n-Simplex circumsphere

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Abstract

We provide a short note on the computation of a n-simplex circumsphere, accompanying the software system *simplex-circumsphere*[1]. The mathematical content is adapted from a blog post by Gautam Manohar and another blog post by G. Westendorp. Please note this is unreviewed work on my part and that I have not checked in depth the claims made on my own.

Revision History

Revision	Date	Author(s)	Description
1.0	June 6, 2022	TH	PDF edition, adjustments, added bibliography.
0.9	August 16, 2021	TH	Draft published in .tex format only.

Contents

1 Notations

We will refer to:

- n the dimensionality
- A simplex with $n+1$ vertices
- The vertices V_i, $i \in [\![0, n]\!]$
- The coordinates of vertex V_i: V_i^j, $j \in [\![1, n]\!]$
- The circumsphere with center C, with coordinates C^j, and radius R

2 Method 1: Circumsphere equation

This method is taken from a blog post by Gautam Manohar [2]. Any vertex V_i is on the circumsphere (Eq. 1),

$$\forall i, \sum_j \left(V_i^j - C^j\right)^2 = R^2 \tag{1}$$

Arbitrarily, we take the first equation, for the first vertex V_0, and subtract it from all the others. After some expansion and cancellation of terms, we obtain Eq. 2.

$$\forall i \in [\![1, n]\!], 2 \sum_j \left(V_0^j - V_i^j\right) \cdot C^j = \sum_j \left(V_0^j\right)^2 - \sum_j \left(V_i^j\right)^2 \tag{2}$$

This is readily expressed in matrix format, with i indexing the rows in a linear system of equations (Eq. 3).

$$A \cdot x = b \tag{3}$$

With:

- A a square matrix with elements $A_{i,j}$, of size n (Eq. 4)
- x the vector of C^j coordinates, of length n.
- b a right hand side vector defined by Eq. 5, of length n.

$$A_{i,j} = 2\left(V_0^j - V_i^j\right) \tag{4}$$

$$b_i = \sum_j \left(V_0^j\right)^2 - \sum_j \left(V_i^j\right)^2 \tag{5}$$

We can solve for $x = C$ using any linear equation solver. Next, we can retrieve R from the distance of any vertex from the center, for example eq (Eq. 6).

$$R = \sqrt{\sum_j \left(V_0^j - C^j\right)^2} \tag{6}$$

Thus, we have computed the center C of the circumsphere, and R its radius.

3 Method 2: Cayley-Menger matrix

As noted by Westendorp [3], building on a work by Coxeter [4], we can compute the circumsphere of a simplex with the aid of the Cayley-Menger matrix. The Cayley-Menger matrix is given by Eq. 7.

$$CM = \begin{bmatrix} 0 & 1 & 1 & 1 & \dots \\ 1 & 0 & d_0^1 & d_0^2 & \dots \\ 1 & d_1^0 & 0 & d_1^2 & \dots \\ 1 & d_2^0 & d_2^1 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \tag{7}$$

with $d_i^j = \sum_k \left(V_i^k - V_j^k\right)^2$, the squared distance between vertices V_i and V_j.
Then, the radius of the circumsphere is given by Eq. 8, the circumcenter by Eq. 9 (please refer to [3] for the proof).

$$R = \sqrt{-\frac{1}{2} \cdot {CM^{-1}}_{1,1}} \tag{8}$$

$$x_j = {CM^{-1}}_{1,j+1} \tag{9}$$

Note that we only need the first row of the inverse CM matrix, not the whole inverse. Also note that CM is symmetric, which enables simpler decompositions for the inversion operation. CM is *indefinite* (proof omitted). Since CM is square symmetric, but not positive-definite, the most efficient decomposition to perform the inverse, to the best of my knowledge, is the Bunch–Kaufman decomposition [5], which is only slightly better than LUP [6].

See also the Cayley-Menger determinant [7] for the link between the Cayley-Menger matrix and the volume (or *content*) of n-simplices.

4 Method tradeoff

Starting from a list of vertices coordinates V_i^j, which method is the most efficient computationally? Let's count operations to make sure.

- Method 1:
  - A: n^2 subtractions
  - b: $n(n+1)$ squares, $(n-1)(n+1)$ sums, n subtractions
  - LUP decomposition [6] and solve.
- Method 2:
  - Distance squared for one pair of vertices: $(n-1)$ subtractions, $(n-1)$ squares, $(n-1)$ sums.
  - Number of unique pairs with non-zero distance: $n(n-1)/2$
  - Bunch-Kaufman decomposition [5] and solve.

Long story short, the setup for the first method is $\mathcal{O}(n^2)$ in time, the second method is $\mathcal{O}(n^3)$. Both decompositions are $\mathcal{O}(n^3)$ with a slight advantage for Bunch-Kaufman. Method 1 is preferable.

References

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