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3D Malfatti's constrained optimization problem

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Abstract: In 1803, the Italian mathematician Malfatti posed a problem of packing three non-overlapping circles of maximum total area within a given triangle. Malfatti initially believed that the optimal solution involved three circles inscribed within the triangle, each tangent to the other two and touching two sides of the triangle. However, it is now widely recognized that this solution is not optimal. The problem for the first time was formulated as a global optimization problem in [9]. In this paper, we introduce a new formulation of Malfatti's problem, referred to as the $3D$ Malfatti's constrained optimization problem in three-dimensional space. The problem is presented as a nonconvex optimization problem with nonlinear constraints, and numerical experiments were conducted using Python for various cases.

Key words: Malfatti's problem, Nonconvex optimization, sphere

1. Introduction

In 1803, Gian Francesco Malfatti posed a now-classic optimization problem: determining the best way to pack three non-overlapping circles within a given triangle, maximizing their total area. Malfatti's initial hypothesis was that the optimal solution would involve three circles, each tangent to the other two and touching two sides of the triangle. This configuration, which became known as "Malfatti's Circles,"was long assumed to be the solution. However, subsequent mathematical research revealed that this arrangement did not, in fact, yield the maximal total area.

Over the past two centuries, Malfatti's problem has intrigued mathematicians and evolved considerably. Numerous studies have explored alternative solutions using advanced algebraic and geometric methods $[2-9]$. For example, Zalgaller and Los (1994) demonstrated that a "greedy"algorithm, which incrementally maximizes each circle's area, can achieve a better total area than the classic Malfatti solution [4]. Such insights have broadened our understanding of the problem, showing that optimal solutions can differ significantly from intuitive geometric arrangements.

Recent developments have recast Malfatti's problem as a global optimization task, leveraging more rigorous mathematical techniques. One of the notable extensions in the field is presented by Barkova and Strekalovsky (2016), who formulated Malfatti's problem in higher-dimensional spaces through global optimization methods. Their work demonstrated the effectiveness of global optimization in addressing complex constraints and revealed new possibilities for solving high-dimensional variants of Malfatti's classical problem [10].

In 2017, Anikin and Gornov further extended this idea by reducing the generalized Malfatti problem to a global optimization framework. They proposed a reduction technique that simplified the computational complexity, making it easier to achieve more precise solutions in generalized contexts [11]. This reduction framework has provided a solid foundation for exploring other complex geometric optimization problems.

Building on these advancements, Enkhbat (2020) formulated the generalized sphere packing problem as a convex maximization problem. This work introduced new optimization formulations, bridging the gap between classical geometric packing problems and modern convex optimization techniques [12].

A multi-objective optimization approach to Malfatti's problem was proposed by Battur (2021). In this study, they employed multi-objective optimization techniques to extend the problem and explored trade-offs between different optimization objectives, contributing a new dimension to the problem's complexity [13].

In addition to these extensions, they formulated the generalized Malfatti problem as a Generalized Nash Equilibrium (GNE) problem. Their approach integrated game theory into the classical optimization problem, offering novel insights into strategic interactions and equilibrium solutions in geometric contexts [14].

The High dimensional Malfatti's problem has found an economic application in [18]. In this paper, one-sphere packing problem was used in a profitability analysis of a company.

In this paper, we extend Malfatti's problem into three-dimensional space, resulting in what we refer to as the $3D$ Malfatti's constrained optimization problem. In this extended problem, the aim is to inscribe three non-overlapping spheres within a given tetrahedron to maximize their total volume while centers of spheres belong to given hyperplanes. This three-dimensional variation adds new layers of complexity, as the spheres' positioning must consider not just two, but three axes of interaction, introducing nonlinear constraints within a nonconvex optimization framework.

2. Methodology

2.1. Malfatti's problem and convex maximization

In the process of transforming Malfatti's problem into an optimization problem, several key steps must be undertaken. Initially, it is imperative to express the problem in equivalent terms, which involves the utilization of convex sets, notably a ball and a triangle set. Subsequently, the focus shifts towards establishing the conditions that govern the inscribed placement of balls within a triangle set. To facilitate this endeavor, a set of relevant sets is introduced, serving as foundational components for further analysis and problem formulation.

Let $B(x,r)$ be a ball with a center $x \in \mathbb{R}^n$ and radius $r \in \mathbb{R}$,

$$B\,(x,r) = \{y \in \mathbb{R}^n | \|y - x\| \le r\}. \tag{2.1}$$

Let D be a polyhedral set given by the following linear inequalities.

$$D = \{x \in \mathbb{R}^n | \langle a^i, x\rangle \le b_i,\ i = \overline{1,m}\}, \quad a^i \in \mathbb{R}^n, \quad b_i \in \mathbb{R}, \tag{2.2}$$

here $\langle , \rangle$ denotes the scalar product of two vectors in $\mathbb{R}^n$, and $\|\cdot\|$ is Euclidean norm, $a^i \ne a^j,\ i \ne j;\ i,j = \overline{1,m}$ and int $D \ne \emptyset$. Assume that D is a compact set. Clearly, D is convex set in $\mathbb{R}^n$.

Theorem 2.1. *[9, 10] $B\,(x,r) \subset D$ if and only if*

$$\langle a^i, x\rangle + r\|a^i\| \le b_i, \quad i = \overline{1,m}. \tag{2.3}$$

Now, we formulate the conditions for packing three spheres within a polyhedral set with constraints imposed on centers. Assume that the interiors of these spheres do not overlap.

One of the spheres is tangent to the other two, but their centers do not lie on the same plane. Simultaneously, the latter two spheres do not intersect with each other.

Denote by $u(x_1, x_2, \dots, x_n)$, $v(x_{n+1}, x_{n+2}, \dots, x_{2n})$, and $p(x_{2n+1}, x_{2n+2}, \dots, x_{3n})$ the centers of the three balls inscribed in a polyhedral set D as given by (2.2). Let x_{3n+1}, x_{3n+2} and x_{3n+3} be their corresponding radii. 3D Malfatti's constrained optimization problem is then formulated as follows:

$$\max f(x) = \frac{\pi^{\frac{n}{2}}}{\Gamma(\frac{n}{2}+1)}(x_{3n+1}^n + x_{3n+2}^n + x_{3n+3}^n), \tag{2.4}$$

$$\langle a^i, u\rangle + x_{3n+1}\|a^i\| \le b_i, \quad u = (x_1, x_2, x_3), \quad i = 1, 2, 3, \tag{2.5}$$

$$\langle a^i, v\rangle + x_{3n+2}\|a^i\| \le b_i, \quad v = (x_4, x_5, x_6), \quad i = 1, 2, 3, \tag{2.6}$$

$$\langle a^i, p\rangle + x_{3n+3}\|a^i\| \le b_i, \quad p = (x_7, x_8, x_9), \quad i = 1, 2, 3, \tag{2.7}$$

$$\|u - v\|^2 \le (x_{3n+1} + x_{3n+2})^2, \tag{2.8}$$

$$\|u - p\|^2 \le (x_{3n+1} + x_{3n+3})^2, \tag{2.9}$$

$$\|p - v\|^2 \le (x_{3n+2} + x_{3n+3})^2, \tag{2.10}$$

$$x_{3n+1} \ge 0, \quad x_{3n+2} \ge 0, \quad x_{3n+3} \ge 0. \tag{2.11}$$

Additional constraints for the centers are:

$$g_1(u) = 0, \quad g_2(v) = 0, \quad g_3(p) = 0. \tag{2.12}$$

$\Gamma(x)$ be the gamma-function. Let g_1, g_2 and g_3 be linear functions defined on a set in $\mathbb{R}^3$. The function f in (2.4) represents the total area of the three spheres. Thus, problem (2.5) – (2.12) becomes a convex maximization problem over a nonconvex set.

2.2. The Gekko Optimization Algorithm

The Gekko optimization algorithm is a powerful and versatile tool for solving a wide range of optimization problems in fields such as engineering, finance, operations research, and more. Gekko is a Python library specifically designed for optimization and modeling of dynamic systems. It effectively addresses both constrained and unconstrained optimization problems, making it suitable for diverse applications. In particular, it is known for handling complex mathematical problems that involve differential equations and dynamic simulations, which are often challenging for traditional optimization techniques [15]. In our study, we utilized the APOPT solver, an integral part of the Gekko suite, to tackle a large-scale nonlinear programming problem. APOPT stands out for its ability to solve nonlinear programming (NLP) problems, including mixed-integer nonlinear programming (MINLP) scenarios [16]. This solver is particularly adept at handling large, intricate problems where both integer and continuous variables are present. The APOPT solver employs the interior point optimization technique, which explores the feasible region's interior by iteratively refining the search direction to converge on optimal solutions [17].

Key Aspects of the Interior Point Method:

1. Barrier Function: This technique involves a barrier function that penalizes infeasible points, thereby guiding the optimization process toward the interior of the feasible region. This helps ensure that the solution remains within bounds and respects all constraints.
2. Central Path: The solver follows a central path during optimization. This means it maintains a trajectory within the feasible region, balancing between the need to satisfy constraints and the drive toward optimizing the objective function.
3. Optimality Conditions: APOPT is designed to find points that satisfy the Karush-Kuhn-Tucker (KKT) conditions, representing the first-order optimality criteria for constrained optimization problems.

4. Iterative Refinement: The method involves iteratively adjusting penalty parameters and search directions, which allows the solver to refine the solution with each step until it reaches convergence, providing both accuracy and efficiency.

3. The numerical results

To test the capabilities of the Gekko algorithm, we applied it to a challenging geometric optimization problem involving a tetrahedron with vertices at A(1,1,0), B(4,1,0), C(3,3,0) and D(5,4,3). This configuration presented a complex scenario for evaluating the solver's performance due to the geometric properties and constraints involved. The task required solving a convex maximization problem, involving a reduction of Malfatti's problem into a three-dimensional space with added constraints. Now we have the following problem:

$$
\begin{aligned}
\max f = \frac{4}{3}\pi(x_{10}^3 + x_{11}^3 + x_{12}^3),\\
-x_3 + x_{10} \le 0,\\
-3x_1 + 3x_2 + x_3 + \sqrt{19}x_{10} \le 0,\\
-3x_2 + 3x_3 + \sqrt{18}x_{10} \le -3,\\
6x_1 + 3x_2 - 5x_3 + \sqrt{70}x_{10} \le 27,\\
-x_6 + x_{11} \le 0,\\
-3x_4 + 3x_5 + x_6 + \sqrt{19}x_{11} \le 0,\\
-3x_5 + 3x_6 + \sqrt{18}x_{11} \le -3,\\
6x_4 + 3x_5 - 5x_6 + \sqrt{70}x_{11} \le 27,\\
-x_9 + x_{12} \le 0,\\
-3x_7 + 3x_8 + x_9 + \sqrt{19}x_{12} \le 0,\\
-3x_8 + 3x_9 + \sqrt{18}x_{12} \le -3,\\
6x_7 + 3x_8 - 5x_9 + \sqrt{70}x_{12} \le 27,\\
(x_4 - x_1)^2 + (x_5 - x_2)^2 + (x_6 - x_3)^2 - (x_{10} + x_{11})^2 \ge 0,\\
(x_7 - x_4)^2 + (x_8 - x_5)^2 + (x_9 - x_6)^2 - (x_{11} + x_{12})^2 \ge 0,\\
(x_7 - x_1)^2 + (x_8 - x_2)^2 + (x_9 - x_3)^2 - (x_{10} + x_{12})^2 \ge 0,\\
x_{10} \ge 0,\ x_{11} \ge 0,\ x_{12} \ge 0.
\end{aligned}
$$

Additional constraints for centers:

$$
\begin{aligned}
&Case\ 1: \quad x_3 - 1.1138 = 0, \quad x_6 - 0.5026 = 0, \quad x_9 - 0.3336 = 0,\\
&Case\ 2: \quad x_2 - 2.9808 = 0, \quad x_5 - 2.2134 = 0, \quad x_8 - 2.6506 = 0,\\
&Case\ 3: \quad x_2 - 3x_3 = 0, \quad x_4 - 3x_6 = 0, \quad x_7 - 2x_8 + 1 = 0.
\end{aligned}
$$

The performance of the proposed algorithm was tested on the above constrained 3D Malfatti's problem. The programming code for the algorithm was written in Python. The optimal solution results are shown in Figures 1, 2 and 3.

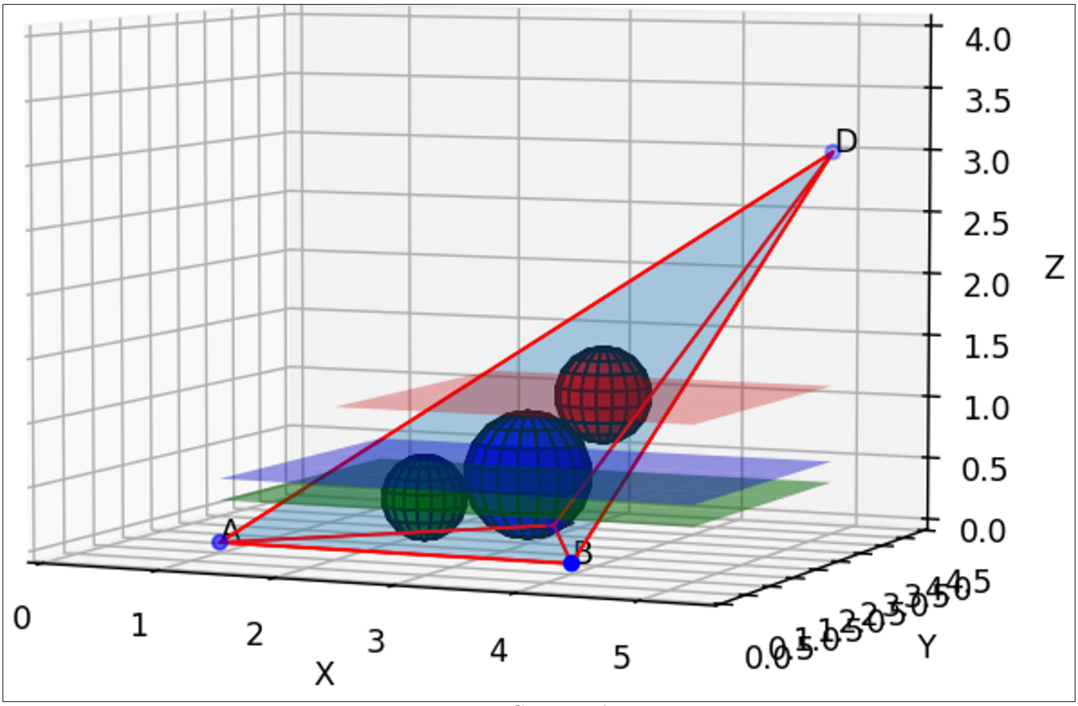

Figure 1: Case 1 solution.

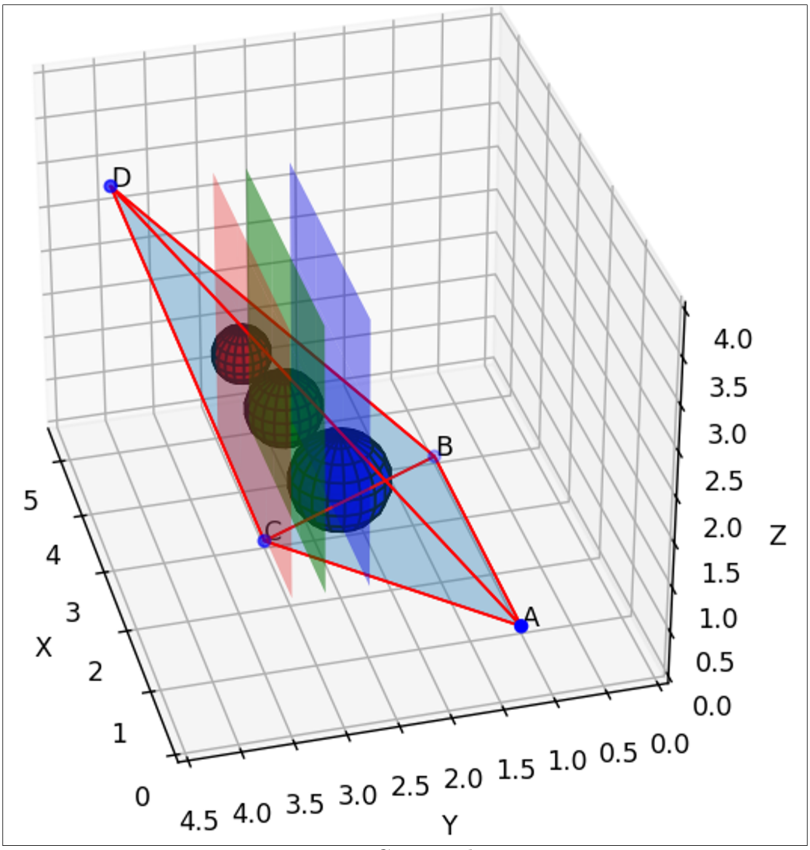

Figure 2: Case 2 solution.

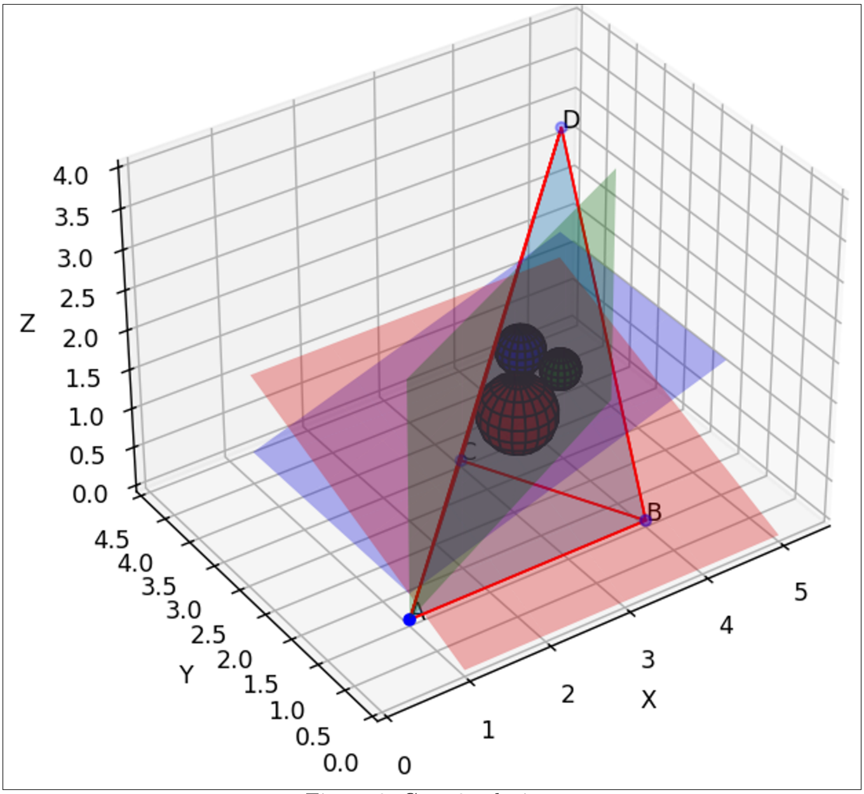

Figure 3: Case 3 solution.

For additional constraints, three planes were selected to be parallel along the Z and X axes (Case 1 and Case 2) and to intersect (Case 3).

The use of Gekko proved effective in addressing the intricacies of the 3D Malfatti's constrained optimization problem. Through its iterative interior point methods, the solver managed to find an optimal solution that respects the constraints, which was verified by ensuring that the KKT conditions were satisfied. This success demonstrates Gekko's robustness in solving complex nonlinear optimization problems with mixed constraints, even within the realm of geometric and spatial challenges. We have tested three cases of 3D Malfatti's problem. The results are given for each case in Table 1. From the table 1, we can see that case 1 provides the better result that case 2, 3.

Table 1: Numerical results (tetrahedron volume = 3).

Case	Total Volume of balls	Packed Volume (%)
Case 1	0.916	30.5
Case 2	0.859	28.7
Case 3	0.488	16.3

4. Conclusions

This study successfully extended Malfatti's classical optimization problem into a three-dimensional domain, yielding the 3D Malfatti constrained optimization problem. This reformulation involved the introduction of additional nonlinear constraints and complex geometric interactions within a nonconvex optimization framework, specifically addressing the challenge of maximizing the volume of three non-overlapping spheres inscribed within a given tetrahedron.

In conclusion, the extension of Malfatti's problem to three dimensions not only enriches the mathematical framework of classical geometric optimization but also highlights the adaptability of contemporary optimization algorithms to multidimensional, nonlinear challenges.

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