OPTIMAL CLUSTERING PROBLEMS

Optimal clustering problem. Given two (irregular) objects bounded by circular arcs and/or straight line segments where free continuous rotations of the objects are permitted, find the minimal sizes of a given containing region (rectangle, circle, or convex polygon) according to a given objective (a polynomial function) and placement parameters of two objects such that the objects are placed completely inside the containing region without overlap and taking into account allowable distances between objects. We consider a number of frequently occurring objectives, i.e. minimum area, perimeter, and homothetic coefficient of a given container.

We assume that the object frontier is given by an ordered collection of frontier elements \( l_1, l_2, \ldots, l_n \), (in counter clockwise order). Each element \( l_i \) is given by tuple \((x_i, y_i, r_i, x_{c_i}, y_{c_i})\) if \( l_i \) is an arc or by tuple \((x_i, y_i, r_i)\) if \( l_i \) is a line segment, where \((x_i, y_i)\) is the starting point of \( l_i \), \((x_{c_i}, y_{c_i})\) is the centre point of an arc. We assume that element \( l_i \) is a line segment, if \( r_i = 0 \); \( l_i \) is a "convex" arc, if \( r_i > 0 \); \( l_i \) is a "concave" arc, if \( r_i < 0 \).

We consider the following containing regions:

a) an axis-parallel rectangle: \( R = \{(x, y): 0 \leq x \leq a, 0 \leq y \leq b\} \) of variable \( a \) and \( b \) in fixed position (Fig. 1.a),

b) a circle of variable radius \( r \): \( C = \{(x, y): x^2 + y^2 \leq r\} \) with origin at the center point (Fig. 1.b),

c) a convex polygon \( K \):

- \( K \) is given by its variable sides \( e_i, \ i = 1, \ldots, m \) (Fig. 1.c), where each side \( e_i = [v_i, v_{i+1}] \) of variable length \( t_i \) is defined by two variable vertices \( v_i = (x_i, y_i) \) and \( v_{i+1} = (x_{i+1}, y_{i+1}) \), \( x_{i+1} = x_i + t_i \cdot \cos \theta_i, y_{i+1} = y_i + t_i \cdot \sin \theta_i \). Therefore, each side \( e_i \) may be given by variable vector \((x_i, y_i, \theta_i, t_i)\),

- \( \alpha K \) is given by its vertices \( \alpha v_i = (\alpha x_i, \alpha y_i), \ i = 1, \ldots, m \), where \( \alpha \) is a variable homothetic coefficient and \( x_i \) and \( y_i \) are constant (Fig. 1.d), subject to for original polygon \( \alpha = 1 \).
We consider six realizations of the optimal clustering problem, denoted by P1, .., P6, with respect to the shape of the containing region $\Omega$ and the form of the objective function $F(u)$:

- **P1**: $\Omega \equiv R$, $F_1(u) = ab$ (area of $R$),
- **P2**: $\Omega \equiv R$, $F_2(u) = a + b$ (half-perimeter of $R$),
- **P3**: $\Omega \equiv C$, $F_3(u) = r$ (radius of $C$),
- **P4**: $\Omega \equiv K$, $F_4(u) = \sum_{i=1}^{m} t_i$ (perimeter of $K$),
- **P5**: $\Omega \equiv K$, $F_5(u) = \sum_{i=1}^{m} (x_{i1}y_{i+1} - y_{i1}x_{i+1})$ s.t. $m + 1 \equiv 1$, (doubled area of $K$),
- **P6**: $\Omega \equiv \alpha K$, $F_6(u) = \alpha$ (homotetic coefficient of $K$).

**Fig. 1** Containing region $\Omega$ of variable metrical characteristics.
Computational experiments

In all cases the input data of the example has been provided in Appendix. For local optimisation in our programs we use IPOPT (https://projects.coin-or.org/Ipopt) developed by [1]. We use computer AMD Athlon 64 X2 5200+.

Example 1. We consider two triangles $A$ and $B$ and problem $P2$. The task is to find the enclosing rectangle of minimal perimeter, i.e. $F(u) = a + b$.

Example 1.1. Non-rotatable case. In this example we demonstrate the approach for computing the global solution. We use Algorithm 1 to relise model (6)-(7). Figure 2 shows the optimal arrangements of $A$ and $B$ which correspond to six local minima of problem (4)-(5) arising from the solution tree. Since all subproblems (7) are linear, we can find the global

![Diagram showing arrangements of A and B](image)

Fig. 2 Arrangements of $A$ and $B$ of Example 1.1, corresponding to points $u_s^*$, $s = 1, \ldots, 6$
minima $F(u^*)$ of problem (6)-(7). In Figure 5, each solution point $u^{s*}$ is the global minimum of subproblem (5), $s = 1, \ldots, 6$. Solution $u^* = u^{4*}$ is the point of the global minimum of problem (4)-(5). $F(u^*) = \min \{F(u^{1*}), F(u^{2*}), F(u^{3*}), F(u^{4*})\} = F(u^{4*}) = 7.6667$. Running time is 0.06 sec.

**Example 1.2.** Continuous rotations are allowed, $F(u^*) = a + b = 6.3640$. Running time is 0.109 sec, see Figure 3. We use Algorithm 1 to realize model (6)-(7).

**Example 2.** We consider two rotated objects $A$ and $B$, see Figure 4. We use Algorithm 2.

**Example 2.1** Clustering of objects $A$ and $B$ into a rectangle $R$ which looks like the optimal, problem $P1$ (Figure 4a), $F(u^*) = a^* \cdot b^* = 23.2253$. Running time is 0.431 sec.

**Example 2.2** Clustering of objects $A$ and $B$ into a circle $C$, which looks like the optimal, problem $P3$ (Figure 4b), $F(u^*) = r^* = 3.2599$. Running time is 0.387 sec.

**Example 2.3** Clustering of objects $A$ and $B$ into a rectangle $R$ taking into account minimal allowable distance $\rho = 0.6$ between objects, which looks like the optimal, problem $P1$ (Figure 4c). $F(u^*) = a^* \cdot b^* = 27.685$. Running time is 0.407 sec.

**Example 2.4** Polygonal approximation to the minimal convex hull of objects $A$ and $B$, problem $P5$ (Figure 4d). $F(u^*) = S^* = 42.6835$. Running time is 0.589 sec.

**Example 2.5** Clustering of objects $A$ and $B$ into a convex pentagon $K$ of minimal homotetic coefficient, which looks like the optimal, problem $P6$ (Figure 7e). $F(u^*) = a^* = 0.5259$. Running time is 0.401 sec.

---

**Fig. 3** Arrangement of polygons $A$ and $B$ corresponding to point $u^*$, Example 1.2
Fig. 4. Arrangement of objects $A$ and $B$ as described in Example 2: a) minimal enclosing rectangle, b) minimal enclosing circle, c) minimal enclosing rectangle taking into account distance constraints, d) minimal enclosing m-polygon, e) minimum homottetic coefficient

**Example 3.** We consider two irregular objects $A$ and $B$, see Figure 5. We use Algorithm 2.

**Example 3.1.** Optimal clustering of objects $A$ and $B$ in a circle of minimal radius, which looks like the optimal, problem $P3$, (Figure 5a). $F(u^*)=8.5826$. Running time is 0.531 sec

**Example 3.2.** Clustering of objects $A$ and $B$ in a circle of minimal radius with allowable distance $\rho = 0.3$, which looks like the optimal, problem $P3$, (Figure 5b). $F(u^*)=r^*=11.3709$. Running time is 1.235 sec

**Example 3.3.** Clustering of objects $A$ and $B$ in a convex polygon of minimal area, which looks like the optimal, problem $P5$, (Figure 5c). $F(u^*)=S^*=439.8638$. Running time is 5.06 sec.
Fig 5. Minimal enclosing container of objects $A$ and $B$ as described in Example 3: a) circle, without distance constraints, b) circle, with distance constraints, c) convex $m$-polygon

Example 4. We consider two irregular objects $A$ and $B$, see Figure 6. We use Algorithm 2.

Example 4.1 Clustering of objects $A$ and $B$ in a circle of minimal radius, which looks like the optimal, problem $P3$, (Figure 6a). $F(u^*)=17.7674$. Running time is 5.031 sec.

Example 4.2 Clustering of objects $A$ and $B$ in a rectangle of minimal area, which looks like optimal, problem $P1$, (Figure 6b). $F(u^*)=1121.6867$. Running time is 2.938 sec.

Example 4.3 Optimal clustering of objects $A$ and $B$ in a convex $m$-polygon, which looks like optimal, problem $P5$, (Figure 6c). $F(u^*)=1736.6091$. Running time is 10.375 sec.

Fig 6. Minimal enclosing regions for objects $A$ and $B$ of Example 4: a) rectangle, b) circle, c) convex $m$-polygon

Example 5. The convex hull of two rotated convex polygons $A$ and $B$, the optimal solution, problem $P5$, see Figure 10a. $F(u^*)=387.5215$. Running time is 0.14 sec. We use Algorithm 1.
Fig. 7 The convex hull for objects A and B: (a) two convex polygons, Example 5, (b) two non-convex arc objects, Example 6.

Example 6. The convex hull for two rotated objects A and B, which looks like optimal, problem P5, see Figure 9b. $F(u^*) = 51.0228$. Running time is 0.484 sec. We use Algorithm 2.

Example 7. An approximation of the convex hull for two convex polygons considering distance constraints, which looks like the optimal, problem P5, see Figure 8. Data of polygons A and B, are given for Example 1 in Appendix D. $F(u^*) = 11.3211$. Running time is 0.58 sec. We use Algorithm 1.

Fig. 8. An approximation of the m-polygonal convex hull for two convex polygons of Example 1.

Example 8. An approximation of the convex hull for two non-convex objects, see Figure 12. We use Algorithm 2.

Example 8. 1. An approximation of the convex hull of minimal area for two non-convex objects, which looks like the optimal, problem P5, (Figure 9 a ), $F(u^*) = 373.5249$. Running time is 0.56 sec

Example 8. 2. An approximation of the convex hull of minimal perimeter for two non-convex objects, which looks like the optimal, problem P4, (Figure 9b), $F(u^*) = 55.0508$. Running time is 0.57 sec
Fig 9. An approximation of the m-polygonal convex hull for two non-convex objects of Example 8: (a) area of the convex hull, m=6, (b) perimeter of the convex hull, m=8


APPENDIX: Objects data and output data for examples

Example_1. INPUT DATA

OBJECT A EX_1

$l_A = (2, -1, 0, 0, 2, 0, -2, 0, 0)$

OBJECT B EX_1

$l_B = (0, 0, 0, 3, 2, 0, 0, 2, 0)$

Example_1 OUTPUT DATA

Example 1.1. $u^* = (a^*, b^*, x_1^*, y_1^*, x_2^*, y_2^*) = (4.0, 3.6667, 2.0, 1.0, 0.0, 1.6667)$.

Example 1.2. $u^* = (a^*, b^*, x_1^*, y_1^*, x_2^*, y_2^*, \theta_1^*, \theta_2^*) = (3.5355, 2.8284, 2.1213, 1.4142, 2.3562, 0.0791, 0.7591, 6.3087)$

Example_2. INPUT DATA

OBJECT A EX_2

$l_A = (-1.605, -2.125, -2.693, 0.829, -3.278, 1.892, -0.804, 0, 2.039, 1.369, 0, -0.2372, 2.0661, 0)$

OBJECT B EX_2

$l_B = (2.022, -1.281, 1.843, 1.1539, 0.3449, 0.708, 2.133, 12.743, 7.836, -8.429, -2.934, -1.619, -3.632, -0.276, -4.0936)$

Example_2. OUTPUT DATA

Example 2.1.
\[ u^* = (a^*, b^*, x_1^*, y_1^*, \theta_1^*, x_2^*, y_2^*, \theta_2^*) = (6.0977, 3.8089, 4.1637, 2.9426, 1.2554, 2.8937, 1.2500, -2.3398) \]

**Example 2.2**.

\[ u^* = (r^*, x_1^*, y_1^*, \theta_1^*, x_2^*, y_2^*, \theta_2^*) = (3.2599, -0.2514, 1.4905, -5.4582, -0.1020, -0.7134, -9.01344) \]

**Example 2.3**.

\[ u^* = (a^*, b^*, x_1^*, y_1^*, \theta_1^*, x_2^*, y_2^*, \theta_2^*) = (4.4249, 6.2566, 0.8663, 4.3227, 5.9678, 3.1659, 2.8858, 2.3858) \]

**Example 2.4**. \( m=11, \)

\[ u^* = (x_1^*, y_1^*, \theta_1^*, \theta_1^*, t_1^*; \ldots; x_{11}^*, y_{11}^*, \theta_{11}^*, t_{11}^*; x_A^*, y_A^*, \theta_A^*, x_B^*, y_B^*, \theta_B^*) = (3.7724, 0.0000, 2.3683, 0.8404, 3.1711, -0.5870, 2.8165, 0.8404, 2.3747, -0.8554, -3.0185, 0.8404, 1.5408, -0.7522, -2.5702, 0.8404, 0.8339, -0.2977, -2.1220, 1.1793, 0.70686, 1.5251, 2.6428, 4.0045, 1.4298, 1.7318, 1.4485, 0.9580, 3.2641, 5.9187, 2.7233, 2.1026, 2.3254) \]

**Example 2.5**.

Pentagon \( K \) is given by a vector of coordinates of its vertices:

\[ (7.0190, 1.4637, 0, 1.8053, 7.2809, 0, -5.3382, 4.1200, 0, -4.5396, -3.6507, 0, 3.0977, -5.2924, 0) \]

\( m=5, \)

\[ u^* = (\alpha^*, x_A^*, y_A^*, \theta_A^*, x_B^*, y_B^*, \theta_B^*) = (0.5259, 1.6035, 1.1955, 8.1947, -0.3486, -0.0779, 10.8685) \]

**Example 3** INPUT DATA

**OBJECT A EX_3**

\[ I_A = (4.326, 6.395, -1.433, 2.914, 6.639, 1.56, 6.169, -2.405, 3.738, 7.189, 1.333, 7.212, 1.507, -0.143, 6.908, -0.553, 8.358, 3.78, 3.226, 8.266, 2.139, 4.645, -1.335, 1.574, 3.436, 0.749, 2.385, -41.479, 26.033, 35.267, -4.337, 7.015, 0.69, -4.999, 6.826, -4.974, 6.137, -11.293, -10.967, -3.435, -1.594, 2.865, -2.1027, -3.484, 1.944, -1.523, 1.186, -3.278, -1.925, 4.439, -4.36, 2.245, 18.437, -17.211, -10.975, -8.242, 5.133, -19.365, -19.496, -10.626, -3.431, 0.187, -0.727, -4.157, 0.218, -4.551, -0.393, -6.038, -1.879, 5.022, -6.914, 1.689, 1.485, -8.213, 0.971, -9.274, 2.01, -1.738, -8.923, 0.308, -8.055, -1.197, 7.273, -2.074, 2.942) \]

**OBJECT B EX_3**

\[ I_B = (2.493, 6.764, 1.771, 2.143, 5.028, 0.38, 5.191, -4.788, 1.364, 0.506, 4.149, 4.399, -1.876, 2.274, 4.368, 1.795, 2.554, 10.681, -0.594, -7.857, -1.702, 2.767, 8.905, 2.509, 10.614, 4.229, 1.877, -0.496, 4.671, 1.651, 4.781, 1.167, -16.555, 1.111, 17.31, -1.293, 0.931, 0.944, -1.623,
Example 3. OUTPUT DATA

Example 3.1. \( u^* = (r^*, x_1^*, y_1^*, \theta_1^*, x_2^*, y_2^*, \theta_2^*) = (8.5826, 2.6036, 4.1595, -1.9849, 1.1292, -0.5965, -4.4319) \)

Example 3.2. \( u^* = (r^*, x_1^*, y_1^*, \theta_1^*, x_2^*, y_2^*, \theta_2^*) = (5.6452, 4.7846, -1.3617, -1.1846, -3.5867, -3.6332) \)

Example 3.3.

\[
m=24, \quad u^* = (x_1^*, y_1^*, \theta_1^*, t_1^*, \ldots, x_{24}^*, y_{24}^*, \theta_{24}^*, t_{24}, x_A^*, y_A^*, \theta_A^*, x_B^*, y_B^*, \theta_B^*) = (-5.3369, -8.5664, -2.6532, 2.4302, -7.4829, -7.4261, -2.3683, 2.4302, -9.2220, -5.7287, -2.0835, 2.4302, -10.4141, -3.6120, -1.7987, 2.4302, -10.9631, -1.2436, -1.5138, 2.4302, -10.8247, 1.1826, -1.2290, 2.4302, -10.0101, 3.4722, -0.9441, 1.2151, -9.2975, 4.4564, -0.8760, 0.9460, -8.6918, 5.1831, -0.6355, 1.8920, -7.1669, 6.3030, -0.3909, 1.8920, -5.4177, 7.0239, -0.2271, 1.3731, -4.0798, 7.3330, 0.0182, 4.0874, 0.00688, 7.2587, 0.3034, 2.2215, 2.1269, 6.5950, 0.6065, 2.2215, 3.9522, 5.3288, 0.9096, 2.2215, 5.3164, 3.5755, 1.2127, 2.2215, 6.0950, 1.4949, 1.5158, 2.2215, 6.2171, -0.7232, 1.8189, 2.2215, 5.6716, -2.8767, 2.1220, 2.2215, 4.5081, -4.7695, 2.3619, 4.8634, 1.0496, -8.1884, 2.6565, 0.5084, 0.5998, -8.4255, 2.7755, 1.2151, -0.5346, -8.8605, 3.0603, 2.4302, -2.9569, -9.0577, -2.9380, 2.4302, 2.1774, 1.4609, 4.9044, -1.7436, -1.6084, 2.4573)\]

Example 4 INPUT DATA

OBJECT A EX_4

Example 4. OUTPUT DATA

Example 4.1. $u^* = (r^*, x_1^*, y_1^*, \theta_1^*, x_2^*, y_2^*, \theta_2^*) = (17.7674, -1.2785, 5.0441, -2.7258, -0.2362, -2.6272, 1.8515)$

Example 5. INPUT DATA

OBJECT A EX_5
\[ l_A = (-7.2662, 1.5935, 0, -5.9413, -6.8803, 0, -3.2915, -2.885, 3.884, 0, 0.83, 0.55, 0, -1.443, 2.605, -5.001, -4.7927, -1.107, 8.011, -0.12, -5.0, -2.885, 3.884, -2.879, -1.116, 0, 0.21, -1.116, -5.0, -4.7927, -1.109) \]

Example 5. OUTPUT DATA

\[ m = 10, \quad u^* = (x_1^*, y_1^*, \theta_1^*, t_1^*, \ldots, x_m^*, y_m^*, \theta_m^*, t_m^*, u_A^*, u_B^*) = (10.0238, -2.2864, 3.0242, 3.2338, 6.8123, -2.6651, -2.4537, 8.5767, 0.186, 2.7454, 5.925, 6.6713, 6.4244, 5.5554, 6.6713, 6.4244, 5.5554) \]

Example 6. INPUT DATA

OBJECT A EX_6
\[ l_A = (-1.4427, -4.8186, 0, 2.6700, -1.1068, 0, 2.089, 4.4005, -1, 0.830000, 0.5500, 0, -1.4427, 2.6050, 0, -0.1100, -0.1100, -1, -2.8787, -1.1163, -1, 0.2100, -1.1163, 0, -1.4427, -4.8186, -1) \]

OBJECT B EX_6
\[ l_B = (-1.4427, -4.8186, 0, 2.6700, -1.1068, 0, 2.0887, 4.4005, -1, 0.8300, 0.5500, 0, -1.4427, 2.6050, 0, -0.1100, -0.1100, -1, -2.8787, -1.1163, -1, 0.2100, -1.1163, 0, -1.4427, -4.8186, -1) \]

Example 6. OUTPUT DATA

\[ m = 6, \quad u^* = (x_1^*, y_1^*, \theta_1^*, t_1^*, \ldots, x_m^*, y_m^*, \theta_m^*, t_m^*, u_A^*, u_B^*) = (0.0889, 5.3038, -1.5932, 3.9616, 0, 9.2643, 0.3428, 5.5377, 5.2157, 7.4031, 1.2794, 5.5372, 6.8065, 2.099, 1.5484, 3.9615, 6.896, -1.8612, -2.7988, 5.5379, 1.6797, 0, -1.8622, 5.5372, 3.0618, 5.4759, 5.1604, 3.8337, 1.9273, 2.019) \]

Example 7.

INPUT DATA
\[ \rho = 0.2 \] is allowable distance between polygons A and B (see input data on polygons of example 1).

OUTPUT DATA
Example 8. INPUT DATA

OBJECT A EX_8 and OBJECT B EX_8

\[ l_A = l_B = (2.0, 7.0, 0, -4.0, -3.0, 0, 0, -5.0, -2.5, -1.5, -3.0, 3.0, -5.0, 0, 11.0, 0, -8.0623, 10.0, 8.0) \]

Example 8. OUTPUT DATA

Example 8.1. \( m = 6, u^* = (x_1^*, y_1^*, \theta_1^*, t_1^*, \ldots, x_m^*, y_m^*, \theta_m^*, t_m^*, u_A^*, u_B^*) = (20.2289, -2.57832, 1.49784, 4.4721, 20.5550, -7.0386, 3.1454, 11.6619, 8.8932, -6.9943, -2.4381, 11.6619, 0.0000, 0.5497, -0.7467, 11.4018, 8.3684, 8.2938, 0.6766, 13.2450, 18.6952, 0.0000, 1.0342, 3.0000, 15.9317, -5.1345, 4.1758, 6.5824, -2.5603, 4.8755) \)

Example 8.2. \( m = 8, u^* = (x_1^*, y_1^*, \theta_1^*, t_1^*, \ldots, x_m^*, y_m^*, \theta_m^*, t_m^*, u_A^*, u_B^*) = (0, 4.4189, -0.3471, 10.6193, 9.9858, 8.0318, 0.3941, 9.4340, 18.696, 4.4093, 0.9527, 3, 20.435, 1.9643, 1.4164, 4.4721, 21.123, -2.4546, 2.794, 10.6193, 11.1372, -6.0674, -2.7475, 9.434, 2.4264, -2.445, -2.1889, 3, 0.688, 0, -1.7252, 4.4721, 16.3601, -0.9331, 4.0943, 4.7629, 2.8974, 0.9527) \)