`compGeometeR`: an `R` package for computational geometry

Thomas R. Etherington
Manaaki Whenua – Landcare Research

O. Pascal Omondiagbe
Manaaki Whenua – Landcare Research

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Abstract

Computational geometry algorithms and data structures are widely applied across numerous scientific domains, and there a variety of `R` packages that apply computational geometry. However, these packages often work in specific numbers of dimensions, have incompatible data structures, and include additional non-computational geometry functionality that can be domain specific. Our objective in developing the `compGeometeR` package is to produce a systematic implementation of the most commonly used computational geometry algorithms so that they can be easily integrated into domain specific scientific workflows. We briefly explain the algorithms available in `compGeometeR`, and identify priorities for future development.

Keywords: alpha complex, alpha shape, convex hull, convex layers, Delaunay triangulation, digital, discrete.

1 Introduction

Computational geometry seeks to develop algorithms and data structures for geometric objects, and the results are widely applied across numerous scientific domains (de Berg et al., 2008). Given the importance of computational geometry it is no surprise that within the R computing ecosystem there are a variety of options for applying various computational geometry algorithms in a variety of dimensions. However, these packages often work in specific numbers of dimensions, have incompatible data structures, and include additional non-computational geometry functionality that can be domain specific.

Our objective in developing the `compGeometeR` package is to produce a systematic implementation of some of the most commonly used computational geometry algorithms across various of branches of geometry so that they can be easily integrated into domain specific scientific workflows. The functionality of `compGeometeR` is entirely dependent on computational foundations provided by the `Qhull` C++ interface software (Barber et al., 1996).

Table 1: Computational geometry software options in R. For each computational geometry function, the R software (and version) that can apply this algorithm is noted by reference to the number of dimensions in which the algorithm will work.

	compGeometeR (1.0.0)	R (3.5.3)	alphahull (2.2)	alphashape3d (1.3.1)	deldir (0.1-25)	geometry (0.4.5)	spatstat (1.63-3)	tripack (1.3-9.1)
Discrete geometry								
Alpha complex	n							
Alpha shape			2	3				
Convex hull	n	2				n	2	2
Convex layers	n							
Delaunay triangulation	n		2		2	n	2	2
Voronoi diagram			2		2	n	2	2
Digital geometry								
Alpha complex	n							
Alpha shape	n							
Convex hull	n							

2 Algorithms

There are a variety of computational geometry algorithms available in `compGeometeR`, some of which are replicated in other R packages. By documenting these differences (Table 1) we hope to help potential users to assess if `compGeometeR` is the best option for their needs as there may be other options that are more suitable.

2.1 Discrete geometry

Discrete geometry studies the shapes and interactions between sets of discrete objects such as points, lines, circles, and polygons in 2-dimensional space. All of the discrete computational geometry algorithms in `compGeometeR` take as an input a set of points P in n-dimensional Euclidean space $\mathbb{R}^n$.

A convex hull defines the smallest subset of $\mathbb{R}^n$ that contains P and for which the subset is convex so any two points within the convex hull can be connected by a straight line also contained by the convex hull (Figure 1a).

Convex layers were first presented by Huber (1972) and Barnett (1976) who both gave unreferenced credit for this idea to Tukey. Convex layers are a nested sequence of convex hulls produced by repeating the process of constructing a convex hull for P and then removing the points forming the vertices of the convex hull from P before producing the next convex layer. The first convex layer is equivalent to the convex hull, with each successive convex layer representing ever smaller region of space (Figure 1b).

The Delaunay triangulation (Delaunay, 1934) produces a set of simplices (triangles in

2-dimensions or tetrahedrons in 3-dimensions) for which no point in P is inside the the circumhypersphere (a circle in 2-dimensions or a sphere in 3-dimensions) of each simplex (Figure 1c).

The alpha complex (Edelsbrunner and Mücke, 1994) is a subset of the Delaunay triangulation that contains only those simplices for whose circumhypersphere radius is smaller than a specified α parameter value ranging $0 < \alpha < \infty$ (Figure 1d).

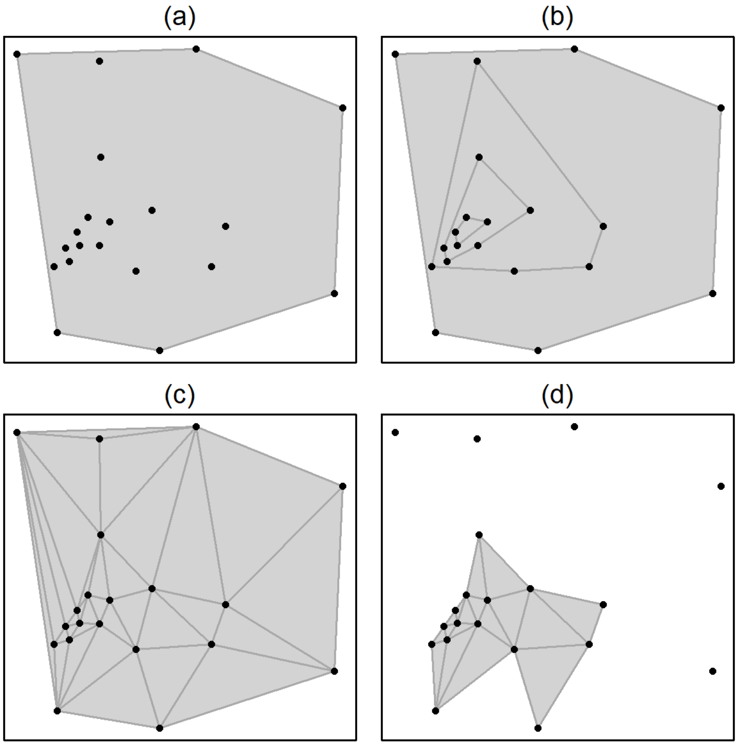

Figure 1: Two-dimensional examples of discrete geometry algorithms currently available in `compGeometeR`. (a) Convex hull, (b) convex layers, (c) Delaunay triangulation, and (d) alpha complex.

2.2 Digital geometry

Digital geometry is a branch of geometry that studies the geometric properties of a grid (or lattice) of points in Euclidean space, and usually involves the digitisation of discrete lines and regions (Rosenfeld and Melter, 1989). Digitisation occurs by representing Euclidean space $\mathbb{R}^n$ as a a rectangular orthogonal grid $\mathbb{G}^n$. The elements of $\mathbb{G}^2$ are called pixels, and the elements of $\mathbb{G}^3$ are called voxels, and each element in $\mathbb{G}^n$ has a grid coordinate for its centre (Klette and Rosenfeld, 2004) and a value that denotes if the element belongs to a digitised geometric object, or when required, which part of the digitised geometric object .

3 Future work

`compGeometeR` is very much a work in progress, and while there is sufficient functionality for it to be of wide use in the computational sciences, there is some functionality that has been identified as being particularly useful for future development.

The Voronoi diagram (Voronoï, 1908; Okabe et al., 2000) partitions n-dimensional space into a set of polytopes for which each polytope delineates the region of n-dimensional space that is closest to each point in P. The Voronoi diagram would be an obvious addition for the discrete geometry algorithms given its wide implementation in other R geometry packages (Table 1).

As well as expanding the number of discrete geometry algorithms, and implementing more discrete algorithms in digital form, there are other kinds of computational geometry algorithms that we think would be of particular value.

There are a variety of useful graph structures that can be produced based on geometric principles. For example, the Delaunay triangulation (Delaunay, 1934) can also be represented as a graph structure, and for which there are several useful subgraphs such as the Gabriel graph (Gabriel and Sokal, 1969), Urquhart graph (Urquhart, 1980), and relative neighbourhood graph (Toussaint, 1980).

In some contexts it will be important to recognise that there is uncertainty in the position of points in space and the parameters defining a given algorithm. In such situations it may be helpful to adopt fuzzy geometry (Rosenfeld, 1998) view in which, foe example, memberships of points in space are not crisp being either 0 or 1, but rather are fuzzy on a scale from 0 to 1. Creating fuzzy versions of the `compGeometeR` algorithms could result in very useful functionality where quantifying uncertainty of any computational geometry is important. The existing digital geometric algorithms could be easily extended to fuzzy forms as all that is required is to assign a membership value to each pixel (Klette and Rosenfeld, 2004).

All the algorithms in `compGeometeR` work in Euclidean space, but computational geometry algorithms can also be usefully applied in spherical or hyperbolic space (Gowers, 2003). For example, the Fortran `STRIPACK` software (Renka, 1997) could be wrapped by R to provide functionality to compute Delaunay triangulations and Voronoi diagrams on the surface of a sphere.

4 Code availability

`compGeometeR` is open source software made available under a General Public License license. Installation instructions can be found at the GitHub repository `https://github.com/manaakiwhenua/compGeometeR`.

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References

Barber CB, Dobkin DP, Huhdanpaa H (1996) The Quickhull algorithm for convex hulls. ACM Transactions on Mathematical Software 22: 469–483

Barnett V (1976) The ordering of multivariate data. Journal of the Royal Statistical Society. Series A 139: 318–355 de Berg M, Cheong O, van Kreveld M, Overmars M (2008) Computational Geometry, 3rd edition. Springer, Berlin

Delaunay B (1934) Sur la sphère vide. Bulletin de l'Académie des Sciences de l'URSS, Classe des Sciences Mathématiques et Naturelles 6: 793–800

Edelsbrunner H, Mücke EP (1994) Three-dimensional alpha shapes. ACM Transactions on Graphics 13: 43–72

Gabriel KR, Sokal RR (1969) A new statistical approach to geographic variation analysis. Systematic Biology 18: 259–278

Gowers T (2003) Mathematics: a very short introduction. Oxford University Press, New York

Huber PJ (1972) Robust statistics: a review. The Annals of Mathematical Statistics 43: 1041–1067

Klette R, Rosenfeld A (2004) Digital Geometry. Morgan Kaufmann, San Francisco

Okabe A, Boots B, Sugihara K, Chiu SN (2000) Spatial Tessellations: concepts and applications of Voronoi diagrams, second edition edition. John Wiley & Sons, Chichester

Renka RJ (1997) Algorithm 772: Stripack: Delaunay triangulation and voronoi diagram on the surface of a sphere. ACM Transactions on Mathematical Software 23: 416–434

Rosenfeld A (1998) Fuzzy geometry an updated overview. Information Sciences 110: 127–133

Rosenfeld A, Melter RA (1989) Digital geometry. The Mathematical Intelligencer 11: 69–72

Toussaint GT (1980) The relative neighbourhood graph of a finite planar set. Pattern Recognition 12: 261–268

Urquhart RB (1980) Algorithms for computation of relative neighbourhood graph. Electronics Letters 16: 556–557

Voronoï G (1908) Nouvelles applications des paramètres continus à la théorie des formes quadratiques. Premier mémoire. Sur quelques propriétés des formes quadratiques positives parfaites. Journal für die reine und angewandte Mathematik 133: 97–102