} \end{bmatrix}_{:,k} + \frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v} \begin{bmatrix} \left(\frac{\partial V_{ij}}{\partial \omega}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \omega} \right) \mathcal{X}_{ij} \\ 0 \end{bmatrix} + \begin{bmatrix} \mathcal{U}_{ij} \left(\frac{\partial V_{ij}}{\partial \omega}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \omega} \right) \\ \mathcal{X}_{ij}^\top \left(\frac{\partial V_{ij}}{\partial \omega}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \omega} \right) \end{bmatrix} \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}v} +$$
$$\begin{bmatrix} S_{ij} \left(\frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}u} \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}v} + \frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v} \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}u} \right) \\ 0 \end{bmatrix} + \begin{bmatrix} \mathbf{0}_{n,1} \\ \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}v}^\top S_{ij} \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}u} \end{bmatrix}.$$

Let $u = \omega \in \mathcal{O}_j$ and $v = [c_i]_k$ or $v = [c_j]_k$ for some $k \in \{1, \dots, n\}$. We have

$$b^{u,v} = \frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v} \begin{bmatrix} \left(\frac{\partial V_{ij}}{\partial \omega}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \omega} \right) \mathcal{X}_{ij} \\ 0 \end{bmatrix} + \begin{bmatrix} \mathcal{U}_{ij} \left(\frac{\partial V_{ij}}{\partial \omega}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \omega} \right) \\ \mathcal{X}_{ij}^\top \left(\frac{\partial V_{ij}}{\partial \omega}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \omega} \right) \end{bmatrix} \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}v} +$$

$$\begin{bmatrix} S_{ij} \left(\frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}u} \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}v} + \frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v} \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}u} \right) \\ 0 \end{bmatrix} + \begin{bmatrix} \mathbf{0}_{n,1} \\ \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}v}^\top S_{ij} \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}u} \end{bmatrix}.$$

Let $u = \omega \in \mathcal{O}_i \cup \mathcal{O}_j$ and $v = \sigma \in \mathcal{O}_i \cup \mathcal{O}_j$. We have

$$b^{u,v} = \begin{bmatrix} \mathcal{U}_{ij} \left(\frac{\partial^2 V_{ij}}{\partial \sigma \partial \omega}^\top V_{ij} + \frac{\partial V_{ij}}{\partial \omega}^\top \frac{\partial V_{ij}}{\partial \sigma} + \frac{\partial V_{ij}}{\partial \sigma}^\top \frac{\partial V_{ij}}{\partial \omega} + V_{ij}^\top \frac{\partial^2 V_{ij}}{\partial \sigma \partial \omega} \right) \mathcal{X}_{ij} - P_i^{-\frac{1}{2}} \frac{\partial^2 Q_i}{\partial \sigma \partial \omega}^\top (c_i - c_j) \\ \left[\left(\frac{\partial V_{ij}}{\partial \sigma} \mathcal{X}_{ij} \right)^\top \frac{\partial V_{ij}}{\partial \omega} + \left(V_{ij} \mathcal{X}_{ij} \right)^\top \frac{\partial^2 V_{ij}}{\partial \sigma \partial \omega} \right] \mathcal{X}_{ij} \end{bmatrix} +$$

$$\frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v} \begin{bmatrix} \left(\frac{\partial V_{ij}}{\partial \omega}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \omega} \right) \mathcal{X}_{ij} \\ 0 \end{bmatrix} + \begin{bmatrix} \mathcal{U}_{ij} \left(\frac{\partial V_{ij}}{\partial \omega}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \omega} \right) \\ \mathcal{X}_{ij}^\top \left(\frac{\partial V_{ij}}{\partial \omega}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \omega} \right) \end{bmatrix} \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}v} +$$

$$\frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}u} \left(\begin{bmatrix} \left(\frac{\partial V_{ij}}{\partial \sigma}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \sigma} \right) \mathcal{X}_{ij} \\ 0 \end{bmatrix} + \begin{bmatrix} S_{ij} \\ \mathbf{0}_{1,n} \end{bmatrix} \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}v} \right) +$$

$$\left(\begin{bmatrix} \mathcal{U}_{ij} \left(\frac{\partial V_{ij}}{\partial \sigma}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \sigma} \right) \\ \mathcal{X}_{ij}^\top \left(\frac{\partial V_{ij}}{\partial \sigma}^\top V_{ij} + V_{ij}^\top \frac{\partial V_{ij}}{\partial \sigma} \right) \end{bmatrix} + \frac{\mathrm{d}\mathcal{U}_{ij}}{\mathrm{d}v} \begin{bmatrix} S_{ij} \\ \mathbf{0}_{1,n} \end{bmatrix} + \begin{bmatrix} \mathbf{0}_{n,n} \\ \left(S_{ij} \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}v} \right)^\top \end{bmatrix} \right) \frac{\mathrm{d}\mathcal{X}_{ij}}{\mathrm{d}u}.$$

Bibliography

[1] B. J. Alder and T. E. Wainwright. Phase transition for a hard sphere system. *Journal of Chemical Physics*, 27(5):1208–1209, 1957.

[2] R. Andreani, E. G. Birgin, J. M. Martínez, and M. L. Schuverdt. On Augmented Lagrangian methods with general lower-level constraints. *SIAM Journal on Optimization*, 18:1286–1309, 2007.

[3] M. Andretta, E. G. Birgin, and J. M. Martínez. Practical active-set Euclidian trust-region method with spectral projected gradients for bound-constrained minimization. *Optimization*, 54(3):305–325, 2005.

[4] J. D. Bernal. Geometrical Approach to the Structure of Liquids. *Nature*, 183(4655):141–147, 1959.

[5] D. P. Bertsekas. *Nonlinear Programming.* Athena Scientific, Belmont, MA, USA, 2nd edition, 1999.

[6] E. G. Birgin, L. H. Bustamante, H. F. Callisaya, and J. M. Martínez. Packing circles within ellipses. *International Transactions in Operational Research*, 20(3):365–389, 2013.

[7] E. G. Birgin, L. H. Bustamante, H. F. Callisaya, and J. M. Martínez. Packing circles within ellipses. *International Transactions in Operational Research*, 20(3):365–389, 2013.

[8] E. G. Birgin, C. A. Floudas, and J. M. Martínez. Global minimization using an Augmented Lagrangian method with variable lower-level constraints. *Mathematical Programming*, 125(1):139–162, 2010.

[9] E. G. Birgin and J. M. Gentil. New and improved results for packing identical unitary radius circles within triangles, rectangles and strips. *Computers & Operations Research*, 37(7):1318 – 1327, 2010.

[10] E. G. Birgin and R. D. Lobato. Orthogonal packing of identical rectangles within isotropic convex regions. *Computers & Industrial Engineering*, 59(4):595 – 602, 2010.

[11] E. G. Birgin and J. M. Martínez. A box-constrained optimization algorithm with negative curvature directions and spectral projected gradients. *Computing [Suppl]*, 15:49–60, 2001.

[12] E. G. Birgin and J. M. Martínez. Large-scale active-set box-constrained optimization method with spectral projected gradients. *Computational Optimization and Applications*, 23:101–125, 2002.

[13] E. G. Birgin and J. M. Martínez. *Practical Augmented Lagrangian Methods for Constrained Optimization*. Society for Industrial and Applied Mathematics, Philadelphia, PA, 2014.

[14] E. G. Birgin, J. M. Martínez, F. H. Nishihara, and D. P. Ronconi. Orthogonal packing of rectangular items within arbitrary convex regions by nonlinear optimization. *Computers & Operations Research.*, 33(12):3535–3548, December 2006.

[15] E. G. Birgin, J. M. Martínez, and M. Raydan. Nonmonotone Spectral Projected Gradient Methods on Convex Sets. *SIAM Journal on Optimization*, 10(4):1196–1211, 2000.

[16] E. G. Birgin, J. M. Martínez, and M. Raydan. Algorithm 813: SPG–Software for Convex-Constrained Optimization. *ACM Transactions on Mathematical Software*, 27(3):340–349, September 2001.

[17] E. G. Birgin, J. M. Martínez, and D. P. Ronconi. Optimizing the packing of cylinders into a rectangular container: A nonlinear approach. *European Journal of Operational Research*, 160(1):19 – 33, 2005.

[18] E. G. Birgin and F. N. C. Sobral. Minimizing the object dimensions in circle and sphere packing problems. *Computers & Operations Research*, 35(7):2357 – 2375, 2008.

[19] I. Castillo, F. J. Kampas, and J. D. Pintér. Solving circle packing problems by global optimization: Numerical results and industrial applications. *European Journal of Operational Research*, 191(3):786 – 802, 2008.

[20] P. Chaikin. Thermodynamics and hydrodynamics of hard spheres: the role of gravity. In M. E. Cates and M. R. Evans, editor, *Soft and Fragile Matter: Nonequilibrium Dynamics, Metastability and Flow*, volume 53, pages 315–348, Bristol, UK, 2000. Institute of Physics Publishing.

[21] Z. D. Cheng, W. B. Russell, and P. M. Chaikin. Controlled growth of hard-sphere colloidal crystals. *Nature*, 401(6756):893–895, 1999.

[22] J. H. Conway and N. J. A. Sloane. *Sphere packings, lattices and groups*, volume 290 of *Grundlehren der math. Wissenschaften*. Springer-Verlag New York, 1999.

[23] A. Donev, I. Cisse, D. Sachs, E. Variano, F. H. Stillinger, R. Connelly, S. Torquato, and P. M. Chaikin. Improving the density of jammed disordered packings using ellipsoids. *Science*, 303(5660):990–993, 2004.

[24] S. F. Edwards. The Role of Entropy in the Specification of a Powder. In A. Mehta, editor, *Granular Matter: An Interdisciplinary Approach*, pages 121–140, New York, 1994. Springer–Verlag.

[25] R. Fourer, D. M. Gay, and B. W. Kernighan. *AMPL – A Modeling Language for Mathematical Programming*. Duxbury Press, 2nd edition, 2002.

[26] Sh. I. Galiev and M. S. Lisafina. Numerical optimization methods for packing equal orthogonally oriented ellipses in a rectangular domain. *Computational Mathematics and Mathematical Physics*, 53(11):1748–1762, 2013.

[27] G. H. Golub and C. F. Van Loan. *Matrix computations (3rd ed.)*. Johns Hopkins University Press, Baltimore, MD, USA, 1996.

[28] T. C. Hales. A proof of the Kepler conjecture. *Annals of Mathematics*, 162(3):1065–1185, 2005.

[29] T. C. Hales. Historical Overview of the Kepler Conjecture. *Discrete & Computational Geometry*, 36(1):5–20, 2006.

[30] S. He and H.-K. Xu. Uniqueness of supporting hyperplanes and an alternative to solutions of variational inequalities. *Journal of Global Optimization*, 55(4):1375–1384, 2012.

[31] G. B. Hughes and M. Chraibi. Calculating ellipse overlap areas. *Computing and Visualization in Science*, 15(5):291–301, 2012.

[32] A. F. Izmailov, M. V. Solodov, and E. I. Uskov. Global Convergence of Augmented Lagrangian Methods Applied to Optimization Problems with Degenerate Constraints, Including Problems with Complementarity Constraints. *SIAM Journal on Optimization*, 22(4):1579–1606, 2012.

[33] A.F. Izmailov, M.V. Solodov, and E.I. Uskov. Combining stabilized SQP with the augmented Lagrangian algorithm. *Computational Optimization and Applications*, 62(2):405–429, 2015.

[34] H. M. Jaeger and S. R. Nagel. Physics of the granular state. *Science*, 255(5051):1523–1531, 1992.

[35] H. M. Jaeger, S. R. Nagel, and R. P. Behringer. Granular solids, liquids, and gases. *Reviews of Modern Physics*, 68(4):1259–1273, 1996.

[36] J. Kallrath. Packing ellipsoids into volume-minimizing rectangular boxes. *Journal of Global Optimization*. doi:10.1007/s10898-015-0348-6.

[37] J. Kallrath. Cutting circles and polygons from area-minimizing rectangles. *Journal of Global Optimization*, 43(2-3):299–328, 2009.

[38] J. Kallrath and S. Rebennack. Cutting ellipses from area-minimizing rectangles. *Journal of Global Optimization*, 59(2-3):405–437, 2014.

[39] Y. Lin and L. Schrage. The global solver in the LINDO API. *Optimization Methods and Software*, 24(4-5):657–668, 2009.

[40] L.-Z. Lu and C. E. M. Pearce. Some new bounds for singular values and eigenvalues of matrix products. *Annals of Operations Research*, 98(1):141–148, 2000.

[41] B. D. Lubachevsky and F. H. Stillinger. Geometric properties of random disk packings. *Journal of Statistical Physics*, 60(5-6):561–583, 1990.

[42] J. M. Martínez. Local minimizers of quadratic functions on euclidean balls and spheres. *SIAM Journal on Optimization*, 4(1):159–176, 1994.

[43] L. Martínez, R. Andrade, E. G. Birgin, and J. M. Martínez. Packmol: A package for building initial configurations for molecular dynamics simulations. *Journal of Computational Chemistry*, 30(13):2157–2164, 2009.

[44] C. D. Meyer. *Matrix Analysis and Applied Linear Algebra*. Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 2000.

[45] R. Misener and C. A. Floudas. GloMIQO: Global mixed-integer quadratic optimizer. *Journal of Global Optimization*, 57(1):3–50, 2013.

[46] H. D. Mittelmann and F. Vallentin. High-accuracy semidefinite programming bounds for kissing numbers. *Experimental Mathematics*, 19(2):175–179, 2010.

[47] A. Pankratov, T. Romanova, and O. Khlud. Quasi-phi-functions in packing of ellipsoids. *Radioelectronics & Informatics*, 68:37–42, 2015.

[48] P. N. Pusey. Colloidal Suspensions. In J. P. Hansen and D. Levesque and J. Zinnjustin, editor, *Liquids, Freezing and Glass Transition, PT 2*, volume 51 of *Les Houches Summer School Session*, pages 763–942, Amsterdam, 1991. Elsevier Science Publishers B. V.

[49] M. D. Rintoul and S. Torquato. Metastability and crystallization in hard-sphere systems. *Physical Review Letters*, 77(20):4198–4201, Nov 1996.

[50] R. T. Rockafellar. *Convex Analysis*, volume 28 of *Princeton Mathematical Series*. Princeton University Press, Princeton, NJ, USA, 1970.

[51] N. V. Sahinidis. *BARON 14.3.1: Global Optimization of Mixed-Integer Nonlinear Programs,* User's Manual, 2014.

[52] Y. G. Stoyan, A. Pankratov, and T. Romanova. Quasi-phi-functions and optimal packing of ellipses. *Journal of Global Optimization*, 65(2):283–307, 2016.

[53] Y. G. Stoyan and G. Yas'kov. A mathematical model and a solution method for the problem of placing various-sized circles into a strip. *European Journal of Operational Research*, 156(3):590 – 600, 2004.

[54] Y. G. Stoyan and G. Yas'kov. Packing congruent hyperspheres into a hypersphere. *Journal of Global Optimization*, 52(4):855–868, 2012.

[55] Y. G. Stoyan and G. Yas'kov. Packing equal circles into a circle with circular prohibited areas. *International Journal of Computer Mathematics*, 89(10):1355–1369, 2012.

[56] Y. G. Stoyan, M. V. Zlotnik, and A. Chugay. Solving an optimization packing problem of circles and non-convex polygons with rotations into a multiply connected region. *Journal of the Operational Research Society*, 63(3):379–391, 2012.

[57] C. Uhler and S. J. Wright. Packing Ellipsoids with Overlap. *SIAM Review*, 55(4):671–706, 2013.