

A shape optimization approach to the problem of covering a two-dimensional region with minimum-radius identical balls

Antoine Laurain

Instituto de Matemática e Estatística, Universidade de São Paulo.

joint work with: Ernesto G. Birgin, Rafael Massambone, Arthur G. Santana

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Packing of spheres and covering problem

- ▶ *Sphere packings, lattices and groups*
J.H. Conway and N.J.A. Sloane.
- ▶ The packing and covering problems in the whole space are kind of dual.
- ▶ The solutions to these problems often involve lattices.
- ▶ Kepler conjecture (3D) solved by Thomas Hales in 1998.
- ▶ Optimal packing in 8D solved by Maryna Viazovska in 2016.

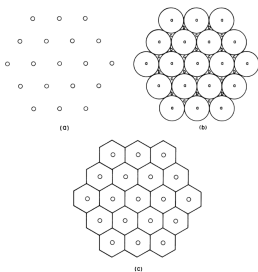


Figure 1.3. (a) The hexagonal lattice in the plane. (b) The corresponding sphere-packing (in this case a circle-packing). The points labeled a are the lattice points; the points labeled b and c are the "deep holes" in this lattice, the points of the plane furthest from the lattice. (c) The Voronoi cells are regular hexagons. (d) An enlargement of (b) and (c), showing the packing radius μ of the lattice (the radius of the circles in (b)), and the covering radius R , the distance from a lattice point to a deep hole. For this lattice $R = 2\mu/\sqrt{3}$.

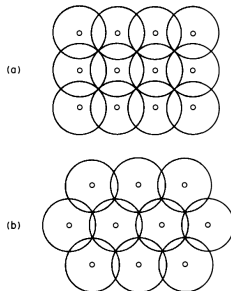


Figure 2.1. Covering the plane with circles. In (a) the centers belong to the square lattice Z^2 , in (b) they belong to the hexagonal lattice. (b) is a more efficient or *thinner* covering.

Covering problem

- ▶ We consider the problem of covering a subset A of \mathbb{R}^2 (not the whole plane).
- ▶ $A \subset \mathbb{R}^2$ and $\Omega(\mathbf{x}, r) = \cup_{i=1}^m B(x_i, r)$ with $\mathbf{x} := \{x_i\}_{i=1}^m$.
- ▶ Find $(\mathbf{x}, r) \in \mathbb{R}^{2m+1}$ such that $A \subset \Omega(\mathbf{x}, r)$ with minimum r .
- ▶ Optimization formulation:

$$\text{Minimize}_{(\mathbf{x}, r) \in \mathbb{R}^{2m+1}} r \text{ subject to } G(\mathbf{x}, r) = 0,$$

where

$$G(\mathbf{x}, r) := \text{Vol}(A) - \text{Vol}(A \cap \Omega(\mathbf{x}, r))$$

- ▶ $G(\mathbf{x}, r) = 0$ if and only if $A \subset \Omega(\mathbf{x}, r)$ up to a set of zero measure, i.e., when $\Omega(\mathbf{x}, r)$ covers A .

Covering problem

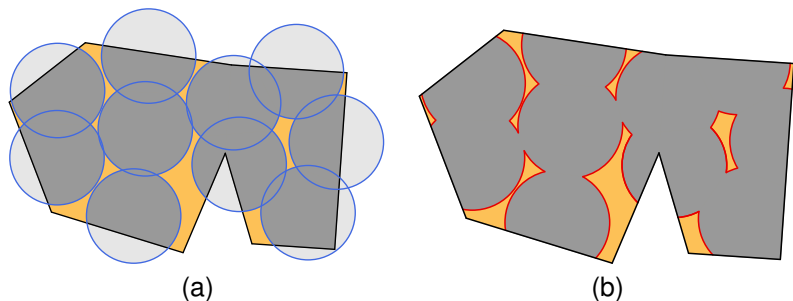


Figure: (a) represents a region A (orange color) to be covered by a union of balls $\Omega(\mathbf{x}, r)$. (b) represents, in red, $\partial\Omega(\mathbf{x}, r) \cap A$. Each $\mathcal{A}_i := \partial B(x_i, r) \cap \partial\Omega(\mathbf{x}, r) \cap A$ corresponds to the red arcs intersecting $\partial B(x_i, r)$. In this example, most sets \mathcal{A}_i contain two or three maximal arcs and there is only one \mathcal{A}_i with four maximal arcs.

Some important notations

- ▶ Given $x, y \in \mathbb{R}^n$, $x \cdot y = x^\top y \in \mathbb{R}$ and $x \otimes y = xy^\top \in \mathbb{R}^{n \times n}$.
- ▶ $B(x_i, r)$ denotes an open ball with center $x_i \in \mathbb{R}^2$ and radius r .
- ▶ For a sufficiently smooth set $S \subset \mathbb{R}^2$, $\nu_S(z)$ denotes the unitary-norm outwards normal vector to S at z .
- ▶ $\tau_S(z)$ is the unitary-norm tangent vector to ∂S at z (pointing counter-clockwise).
- ▶ When $S = B(x_i, r)$ we use $\nu_i(z) := \nu_{B(x_i, r)}$ and $\tau_i(z) := \tau_{B(x_i, r)}$.
- ▶ For intersection points $z \in \partial S \cap B(x_i, r)$, we also use the notation $\nu_{-i}(z) := \nu_S(z)$.

Second-order derivative of G

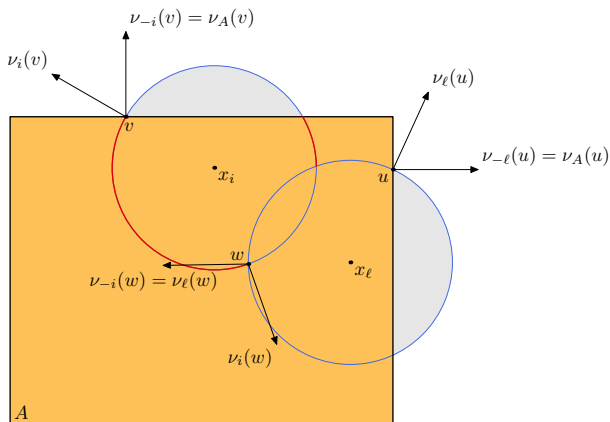


Figure: The set $\mathcal{A}_i = \partial B(x_i, r) \cap \Omega(\mathbf{x}, r) \cap A$ is composed of two arcs (in red). If $z \in \partial B(x_i, r) \cap \partial B(x_\ell, r)$ for some $\ell \neq i$, as for $z = w$, then $\nu_{-i}(z) = \nu_\ell(z)$, while if $z \in \partial B(x_i, r) \cap \partial A$, as for $z \in \{u, v\}$, then $\nu_{-i}(z) = \nu_A(z)$.

First and second-order derivative of G

- ▶ The derivatives of G can be computed using techniques of shape calculus [Delfour, Henrot, Murat, Pierre, Simon, Sokolowski, Zolésio].
- ▶ Assuming (\mathbf{x}, r) is non-degenerate:

$$\nabla G(\mathbf{x}, r) = - \left(\int_{\mathcal{A}_1} \nu_1(z) dz, \dots, \int_{\mathcal{A}_m} \nu_m(z) dz, \int_{\partial\Omega(\mathbf{x}, r) \cap A} dz \right)^\top,$$

with $\mathcal{A}_i := \partial B(x_i, r) \cap \partial\Omega(\mathbf{x}, r) \cap A$.

- ▶ The Hessian of G is given by:

$$\nabla^2 G(\mathbf{x}, r) = \begin{pmatrix} \nabla_{\mathbf{x}}^2 G(\mathbf{x}, r) & \nabla_{\mathbf{x}, r}^2 G(\mathbf{x}, r) \\ \nabla_{\mathbf{x}, r}^2 G(\mathbf{x}, r)^\top & \nabla_r^2 G(\mathbf{x}, r) \end{pmatrix},$$

with the blocks $\nabla_{\mathbf{x}}^2 G(\mathbf{x}, r) \in \mathbb{R}^{2m \times 2m}$, $\nabla_{\mathbf{x}, r}^2 G(\mathbf{x}, r) \in \mathbb{R}^{2m}$, and $\nabla_r^2 G(\mathbf{x}, r) = \partial_r^2 G(\mathbf{x}, r) \in \mathbb{R}$.

Second-order derivative of G

- ▶ \mathcal{A}_i is a finite union of arcs of the circle $\partial B(x_i, r)$.
- ▶ \mathbb{A}_i denotes the set of pairs (v, w) that represent the arcs in \mathcal{A}_i .
- ▶ $\mathbb{A}_i = \emptyset$ if \mathcal{A}_i is a full circle.
- ▶ The scalar $\nabla_r^2 G(\mathbf{x}, r)$ is given by:

$$\nabla_r^2 G(\mathbf{x}, r) = -\frac{\text{Per}(\partial\Omega(\mathbf{x}, r) \cap \mathcal{A})}{r} - \sum_{i=1}^m \sum_{(v, w) \in \mathbb{A}_i} \left[\left[\frac{|L(z)| \cdot \nu_{-i}(z) \cdot \nu_i(z)}{\nu_{-i}(z) \cdot \tau_i(z)} \right] \right]_v^w$$

- ▶ $\left[\left[\Phi(z) \right] \right]_v^w := \Phi(w) - \Phi(v)$
- ▶ For an extreme z of an arc represented by $(v, w) \in \mathbb{A}_i$,

$$L(z) = \{\ell \in \{1, \dots, m\} \setminus \{i\} \mid z \in \partial B(x_\ell, r)\}.$$

Second-order derivative of G

- ▶ Matrix $\nabla_{\mathbf{x}}^2 G(\mathbf{x}, r)$ is given by the 2×2 diagonal blocks

$$\begin{aligned} \partial_{x_i x_i}^2 G(\mathbf{x}, r) &= \frac{1}{r} \int_{\mathcal{A}_i} -\nu_i(\mathbf{z}) \otimes \nu_i(\mathbf{z}) + \tau_i(\mathbf{z}) \otimes \tau_i(\mathbf{z}) \, d\mathbf{z} \\ &\quad + \sum_{(\mathbf{v}, \mathbf{w}) \in \mathbb{A}_i} \left[\left[\frac{\nu_{-i}(\mathbf{z}) \cdot \nu_i(\mathbf{z})}{\nu_{-i}(\mathbf{z}) \cdot \tau_i(\mathbf{z})} \nu_i(\mathbf{z}) \otimes \nu_i(\mathbf{z}) \right] \right]_{\mathbf{v}}^{\mathbf{w}} \end{aligned}$$

and the 2×2 off-diagonal blocks

$$\partial_{x_i x_\ell}^2 G(\mathbf{x}, r) = \sum_{\mathbf{v} \in \mathcal{I}_{i\ell}} \frac{\nu_i(\mathbf{v}) \otimes \nu_\ell(\mathbf{v})}{\nu_\ell(\mathbf{v}) \cdot \tau_i(\mathbf{v})} - \sum_{\mathbf{w} \in \mathcal{O}_{i\ell}} \frac{\nu_i(\mathbf{w}) \otimes \nu_\ell(\mathbf{w})}{\nu_\ell(\mathbf{w}) \cdot \tau_i(\mathbf{w})},$$

- ▶ $\mathcal{I}_{i\ell} = \{\mathbf{v} \in \partial B(x_\ell, r) \mid (\mathbf{v}, \cdot) \in \mathbb{A}_i\}$
- ▶ $\mathcal{O}_{i\ell} = \{\mathbf{w} \in \partial B(x_\ell, r) \mid (\cdot, \mathbf{w}) \in \mathbb{A}_i\}$
- ▶ Note that $\mathcal{I}_{i\ell} = \mathcal{O}_{i\ell} = \emptyset$ for all $\ell \neq i$ if $\mathbb{A}_i = \emptyset$.

Second-order derivative of G

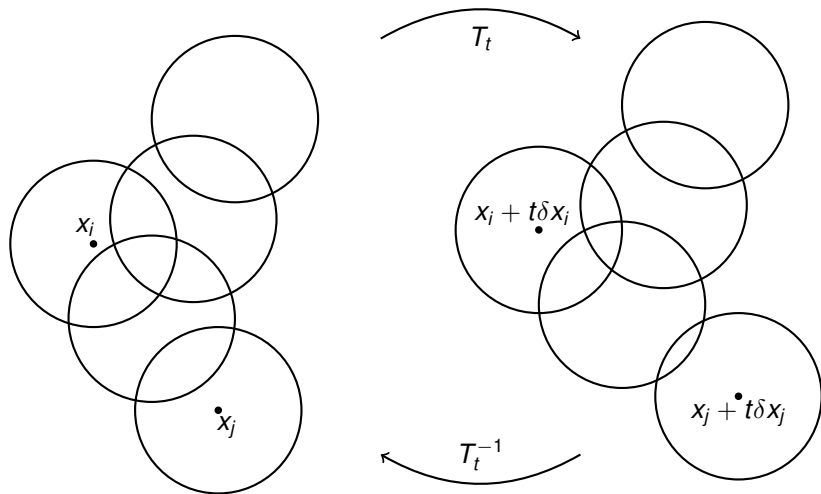
- ▶ $\nabla_{\mathbf{x}, r}^2 G(\mathbf{x}, r)$ is given by the 2-dimensional arrays

$$\begin{aligned} \partial_{x_i r}^2 G(\mathbf{x}, r) = & -\frac{1}{r} \int_{\mathcal{A}_i} \nu_i(z) dz \\ & + \sum_{(v, w) \in \mathbb{A}_i} \left[\frac{\nu_{-i}(z) \cdot \nu_i(z)}{\nu_{-i}(z) \cdot \tau_i(z)} \nu_i(z) - \sum_{\ell \in L(z)} \frac{\nu_i(z)}{\tau_i(z) \cdot \nu_\ell(z)} \right]_{v, w} \end{aligned}$$

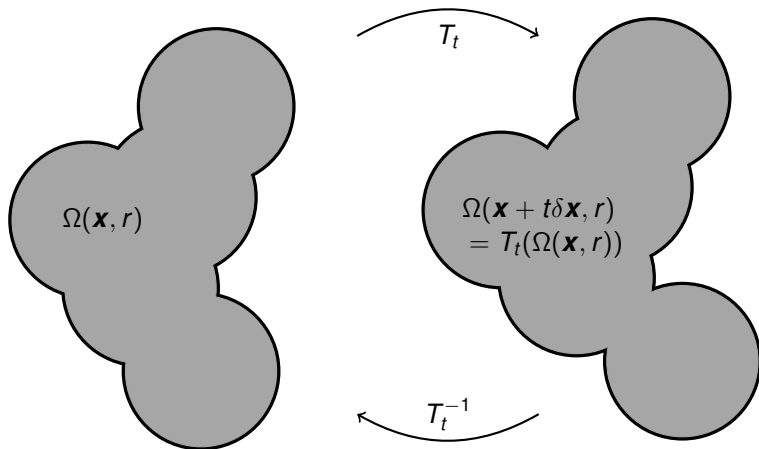
- ▶ For an extreme z of an arc represented by $(v, w) \in \mathbb{A}_i$,

$$L(z) = \{\ell \in \{1, \dots, m\} \setminus \{i\} \mid z \in \partial B(x_\ell, r)\}.$$

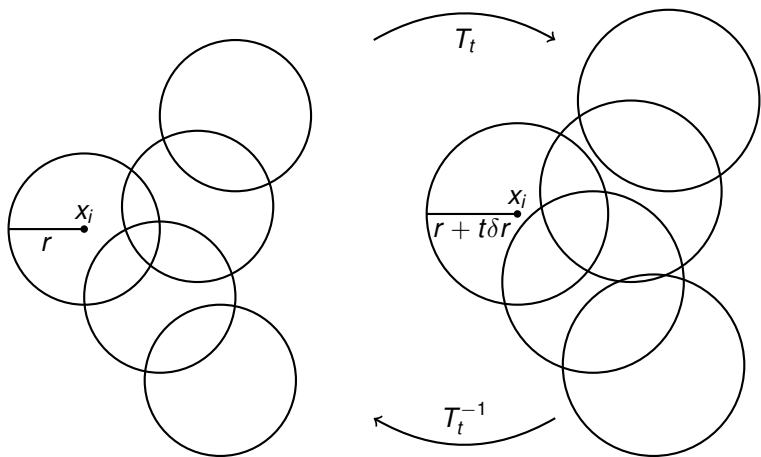
Center perturbations



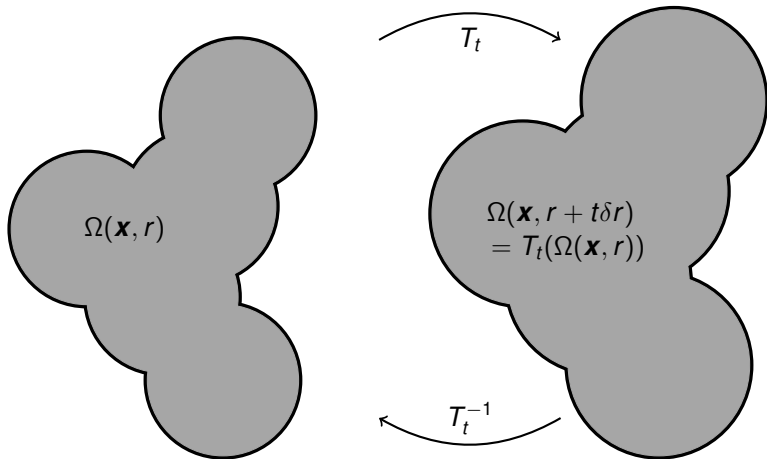
Center perturbations



Radius perturbations



Radius perturbations



Construction of bi-Lipschitz mappings T_t

- ▶ How can we build bi-Lipschitz mappings $T_t : \Omega(\mathbf{x}, r) \rightarrow \Omega(\mathbf{x} + t\delta\mathbf{x}, r)$ and $T_t : \Omega(\mathbf{x}, r) \rightarrow \Omega(\mathbf{x}, r + t\delta r)$?
- ▶ First, we observe that $\partial\Omega(\mathbf{x}, r)$ contains singular points (the circle intersections) and regular points.
- ▶ The motion of the singular points is **fully determined** by the center or radius perturbations.
- ▶ For instance, the motion of an intersection point in $\partial B(\mathbf{x}_i + t\delta\mathbf{x}_i, r) \cap \partial B(\mathbf{x}_j + t\delta\mathbf{x}_j, r)$ can be fully determined, for sufficiently small t , using the implicit function theorem.
- ▶ The motion of the regular points is **underdetermined**. Roughly speaking, one direction of T_t is prescribed (such as $t\delta\mathbf{x}_i$ for center perturbations), while the orthogonal direction can be chosen “freely”.

Construction of bi-Lipschitz mappings T_t

- ▶ Thus, we are free to choose this orthogonal direction of T_t at regular points, as long as these constraints are satisfied:
 - T_t must be bi-Lipschitz
 - The value of T_t is prescribed at the singular points.
 - $T_t(\Omega(\mathbf{x}, r) \cap A) = \Omega(\mathbf{x} + t\delta\mathbf{x}, r) \cap A$ or
 $T_t(\Omega(\mathbf{x}, r) \cap A) = \Omega(\mathbf{x}, r + t\delta r) \cap A$.
- ▶ Since $\partial\Omega(\mathbf{x}, r)$ is a union of arcs, we can use local polar coordinates on each $B(x_i, r)$ to define the missing direction of T_t at regular points.
- ▶ Then we extend T_t to $\Omega(\mathbf{x}, r) \cap A$, in a way that preserves the bi-Lipschitz property of T_t .

Shape derivative for radius perturbations

- ▶ We can actually build a bi-Lipschitz mapping

$$T_t : \Omega(\mathbf{x}, r) \cap A \rightarrow \Omega(\mathbf{x}, r + t\delta r) \cap A.$$

- ▶ T_t allows us to use the following change of variables:

$$\begin{aligned} G(\mathbf{x}, r + t\delta r) &= \text{Vol}(A \setminus \Omega(\mathbf{x}, r + t\delta r)) \\ &= \text{Vol}(A) - \text{Vol}(A \cap \Omega(\mathbf{x}, r + t\delta r)) \\ &= \text{Vol}(A) - \int_{T_t(\Omega(\mathbf{x}, r) \cap A)} dz \\ &= \text{Vol}(A) - \int_{\Omega(\mathbf{x}, r) \cap A} |\det DT_t(z)| dz. \end{aligned}$$

- ▶ Then the derivative is, with $V := \partial_t T_t|_{t=0}$,

$$\begin{aligned} \left. \frac{d}{dt} G(\mathbf{x}, r + t\delta r) \right|_{t=0} &= - \int_{\Omega(\mathbf{x}, r) \cap A} \text{div } V(z) dz \\ &= - \int_{\partial(\Omega(\mathbf{x}, r) \cap A)} V(z) \cdot \nu(z) dz = -\delta r \int_{\partial\Omega(\mathbf{x}, r) \cap A} dz \end{aligned}$$

Other shape derivatives

- ▶ The property $V(z) \cdot \nu(z) = \delta r$ on $\partial\Omega(\mathbf{x}, r) \cap A$ comes from the explicit construction of T_t on $\partial(\Omega(\mathbf{x}, r) \cap A)$.
- ▶ The calculation works in a similar way for center perturbations and for second-order derivatives.
- ▶ The main task is to build the appropriate T_t for each type of perturbation, and compute the corresponding $V := \partial_t T_t|_{t=0}$.

Other shape derivatives

- ▶ These derivatives were obtained assuming (\mathbf{x}, r) is non-degenerate, i.e., when the following assumptions hold.
- ▶ **Assumption 1.** The centers $\{x_i\}_{i=1}^m$ satisfy $\|x_i - x_j\| \notin \{0, 2r\}$ for all $1 \leq i, j \leq m$, $i \neq j$ and $\partial B(x_i, r) \cap \partial B(x_j, r) \cap \partial B(x_k, r) = \emptyset$ for all $1 \leq i, j, k \leq m$ with i, j, k pairwise distinct.
- ▶ **Assumption 2.** $\Omega(\mathbf{x}, r)$ and A are compatible.
- ▶ This yields the following decomposition, with \bar{k} independent of t :

$$\partial\Omega(\mathbf{x} + t\delta\mathbf{x}, r) \cap A = \bigcup_{k=1}^{\bar{k}} \mathcal{S}_k(t),$$

where $\mathcal{S}_k(t)$ are arcs parameterized by an angle aperture $[\theta_{k,v}(t), \theta_{k,w}(t)]$, and $t \mapsto \theta_{k,v}(t)$, $t \mapsto \theta_{k,w}(t)$ are continuous.

Compatibility

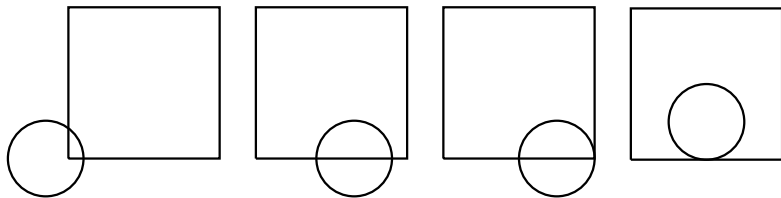


Figure: Compatibility of a ball and a square. From left to right: (a) compatible (b) compatible (c) not compatible (d) not compatible.

Example of degenerate case: two tangent disks

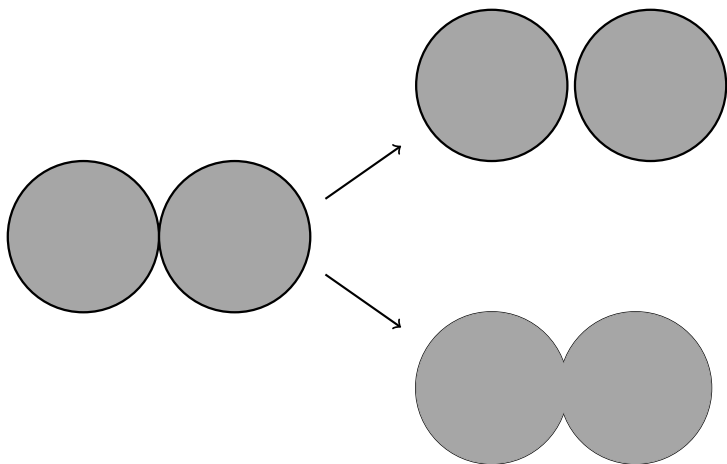
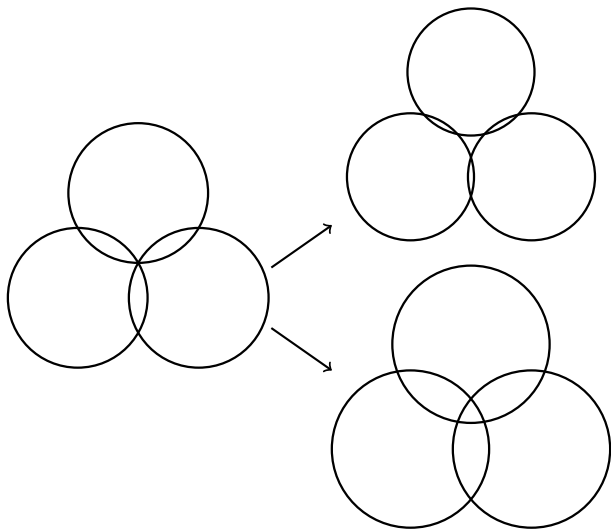


Figure: Two tangent disks $B(x_1, r)$ and $B(x_2, r)$ may either merge if $(x_1 - x_2) \cdot (\delta x_1 - \delta x_2) < 0$ or have an empty intersection if $(x_1 - x_2) \cdot (\delta x_1 - \delta x_2) > 0$.

Example of degenerate case: three disks



Analysis of singular cases

- ▶ Other singular cases: two superposed disks, a disk tangent to ∂A , etc ...
- ▶ Singular cases can be investigated using asymptotic analysis: G is sometimes differentiable, but seems to never be twice differentiable.
- ▶ Gateaux semidifferentiability of the components of ∇G can often be proved.

Algorithm 1

- ▶ After discretization, the problem becomes a constrained nonlinear programming problem (with a linear objective function and a single difficult nonlinear constraint) of the form

Minimize $f(\mathbf{x}, r) := r$ subject to $G_h(\mathbf{x}, r) = 0$ and $r \geq 0$

- ▶ We considered the safeguarded Augmented Lagrangian (AL) method Algencan [Andreani, Birgin, Martínez, Schuverdt].
- ▶ Algencan is based on the PHR AL function, in this case:

$$L_\rho(\mathbf{x}, r, \lambda) = f(\mathbf{x}, r) + \frac{\rho}{2} \left[G_h(\mathbf{x}, r) + \frac{\lambda}{\rho} \right]^2, \quad (1)$$

for all $\rho > 0$, $r \geq 0$, and $\lambda \in \mathbb{R}$.

- ▶ Each iteration of the method consists in the approximate minimization of (1) subject to $r \geq 0$ followed by the update of the Lagrange multiplier λ and the penalty parameter ρ .

Numerical results for Algorithm 1

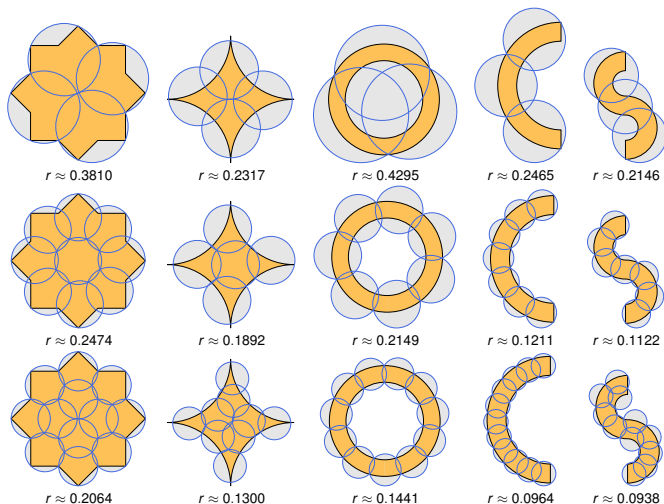


Figure: Solutions found for covering two-squares region with $m = 4, 9, 12$, peaked star region with $m = 4, 5, 9$, ring, half-ring, and two-half-rings regions with $m = 3, 7, 11$, and disconnected region with $m = 3, 7, 15$.

Numerical results for Algorithm 1

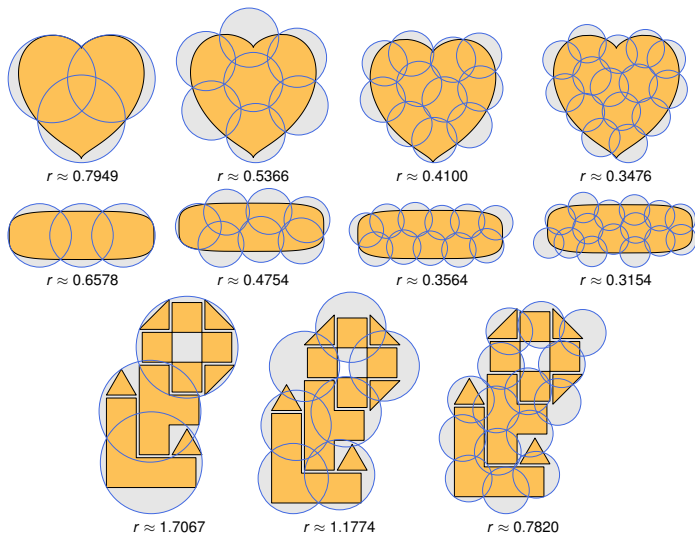







Figure: Solutions found for covering heart-shape and soap-shape regions with $m = 3, 7, 11, 15$, and disconnected region with $m = 3, 7, 15$.

Performance metrics for Algorithm 1

Alg. 1.1 computes G (complexity $O(1/h^2)$), Alg. 1.2 computes ∇G (complexity $O(1/h)$), “trial” is the number of the initial guess yielding the best solution, “outit” and “innit” are the number of outer and inner iterations of the AL optimization method.

Region A	m	r^*	trial	outit	innit	Alg. 1.1	Alg. 1.2	CPU Time
	3	0.7949	100	20	155	2188	249	59.08
	7	0.5366	69	15	50	214	117	7.92
	11	0.4100	89	12	68	303	130	12.77
	15	0.3476	78	13	77	311	138	15.46
	3	0.6578	70	12	76	402	134	4.61
	7	0.4754	30	13	119	1228	185	20.11
	11	0.3564	61	13	72	261	132	6.12
	15	0.3154	69	13	80	447	140	12.77
	4	0.3810	91	11	40	222	90	2.78
	9	0.2474	70	11	45	197	94	3.18
	12	0.2064	32	10	66	346	112	6.16
	4	0.2317	82	20	136	2221	230	14.55
	5	0.1892	32	10	61	251	107	1.70
	9	0.1300	59	10	56	248	107	1.84
	3	0.4295	12	10	40	186	86	0.49
	7	0.2149	36	10	35	155	78	0.58
	11	0.1441	23	12	94	337	152	1.50

Algorithm 1

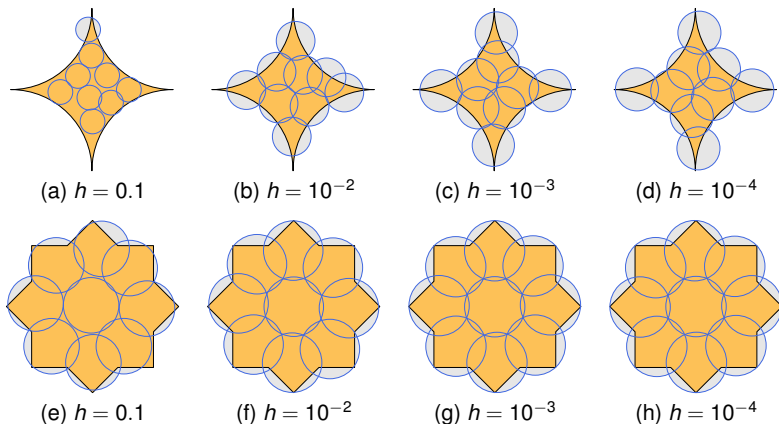


Figure: Solutions found varying $h \in \{0.1, 10^{-2}, 10^{-3}, 10^{-4}\}$ in problems (a–d) “two squares” and (e–h) “peaked star” with $m = 9$. The peaked star requires a smaller h to cover its small thin features.

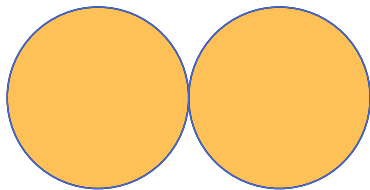


Figure: An example of a degenerate case: A is the union of two tangent unitary-diameter balls to be covered by $m = 2$ balls. In this case, ∇G does not exist. Even though this singular case is not covered by the theory, the solution, which is the set A itself, was found with a single run of the method.

Algorithm 2

- ▶ Algorithm 1 allows to find coverings of general shapes A , but is relatively slow when a fine discretization is required (i.e., a small h). This occurs when A presents small thin features. Algorithm 1 only uses G and ∇G .
- ▶ Algorithm 2 deals with the case $A = \cup_{j=1}^p A_j$ and $\{A_j\}_{j=1}^p$ are non-overlapping convex polygons. Algorithm 2 uses G , ∇G and $\nabla^2 G$. In this case G , ∇G and $\nabla^2 G$ can be computed analytically which leads to a fast and accurate algorithm.

Algorithm 2

- ▶ Compute Voronoi diagram with cells $\{V_i\}_{i=1}^m$ associated with the balls centers x_1, \dots, x_m .
- ▶ Compute convex polygons $W_{ij} = A_j \cap V_i$ and $S_{ij} = W_{ij} \cap B(x_i, r)$ for $j = 1, \dots, p$ and $i = 1, \dots, m$.
- ▶ $\mathcal{K}_{A_j} = \{i \in \{1, \dots, m\} \mid S_{ij} \neq \emptyset\}$
- ▶ Partition $A_j \cap \Omega(\mathbf{x}, r) = \bigcup_{i \in \mathcal{K}_{A_j}} S_{ij}$, $j = 1, \dots, p$.

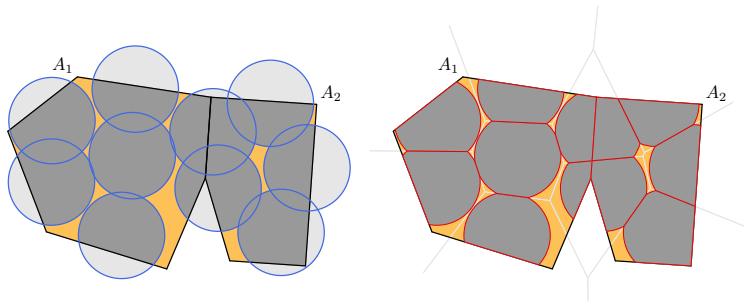


Figure: (left) $A = \bigcup_{j=1}^p A_j$ with $p = 2$ and $\Omega(\mathbf{x}, r) = \bigcup_{i=1}^m B(x_i, r)$ with $m = 10$. (right) Voronoi diagram and sets S_{ij} .

Algorithm 2

- ▶ Using the sets S_{ij} , G , ∇G and $\nabla^2 G$ can be computed analytically.
- ▶ $G(\mathbf{x}, r) = \text{Vol}(A) - \text{Vol}(A \cap \Omega(\mathbf{x}, r)) = \text{Vol}(A) - \sum_{(i,j) \in \mathcal{K}} \text{Vol}(S_{ij})$.
- ▶ Using Green's Theorem,

$$\begin{aligned} \text{Vol}(S_{ij}) &= \int_{S_{ij}} dx dy = \int_{\partial S_{ij}} x dy \\ &= \sum_{[v,w] \in \mathbb{E}(S_{ij})} \int_0^1 x_{\mathcal{E}}(t) dy_{\mathcal{E}}(t) + \sum_{(v,w) \in \mathbb{A}(S_{ij})} \int_{\theta_v}^{\theta_w} x_{\mathcal{A}}(\theta) dy_{\mathcal{A}}(\theta) \end{aligned}$$

and this can be computed analytically.

- ▶ Here $\mathbb{E}(S_{ij})$ is the set of edges of ∂S_{ij} , and $\mathbb{A}(S_{ij})$ is the set of arcs of ∂S_{ij} .
- ▶ Works in a similar way for ∇G and $\nabla^2 G$.

Algorithm 2

- ▶ The algorithms for computing G , ∇G and $\nabla^2 G$ depend on the computation of \mathbb{E}_i and \mathbb{A}_i for $i = 1, \dots, m$.
- ▶ Computing \mathbb{E}_i and \mathbb{A}_i requires to compute the Voronoi diagram (using Fortune's algorithm) and to compute $W_{ij} = V_i \cap A_j$ and $S_{ij} = W_{ij} \cap B(x_i, r)$.
- ▶ The worst-case time complexity of Algorithm 2 is $\mathcal{O}(m \log m + m \sum_{j=1}^p e_{A_j})$, where e_{A_j} is the number of sides of A_j .

Numerical results for Algorithm 2

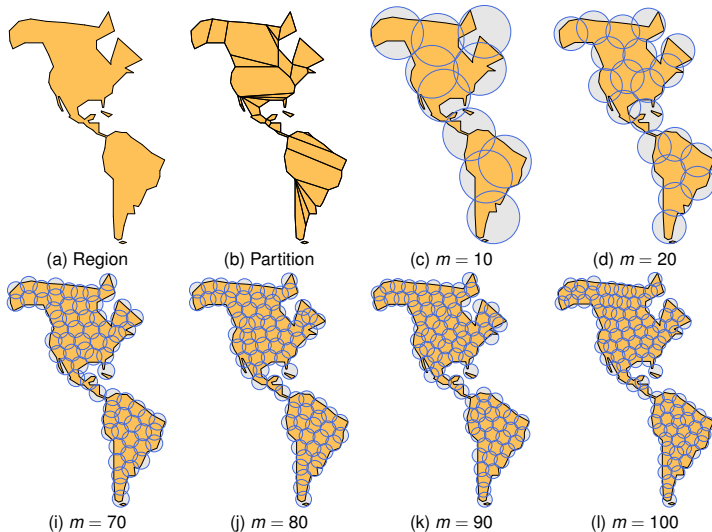
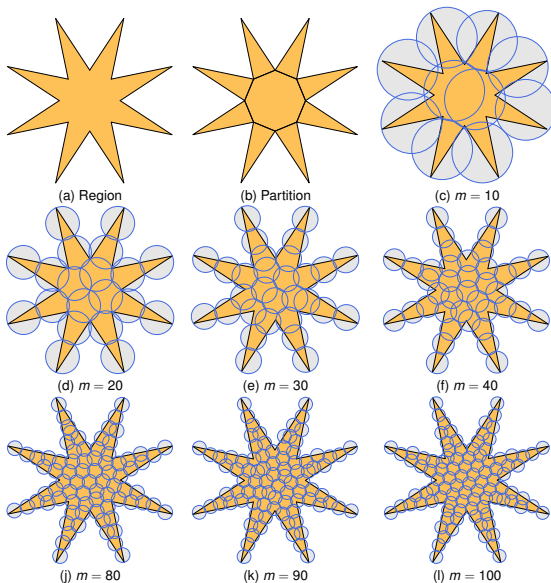


Figure: (a) Sketch of America, partitioned into $p = 34$ convex polygons. Pictures from (c) to (l) display the solutions for $m \in \{10, \dots, 100\}$.

Numerical results for Algorithm 2



Conclusion

- ▶ Shape-Newton method in a nonsmooth setting.
- ▶ Algorithm 1 is based on first-order derivative and works for general shapes A .
- ▶ Algorithm 2 is based on first- and second-order derivatives and works for the union of non-overlapping convex polygons. Much faster and more accurate than Algorithm 1.
- ▶ It seems that the assumptions used to derive $\nabla^2 G$ cannot be weakened.
- ▶ *A shape optimization approach to the problem of covering a two-dimensional region with minimum-radius identical balls*
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- ▶ *A Shape-Newton approach to the problem of covering with identical balls.*
E. G. Birgin, A. Laurain, R. Massambone, and A. G. Santana
arXiv:2106.03641, 2021

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THANKS FOR YOUR ATTENTION!