Applications of nonlinear programming to packing problems

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Abstract The problem of packing items within bounded regions in the Euclidean space has multiple applications in a variety of areas, such as, Physics, Chemistry, and Engineering. Problems of this type exhibit various levels of complexity. Nonlinear programming formulations and methods had been successfully applied to a wide range of packing problems. In this review paper, a brief description of the state-of-the-art and an illustrated overview of packing nonlinear programming techniques and applications will be presented.

1 Introduction

The problem of packing items within bounded areas has been widely studied over the last decades. Due to the amount of publications dedicated to packing and cutting problems, making a comprehensive review of the recent literature may be impossible. A simple search by the words "circle packing" in the Google Images search engine displays a myriad of amazing pictures describing theoretical results and applications. In this work we focus on models and techniques based on nonlinear programming.

Among the packing problems that can be addressed by nonlinear models and methods, the problem of packing identical or non-identical circular and spherical items presents several applications, such as origami design [17], analysis of concrete properties [23], study of the properties of forest soils and its influence in the development of roots [22], Gamma Knife radiosurgery [24], molecular dynamics simulations [19, 20], and industrial problems like facility location [13] and container loading [14], among others. More recently, the packing of three-dimensional polygons, such as thetrahedra, has also gained attention due to its applications to model

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low-temperature states of matter, including liquids, crystals, glasses, and powders (see, [12] and the references therein). In [8, 21] the concept of *sentinels* has been introduced as a tool to model the overlapping between polygons through the satisfaction of a finite set of continuous and differentiable constraints, that is one of the key ingredients to model packing problems as tractable nonlinear programming problems.

Nonlinear programming models include, in the objective function or the constraints, functions that "measure" the overlapping between every pair of items. As described in [26], these functions were named Φ-functions in [25]. Given a pair of items i and j, a function $\Phi_{ij}(\cdot)$ is said a Φ-function if its value is negative whenever items i and j overlap, null if they are tangent, and positive if they do not overlap. Every mathematical model related to a packing problem needs to deal with the items' overlapping and, in some way or another, makes use of and objective function or a set of constraints that can be seen as Φ-functions.

2 Packing of circles and spheres

The problem of packing a given set of items within an object with fixed dimensions may be modeled as a nonlinear (continuous and differentiable) feasibility problem. As an example, the problem of packing N circular items with radii $r_1, r_2, \dots, r_N$ within a circular object with radius R (with $R \geq r_i$ for all i) can be modeled as finding $(x_i, y_i)^T \in \mathbb{R}^2$ (for $i = 1, \dots, N$) such that

$$\begin{aligned} (x_i - x_j)^2 + (y_i - y_j)^2 &\geq (r_i + r_j)^2, \text{ for all } j > i, \\ x_i^2 + y_i^2 &\leq (R - r_i)^2, \text{ for all } i. \end{aligned} \tag{1}$$

In the problem described above, without loss of generality, it is assumed that the circular object is centered at the origin of the Cartesian coordinate system. The first set of equations says that the circular items must not overlap; while the second set of equations says that the items must be placed within the object. Both sets of equations are based on computing distances; and distances are squared to avoid the nondifferentiability of the square root at $x = 0$. Analogous models can be considered for different kinds of items and objects.

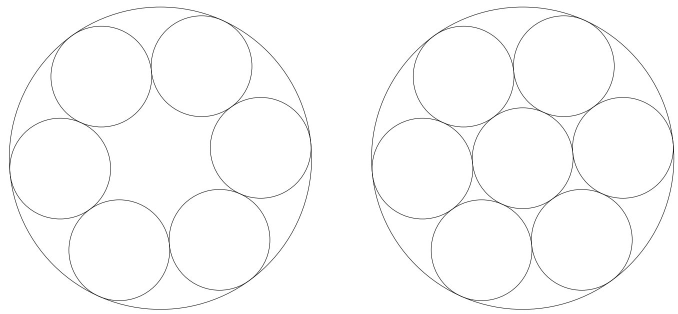
When the items to be packed are all identical, the considered goal may be maximizing the number of packed items within an object with fixed dimensions. In this case, the feasibility problem (1) may be used to solve the problem if an increasing number of items N is considered. More specifically, we may try to solve the feasibility problem (1) with $N = 1$. If we manage to find a solution, then we try with $N + 1$ until finding that for, let say, $N = \widehat{N}$, problem (1) is infeasible. In this case, the maximum number of identical items that can be packed is $\widehat{N} - 1$. In practice, guaranteeing that a nonlinear feasibility problem is infeasible is a very hard task. Therefore, we may fix some maximum effort we are able to do and, if within this limited amount of effort we are unable to find a solution, we may heuristically say that the problem is infeasible. At this point, many readers may think that it would be better to try some kind of bisection scheme instead of increasing N one by one. Assume that the maximum number of items that can be packed is N^*. Feasibility problems with $N < N^*$ are feasible and use to be simple (can be solved with a small computational effort). On the other hand, feasibility problems with $N > N^*$ are infeasible and detecting infeasibility may be very hard. For that reason, it is easier (cheaper) to approach N^* from below increasing N slowly. Of course, there is no need to start with $N = 1$ if it is known that the feasibility problem is feasible for some value $N = N_{\text{LB}}$. The described strategy was considered in [10] to pack identical circles within circles, in [3] to pack identical circles within ellipses, and in [9, 8, 5] to pack identical rectangles (with different types of constraints related to the rectangular items' angle of rotation) within arbitrary convex regions.

If the items to be packed are different and each item has an associated value (that may be proportional to the item's area), the goal may be maximizing the value of the packed items [18]. In this case, packing an increasing number of items as described in the paragraph above does not provide an optimal strategy. Selecting the subsets of items for which a feasibility nonlinear (sub)problem may be modeled and solved is a combinatorial problem for which heuristic strategies may be considered in practice. On the other hand, independently of the items being identical or not, if the object dimensions are not fixed, the goal may be finding the smallest object of a certain type (circle, square, equilateral triangle, rectangle with smallest perimeter or area, etc) within which a given set of items can be packed. In this case the problem can be modeled as an optimization problem. As an example, consider again the problem of packing a fixed number N circular items with radii $r_1, r_2, \dots, r_N$ within a circular object with variable radius R and assume that the problem is to minimize R. This problem can be easily formulated as

$$\begin{aligned} &\text{Minimize } R \\ &\text{subject to } (x_i - x_j)^2 + (y_i - y_j)^2 \geq (r_i + r_j)^2, \quad \text{for all } j > i, \\ &\qquad\qquad x_i^2 + y_i^2 \leq (R - r_i)^2, \qquad\qquad\quad \text{for all } i, \\ &\qquad\qquad R \geq \bar{r}, \end{aligned} \tag{2}$$

where $\bar{r} = \max_{1 \leq i \leq N}\{r_i\}$. Figure 1a shows the solution to the problem of finding the smallest circle within which $N = 6$ identical unitary-radius circular items can be packed. The solution corresponds to $R^* = 3$ [16, 15]. It is interesting to note that, within the circular object with $R = 3$, $N = 7$ identical unitary-radius circular items can also be packed (see Figure 1b). This means that there is no equivalence between the problem of minimizing the object dimensions and the problem of packing as many items as possible. Variations of the model (2) were considered in [4, 11] for packing identical circular items within circles, squares, equilateral triangles, and strips, among others. Models and methodology presented in [11] also deal with 3D problems. See Figure 2.

In [7, p.171], sphere packing problems with up to 1,000,000 spheres are considered as an illustration of the capabilities of a nonlinear programming solver named



(a) (b)

Fig. 1 Graphical representation of (a) the smallest circle (that has $R^* = 3$) within which 6 unitary-radius circles can be packed and (b) the maximum number of unitary-radius circles that can be packed within a circle with radius $R = 3$.

(a) (b) (c)

Fig. 2 Graphical representation of (a) smallest cube, (b) cylinder of minimal surface, and (c) smallest regular tetrahedron within which 100 unitary-radius spheres can be packed. See [11] for details.

Algencan [1, 2]. Those problems are an oversimplification of the problem of packing molecules considered in [19, 20]. One of the characteristics of this problem that makes it tractable is that the density (proportion of occupied volume of the object) is relatively low. The first step in a molecular dynamics simulation consists of obtaining initial coordinates for all the atoms of the system. Since molecular dynamics force-fields contain repulsive terms that increase abruptly for short atom-to-atom distances, the distances between atoms from different molecules must be large enough so that repulsive potentials do not disrupt the simulations. Finding adequate initial configurations was modeled as a packing problem in [19] and [20], giving rise to the software Packmol[1].

Let us call *nmol* the total number of molecules that we want to place in a region $\mathscr{R}$ of the three-dimensional space. For each $i = 1, \ldots, nmol$, let $natom(i)$ be the number of atoms of the i-th molecule. Each molecule is represented by the orthog-

[1] http://www.ime.unicamp.br/∼martinez/packmol/

onal coordinates of its atoms. To facilitate the visualization, assume that the origin is the barycenter of all the molecules. For all $i = 1, \dots, nmol$, $j = 1, \dots, natom(i)$, let $A(i,j) = (a_1^{ij}, a_2^{ij}, a_3^{ij})$ be the coordinates of the j-th atom in the i-th molecule. Suppose that one rotates the i-th molecule sequentially around the axes x_1, x_2, and x_3, being $\gamma^i = (\gamma_1^i, \gamma_2^i, \gamma_3^i)$ the angles that define such rotations. Moreover, suppose that, after these rotations, the whole molecule is displaced so that its barycenter, instead of the origin, becomes $t^i = (t_1^i, t_2^i, t_3^i)$. These movements transform the atom of coordinates $A(i,j)$ in a displaced atom of coordinates $P(i,j) = (p_1^{ij}, p_2^{ij}, p_3^{ij})$. Observe that $P(i,j)$, $j = 1, \dots, natom(i)$, is a function of (t^i, γ^i), the relation being $P(i,j) = t^i + R(\gamma^i)A(i,j)$, $j = 1, \dots, natom(i)$, where

$$R(\gamma^i) = \begin{pmatrix} c_1^i c_2^i c_3^i - s_1^i s_3^i & s_1^i c_2^i c_3^i + c_1^i s_3^i & -s_2^i c_3^i \\ -c_1^i c_2^i s_3^i - s_1^i c_3^i & -s_1^i c_2^i s_3^i + c_1^i c_3^i & -s_2^i s_3^i \\ c_1^i s_2^i & s_1^i s_2^i & c_2^i \end{pmatrix}, \tag{3}$$

in which $s_k^i \equiv \sin \gamma_k^i$ and $c_k^i \equiv \cos \gamma_k^i$, for $k = 1, 2, 3$.

In [19, 20], the objective is to find angles γ_i and displacements t_i, $i = 1, \dots, nmol$, in such a way that, whenever $i \neq i'$,

$$\|P(i,j) - P(i',j')\|_2^2 \geq d^2, \tag{4}$$

for all $j = 1, \dots, natom(i)$, $j' = 1, \dots, natom(i')$, where $d > 0$ is the required minimum distance, and

$$P(i,j) \in \mathscr{R}, \tag{5}$$

for all $i = 1, \dots, nmol$, $j = 1, \dots, natom(i)$. In other words, the rotated and displaced molecules must remain in the specified region and the distance between any pair of atoms must not be less than d. Problem (4,5) is a nonlinear feasibility problem similar to (1). With some reformulations related to specific characteristics of the problem, using heuristics to construct initial guesses, and using a nonlinear programming solver [6], Packmol is able to solve practical problems like the ones illustrated in Figure 3.

3 Packing of polygons

The packing of rectangular items within rectangular objects is a particular case of the packing of polygons within polygons that has many practical applications in Logistics and Engineering. A large variety of problems exists, depending on the imposition of “cutting patterns”, the possibility of allowing rotations of the items or not, the fact of the items being identical or not, etc. In many cases, the problem can be modeled as a mixed-integer linear programing problem and solved by dedicated exact or heuristic methods. On the other hand, when the rectangular items can be freely rotated or the the items are other kind of polygons and the object within which

Fig. 3 Graphical representation of a double layered spherical vesicle with water inside and outside. The depicted configuration, obtained by solving a packing problem, can be used as initial point for molecular dynamics simulations. (This figure was extracted from the Packmol web site, where additional information can be found.) In practice, the region $\mathscr{R}$ in (5) is replaced for potentially different regions $\mathscr{R}_{ij}$ for each atom i of each molecule j.

the items must be placed is an arbitrary convex region, the problem may be modeled as a nonlinear programming problem.

In [8, 21] the concept of *sentinels* was introduced. Let I_1 and I_2 be nonempty, open, bounded, and convex sets of $\mathbb{R}^n$. Define $J_1 = \bar{I}_1$ the closure of I_1 and $J_2 = \bar{I}_2$ the closure of I_2 (J_1 and J_2 place the role of the items to be packed). Let $D_1, D_2 : \mathbb{R}^n \to \mathbb{R}^n$ be two displacement operators. So, D_1 and D_2 transform items in items preserving distances, angles, and orientation. If $D_1(I_1) \cap D_2(I_2) \neq \emptyset$ then we say that $D_1(J_1)$ and $D_2(J_2)$ (or $D_1(I_1)$ and $D_2(I_2)$) are superposed. Let S_1 and S_2 be finite subsets of J_1 and J_2, respectively. We say that S_1 and S_2 are *sentinels sets* relatively to J_1 and J_2 if the following property holds: *for all displacements D_1 and D_2, if $D_1(J_1)$ and $D_2(J_2)$ are superposed then $D_1(S_1) \cap D_2(I_2) \neq \emptyset$ or $D_2(S_2) \cap D_1(I_1) \neq \emptyset$.* Roughly speaking, if, after the displacements, the items J_1 and J_2 are superposed then at least one sentinel of J_1 becomes interior to J_2 or one sentinel of J_2 becomes interior to J_1. The concept of sentinels can be easily extended to any family of (potentially non-identical) $m \geq 2$ "items", the key point being to define the (finite) sentinels sets for a given family of polygons (or to determine that they do not exist). In [21], minimal sets of sentinels for rectangles are exhibited (see Figure 4), as well as sentinels sets for other types of polygons; while it is also shown that no finite sets of sentinels do not exist for triangles.

We now describe how the sentinels concept can be used to formulate a polygons packing problem as a nonlinear programming problem. This description follows [8] very closely. Let $I_1, \dots, I_m \subset \mathbb{R}^n$ be nonempty, open, bounded, and convex sets, $\Omega \subset \mathbb{R}^n$, and assume that we want to pack the items $I_1, \dots, I_m$ (or, equivalently, they closures $J_1, \dots, J_m$) into the region Ω. This means that we want to find displacements $D_1, \dots, D_m$ such that

$$D_i(J_i) \subset \Omega \text{ for } i = 1, \dots, m \tag{6}$$

and

$$D_i(J_i) \text{ and } D_j(J_j) \text{ are not superposed for all } i \neq j. \tag{7}$$

Let $S_1 \subset J_1, \ldots, S_m \subset J_m$ be such that $S_1, \ldots, S_m$ are *sentinels sets* relatively to $J_1, \ldots, J_m$. Given $i, j \in \{1, \ldots, m\}$, $i \neq j$, define

$$\kappa(D_i, D_j) = \#\{[D_i(S_i) \cap D_j(I_j)] \cup [D_j(S_j) \cap D_i(I_i)]\}. \tag{8}$$

This means that condition (7) can be formulated as

$$\kappa(D_i, D_j) = 0 \text{ for all } i \neq j \tag{9}$$

and, thus, the packing problem defined by (6,7) can be formulated as the optimization problem

$$\text{Minimize} \sum_{i \neq j} \kappa(D_i, D_j) \text{ subject to } D_i(J_i) \subset \Omega \text{ for } i = 1, \ldots, m. \tag{10}$$

The objective function of (10) represents the total number of sentinels of one item that, after the displacements, fall in the interior of some other item. If a global solution of (10) is found such that the objective function vanishes then the packing problem (6,7) is solved.

The optimization problem (10) defines the *Method of Sentinels*. However, this minimization problem needs to be reformulated in order to be transformed into a solvable nonlinear programming problem. Let us consider the case in which Ω is a closed and convex set defined by a set of inequalities, i.e.

$$\Omega = \{x \in \mathbb{R}^n \mid g_k(x) \leq 0,\ k = 1, \ldots, p\}. \tag{11}$$

Moreover, assume that each item J_i is a bounded polytope, so it is the convex hull of its vertices $V_1(J_i), \ldots, V_{\nu(i)}(J_i)$. Then, the constraints of (10) take the form

$$g_k(D_i[V_\ell(J_i)]) \leq 0 \text{ for } i = 1, \ldots, m,\ \ell = 1, \ldots, \nu(i),\ k = 1, \ldots, p. \tag{12}$$

The displacements D_i can always be described by a finite set of parameters. For example, displacements in $\mathbb{R}^2$ are given by three parameters, the first two representing a translation and the third the angle of rotation. Therefore, the constraints (12) have the usual form adopted in nonlinear programming problems.

The objective function of (10) depends on the continuous variables that define the displacements but it takes only discrete integer nonnegative values. For nonlinear programming reformulations we need to replace it by a continuous function of the displacement variables. As before, we restrict ourselves to the case in which the sets J_i are bounded polytopes. In this case, each J_i is described by a set of linear inequalities of the form

$$\langle c_{ik}, x \rangle \leq b_{ik} \text{ for } k = 1, \ldots, \mu(i). \tag{13}$$

If $s \in S_j \subset J_j$ is a sentinel of I_j and $D_j(s)$ is in $D_i(I_i)$ with $i \neq j$ then $D_i^{-1} D_j(s)$ belongs to I_i and, therefore, it satisfies

$$\langle c_{ik}, D_i^{-1} D_j(s) \rangle < b_{ik} \text{ for } k = 1, \ldots, \mu(i). \tag{14}$$

Thus, the displaced sentinel s belongs to the displaced I_i if, and only if,

$$\prod_{k=1}^{\mu(i)} \max\{0, b_{ik} - \langle c_{ik}, D_i^{-1} D_j(s) \rangle\} > 0. \tag{15}$$

Therefore, a degree of the superposition of I_i and I_j (or J_i and J_j) under the displacements D_i and D_j is given by

$$\begin{aligned} \Phi(D_i, D_j) = & \textstyle\sum_{s \in S_i} \prod_{k=1}^{\mu(j)} \max\{0, b_{jk} - \langle c_{jk}, D_j^{-1} D_i(s) \rangle\}^2 \\ & + \textstyle\sum_{s \in S_j} \prod_{k=1}^{\mu(i)} \max\{0, b_{ik} - \langle c_{ik}, D_i^{-1} D_j(s) \rangle\}^2. \end{aligned} \tag{16}$$

The function $\Phi(D_i, D_j)$ is nonnegative and continuously differentiable with respect to the parameters that define the displacements D_i and D_j; and it vanishes if, and only if, $D_i(J_i)$ and $D_j(J_j)$ are not superposed. Therefore, it can replace the function $\kappa(D_i, D_j)$ in the optimization problem (10).

Summing up, in the case in which Ω is a convex set defined by inequalities and the items are bounded polytopes, the packing problem can be formulated as the continuous and differentiable nonlinear programming problem

$$\text{Minimize } \sum_{i \neq j} \Phi(D_i, D_j) \tag{17}$$

subject to (12). Moreover, since we are only interested in global solutions of (17) where the objective function must vanish, the problem can be reformulated as the feasibility problem given by

$$\begin{aligned} & \textstyle\sum_{i \neq j} \Phi(D_i, D_j) = 0, \\ & g_k(D_i[V_\ell(J_i)]) \leq 0, \; i = 1, \ldots, m, \ell = 1, \ldots, \nu(i), k = 1, \ldots, p. \end{aligned} \tag{18}$$

Finally, (18) is equivalent to the following unconstrained continuously differentiable global optimization problem

$$\text{Minimize } \sum_{i \neq j} \Phi(D_i, D_j) + \sum_{i=1}^{m} \sum_{\ell=1}^{\nu(i)} \sum_{k=1}^{p} \max\{0, g_k(D_i[V_\ell(J_i)])\}^2. \tag{19}$$

A few examples of the solutions that can be obtained by solving (17), (18), or (19) can be seen in Figure 5. In general, the nonlinear programming problems are nonconvex with many spurious stationary points that are not solutions to the packing problem they represent (only global solutions are of interest). Because of that, clever heuristics need to be developed to determine promising starting points for the iterative optimization process. One possibility explored in [8] for packing rectangular items was to consider, for each rectangle, a partial covering with varied-sized circles (see Figure 6). In a first phase, a circle packing problem is solved (with models similar to the one described in the previous section) to place the circles within the object and avoiding the overlapping of the circles that cover different items. In a second phase the circles are dismissed and the placement of the rectangular items is used as an initial guess to the rectangular items packing problem.

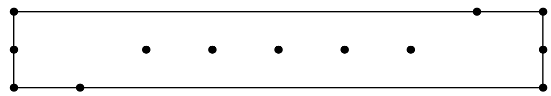


Fig. 4 Minimal set of sentinels for a family of m identical rectangular items with smallest side s and largest side $7s$. The distance between the sentinels in the smallest side is $s/2$ while the "horizontal distance" between the sentinels in the largest side and in the central line is smaller that s. (Enjoy yourself: make two copies of the rectangle in the figure and try to overlap them without having a sentinel of one rectangle in the interior of the other. Free rotations are allowed.)

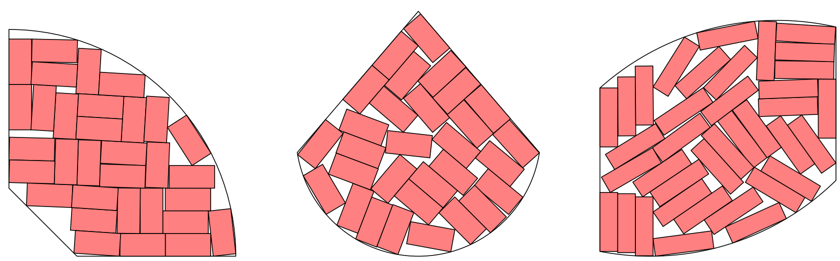


Fig. 5 Examples of solutions found in [8] to the problem of packing freely-rotated rectangular items within arbitrary convex regions.

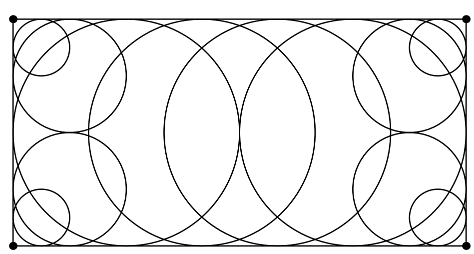


Fig. 6 Arbitrary partial covering of a rectangular item by circles. In a first phase, a packing problem with the circular items is solved (avoiding overlapping between the circles that cover different rectangles). The position of the rectangular items inherited by the solution of the problem of the first phase is used as initial guess to the original packing problem with rectangular items.

4 Concluding remarks

There are packing problems that, by its nature, are combinatorial problems. Examples of those problems are one-dimensional bin packing problems, two-dimensional bin packing or stock cutting problems involving rectangular items (that can not be freely rotated) and rectangular objects, and some two- or three-dimensional puzzle problems, among many others. There are other packing problems, like for example finding the densest packing of circles or spheres in the infinite Euclidean space, that can be solved using lattices. On the other hand, there are also packing problems that can be naturally addressed with nonlinear programming techniques. The packing of circles or spheres within restricted domains or the packing of irregular shape items or arbitrary varied polygons are some of the many possible examples. In these cases, discretizing the problem domain may produce sub-optimal solutions (by reducing the feasible region) and nonlinear programming models and solution methods should be considered. In most of the cases, global solutions are sought and problems are very challenging and provide a nice source for benchmarking.

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