A. V. Pankratov,
Doctor of Engineering Science
T. E. Romanova,
Doctor of Engineering Science
A. M. Chugay,
Ph.D of Engineering Science

A. N. Podgorny Institute for Mechanical Engineering Problems, National Academy of Sciences of Ukraine,
Kharkiv, e-mail: impankratov@mail.ru, sherom@kharkov.ua, chugay@ipmach.kharkov.ua

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OPTIMAL PACKING OF CONVEX POLYTOPES USING QUASI-PHI-FUNCTIONS

Розглядається задача упаковки опуклих багатогранників у прямокутний контейнер мінімального об'єму. При цьому багатогранники припускають безперервні повороти та трансляції. Крім того, враховуються мінімально припустимі відстані між багатогранниками. Для побудови математичної моделі задачі як задачі нелінійного програмування використовуються вільні від радикалів квазі-phi-функції. Розроблено ефективний алгоритм розв'язання, який дозволяє зменшити розмірність задачі і обчислювальні витрати. Наведено числові приклади.

Introduction

Optimal packing problem is a part of operational research and computational geometry [1]. It has a wide spectrum of applications in modern biology, mineralogy, medicine, materials science, nanotechnology, robotics, pattern recognition systems, control systems, space apparatus control systems, as well as in the chemical industry, power engineering, mechanical engineering, shipbuilding, aircraft construction, civil engineering, etc. At present, the interest in finding effective solutions for packing problems is growing rapidly. This is due to a large and growing number of applications and an extreme complexity of methods used to handle many of them.

These problems are NP-hard [2], and, as a result, solution methodologies generally employ heuristics e. g., [3–13]. Some researchers develop approaches based on mathematical modeling and general optimization procedures; e. g., [14–19].

We consider a practical problem of packing a collection of a given non-identical convex polytopes into a rectangular container of minimal volume.

In the paper [16] authors present an efficient solution method for packing polytopes within the bounds of a polytope container. The central geometric operation of the method is an exact one-dimensional translation of a given polytope to a position which minimizes its volume of overlap with all other polytopes. The translation algorithm is used as part of a local search heuristic and a meta-heuristic technique, guided local search, is used to escape local minima. Additional details are given for the three-dimensional case and results are reported for the problem of packing polytopes in a rectangular parallelepiped. Utilization of container space is improved by an average of more than 14 percentage points compared to previous methods proposed in [20]. However, in the experiments the largest total volume of overlap allowed in a solution corresponds to one percent of the total volume of all polytopes for the given problem.

Our approach is based on mathematical modeling of relations between geometric objects and thus reducing the packing problem to a nonlinear programming problem. To this end we use the phi-function technique (see e. g. [21]) for analytic description of objects placed in a container taking into account their *continuous rotations* and *translations*. At present phi-functions for the simplest 3D-objects, such as parallelepipeds, convex polytopes and spheres are considered in [22, 23]. Some of phi-functions (especially for 3D-objects, i.e. polytopes) happen to be *rather complicated*, analytically (involve a lot of radicals, operations of maximum), and difficult in practical use (to apply NLP-solvers).

In this paper we apply the concept of phi-functions, extending their domains by including auxiliary variables. The new functions, called *quasi-phi-functions*, can be described by analytical formulas that are substantially simpler than those used for phi-functions, for some types of objects, in particular, for polytopes. In addition we construct an adjusted phi-function for describing distance constraints for a pair of polytopes.

One way to tackle the packing problem is use the existing phi-functions for rotating polytopes described in [22]. In the paper we propose alternative way to solve the problem which is based on quasi-phi-functions [24], is capable of finding a good local-optimal solution in reasonable computational time. The use of quasi-phi-functions, instead of phi-functions, allows us to simplify non-overlapping, as well as, to describe distance constraints, but there is a price to pay: now the optimization has to be performed over a larger set of parameters, including the extra variables used by our new functions, but this is a small price. We believe our quasi-phi-functions and our optimization algorithm described below are more flexible and efficient than other techniques.

The paper is organized as follows: in Section 2 we formulate the polytope packing problem. In Section 3 we define our quasi-phi-functions (adjusted-quasi-phi-functions) for an analytical description of non-overlapping, containment and distance constraints in the problem. In Section 4 we propose a mathematical model as a nonlinear programming problem by means of quasi-phi-functions. In Section 5 we develop a solution algorithm, which involves a fast starting point algorithm and efficient local optimization procedures. In Section 6 we present our computational results for some new instances and several instances studied before. In Section 7 we give some conclusions.

2. Problem formulation

We consider here a packing problem in the following setting. Let Ω denote a rectangular domain $\Omega = \{(x, y, z) \in R^3 : 0 \le x \le l, 0 \le y \le w, 0 \le z \le h\}$. It should be noted that each of the three dimensions (l or w or h) may be fixed. In particular three of dimensions of l, w, h may be variable. Suppose a set of polytopes K_i, $i \in \{1, 2, \ldots, n\} = I_n$, is given to be placed in Ω without overlaps. Each polytope K_i is defined by its vertices p^i_j, $j = 1, \ldots, m_i$, whose values are fixed. With each polytope K_i we associate its local coordinate system whose origin is called a pole of the polytope. Without loss of generality, we assume that the pole of a polytope K_i coincides with the center point of its circumscribed sphere S_i of radius r_i. We also use a fixed coordinate system attached to the container Ω.

The location and orientation of polytope K_i is defined by a variable vector of its placement parameters (v_i, θ_i). Here $v_i = (x_i, y_i, z_i)$ is a translation vector, $\theta_i = (\theta_i^1, \theta_i^2, \theta_i^3)$ is a vector of rotation parameters, where $\theta^1{}_i$, $\theta^2{}_i$, $\theta^3{}_i$ are appropriate angels from axis OX to OY, from axis OY to OZ and from axis OX to OZ from axis OX to OY, from axis OY to OZ and from axis OX to OZ in the local coordinate system of polytope K_i.

The translation of polytope K_i by vector v_i, the rotation of polytope K_i by vector θ_i is defined by $K_i(u_i) = \{p \in R^3 : p = v_i + M(\theta_i) \cdot p^0, \forall p^0 \in K_i^0\}$, K_i^0 denotes the non-translated and non-rotated polytope K_i with $\lambda_i = 1$, $M(\theta_i) = M_1(\theta_i^1) \cdot M_2(\theta_i^2) \cdot M_3(\theta_i^3)$ is a rotation matrix, where

$$M_1(\theta_i^1) = \begin{pmatrix} \cos\theta_i^1 & -\sin\theta_i^1 & 0 \\ \sin\theta_i^1 & \cos\theta_i^1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad M_2(\theta_i^2) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta_i^2 & -\sin\theta_i^2 \\ 0 & \sin\theta_i^2 & \cos\theta_i^2 \end{pmatrix}, \qquad M_3(\theta_i^3) = \begin{pmatrix} \cos\theta_i^3 & 0 & \sin\theta_i^3 \\ 0 & 1 & 0 \\ -\sin\theta_i^3 & 0 & \cos\theta_i^3 \end{pmatrix}.$$

Between each pair of polytopes K_i and K_j, as well as, between polytope K_i and the walls of domain Ω appropriate minimal allowable distances ρ_{ij}^- and ρ_i^- may be given.

Polytope packing optimization problem. Pack the set of polytopes $K_i(u_i)$, $i \in I_n$, within a rectangular domain Ω of minimal volume $F = l \cdot w \cdot h$ taking into account minimal allowable distances.

3. Mathematical modeling of placement constraints

To describe non-overlapping and containment constraints we use quasi-phi-functions and phi-functions. To describe distance constraints we apply adjusted quasi-phi-functions and adjusted phi-functions. Clear definitions of a phi-function (a quasi-phi-function), an adjusted phi-function (an adjusted quasi-phi-function) one can find in papers [21, 24].

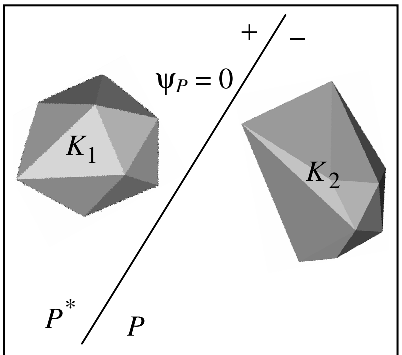

Fig. 1. A separating plane for two convex polytopes K_1 and K_1

To describe *non-overlapping* constraint $\operatorname{int} K_1 \cap \operatorname{int} K_2 = \varnothing$, we use quasi-phi-function $\Phi'^{K_1K_2}$ for two convex polytopes K_1 and K_2.

Let $K_1(u_1)$ and $K_2(u_2)$ be convex polytopes, given by their vertices p_i^1, $i = 1, \ldots, m_1$, and p_j^2, $j = 1, \ldots, m_2$.

Let $P(u_P) = \{(x, y, z) : \psi_P = \alpha \cdot x + \beta \cdot y + \gamma \cdot z + \mu_P \le 0\}$ be a half-space, where $\alpha = \sin\theta_{yP}$, $\beta = -\sin\theta_{xP} \cdot \cos\theta_{yP}$, $\gamma = \cos\theta_{xP} \cdot \cos\theta_{yP}$ (note that $\alpha^2 + \beta^2 + \gamma^2 = 1$) and $u_P = (\theta_{xP}, \theta_{yP}, \mu_P)$.

Suppose $\Phi^{K_1P}(u_1, u_P)$ is the normalised phi-function for $K_1(u_1)$ and a half-space $P(u_P)$ [21] and $\Phi^{K_2P^*}(u_2, u_P)$ is the normalised phi-function for $K_2(u_2)$ and $P^*(u_P) = R^3 \setminus \operatorname{int} P(u_P)$, where $\Phi^{K_1P}(u_1, u_P) = \min_{1 \le i \le m_1} \psi_P(p_i^1)$ and $\Phi^{K_2P^*}(u_2, u_P) = \min_{1 \le j \le m_2} (-\psi_P(p_j^2))$.

A function defined by

$$\Phi'^{K_1K_2}(u_1, u_2, u_P) = \min\{\Phi^{K_1P}(u_1, u_P), \Phi^{K_2P^*}(u_2, u_P)\}, \tag{1}$$

is a *quasi-phi-function* for $K_1(u_1)$ and $K_2(u_2)$ [24].

Figure 1 shows that if two convex polytopes K_1 and K_2 do not have common points then there is always exist additional variables $u_P = (\theta_{xP}, \theta_{yP}, \mu_P)$ such that $\max_{u_P} \Phi'^{K_1K_2} > 0$.

Thus, $\max_{u_P} \Phi'^{K_1K_2} \ge 0 \Leftrightarrow \operatorname{int} K_1 \cap \operatorname{int} K_2 = \varnothing$. We follow here the important characteristic of a *quasi-phi-function*: if $\Phi'^{K_1K_2} \ge 0$ for some u_P, then $\operatorname{int} K_1 \cap \operatorname{int} K_2 = \varnothing$.

Let $\operatorname{dist}(K_1, K_2) = \min_{a \in K_1, b \in K_2} d(a, b)$, where $d(a, b)$ stands for the Euclidean distance between points $a, b \in R^3$ and let $\rho_{12}^- > 0$ denote minimal allowable distances between polytopes $K_1(u_1)$ and $K_2(u_2)$.

To describe *distance* constraint $\operatorname{dist}(K_1, K_2) \ge \rho_{12}^-$, we use adjusted quasi-phi-function $\widehat{\Phi}'_{12}$ for polytopes $K_1(u_1)$ and $K_2(u_2)$.

An adjusted quasi-phi-function for convex polytopes $K_1(u_1)$ and $K_2(u_2)$ is derived by

$$\widehat{\Phi}'^{K_1K_2}(u_1, u_2, u_P) = \Phi'^{K_1K_2}(u_1, u_2, u_P) - 0.5\rho_{12}^-. \tag{2}$$

Thus, $\max_{u' \in U} \widehat{\Phi}'^{K_1K_2} \ge 0 \Leftrightarrow \operatorname{dist}(K_1, K_2) \ge \rho_{12}^-$.

It follows from (2) that $\Phi'^{K_1K_2}(u_1, u_2, u_P) - 0.5\rho_{12}^- \ge 0 \Rightarrow \operatorname{dist}(K_1, K_2) \ge \rho_{12}^-$.

To describe containment constraint $K_1 \subset \Omega \Leftrightarrow \operatorname{int} K_1 \cap \Omega^* = \varnothing$ we use phi-function $\Phi^{K_1\Omega^*}$ *for a convex polytope $K_1(u_1)$ and object* $\Omega^* = R^3 \setminus \operatorname{int}\Omega$.

Let $K_1(u_1)$ be convex polytope, given in its local coordinate system by their vertices p_i^1, $i = 1, \ldots, m_1$, where $p_i^1 = (p_{xi}^1, p_{yi}^1, p_{zi}^1)$.

A phi-function for a convex polytope $K_1(u_1)$ and object Ω^* may be defined as

$$\Phi^{K_1\Omega^*}(u_1) = \min\{\min_{1 \le i \le m_1} \varphi_{1j}(p_i^1), j = 1, \ldots, 6\}. \tag{3}$$

$$\varphi_{11}(p_i^1) = x_1 + p_{xi}^1, \qquad \varphi_{12}(p_i^1) = -(x_1 + p_{xi}^1) + l, \qquad \varphi_{13}(p_i^1) = y_1 + p_{yi}^1,$$

$$\varphi_{14}(p_i^1) = -(y_1 + p_{yi}^1) + w, \qquad \varphi_{15}(p_i^1) = z_1 + p_{zi}^1, \qquad \varphi_{16}(p_i^1) = -(z_1 + p_{zi}^1) + h.$$

To describe *containment* constraint taking into account minimal allowable distance $\operatorname{dist}(K_1,\Omega^*) \ge \rho_1^-$ we use adjusted phi-function $\widehat{\Phi}_1'$ for *a convex polytope* $K_1(u_1)$ *and object* Ω^*.

An adjusted phi-function for a convex polytope $K_1(u_1)$ *and object* Ω^* is defined by

$$\widehat{\Phi}^{K_1\Omega^*}(u_1) = \Phi^{K_1\Omega^*}(u_1) - \rho_1^-. \tag{4}$$

4. Mathematical model

First we assemble a complete set of variables for our optimization problem. The vector $u \in R^\sigma$ of all our variables can be described as follows: $u = (l, w, h, u_1, u_2, ..., u_n, \tau) \in R^\sigma$, where (l, w, h) denote the variable dimensions (length, width and height) of the rectangular container Ω and $u_i = (v_i, \theta_i) = (x_i, y_i, z_i, \theta_i^1, \theta_i^2, \theta_i^3)$ is the vector of placement parameters for the polytope K_i, $i \in I_n$. Here $\tau = (u_p^1, ..., u_p^m)$ denotes the vector of additional variables, where $u_p^k = (\theta_{x_p}^k, \theta_{y_p}^k, \mu_p^k)$, are additional variables for the k^{th} pair of polytopes, according to (1)–(4), $k = 1, \dots, m$, $m = 0.5(n-1)n$. Lastly we derive the number of the problem variables $\sigma = 3 + 6n + 3m$.

Now a mathematical model of the *polytope packing optimization problem* may be stated in the form

$$\min_{u \in W \subset R^\sigma} F(u), \tag{5}$$

$$W = \{u \in R^\sigma : \widehat{\Phi}_{ij}' \ge 0, \widehat{\Phi}_i \ge 0, i = 1,2,...,n, j = 1,2,...,n, j > i\}, \tag{6}$$

where $F(u) = l \cdot w \cdot h$, $\widehat{\Phi}_{ij}'$ is a radical free adjusted quasi phi-function (2) defined for the pair of polytopes K_i and K_j, taking into account minimal allowable distance ρ_{ij}^-, Φ_i' is a radical free adjusted phi-function (4) defined for the polytope K_i and the object Ω^* (to hold the *containment* constraint), also taking into account minimal allowable distance ρ_i^-.

If $\rho_{ij}^- = 0$ and $\rho_i^- = 0$ we replace the adjusted quasi-phi-function $\widehat{\Phi}_{ij}'$ by a radical free quasi-phi-function Φ_{ij}' defined by (1) for each pair of polytopes to enforce the *non-overlapping* constraint and the adjusted phi-function $\widehat{\Phi}_i'$ with a radical free phi-function Φ_i defined by (3) for each polytope and the object Ω^* to enforce the *containment* constraint.

Our problem (5)–(6) is a constrained multiextremal optimization problem. Each quasi-phi-function inequality in (6) is presented by a system of inequalities with infinitely differentiable functions. The frontier of W is made of nonlinear surfaces containing valleys and ravines. Our model is non-convex and continuous nonlinear programming problem. Problem (5)–(6) is an exact formulation for the *polytope packing optimization problem*.

5. A solution strategy

Our solution strategy involves the following steps:

1) Generate a number of starting points from the feasible set of the problem (5)–(6). We employ a new starting point algorithm (SPA). See Subsection 5.1.

2) Search for a local minimum of the objective function $F(u)$ of problem (5)–(6), starting from each point obtained at Step 1. We employ a special optimisation procedure – Local Optimization with Feasible Region Transformation (LOFRT-3D). See Subsection 5.2.

3) Choose the best local minimum from those found at Step 2. This is our best solution of the problem (5)–(6).

An essential part of our local optimization scheme (Step 2) is the LOFRT procedure that reduces the dimension of the problem and computational time. The reduction scheme used by our LOFRT algorithm is described below. The actual search for a local minimum is performed by a standard IPOPT algorithm [25], which is available at an open access noncommercial software depository (https://projects.coin-or.org/Ipopt) .

5.1 Starting point algorithm (SPA)

In order to find a starting point u^0 that belongs to the feasible set W we apply the following algorithm based on homothetic transformation of polytopes.

The algorithm consists of the following steps:

1. Choose starting dimensions (length and width) for the container Ω^0. They must be sufficiently large to allow for a placement of all our polytopes with required distance constraints within Ω^0. For example, we can set

$$l^0 = w^0 = l^0 = h^0 = 2\sum_{i=1}^{n} r_i + (n+1)\rho^-, \qquad \rho^- = \max\{\max_{i,j\in I_n} \rho_{ij}^-, \max_{i\in I_n} \rho_i^-\}.$$

2. Generate randomly, within Ω^0, a set of n randomly chosen center points $(x_i^{'0}, y_i^{'0}, z_i^{'0})$, $i = 1, 2, \ldots, n$ of circumbsribed spheres S_i of radius λr_i. We assume here that λ is a homothetic coefficient for all our spheres S_i and $0 \le \lambda \le 1$.

3. Take the starting point $u^{'0} = (x_1^{'0}, y_1^{'0}, z_1^{'0}, \ldots, x_n^{'0}, y_n^{'0}, z_n^{'0}, \lambda^{'0} = 0)$ and solve the following auxiliary optimization problem, assuming that $l = l^0$, $w = w^0$ and $h = h^0$:

$$\max_{u'\in W'} \lambda\,, \tag{7}$$

$$W' = \{u' \in \mathrm{R}^{3n+1} : \hat{\Phi}^{S_iS_j} \ge 0, \hat{\Phi}^{S_i\Omega^*} \ge 0, i < j = 1,2,\ldots,n, 1-\lambda \ge 0, \lambda \ge 0\}, \tag{8}$$

where $u' = (x_1, y_1, z_1, \ldots, x_n, y_n, z_n, \lambda)$,

$$\hat{\Phi}^{S_iS_j} = (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2 - (\lambda r_i + \rho^- + \lambda r_j)^2,$$

is an adjusted phi-function for sphere S_i of radius λr_i and sphere S_j of radius λr_j,

$$\hat{\Phi}^{S_i\Omega^*} = \min\{\varphi_{ki}, k = 1,\ldots,6\},$$

$$\varphi_{1i} = -x_i + l^0 - \lambda r_i - \rho_i^-, \qquad \varphi_{2i} = x_i - \lambda r_i - \rho_i^-, \qquad \varphi_{3i} = -y_i + w^0 - \lambda r_i - \rho_i^-,$$

$$\varphi_{4i} = y_i - \lambda r_i - \rho_i^-, \qquad \varphi_{5i} = -z_i + h^0 - \lambda r_i - \rho_i^-, \qquad \varphi_{4i} = z_i - \lambda r_i - \rho_i^-$$

is an adjusted phi-function for sphere S_i of radius λr_i and object Ω^*.

We denote the point of global maximum of problem (7)–(8) by $u^{'*} = (x_1^{'*}, y_1^{'*}, z_1^{'*}, \ldots, x_n^{'*}, y_n^{'*}, z_n^{'*}, \lambda^{'*})$.

Remark. Note that if an optimal global solution point is found, then $\lambda^{'*} = 1$. The solution automatically respects all the non-overlapping and containment constraints.

Our use of homothetic transformations of spheres here is similar to the use of variable radii for optimal packing of nD-spheres, which was proposed in [26].

4. Form feasible starting point $u^0 = (l^0, w^0, h^0, u_1^0, u_2^0, \ldots, u_n^0, \tau^0)$ for problem (5)–(6):

– Form a vector of starting placement parameters $u_i^0 = (x_i^0, y_i^0, z_i^0, \theta_i^0)$ for each polytope K_i, $i = 1, \ldots, n$, where $(x_i^0, y_i^0, z_i^0) = (x_i^{'*}, y_i^{'*}, z_i^{'*})$ and $\theta_i^0 = (\theta_{i\,z}^0, \theta_{i\,x}^0, \theta_{i\,y}^0)$ are randomly generated rotation parameters.

– Find values for the vector of additional variables $\tau^0 = (u_P^{01}, \ldots, u_P^{0m})$, $u_P^{0k} = (\theta_{x_P}^{0k}, \theta_{y_P}^{0k}, \mu_P^{0k})$ by a special optimization procedure that solves an auxiliary problem of searching for $\max_{u_P^k \in R^3} \hat{\Phi}'_{ij}(u_i^0, u_j^0, u_P^k)$ for each quasi-phi-function (or, respectively, adjusted phi-function) that is involved in (6), under fixed parameters $u_i^0 = (x_i^0, y_i^0, z_i^0, \theta_i^0)$, $i = 1, 2, \ldots, n$.

To solve the above auxiliary problem we use the following model:

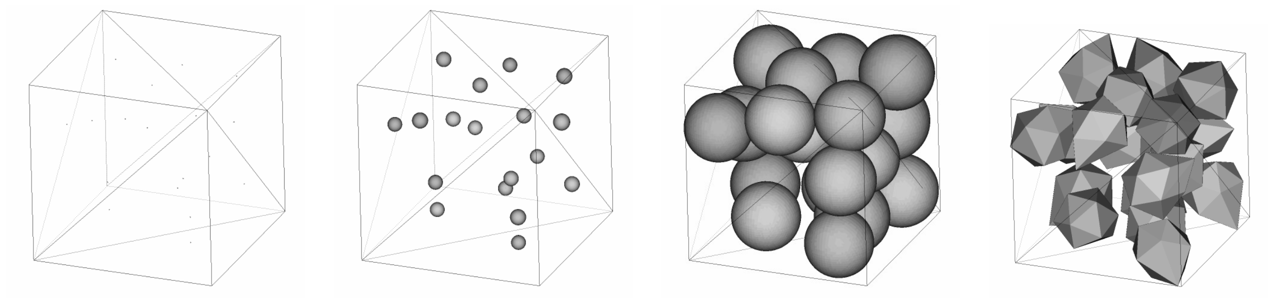

Fig. 2. Illustration of steps 1)-4) in SPA:
a) – step 1; b) – step 2; c) – step 3; d) – step 4

$$\max \mu,\ s.t.\, u' \in W'_{\mu},$$

where $W'_{\mu} = \{(u^k_p, \mu) \in R^4 : \hat{\Phi}'_{ij}(u^0_i, u^0_j, u^k_p) \geq \mu\}$, $\mu \in R^1$, is a new auxiliary variable, u^k_p is the vector of auxiliary variables and (u^0_i, u^0_j) are fixed placement parameters for our adjusted phi-functions (respectively, quasi-phi-functions), $k = 1, \ldots, m$.

As a result we form a feasible starting point $u^0 = (l^0, w^0, h^0, u^0_1, u^0_2, \ldots, u^0_n, \tau^0)$. Thus all our adjusted quasi-phi-functions (or quasi-phi-functions) and adjusted phi-functions (or phi-functions) for our polytopes at the point u^0 take non-negative values.

Figure 2 gives illustrations to steps 1)–4) in our starting point algorithm SPA.

Lastly, our algorithm returns the vector u^0 as a starting point for a subsequent search for a local minimum of the problem (5)–(6).

5.2 Algorithm of Local Optimization with Feasible Region Transformation for 3D packing (LOFRT-3D)

The algorithm based on LOFRT procedure proposed in [27] for optimal ellipse packing problem. We extended the algorithm to 3D case for packing of convex polytopes.

Let $u^0 \in W$ be one of the starting points found by SPA. The main idea of the LOFRT-3D algorithm is as follows.

First we take sphere S_i of radius r_i circumscribed around each polytope K_i, $i = 1, 2., \ldots, n$. Then we extend the radius of each sphere S_i by $0.5\rho^-$ (derived above at step 1 of SPA) and for each extended sphere S_i construct an "individual" rectangular container $\Omega_i \supset S_i \supset K_i$ with equal half-sides of length $r_i + 0.5\rho^- + \varepsilon$, $i = 1, 2, \ldots, n$, so that S_i, K_i and Ω_i have the same center (x^0_i, y^0_i, z^0_i). We take the epsilon parameter of the LOFTR-3D procedure as $\varepsilon = \sum_{i=1}^{n} r_i / n$. Further we fix the position of each individual container Ω_i and let the local optimization algorithm move the extended sphere S_i (and the appropriate polytope K_i) only within the individual container Ω_i. It is clear that if Ω_i and Ω_j do not overlap each other (i. e. $\Phi^{\Omega_i \Omega_j} \geq 0$), then we do not need to check the non-overlapping constraint for the corresponding pair of polytopes K_i and K_j, taking into account distance constraints. Here

$$\Phi^{\Omega_i \Omega_j} = \max\{\varphi^k_{ij}, k = 1, \ldots, 6\},$$

where, assuming $R_{ij} = (r_i + r_j) + \rho^- + 2\varepsilon$,

$$\varphi^1_{ij} = (x^0_i - x^0_j) - R_{ij}, \qquad \varphi^2_{ij} = (y^0_i - y^0_j) - R_{ij}, \qquad \varphi^3_{ij} = (z^0_i - z^0_j) - R_{ij},$$

$$\varphi^4_{ij} = -(x^0_i - x^0_j) - R_{ij}, \qquad \varphi^5_{ij} = -(y^0_i - y^0_j) - R_{ij}, \qquad \varphi^6_{ij} = -(z^0_i - z^0_j) - R_{ij}.$$

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By analogy if Ω_i and Ω^*_ε do not overlap each other (i. e. $\Phi^{\Omega_i\Omega^*_\varepsilon} \geq 0$), then we do not need to check the containment constraint for the corresponding polytope K_i and $\Omega_\varepsilon = \{(x,y,z) \in R^3 : \varepsilon \leq x \leq l-\varepsilon, \varepsilon \leq y \leq w-\varepsilon, \varepsilon \leq z \leq h-\varepsilon\}$.

Appropriate phi-function $\Phi^{\Omega_i\Omega^*_\varepsilon}$ for polytope K_i and $\Omega^*_\varepsilon = R^3 \setminus \operatorname{int}\Omega_\varepsilon$ has the form

$$\Phi^{\Omega_i\Omega^*_\varepsilon} = \min\{\psi^k_{ij}, k = 1,...,6\},$$

where assuming $R_i = r_i + \rho^- + 2\varepsilon$,

$$\psi^1_i = x^0_i - R_i, \qquad \psi^2_i = y^0_i - R_i, \qquad \psi^3_i = z^0_i - R_i,$$
$$\psi^4_i = -x^0_i + l - R_i, \qquad \psi^5_i = -y^0_i + w - R_i, \qquad \psi^6_i = -z^0_i + h - R_i.$$

The above key idea allows us to extract subsets of our feasible set W of the problem (5)–(6) at each step of our optimization procedure as follows.

We create an inequality system of additional constraints on the translation vector $v_i = (x_i, y_i, z_i)$ of each polytope K_i in the form: $\Phi^{S_i\Omega^*_{1i}} \geq 0$, $i = 1, 2, \ldots, n$, where

$$\Phi^{S_i\Omega^*_{1i}} = \min\{-x_i + x^0_i + \varepsilon, -y_i + y^0_i + \varepsilon, -z_i + z^0_i + \varepsilon, x_i - x^0_i + \varepsilon, y_i - y^0_i + \varepsilon, z_i - z^0_i + \varepsilon\},$$

is the phi-function for the extended sphere S_i and $\Omega^*_{1i} = R^3 \setminus \operatorname{int}\Omega_{1i}$.

We generate an “artificial” subset Π^ε_1 of the following form:

$$\Pi^\varepsilon_1 = \{u \in R^{\sigma-\sigma_k} : -x_i + x_i^{(0)} + \varepsilon \geq 0,\ -y_i + y_i^{(0)} + \varepsilon \geq 0,\ -z_i + z_i^{(0)} + \varepsilon \geq 0,$$
$$x_i - x_i^{(0)} + \varepsilon \geq 0,\ y_i - y_i^{(0)} + \varepsilon \geq 0,\ z_i - z_i^{(0)} + \varepsilon \geq 0,\ i = 1,...,n\}.$$

Then we form a new subregion $W_1 = W \bigcap \Pi^\varepsilon_1$ defined by

$$W_1 = \{u \in R^{\sigma-\sigma_1} : \hat{\Phi}'_{ij} \geq 0, (i,j) \in \Xi_1, \hat{\Phi}'_i \geq 0, i \in \Xi_2, \Phi^{S_i\Omega^*_{1i}} \geq 0, i = 1,2,...,n, l \geq l_0 - \varepsilon, w \geq w_0 - \varepsilon, h \geq h_0 - \varepsilon\},$$

where $\Xi_1 = \{(i,j) : \Phi^{\Omega_{1i}\Omega_{1j}} < 0, i > j = 1,2,...,n\}$, $\Xi_2 = \{i : \Phi^{\Omega_{1i}\Omega^*} < 0, i = 1,2,...,n\}$.

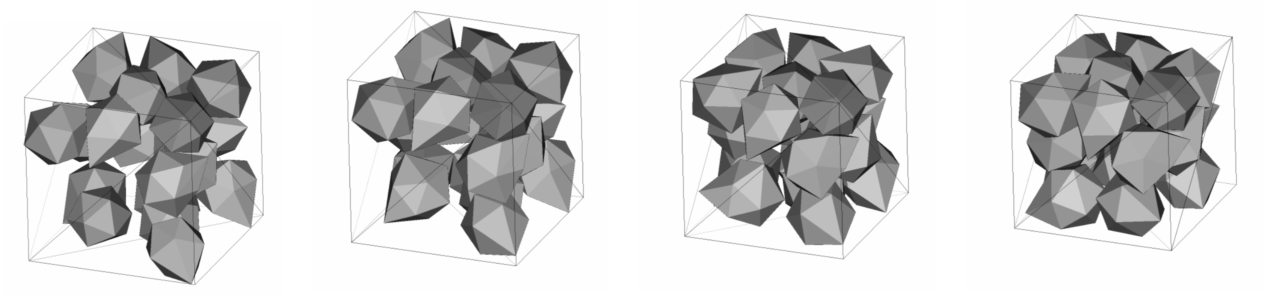
In other words, we *delete* from the system, which describes feasible set W, quasi-phi-function inequalities for all pairs of polytopes whose individual containers do not overlap and we *add* additional inequalities $\Phi^{S_i\Omega^*_{1i}} \geq 0$, which describe the containment of the extended spheres S_i in their individual containers Ω_{1i}, $i = 1, 2, \ldots, n$. Thus, we reduce the number of additional variables by σ_1. Then our algorithm searches for a point of local minimum $u^*_{w_1}$ of the subproblem $\min\limits_{u_{w_1} \in W_1 \subset R^{\sigma-\sigma_1}} F(u_{w_1})$.

When the point $u^*_{w_1}$ is found, it is used to construct a starting point $u^{(1)}$ for the second iteration of our optimization procedure (note that the σ_1 previously deleted additional variables τ_1 have to be redefined by a special procedure used in SPA, assuming $l^0 = 1$).

At that iteration we again identify all the pairs of polytopes with non-overlapping individual containers, form the corresponding subset W_2 (analogously to W_1) and let our algorithm search for a local minimum $u^*_{w_2} \in W_2$. The resulting local minimum $u^*_{w_2}$ is used to construct a starting point $u^{(2)}$ for the third iteration, etc.

On the k^{th} iteration we form starting point $u^{(k-1)}$ from the local minimum $u^*_{w_{(k-1)}}$ and solve the following k^{th} subproblem on a subset $W_k = W \bigcap \Pi^\varepsilon_k$:

$$\min_{u_{w_k} \in W_k \subset R^{\sigma-\sigma_k}} F(u_{w_k}),$$



a) b) c) d)

Fig. 3. Placement of polytopes of LOFRT-3D procedure corresponding to feasible points:
a) – $u^{(0)}$; b) – $u^*_{w_4} = u^{(4)}$; c) – $u^*_{w_8} = u^{(8)}$; d) – $u^*_{w_{20}} = u^{(20)}$

$$W_k = \{u \in R^{\sigma-\sigma_1} : \hat{\Phi}'_{ij} \ge 0, (i,j) \in \Xi_1^k, \hat{\Phi}'_i \ge 0, i \in \Xi_2^k,$$
$$\Phi^{S_i\Omega^*_{ki}} \ge 0, i = 1,2,...,n, l \ge l^{(k-1)} - \varepsilon, w \ge w^{(k-1)} - \varepsilon, h \ge h^{(k-1)} - \varepsilon\},$$

where $\Xi_1^k = \{(i,j) : \Phi^{\Omega_{ki}\Omega_{kj}} < 0, i > j = 1,2,...,n\}$, $\Xi_2^k = \{i : \Phi^{\Omega_{ki}\Omega^*} < 0, i = 1,2,...,n\}$.

If the point $u^*_{w_k}$ of local minimum of the k^{th} subproblem belongs to the frontier of an "artificial" subset

$$\Pi_k^\varepsilon = \{u \in R^{\sigma-\sigma_k} : -x_i + x_i^{(k-1)} + \varepsilon \ge 0, -y_i + y_i^{(k-1)} + \varepsilon \ge 0, -z_i + z_i^{(k-1)} + \varepsilon \ge 0,$$
$$x_i - x_i^{(k-1)} + \varepsilon \ge 0, y_i - y_i^{(k-1)} + \varepsilon \ge 0, z_i - z_i^{(k-1)} + \varepsilon \ge 0, i = 1,...,n\},$$

(i. e. $u^*_{w_k} \in fr\Pi_k^\varepsilon$), we take the point $u^*_{w_k} = u^{(k)}$ as a center point for a new subset Π_{k+1}^ε and continue our optimization procedure, otherwise (i. e. $u^*_{w_k} \in \operatorname{int}\Pi_\varepsilon^k$) we stop our LOFRT-3D procedure.

We note that $\operatorname{dist}(u^*_{w_k}, u^*_{w_{k+1}}) \ge \varepsilon$, if $u^*_{w_{k+1}} \in fr\Pi_\varepsilon^k$, and the value of ε is considerably greater than the accuracy of IPOPT (10^{-8}). Thus, we may conclude that the stopping condition of the LOFRT procedure is always reached in a finite number of iterations.

We claim that the point $u^* = u^{(k)*} = (u^*_{w_k}, \tau^*_k) \in R^\sigma$ is a point of local minimum of the problem (5)–(6), where $u^*_{w_k} \in R^{\sigma-\sigma_k}$ is the last point of our iterative procedure and τ^*_k is a vector of redefined values of the previously deleted additional variables $\tau_k \in R^{\sigma_k}$ (the values can be redefined by the special procedure used in SPA). The assertion comes from the fact that any arrangement of each pair of polytopes K_i and K_j subject to $(i,j) \in \Xi \setminus \Xi_1^k$ guarantees that there always exists a vector τ_k of additional variables such that $\hat{\Phi}'_{ij} \ge 0, (i,j) \in \Xi \setminus \Xi_1^k$ at the point $u^{(k)*}$. Here $\Xi = \{(i,j), i > j = 1,2,...,n\}$. Therefore the values of additional variables of the vector τ_k have no effect on the value of our objective function, i. e $F(u^*_{w_k}) = F(u^{(k)*})$. That is why, indeed, we do not need to redefine the deleted additional variables of the vector τ_k at the last step of our algorithm.

So, while there are $O(n^2)$ pairs of polytopes in the container, our algorithm may in most cases only actively controls $O(n)$ pairs of polytopes (this depends on the sizes of polytopes and the value of ε), because for each polytope only its "ε-neighbors" have to be monitored.

The epsilon parameter provides a *balance* between the number of inequalities in each nonlinear programming subproblem and the number of the subproblems which we need to generate and solve in order to get a local optimal solution of problem (5)–(6). The LOFTR-3D procedure allows us to reduce considerably computational costs (time and memory).

Thus our LOFRT-3D algorithm allows us to reduce the problem (5)–(6) with $O(n^2)$ inequalities and a $O(n^2)$-dimensional feasible set W to a sequence of subproblems, each with $O(n)$ inequalities and a $O(n)$-

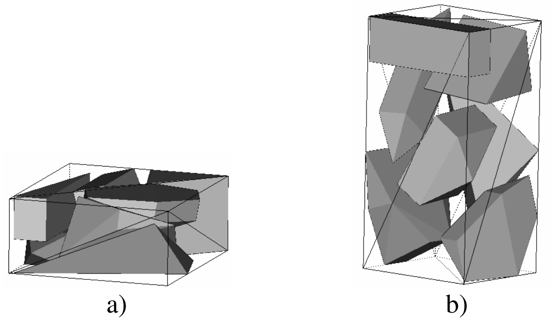


Fig. 4. Local optimal placement of polytopes in Example 1:
a) – $\rho^- = 0$; b) – $\rho^- = 1.5$

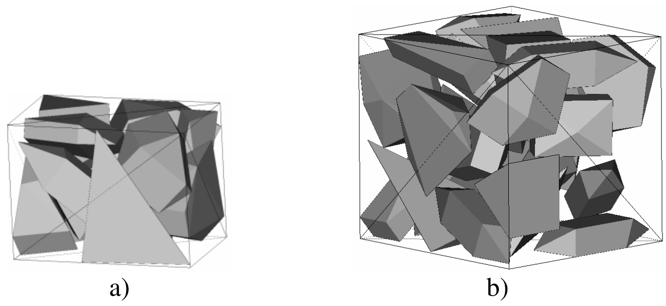


Fig.5. Local optimal placement of polytopes in Example 2:
a) – $\rho^- = 0$; b) – $\rho^- = 1.5$

dimensional solution subset W_k. This reduction is of a paramount importance, since we deal with nonlinear optimization problems.

6. Computational results

Here we present a number of examples to demonstrate the efficiency of our methodology. We have run our experiments on an AMD Athlon 64 X2 5200+ computer, and for local optimization we used the IPOPT code (https://projects.coin-or.org/Ipopt) developed by [25]. We take sizes of polytopes from paper [20] and set $\varepsilon = 5$ for LOFRT-3D procedure in our examples.

Example 1. We consider the collection of polytopes of example 1 given in [20]. Figure 4 shows the local optimal placement of $n = 7$ convex polytopes. The container has dimensions and volume: a) $(l^*, w^*, h^*) = (14.875640, 7.000000, 16.322287)$ and $F(u^*) = 1699.63$ with $\rho^- = 0$ (Fig. 4, a); b) $(l^*, w^*, h^*) = (12.214109, 22.585451, 10.119288)$ and $F(u^*) = 2791.52$ with $\rho^- = 1.5$ (Fig. 4, b).

Example 2. We consider the collection of polytopes of example 2 given in [20]. Figure 5 shows the local optimal placement of $n = 12$ convex polytopes. The container has dimensions and volume: a) $(l^*, w^*, h^*) = (19.062599, 11.588046, 14.178271)$ and $F(u^*) = 3131.96$ with $\rho^- = 0$ (Fig. 5, a); b) $(l^*, w^*, h^*) = (16.474352, 18.375541, 16.930069)$ and $F(u^*) = 5125.15$ with $\rho^- = 1.5$ (Fig. 5, b).

Example 3. We consider the collection of polytopes of example 3 given in [20]. Figure 6 shows the local optimal placement of $n = 25$ convex polytopes. The container has dimensions and volume: a) $(l^*, w^*, h^*) = (17.215330, 18.020337, 18.542389)$ and $F(u^*) = 5752.33$ with $\rho^- = 0$ (Fig. 6, a); b) $(l^*, w^*, h^*) = (21.794149, 22.043191, 20.602907)$ and $F(u^*) = 9897.9$ with $\rho^- = 1.5$ (Fig. 6, b).

For each the example the minimal volume of the container found by our method happens to be smaller than the best solution reported in [20]. The improvement is 65%, 43.7% and 30.3% in Examples 1, 2 and 3 respectively.

Example 4. We generate a collection of $n = 98$ convex polytopes, consisting of the 7 types of polytopes of example 1 given in [20] and taken by 14 of each type. Figure 7 shows the local optimal placement of n=98 convex polytopes. The container has dimensions $(l^*, w^*, h^*) = (30.932420, 28.189778, 26.506470)$ and volume $F(u^*) = 23113.06$.

7. Concluding remarks

Now, using our radical free quasi-phi-functions and phi-functions we can develop exact nonlinear programming model for optimal packing of convex polytopes taking into account distance constraints and applied our methodology to search for “good” local optimal solutions. The values of the objective

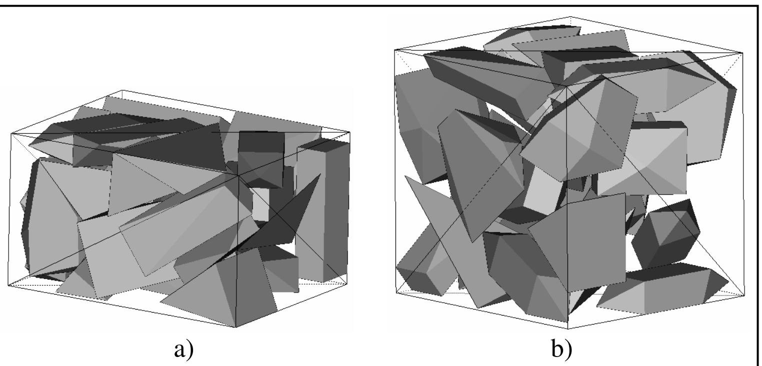


Fig. 6. Local optimal placement of polytopes in Example 3:
a) – $\rho^- = 0$; b) – $\rho^- = 1.5$

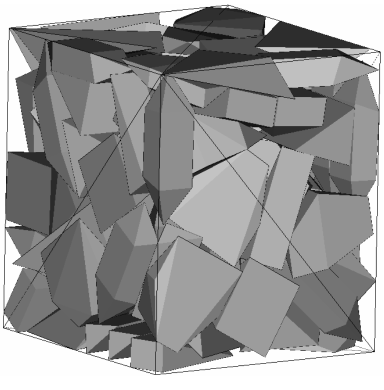


Fig.7. Local optimal placement of polytopes in Example 4

function, as well as, the computational time reported in Section 6 for several examples is achieved presently, but we expect that it will be reduced in the future. The methodology may be extended for a case of non-convex polytopes.

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