The Euclidean InSphere Predicate

Supervisor: Menelaos I. Karavelas

Iordan Marinov Iordanov

Student ID: 780

Thesis committee

Theodoulos Garefalakis Menelaos Karavelas Michael Plexousakis

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Chapter 1

Introduction

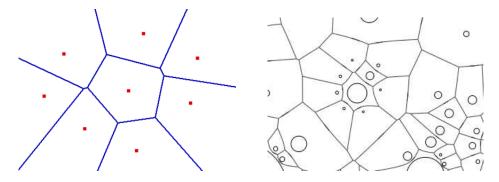
In the area of Computational Geometry, Voronoi diagrams are one of the most studied and researched topics, having numerous applications in various fields of science, ranging from epidemiology (sources of infection) to computer graphics, and from ecology to autonomous robot navigation. In the present work, based upon [3], we present the *InSphere* predicate, allowing us to determine the position of a query sphere in three-dimensional space relative to the tangent sphere of four given spheres.

Initially we present the abstract ideas, as well as practical results in two dimensions. Later on, we generalise our concepts in three dimensions and give a concrete result for the problem at hand.

1.1 General Discussion

We first define what a Voronoi diagram is. Informally, it is a special decomposition of a metric space into subspaces. In the simplest case, it is the partitioning of a plane into n convex regions in such a manner that each region T_q contains exactly one (generating) point p_q , and every point in T_q is closer to p_q than any other point on the plane.

The convex polygons formed in the process are called *Voronoi cells*, and the set of all Voronoi cells form the *Voronoi diagram*. A special case is the *Apollonius diagram*, also known as the *additively weighted Voronoi diagram*, where the cells are defined in relation to a common metric, modified by weights assigned to the generating points. The weighted points comprising an Apollonius diagram can be represented by circles, the center being the point itself, and the radius being the weight of the point. In three dimensions we can think of the sites as spheres, where again the center corresponds to the center of the site, and the radius corresponds to the weight of the given site. The terms *site*, *sphere* and *circle* will be used without discrimination, as long as no confusion is introduced. We examine the case where the metric is the Euclidean norm $\|\cdot\|$, and define the distance $\delta(p, B)$ between



A simple Voronoi diagram for a set of points (left. source: http://www.dma.fi.upm.es/mabellanas/tfcs/fvd/voronoi.html) and a sam-Apollonius diagram a set weighted for of (right, sites source: http://www.cgal.org/Manual/latest/doc_html/cgal_manual/packages.html).

a point p and a site $B = \{b, r\}$ as:

$$\delta(p, B) = ||p - b|| - r,$$

as well as the distance between two sites:

$$\delta(B_i, B_j) = ||b_i - b_j|| - r_i - r_j.$$

Focusing on the case in two dimensions, to construct the Apollonius diagram of a given set of sites, we need to be able to determine the relative position of a query site and a site tangent to any three sites given from the initial set.

1.2 Inversion

The *Inversion mapping* is one of the basic tools presented in [3], and is also the basic tool used in the present work. It is a transformation, a *mapping* which, so to speak, turns a circle "inside-out".

More formally, in two dimensions, let B_i, B_j, B_k be our three given sites, and let them be contained in the complex plane \mathcal{Z} . We define $B_{\nu}^*, \nu = i, j, k$, to be the sites with centers b_{ν} and radii $r_{\nu}^* = r_{\nu} - r_i$. It is obvious that $r_i^* = 0$, and the other two sites may have negative radii. We call the plane containing the sites B_{ν}^* the \mathcal{Z}^* plane. The standard inversion mapping

$$W(z) = \frac{z - z_i}{\|z - z_i\|^2},$$

between the complex planes \mathcal{Z}^* and \mathcal{W} maps circles on the \mathcal{Z}^* plane that do not pass through z_i to circles on the \mathcal{W} plane, and circles that pass through z_i on the \mathcal{Z}^* plane to lines on the \mathcal{W} plane.

This approach proves to be very efficient and simple. We will have a detailed look at the inversion mapping in the next section, where an example is given.

Chapter 2

The case in two dimensions

Please note that all the material in this chapter already exists in [3]. It is presented here to better show how the third dimension is added to our setup and from where do the results emerge.

2.1 General discussion

We have already said a few words about Voronoi diagrams and their applications. We have also noted that to construct the Apollonius diagram of a given set of weighted points (sites), we need to be able to determine the relative position of a query site B_q with respect to the circle tangent to three given sites B_i , B_j and B_k . More precisely, given B_i , B_j and B_k we assume that they define a unique common tritangent circle B_t that has the following properties:

- B_t touches the three sites at the points t_i , t_j and t_k , and the triangle $t_i t_j t_k$ is counterclockwise oriented.
- B_t either lies in the complement of the union of the disks bounded by B_i , B_j and B_k , or lies in the intersection of the three disks bounded by B_i , B_j and B_k .

Notice that, under the conditions above, B_t does not always exist. If, however, it exists, it is also unique. Moreover, we will assume that our sites are disjoint; this is not a restrictive requirement; in fact, the analysis presented throughout this thesis carries over to the general case, i.e., to the case where the sites can possibly intersect, or even have negative weights.

In the sequel we will not discuss at all the problem of existence of B_t ; we will consider it granted that the circle B_t exists, and we will focus on our actual predicate:

Do the disks bounded by B_t and B_q intersect?

This question is equivalent to asking for the sign of the expression $\delta(B_t, B_q)$. There are three possible outcomes to this question:

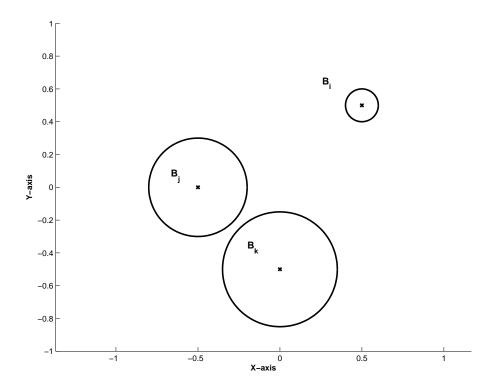


Figure 2.1: Initial experiment setup (\mathcal{Z} -space).

- 1. The sign of $\delta(B_t, B_q)$ is positive; in this case the disk bounded by B_q does not intersect the disk bounded by B_t and the *InCircle* predicate returns *outside*.
- 2. The sign of $\delta(B_t, B_q)$ is zero; in this case B_q is externally tangent to B_t and the *InCircle* predicate returns on.
- 3. The sign of $\delta(B_t, B_q)$ is negative; in this case the disk bounded by B_q intersects the disk bounded by B_t and the *InCircle* predicate returns *inside*.

We will now demonstrate how the Inversion mapping can be employed to help us find an easy and efficient way to answer the *InCircle* predicate. Later on, we will present the mathematics behind the process.

The idea is quite simple, actually. To gain better understanding of the subject, we will present an example. Let us consider the setup presented in Fig. 2.1.

As we can see, the site B_i has the smallest radius, therefore after applying the transformation $r_{\nu}^* = r_{\nu} - r_i$, $\nu = i, j, k$, there will be no negative radii. Subtracting the radius r_i from the radii of all sites, the setup is transformed into the state in Fig. 2.2.

Now, if we had a site tangent to the initial sites, after altering the radii it should remain tangent to all three sites. This means that it would be tangent to the sites B_j and B_k , in Fig. 2.2, and pass through the center of the site B_i , since its radius is now 0. This leads

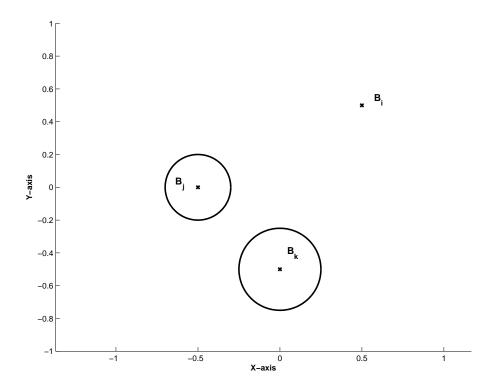


Figure 2.2: Setup after the transformation $r_{\nu}^* = r_{\nu} - r_i, \nu = i, j, k \ (\mathcal{Z}^*\text{-space}).$

us to the conclusion that if we apply the inversion mapping through the center of the site B_i , the tritangent circle would be transformed into a line tangent to the sites B_j and B_k , according to the theory. The site B_i would then be situated at infinity.

There is another way to think about what the inversion mapping does. As we said, the site B_i^* is now situated at infinity, but the tritangent circle, should it exist, would continue to be tritangent. Therefore, we can consider the site B_q^* to be a circle centered at infinity, having a radius of infinity. So the site B_q has such a big radius that when we "zoom in" to be able to see the sites B_i^* and B_k^* , we can consider it to be a line.

Having this in mind, consider another detail: given two circles, we can find four bitangent lines – two internal and two external. Which one do we need to find? The answer is quite clear if we remind ourselves that this is the line which comes from the transformation of the tritangent site B_i . It is then obvious that the sites B_j^* and B_k^* must be situated on the same side of the line, therefore we are searching an external tangent. To select one of the two possible solutions, we define a *orientation* of the line, and request that there is a concrete ordering to the sites. This provides for a unique solution of the problem, and as we will see, it is the solution that proves to be correct.

So, following that train of thought, we apply the inversion mapping, and also find the tangent line to the sites B_j^* and B_k^* which satisfies the aforementioned requirements. The

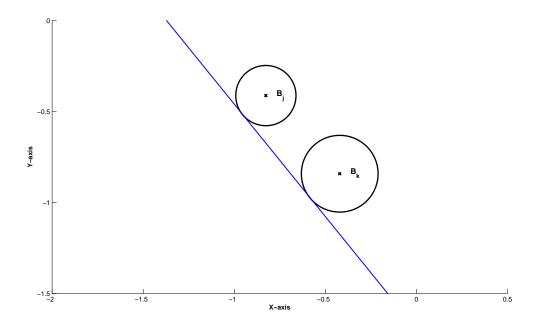


Figure 2.3: Inverted sites and bitangent line (W-space).

result is shown in Fig. 2.3.

What we now have is the line which corresponds to the circle tangent to our three initial sites. According to what we discussed before, it would suffice to calculate the sign of the *signed distance* of a point p from the line, instead of controlling whether the point p is at the internal of the circle B_q . We will see later how this sign is defined and what conventions we make.

To prove our theory that the line corresponds to the site we are searching, we will make one last step and apply the inversion mapping to the line. It sends us back to the initial space \mathcal{Z} , and what it transforms into is a circle whose equation will be presented in a while. Just below is the figure of the initial setup, along with the line mapped into the space \mathcal{Z} through the inversion mapping. We can very well see that it is indeed the tritangent site we are in search of (see Fig. 2.4).

2.2 The DistanceFromBitangent Predicate

Now it's time to become more formal and give austere mathematical explanations for the previous discussion.

We define the site $B = \{b, r\} = \{(b_x, b_y), r\}$ and the line $L := \alpha x + \beta y + \gamma = 0$. The signed distance of B from L is defined as follows:

$$\delta(B, L) = \delta(b, L) - r$$
, where $\delta(b, L) = \frac{\alpha x_b + \beta y_b + \gamma}{\sqrt{a^2 + b^2}}$

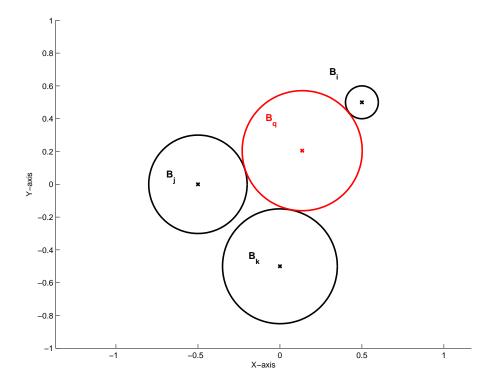


Figure 2.4: Initial setup with the resulting tritangent circle (\mathcal{Z} -space).

We consider three sites B_i , B_j and B_k , and the *oriented* line L_{ij} which has the following properties:

- L_{ij} is tangent to both B_i and B_j
- B_i and B_j are to the left of L_{ij}
- Moving in the positive direction of L_{ij} , we encounter B_i first and B_j next

Our goal is to compute the sign of the distance of B_k from L_{ij} . This is more general than what we discussed previously, as in the previous discussion we assumed that the point p has a weight of 0, for simplicity. We will see how the task is affronted when we want to check the situation of a weighted point in relation to the bitangent line.

Consider $a_{ij}x_{\lambda} + b_{ij}y_{\lambda} + c_{ij} = r_{\lambda}$, $\lambda = i, j$ to be the system of equations the bitangent line satisfies. We need another restriction to be able to determine the coefficients a_{ij}, b_{ij} and c_{ij} , so we will use the condition $a_{ij}^2 + b_{ij}^2 = 1$. The computations necessary are present in [3], and the resulting coefficients are as follows:

$$a_{ij} = \frac{D_{ij}^{x} D_{ij}^{r} + D_{ij}^{y} \sqrt{\Delta_{ij}}}{\left(D_{ij}^{x}\right)^{2} + \left(D_{ij}^{y}\right)^{2}},$$

$$b_{ij} = \frac{D_{ij}^{y} D_{ij}^{r} - D_{ij}^{x} \sqrt{\Delta_{ij}}}{\left(D_{ij}^{x}\right)^{2} + \left(D_{ij}^{y}\right)^{2}},$$

$$c_{ij} = \frac{D_{ij}^{x} D_{ij}^{xr} + D_{ij}^{y} D_{ij}^{yr} + D_{ij}^{xy} \sqrt{\Delta_{ij}}}{\left(D_{ij}^{x}\right)^{2} + \left(D_{ij}^{y}\right)^{2}},$$

where

$$D_{\lambda\nu}^{s} = \begin{vmatrix} s_{\lambda} & 1 \\ s_{\nu} & 1 \end{vmatrix}, \quad D_{\lambda\nu}^{st} = \begin{vmatrix} s_{\lambda} & t_{\lambda} \\ s_{\nu} & t_{\nu} \end{vmatrix}, \quad s,t \in \{x,y,r\}, \quad \lambda,\nu \in \{i,j\},$$

and

$$\Delta_{ij} = (D_{ij}^x)^2 + (D_{ij}^y)^2 - (D_{ij}^r)^2$$
.

Taking into consideration the fact that $a_{ij}^2 + b_{ij}^2 = 1$, and substituting the above equations into the expression for $\delta(B_k, L_{ij})$, we get the following result:

$$\delta(B_k, L_{ij}) = \frac{D_{ij}^x D_{ijk}^{xr} + D_{ij}^y D_{ijk}^{yr} + D_{ijk}^{xy} \sqrt{\Delta_{ij}}}{(D_{ij}^x)^2 + (D_{ij}^y)^2},$$

where

$$D_{\lambda\mu\nu}^{st} = \begin{vmatrix} s_{\lambda} & t_{\lambda} & 1 \\ s_{\mu} & t_{\mu} & 1 \\ s_{\nu} & t_{\nu} & 1 \end{vmatrix}, \quad s, t \in \{x, y, r\}, \quad \lambda, \mu, \nu \in \{i, j, k\}.$$

The sign of the quantity $\delta(B_k, L_{ij})$ clearly depends solely on the numerator, so we need to determine the sign of the quantity $D_{ij}^x D_{ijk}^{xr} + D_{ij}^y D_{ijk}^{yr} + D_{ijk}^{xy} \sqrt{\Delta_{ij}}$.

It is notable that the above quantity is of the form $X_0 + X_1 \sqrt{Y}$, where $X_0 = D_{ij}^x D_{ijk}^{xr} + D_{ij}^y D_{ijk}^{yr}$, $X_1 = D_{ijk}^{xy}$ and $Y = \Delta_{ij}$. The sign of $X_0 + X_1 \sqrt{Y}$ can be determined as follows:

$$\operatorname{sign}(X_0 + X_1 \sqrt{Y}) = \begin{cases} \operatorname{sign}(X_0) & , \text{ if } Y = 0 \\ \operatorname{sign}(X_1) & , \text{ if } X_0 = 0 \\ \operatorname{sign}(X_0) & , \text{ if } X_1 = 0 \\ \operatorname{sign}(X_0) & , \text{ if } \operatorname{sign}(X_0) = \operatorname{sign}(X_1) \\ \operatorname{sign}(X_0) & \operatorname{sign}(X_0^2 - X_1^2 Y) & , \text{ otherwise} \end{cases}$$

where the function sign(X) returns the sign of the quantity X as follows:

$$sign(X) = \begin{cases} -1 & , \text{ if } X < 0 \\ 0 & , \text{ if } X = 0 \\ 1 & , \text{ if } X > 0 \end{cases}.$$

We have shown that the answer to our initial question can be given by calculating the above quantity. It is shown in [3] that the algebraic degree of the **DistanceFrom-Bitangent** predicate is 6. We will now proceed to describe a setup in the 3-dimensional Euclidean space and find a similar method to answer the same question in 3 dimensions.

Chapter 3

The case in three dimensions

To be able to affront the problem in three dimensions, we follow the logic we previously discussed. We must generalize, however, so we need to redefine our setup and follow in the steps presented in the previous chapter.

3.1 Problem formulation

Since we will be working in three dimensions, our sites will now be spheres. A site will be defined as $B = \{b, r\} = \{(b_x, b_y, b_z), r\}$ and we will have four given sites B_i, B_j, B_k and B_m in our initial setup. What we search is the relative position of another, query site B_q , with respect to the site tangent to out initial sites: we need to determine if the ball bounded by the sphere B_t that is tangent to B_i, B_j, B_k and B_m is intersected by the ball bounded by B_q . As in the 2D analogue, this is equivalent to determining the sign of the distance $\delta(B_t, B_q)$. This is our InSphere predicate, and as in two dimensions, it has three possible outcomes:

- 1. The sign of $\delta(B_t, B_q)$ is positive; in this case the ball bounded by B_q does not intersect the ball bounded by B_t and the *InSphere* predicate returns *outside*.
- 2. The sign of $\delta(B_t, B_q)$ is zero; in this case B_q is externally tangent to B_t and the InSphere predicate returns on.
- 3. The sign of $\delta(B_t, B_q)$ is negative; in this case the ball bounded by B_q intersects the ball bounded by B_t and the *InSphere* predicate returns *inside*.

Notice that the three spheres B_i, B_j, B_k and B_m can have may commonly tangent spheres. Among those we are interested in those that satisfy the following conditions:

• The common tangent sphere B_t either lies in the complement of the union of the balls bounded by B_i, B_j, B_k and B_m , or lies in the intersection of the balls bounded by the four spheres.

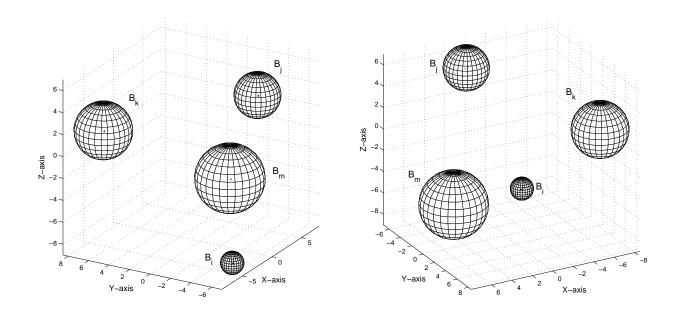


Figure 3.1: Initial experiment setup (\mathcal{Z} -space).

• If t_i, t_j, t_k, t_m are the points of tangency of B_i, B_j, B_k, B_m with B_t , respectively, the tetrahedron $t_i t_j t_k t_m$ is required to be positively oriented.

The sphere B_t that satisfies the above requirements does not always exist; if it exists, however, it is unique. Determining its existence is beyond the scope of this thesis. In what follows we will assume that the four input spheres B_i , B_j , B_k and B_m are such that the sphere B_t , satisfying that conditions above, is indeed defined.

As in the two-dimensional case, affronting the problem directly is quite difficult, more so now that we have to deal with another dimension. We shall see that the inversion mapping is a very handy tool and offers a simple solution.

3.2 Presentation

We saw in the previous chapter that the tangent site in two dimensions was "transformed" into a line. Much alike, in three dimensions, the tangent site is transformed into a plane. Therefore, following the same line of thought, instead of determining the position of our query site in relation to our tangent sphere, we only need to determine its position in relation to a tangent plane, which is much easier to find and calculate. It may be a little too soon, but we will present some experimental results, and later on we will concentrate on the theory.

Fig. 3.1 presents the initial setup for our experiment.

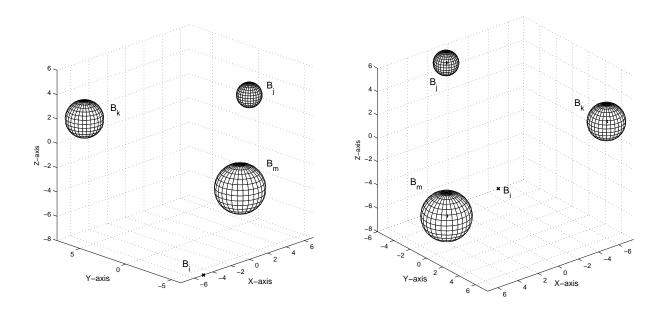


Figure 3.2: Setup after the transformation $r_{\nu}^* = r_{\nu} - r_i, \nu = i, j, k, q$ (\mathcal{Z}^* -space).

As in the previous procedure, we apply the transformation $r_{\nu}^* = r_{\nu} - r_m$, $\nu = i, j, k, m$. Note again that the site B_m has the smallest radius, therefore the transformation will lead to non-negative radii. Applying the transformation of the radii, our system falls into the state shown in Fig. 3.2.

The next step is to apply the Inversion mapping to our whole system. Generalising from the case in two dimensions, it is easy to see that we must apply the mapping through the point b_m^* , the center of B_m^* . Spheres that do not pass through this point will be mapped to spheres on the W-space, and spheres that do pass through b_m^* will be mapped to planes in this space. Therefore, our initial system transforms into a system of three spheres, and the site B_m^* , now merely a point, is situated at infinity. Again, holding in mind that, should we have a sphere tangent to our sites, it would be transformed into a plane (for reasons discussed earlier), we proceed to find the tangent plane. Our results are shown in Fig. 3.3.

Now, to show that the plane we have found in the W-space corresponds to the tangent sphere in the Z-space, we apply the inversion mapping to the plane. We can see in Fig. 3.4 that the results are quite what we hoped for.

So we conclude that the plane we found in the W-space indeed corresponds to the sphere we are searching in the Z-space. Analogously, it is equivalent that we determine the relative position of a query site B_q to the tangent plane in the W-space instead of the tangent sphere in the Z-space. We will show how much simpler expressions we will have to deal with and will present the criteria based on which we proceed during the computations. We must also justify the selection of our plane: given three spheres in general position, there are eight planes tangent to them: which one do we need to choose, and why? The

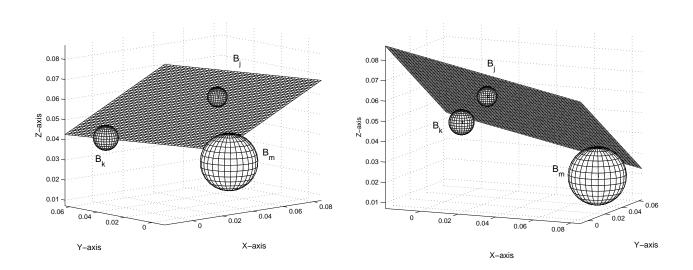


Figure 3.3: Inverted sites and tritangent plane (W-space).

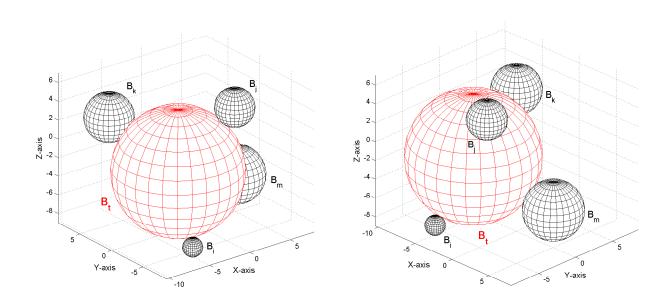


Figure 3.4: Initial setup with resulting quadritangent sphere (\mathcal{Z} -space).

answer follows in the next section.

Application 3.3

Formally, we define the site $B = \{\beta, r\} = \{(\beta_x, \beta_y, \beta_z), r\}$ and the plane $\Pi := ax + ax + ax + ax + bx$ by + cz + d = 0. Now, the signed distance of B from Π is defined by the relation

$$\delta(B,\Pi) = \delta(\beta,\Pi) - r, \text{ where } \delta(\beta,\Pi) = \frac{a\beta_x + b\beta_y + c\beta_z + d}{\sqrt{a^2 + b^2 + c^2}}$$

and $a^2 + b^2 + c^2 = 1$

Consider four sites, B_i, B_j, B_k, B_q , and the (oriented) plane Π_{ijk} such that:

- 1. The centers of the sites B_i, B_j and B_k are not collinear
- 2. Π_{ijk} is tangent to B_i, B_j and B_k
- 3. B_i, B_j and B_k are situated on the positive side of Π_{ijk}
- 4. Moving counter-clockwise on Π_{ijk} we encounter B_i, B_j and B_k in this order

What we seek to compute is the sign of the distance of B_q from Π_{ijk} . Let $a_{ijk}x_{\lambda}$ + $b_{ijk}y_{\lambda} + c_{ijk}z_{\lambda} + d_{ijk} = r_{\lambda}$, $\lambda = i, j, k$, be the equations of the tangent planes in question. Assuming $a_{ijk}^2 + b_{ijk}^2 + c_{ijk}^2 = 1$, we have four equations to determine the four coefficients $a_{ijk}, b_{ijk}, c_{ijk}$ and d_{ijk} of the plane tangent to all three sites.

$$(1) a_{ijk}x_i + b_{ijk}y_i + c_{ijk}z_i = r_i - d_{ijk}$$

(2)
$$a_{ijk}x_j + b_{ijk}y_j + c_{ijk}z_j = r_j - d_{ijk}$$

(3)
$$a_{ijk}x_k + b_{ijk}y_k + c_{ijk}z_k = r_k - d_{ijk}$$

(4) $a_{ijk}^2 + b_{ijk}^2 + c_{ijk}^2 = 1$

$$(4) a_{ijk}^2 + b_{ijk}^2 + c_{ijk}^2 = 1$$

From the first three equations, it is easy to verify by Crammer's rule that the following solution holds:

$$a_{ijk} = \frac{D_{ijk}^{yzr} - dD_{ijk}^{yz}}{D_{ijk}^{xyz}}, \quad b_{ijk} = -\frac{D_{ijk}^{xzr} - dD_{ijk}^{xz}}{D_{ijk}^{xyz}}, \quad c_{ijk} = \frac{D_{ijk}^{xyr} - dD_{ijk}^{xy}}{D_{ijk}^{xyz}},$$

where

$$D_{\lambda\mu\nu}^{pst} = \begin{vmatrix} p_{\lambda} & s_{\lambda} & t_{\lambda} \\ p_{\mu} & s_{\mu} & t_{\mu} \\ p_{\nu} & s_{\nu} & t_{\nu} \end{vmatrix}, \quad D_{\lambda\mu\nu}^{st} = \begin{vmatrix} s_{\lambda} & t_{\lambda} & 1 \\ s_{\mu} & t_{\mu} & 1 \\ s_{\nu} & t_{\nu} & 1 \end{vmatrix}, \quad \lambda, \mu, \nu \in \{i, j, k\}, \quad p, s, t \in \{x, y, z, r\}.$$

From (4) we get that

$$\left(D_{ijk}^{yzr}-dD_{ijk}^{yz}\right)^2+\left(D_{ijk}^{xzr}-dD_{ijk}^{xz}\right)^2+\left(D_{ijk}^{xyr}-dD_{ijk}^{xy}\right)^2=\left(D_{ijk}^{xyz}\right)^2.$$

¹The positive side of Π_{ijk} is defined to be the half-space in the positive direction of the normal to the plane, namely, the vector $[a, b, c]^T$.

Expanding the squares and reordering the terms of the equation leads us to a second order polynomial with respect to d:

$$\left[\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xz} \right)^2 + \left(D_{ijk}^{xy} \right)^2 \right] d^2 - 2 \left[D_{ijk}^{yzr} D_{ijk}^{yz} + D_{ijk}^{xzr} D_{ijk}^{xz} + D_{ijk}^{xyr} D_{ijk}^{xy} \right] d
+ \left[\left(D_{ijk}^{yzr} \right)^2 + \left(D_{ijk}^{xzr} \right)^2 + \left(D_{ijk}^{xyr} \right)^2 - \left(D_{ijk}^{xyz} \right)^2 \right] = 0.$$

Considering the equation to be in the form $Ad^2 + Bd + \Gamma = 0$ with

$$A = (D_{ijk}^{yz})^{2} + (D_{ijk}^{xz})^{2} + (D_{ijk}^{xy})^{2}$$

$$B = -2 \left[D_{ijk}^{yzr} D_{ijk}^{yz} + D_{ijk}^{xzr} D_{ijk}^{xz} + D_{ijk}^{xyr} D_{ijk}^{xy} \right]$$

$$\Gamma = (D_{ijk}^{yzr})^{2} + (D_{ijk}^{xzr})^{2} + (D_{ijk}^{xyr})^{2} - (D_{ijk}^{xyz})^{2}$$

and knowing that $(a+b+c)^2=a^2+b^2+c^2+2ab+2ac+2bc$, we employ the discriminant identity $\Delta'=B^2-4A\Gamma$:

$$B^{2} = 4 \left[\left(D_{ijk}^{yzr} D_{ijk}^{yz} \right)^{2} + \left(D_{ijk}^{xzr} D_{ijk}^{xz} \right)^{2} + \left(D_{ijk}^{xyr} D_{ijk}^{xy} \right)^{2} + 2 D_{ijk}^{yzr} D_{ijk}^{yz} D_{ijk}^{xzr} D_{ijk}^{xz} \right]$$
$$+ 2 D_{ijk}^{yzr} D_{ijk}^{yz} D_{ijk}^{xyr} D_{ijk}^{xy} + 2 D_{ijk}^{xzr} D_{ijk}^{xz} D_{ijk}^{xyr} D_{ijk}^{xy} \right]$$

$$4A\Gamma = 4\left[\left(D_{ijk}^{yzr} D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xzr} D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xyr} D_{ijk}^{yz} \right)^2 - \left(D_{ijk}^{xyz} D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xyr} D_{ijk}^{xz} \right)^2 + \left(D_{ijk}^{xyr} D_{ijk}^{xz} \right)^2 + \left(D_{ijk}^{xyr} D_{ijk}^{xz} \right)^2 - \left(D_{ijk}^{xyz} D_{ijk}^{xz} \right)^2 + \left(D_{ijk}^{xyr} D_{ijk}^{xy} \right)^2 - \left(D_{ijk}^{xyz} D_{ijk}^{xy} \right)^2 \right]$$

After eliminations and regrouping, we get that:

$$\begin{split} \Delta' &= 4 \left[\left(D_{ijk}^{xyz} D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xyz} D_{ijk}^{xz} \right)^2 + \left(D_{ijk}^{xyz} D_{ijk}^{xy} \right)^2 \\ &- \left(D_{ijk}^{xzr} D_{ijk}^{yz} \right)^2 - \left(D_{ijk}^{xyr} D_{ijk}^{yz} \right)^2 - \left(D_{ijk}^{yzr} D_{ijk}^{xz} \right)^2 \\ &- \left(D_{ijk}^{xyr} D_{ijk}^{xz} \right)^2 - \left(D_{ijk}^{yzr} D_{ijk}^{xy} \right)^2 - \left(D_{ijk}^{xzr} D_{ijk}^{xy} \right)^2 \\ &+ 2 D_{ijk}^{yzr} D_{ijk}^{yz} D_{ijk}^{xzr} D_{ijk}^{xz} + 2 D_{ijk}^{yzr} D_{ijk}^{yz} D_{ijk}^{xyr} D_{ijk}^{xy} + 2 D_{ijk}^{xzr} D_{ijk}^{xyr} D_{ijk}^{xy} \right] = \\ 4 \left[\left(D_{ijk}^{xyz} \right)^2 \left[\left(D_{ijk}^{xy} \right)^2 + \left(D_{ijk}^{xz} \right)^2 + \left(D_{ijk}^{yz} \right)^2 \right] - \left(D_{ijk}^{xzr} D_{ijk}^{yz} - D_{ijk}^{yzr} D_{ijk}^{xz} \right)^2 - \\ &- \left(D_{ijk}^{xyr} D_{ijk}^{yz} - D_{ijk}^{yzr} D_{ijk}^{xy} \right)^2 - \left(D_{ijk}^{xyr} D_{ijk}^{xz} - D_{ijk}^{xzr} D_{ijk}^{xy} \right)^2 \right] \end{split}$$

It can be proven that the following relations hold:

$$D_{ij}^{ac}D_{ij}^{b} - D_{ij}^{bc}D_{ij}^{a} = D_{ij}^{ab}D_{ij}^{c}$$

$$D_{ij}^{bd}D_{ij}^{ac} - D_{ij}^{ad}D_{ij}^{bc} = D_{ij}^{ab}D_{ij}^{cd}$$

$$D_{ijk}^{acd}D_{ijk}^{bc} - D_{ijk}^{bcd}D_{ijk}^{ac} = D_{ijk}^{abc}D_{ijk}^{cd}$$

where $a, b, c, d \in \{x, y, z, r\}$.

We are now able to proceed a little further in our simplification and Δ' takes the form

$$\Delta' = 4 \left(D_{ijk}^{xyz} \right)^2 \left[\left(D_{ijk}^{xy} \right)^2 + \left(D_{ijk}^{xz} \right)^2 + \left(D_{ijk}^{yz} \right)^2 - \left(D_{ijk}^{xr} \right)^2 - \left(D_{ijk}^{yr} \right)^2 - \left(D_{ijk}^{zr} \right)^2 \right]$$

We introduce the quantity $\Delta = \left(D_{ijk}^{xy}\right)^2 + \left(D_{ijk}^{xz}\right)^2 + \left(D_{ijk}^{yz}\right)^2 - \left(D_{ijk}^{xr}\right)^2 - \left(D_{ijk}^{yr}\right)^2 - \left(D_{ijk}^{yr}\right)^2$ or, equivalently, $\Delta' = 4\left(D_{ijk}^{xyz}\right)^2 \Delta$, which will prove more useful in the sequel. Supposing that $\Delta' > 0$, the solutions for d should be

$$d_{1,2} = \frac{-B \pm \sqrt{\Delta}}{2A} = \frac{2 \left[D_{ijk}^{yzr} D_{ijk}^{yz} + D_{ijk}^{xzr} D_{ijk}^{xz} + D_{ijk}^{xyr} D_{ijk}^{xy} \right] \pm \sqrt{\Delta'}}{2 \left[\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xz} \right)^2 + \left(D_{ijk}^{xy} \right)^2 \right]}$$
$$= \frac{D_{ijk}^{yzr} D_{ijk}^{yz} + D_{ijk}^{xzr} D_{ijk}^{xz} + D_{ijk}^{xyr} D_{ijk}^{xy} \pm D_{ijk}^{xyz} \sqrt{\Delta}}{\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xy} \right)^2 + \left(D_{ijk}^{xy} \right)^2}$$

From our initial assumptions, it follows that if t_i, t_j and t_k are the common points of the plane Π_{ijk} and the sites B_i , B_j and B_k respectively, then these points are not collinear (since the centers of the sites are not collinear). This translates into the triangle formed by t_i, t_j, t_k having non-zero area, which in turn means that $D_{ijk}^{xyz} \neq 0$. This is a result we will use a little later.

The conditions presented along with the formulation of our problem in \mathcal{Z} -space are equivalent to requiring, in \mathcal{W} -space that:

- 1. The spheres B_i , B_j and B_k must be on the positive side of the plane Π_{ijk} .
- 2. The triangle $t_i t_j t_k$ lying in the plane Π_{ijk} must be properly oriented. The actual requirement in \mathbb{Z} -space is that the tetrahedron $t_i t_j t_k t_m$ is positively oriented. The same must hold for the tetrahedron $t_i^* t_j^* t_k^* b_m$ in \mathbb{Z}^* -space. However, the inversion transformation maps b_m to the point at infinity, which means that the triangle $t_i t_j t_k$ in \mathbb{W} -space must be positively oriented when seen from the point at the infinity. We can see this positive orientation in the following manner: we consider a point $p = (x_p, y_p, z_p)$ in our space. If the point p is on the positive side of the plane Π_{ijk} , then the (signed) volume of the tetrahedron $\{t_i, t_j, t_k, p\}$ is positive. If we let the point p move towards infinity (while staying on the positive halfspace with respect to Π_{ijk} , then sign of the afore-mentioned volume is expressed by the cross-product of the vectors v_{ij} and v_{ik} , which, as we discuss below, in our case is equivalent to the cross-product of the vectors c_{ij} and c_{ik} , with respect to direction.

Recall that we have assumed that moving counter-clockwise on the plane Π_{ijk} , we encounter the sites in the order B_i, B_j, B_k . If we are to define a "positive" side on our plane, we need a way of knowing which side is which. An excellent way of defining the positive side of our plane is the *cross product*. Since we requested that the sites are visited in the order B_i, B_j, B_k while moving counter-clockwise, and having in mind the *right-hand*

rule, let us consider the points t_i, t_j, t_k as defined previously. It has been shown that these points form a triangle, and we can define the vectors connecting them: let the vector $\vec{v_{ij}}$ be the vector beginning at t_i and ending at t_j . Then the quantity we are interested in would be the cross-product of the vectors $\vec{v_{ij}}$ and $\vec{v_{ik}}$. These points can be found, but at this stage they are unknown. We can consider, however, the triangle b_i, b_j, b_k formed by the centers of the sites, and it is evident that the triangle t_i, t_j, t_k is the projection of the triangle b_i, b_j, b_k onto the plane Π_{ijk} . Therefore, instead of calculating the crossproduct of the vectors $\vec{v_{ij}}$ and $\vec{v_{ik}}$, we only need to calculate the cross-product of the vectors $\vec{c_{ij}} = [x_j - x_i, y_j - y_i, z_j - z_i]$ and $\vec{c_{ik}} = [x_k - x_i, y_k - y_i, z_k - z_i]$. If we call this quantity P_{ijk} , i.e.,

$$P_{ijk} = \vec{c_{ij}} \times \vec{c_{ik}},$$

after a few computations we find that $P_{ijk} = \left[D^{yz}_{ijk}, -D^{xz}_{ijk}, D^{xy}_{ijk}\right]^T$. From our discussion above it is clear that the condition that we need to satisfy is that the dot product of the vectors P_{ijk} and \vec{n} be positive, i.e., we require that:

$$P_{ijk} \cdot \vec{n} > 0.$$

It is known that the normal vector to a plane given in the form ax + by + cz + d = 0 is the vector $\begin{bmatrix} a, b, c \end{bmatrix}^T$, hence in our case $\vec{n} = \begin{bmatrix} a_{ijk}, b_{ijk}, c_{ijk} \end{bmatrix}^T$ or, in expanded form

$$\vec{n} = \begin{bmatrix} \frac{D^{yzr}_{ijk} - dD^{yz}_{ijk}}{D^{xyz}_{ijk}}, & -\frac{D^{xzr}_{ijk} - dD^{xz}_{ijk}}{D^{xyz}_{ijk}}, & \frac{D^{xyr}_{ijk} - dD^{xy}_{ijk}}{D^{xyz}_{ijk}} \end{bmatrix}^T$$

In sequel are presented the steps to calculate the inner product $P_{ijk} \cdot \vec{n}$:

$$\begin{split} P_{ijk} \cdot \vec{n} &= \left(D^{yz}_{ijk}, -D^{xz}_{ijk}, D^{xy}_{ijk}\right) \cdot \left(\frac{D^{yzr}_{ijk} - dD^{yz}_{ijk}}{D^{xyz}_{ijk}}, -\frac{D^{xzr}_{ijk} - dD^{xz}_{ijk}}{D^{xyz}_{ijk}}, \frac{D^{xyr}_{ijk} - dD^{xy}_{ijk}}{D^{xyz}_{ijk}}\right)^T \\ &= D^{yz}_{ijk} \frac{D^{yzr}_{ijk} - dD^{yz}_{ijk}}{D^{xyz}_{ijk}} + D^{xz}_{ijk} \frac{D^{xzr}_{ijk} - dD^{xz}_{ijk}}{D^{xyz}_{ijk}} + D^{xy}_{ijk} \frac{D^{xyr}_{ijk} - dD^{xy}_{ijk}}{D^{xyz}_{ijk}} \\ &= \frac{D^{yzr}_{ijk} D^{yz}_{ijk}}{D^{xyz}_{ijk}} - \frac{d \left(D^{yz}_{ijk}\right)^2}{D^{xyz}_{ijk}} + \frac{D^{xzr}_{ijk} D^{xz}_{ijk}}{D^{xyz}_{ijk}} - \frac{d \left(D^{xz}_{ijk}\right)^2}{D^{xyz}_{ijk}} + \frac{D^{xyr}_{ijk} D^{xy}_{ijk}}{D^{xyz}_{ijk}} - \frac{d \left(D^{xy}_{ijk}\right)^2}{D^{xyz}_{ijk}} \\ &= \frac{D^{yzr}_{ijk} D^{yz}_{ijk} + D^{xzr}_{ijk} D^{xz}_{ijk} + D^{xyr}_{ijk} D^{xy}_{ijk}}{D^{xyz}_{ijk}} - d \frac{\left(D^{yz}_{ijk}\right)^2 + \left(D^{xz}_{ijk}\right)^2 + \left(D^{xy}_{ijk}\right)^2}{D^{xyz}_{ijk}}. \end{split}$$

Substitution for d yields:

$$P_{ijk} \cdot \vec{n} = \frac{D_{ijk}^{yzr} D_{ijk}^{yz} + D_{ijk}^{xzr} D_{ijk}^{xz} + D_{ijk}^{xyr} D_{ijk}^{xy}}{D_{ijk}^{xyz}} - \frac{\left[\left[D_{ijk}^{yzr} D_{ijk}^{yz} + D_{ijk}^{xzr} D_{ijk}^{xz} + D_{ijk}^{xyr} D_{ijk}^{xy} \right] \pm D_{ijk}^{xyz} \sqrt{\Delta} \right] \left[\left(D_{ijk}^{yz} \right)^{2} + \left(D_{ijk}^{xz} \right)^{2} + \left(D_{ijk}^{xy} \right)^{2} \right]}{\left[\left(D_{ijk}^{yz} \right)^{2} + \left(D_{ijk}^{xy} \right)^{2} + \left(D_{ijk}^{xy} \right)^{2} \right]}$$

$$\begin{split} &= \frac{D_{ijk}^{yzr}D_{ijk}^{yz} + D_{ijk}^{xzr}D_{ijk}^{xz} + D_{ijk}^{xyr}D_{ijk}^{xy}}{D_{ijk}^{xyz}} \\ &- \frac{D_{ijk}^{yzr}D_{ijk}^{yz} + D_{ijk}^{xzr}D_{ijk}^{xz} + D_{ijk}^{xyr}D_{ijk}^{xy} \pm D_{ijk}^{xyz}\sqrt{\Delta}}{D_{ijk}^{xyz}} \\ &= -\left(\pm\sqrt{\Delta}\right). \end{split}$$

We need the result to be positive, in other words

$$P_{ijk} \cdot \vec{n} > 0 \iff -\left(\pm\sqrt{\Delta}\right) > 0.$$

Since $\Delta > 0$ by hypothesis, we conclude that the solution we are interested in is $d = \frac{-B - \sqrt{\Delta}}{2A}$, or

$$d = \frac{D_{ijk}^{yzr}D_{ijk}^{yz} + D_{ijk}^{xzr}D_{ijk}^{xz} + D_{ijk}^{xyr}D_{ijk}^{xy} - D_{ijk}^{xyz}\sqrt{\Delta}}{\left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xz}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}}.$$

Substituting in the initial relations, we conclude that

$$\begin{split} a_{ijk} &= \frac{D_{ijk}^{yzr} - dD_{ijk}^{yz}}{D_{ijk}^{xyz}} \\ &= \frac{D_{ijk}^{yzr} \left[\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xz} \right)^2 + \left(D_{ijk}^{xy} \right)^2 \right] - D_{ijk}^{yz} \left[D_{ijk}^{yzr} D_{ijk}^{yz} + D_{ijk}^{xzr} D_{ijk}^{xz} + D_{ijk}^{xyr} D_{ijk}^{xy} - D_{ijk}^{xyz} \sqrt{\Delta} \right]}{D_{ijk}^{xyz} \left[\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xy} \right)^2 \right]} \\ &= \frac{D_{ijk}^{yzr} \left[\left(D_{ijk}^{xz} \right)^2 + \left(D_{ijk}^{xy} \right)^2 \right] - D_{ijk}^{yz} \left[D_{ijk}^{xzr} D_{ijk}^{xz} + D_{ijk}^{xyr} D_{ijk}^{xy} \right] + D_{ijk}^{xyz} D_{ijk}^{yz} \sqrt{\Delta}}{D_{ijk}^{xyz} \left[\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xy} \right)^2 + \left(D_{ijk}^{xy} \right)^2 \right]} \\ &= \frac{D_{ijk}^{xz} \left[D_{ijk}^{yzr} D_{ijk}^{xz} - D_{ijk}^{xyz} D_{ijk}^{yz} + D_{ijk}^{xyz} D_{ijk}^{yz} - D_{ijk}^{xyz} D_{ijk}^{yz} + D_{ijk}^{xyz} D_{ijk}^{yz} \sqrt{\Delta}}{D_{ijk}^{xyz} \left[\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xyz} \right)^2 \right]} \\ &= \frac{D_{ijk}^{xz} \left[-D_{ijk}^{xyz} D_{ijk}^{zr} + D_{ijk}^{xyz} D_{ijk}^{yr} + D_{ijk}^{xyz} D_{ijk}^{yz} \sqrt{\Delta}}{D_{ijk}^{yz} \left[\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xyz} \right)^2 \right]} \\ &= \frac{-D_{ijk}^{xz} D_{ijk}^{zr} - D_{ijk}^{xy} D_{ijk}^{yr} + D_{ijk}^{yz} \sqrt{\Delta}}{\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xy} \right)^2}, \end{split}$$

$$b_{ijk} = -\frac{D_{ijk}^{xzr} - dD_{ijk}^{xz}}{D_{ijk}^{xyz}}$$

$$= \frac{-D_{ijk}^{xzr} \left[\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xz} \right)^2 + \left(D_{ijk}^{xy} \right)^2 \right] + D_{ijk}^{xz} \left[D_{ijk}^{yzr} D_{ijk}^{yz} + D_{ijk}^{xzr} D_{ijk}^{xz} + D_{ijk}^{xyr} D_{ijk}^{xy} - D_{ijk}^{xyz} \sqrt{\Delta} \right]}{D_{ijk}^{xyz} \left[\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xy} \right)^2 + \left(D_{ijk}^{xy} \right)^2 \right]}$$

$$= \frac{-D_{ijk}^{xzr} \left[\left(D_{ijk}^{xy} \right)^2 + \left(D_{ijk}^{yz} \right)^2 \right] + D_{ijk}^{xz} \left[D_{ijk}^{xyr} D_{ijk}^{xy} + D_{ijk}^{yzr} D_{ijk}^{yz} \right] - D_{ijk}^{xyz} D_{ijk}^{xz} \sqrt{\Delta}}{D_{ijk}^{xyz} \left[\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xyz} \right)^2 + \left(D_{ijk}^{xyz} \right)^2 \right]}$$

$$= \frac{D_{ijk}^{xy} \left[D_{ijk}^{xyr} D_{ijk}^{xz} - D_{ijk}^{xzr} D_{ijk}^{xy} + \left(D_{ijk}^{xyz} \right)^2 - D_{ijk}^{xyz} D_{ijk}^{xz} \sqrt{\Delta}}{D_{ijk}^{xyz} \left[\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xyz} \right)^2 + \left(D_{ijk}^{xyz} \right)^2 \right]}$$

$$= \frac{D_{ijk}^{xy} \left[D_{ijk}^{xyz} D_{ijk}^{xr} + D_{ijk}^{yz} \left[-D_{ijk}^{xyz} D_{ijk}^{zr} - D_{ijk}^{xyz} D_{ijk}^{xz} \sqrt{\Delta}}{D_{ijk}^{xyz} \left[\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xyz} \right)^2 \right]}$$

$$= \frac{D_{ijk}^{xy} D_{ijk}^{xr} - D_{ijk}^{yz} D_{ijk}^{zr} - D_{ijk}^{xz} \sqrt{\Delta}}{\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xyz} \right)^2}, \text{ and}$$

$$\begin{split} c_{ijk} &= \frac{D_{ijk}^{xyr} - dD_{ijk}^{xy}}{D_{ijk}^{xyz}} \\ &= \frac{D_{ijk}^{xyr} \left[\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xy} \right)^2 + \left(D_{ijk}^{xy} \right)^2 \right] - D_{ijk}^{xy} \left[D_{ijk}^{yzr} D_{ijk}^{yz} + D_{ijk}^{xyr} D_{ijk}^{xy} + D_{ijk}^{xyr} D_{ijk}^{xy} - D_{ijk}^{xyz} \sqrt{\Delta} \right]}{D_{ijk}^{xyz} \left[\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xy} \right)^2 + \left(D_{ijk}^{xy} \right)^2 \right]} \\ &= \frac{D_{ijk}^{xyr} \left[\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xz} \right)^2 \right] - D_{ijk}^{xy} \left[D_{ijk}^{yzr} D_{ijk}^{yz} + D_{ijk}^{xzr} D_{ijk}^{xz} \right] + D_{ijk}^{xyz} D_{ijk}^{xy} \sqrt{\Delta}}{D_{ijk}^{xyz} \left[\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xy} \right)^2 + \left(D_{ijk}^{xy} \right)^2 \right]} \\ &= \frac{D_{ijk}^{yz} \left[D_{ijk}^{xyr} D_{ijk}^{yz} - D_{ijk}^{yzr} D_{ijk}^{xy} \right] + D_{ijk}^{xz} \left[D_{ijk}^{xyz} D_{ijk}^{xy} - D_{ijk}^{xyz} D_{ijk}^{xy} \right]}{D_{ijk}^{xyz} \left[\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xyz} \right)^2 \right]} \\ &= \frac{D_{ijk}^{yz} \left[D_{ijk}^{xyz} D_{ijk}^{yr} \right] + D_{ijk}^{xz} \left[D_{ijk}^{xyz} D_{ijk}^{xr} \right] + D_{ijk}^{xyz} D_{ijk}^{xy} \sqrt{\Delta}}{D_{ijk}^{xyz} \left[\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xy} \right)^2 \right]} \\ &= \frac{D_{ijk}^{yz} D_{ijk}^{yr} + D_{izk}^{xz} D_{ijk}^{xr} + D_{ijk}^{xy} \sqrt{\Delta}}{\left(D_{ijk}^{yz} \right)^2 + \left(D_{ijk}^{xy} \right)^2}. \end{split}$$

Finally, our equations are:

$$a_{ijk} = \frac{-D_{ijk}^{xz}D_{ijk}^{zr} - D_{ijk}^{xy}D_{ijk}^{yr} + D_{ijk}^{yz}\sqrt{\Delta}}{\left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xz}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}},$$

$$b_{ijk} = \frac{D_{ijk}^{xy}D_{ijk}^{xr} - D_{ijk}^{yz}D_{ijk}^{zr} - D_{ijk}^{xz}\sqrt{\Delta}}{\left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xz}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}},$$

$$c_{ijk} = \frac{D_{ijk}^{yz} D_{ijk}^{yr} + D_{ijk}^{xz} D_{ijk}^{xr} + D_{ijk}^{xy} \sqrt{\Delta}}{\left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xz}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}},$$

$$d_{ijk} = \frac{D_{ijk}^{yzr} D_{ijk}^{yz} + D_{ijk}^{xzr} D_{ijk}^{xz} + D_{ijk}^{xyr} D_{ijk}^{xy} - D_{ijk}^{xyz} \sqrt{\Delta}}{\left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xz}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}}.$$

Let us recall that, given $B_q = \{(x_q, x_q, x_q), r_q\}$, the signed distance of B_q and the plane Π_{ijk} is given by

$$\delta(B_q, \Pi_{ijk}) = \frac{a_{ijk}x_q + b_{ijk}y_q + c_{ijk}z_q + d_{ijk}}{\sqrt{a_{ijk}^2 + b_{ijk}^2 + c_{ijk}^2}} - r_q$$

From our initial assumptions, we have that $\sqrt{a_{ijk}^2 + b_{ijk}^2 + c_{ijk}^2} = 1$, so we really need to compute the sign of the expression

$$\begin{split} \delta(B_{q},\Pi_{ijk}) &= & \ a_{ijk}x_{q} + b_{ijk}y_{q} + c_{ijk}z_{q} + d_{ijk} - r_{q} = \\ &= \left[\frac{-D_{ijk}^{xz}D_{ijk}^{zr} - D_{ijk}^{xy}D_{ijk}^{yr} + D_{ijk}^{yz}\sqrt{\Delta}}{\left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}} \right] x_{q} \\ &+ \left[\frac{D_{ijk}^{xy}D_{ijk}^{xr} - D_{ijk}^{yz}D_{ijk}^{zr} - D_{ijk}^{xz}\sqrt{\Delta}}{\left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}} \right] y_{q} \\ &+ \left[\frac{D_{ijk}^{yz}D_{ijk}^{yr} + D_{ijk}^{yz}D_{ijk}^{xr} + D_{ijk}^{xy}\sqrt{\Delta}}{\left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xz}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}} \right] z_{q} \\ &+ \frac{D_{ijk}^{yz}D_{ijk}^{yz} + D_{ijk}^{yz}D_{ijk}^{xz} + D_{ijk}^{xy}D_{ijk}^{xy} - D_{ijk}^{xyz}\sqrt{\Delta}}{\left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}} - r_{q} = \\ &= \frac{\left[-D_{ijk}^{xz}D_{ijk}^{zr} - D_{ijk}^{xy}D_{ijk}^{yr} + D_{ijk}^{yz}\sqrt{\Delta} \right] x_{q}}{\left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}} \\ &+ \frac{\left[D_{ijk}^{xy}D_{ijk}^{xr} - D_{ijk}^{yz}D_{ijk}^{xr} - D_{ijk}^{xy}\sqrt{\Delta} \right] y_{q}}{\left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}} \\ &+ \frac{\left[D_{ijk}^{yz}D_{ijk}^{yr} + D_{ijk}^{xz}D_{ijk}^{xr} + D_{ijk}^{xy}\sqrt{\Delta} \right] z_{q}}{\left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}} \\ &+ \frac{D_{ijk}^{yz}D_{ijk}^{yz} + D_{ijk}^{xz}D_{ijk}^{xr} + D_{ijk}^{xy}\sqrt{\Delta}}{\left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}} \\ &- \frac{\left[\left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xz}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}}{\left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}} \right] r_{q}} \\ &- \frac{\left[\left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xz}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}}{\left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}} \right] r_{q}} \\ &- \frac{\left[\left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xz}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}}{\left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xz}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}} \right] r_{q}} \\ &- \frac{\left[\left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xz}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}}{\left(D_{ijk}^{xy}\right)^{2} + \left(D_{ijk}^{xy}\right)^{2}} \right] r_{q$$

$$= \frac{\left[-D_{ijk}^{yr}x_{q} + D_{ijk}^{xr}y_{q} - D_{ijk}^{xy}r_{q} + D_{ijk}^{xyr}\right]D_{ijk}^{xy}}{\left(D_{ijk}^{xy}\right)^{2} + \left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xz}\right)^{2}} + \frac{\left[-D_{ijk}^{zr}x_{q} + D_{ijk}^{xr}z_{q} - D_{ijk}^{xz}r_{q} + D_{ijk}^{xzr}\right]D_{ijk}^{xz}}{\left(D_{ijk}^{xy}\right)^{2} + \left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xz}\right)^{2}} + \frac{\left[-D_{ijk}^{zr}y_{q} + D_{ijk}^{yr}z_{q} - D_{ijk}^{yz}r_{q} + D_{ijk}^{yzr}\right]D_{ijk}^{yz}}{\left(D_{ijk}^{xy}\right)^{2} + \left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xz}\right)^{2}} - \frac{\left[-D_{ijk}^{yr}x_{q} + D_{ijk}^{xz}y_{q} - D_{ijk}^{xy}z_{q} + D_{ijk}^{xyz}\right]\sqrt{\Delta}}{\left(D_{ijk}^{xy}\right)^{2} + \left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xz}\right)^{2}} = \frac{D_{ijkq}^{xyr}D_{ijk}^{xy} + D_{ijkq}^{xzr}D_{ijk}^{xz} + D_{ijkq}^{yzr}D_{ijk}^{yz} - D_{ijkq}^{xyz}\sqrt{\Delta}}{\left(D_{ijk}^{xy}\right)^{2} + \left(D_{ijk}^{yz}\right)^{2} + \left(D_{ijk}^{xz}\right)^{2}},$$

where the following representations have been used:

$$\begin{vmatrix} u_{\mu} & v_{\mu} & w_{\mu} & m_{\mu} \\ u_{\nu} & v_{\nu} & w_{\nu} & m_{\nu} \\ u_{\lambda} & v_{\lambda} & w_{\lambda} & m_{\lambda} \\ u_{\theta} & v_{\theta} & w_{\theta} & m_{\theta} \end{vmatrix} = D_{\mu\nu\lambda\theta}^{uvwm} \quad , \quad \begin{vmatrix} u_{\mu} & v_{\mu} & w_{\mu} & 1 \\ u_{\nu} & v_{\nu} & w_{\nu} & 1 \\ u_{\lambda} & v_{\lambda} & w_{\lambda} & 1 \\ u_{\theta} & v_{\theta} & w_{\theta} & 1 \end{vmatrix} = D_{\mu\nu\lambda\theta}^{uvw} \quad ,$$

$$u, v, w, m \in \{x, y, z, r\}, \qquad \mu, \nu, \lambda, \theta \in \{i, j, k, q\}.$$

In conclusion:

$$\delta(B_q, \Pi_{ijk}) = \frac{D_{ijkq}^{xyr} D_{ijk}^{xy} + D_{ijkq}^{xzr} D_{ijk}^{xz} + D_{ijkq}^{yzr} D_{ijk}^{yz} - D_{ijkq}^{xyz} \sqrt{\Delta}}{\left(D_{ijk}^{xy}\right)^2 + \left(D_{ijk}^{yz}\right)^2 + \left(D_{ijk}^{xz}\right)^2}.$$

Since the quantity $(D_{ijk}^{xy})^2 + (D_{ijk}^{yz})^2 + (D_{ijk}^{xz})^2$ is strictly positive under the hypothesis that there are no degeneracies, the sign of the distance of the site B_q from the plane Π_{ijk} is determined by the sign of the quantity

$$\mathbf{Q} = D_{ijka}^{xyr} D_{ijk}^{xy} + D_{ijka}^{xzr} D_{ijk}^{xz} + D_{ijka}^{yzr} D_{ijk}^{yz} - D_{ijka}^{xyz} \sqrt{\Delta}$$

where the expressions represent, respectively:

$$\begin{split} D^{uvw}_{\lambda\mu\nu} &= \begin{vmatrix} u_{\lambda} & v_{\lambda} & w_{\lambda} \\ u_{\mu} & v_{\mu} & w_{\mu} \\ u_{\nu} & v_{\nu} & w_{\nu} \end{vmatrix} \quad , \qquad D^{uv}_{\lambda\mu\nu} &= \begin{vmatrix} u_{\lambda} & v_{\lambda} & 1 \\ u_{\mu} & v_{\mu} & 1 \\ u_{\nu} & v_{\nu} & 1 \end{vmatrix} \quad , \\ D^{uvwm}_{\kappa\lambda\mu\nu} &= \begin{vmatrix} u_{\kappa} & v_{\kappa} & w_{\kappa} & m_{\kappa} \\ u_{\lambda} & v_{\lambda} & w_{\lambda} & m_{\lambda} \\ u_{\mu} & v_{\mu} & w_{\mu} & m_{\mu} \\ u_{\nu} & v_{\nu} & w_{\nu} & m_{\nu} \end{vmatrix} \quad , \qquad D^{uvw}_{\kappa\lambda\mu\nu} &= \begin{vmatrix} u_{\kappa} & v_{\kappa} & w_{\kappa} & 1 \\ u_{\lambda} & v_{\lambda} & w_{\lambda} & 1 \\ u_{\mu} & v_{\mu} & w_{\mu} & 1 \\ u_{\nu} & v_{\nu} & w_{\nu} & 1 \end{vmatrix} \quad , \\ u, v, w, m &\in \{x, y, z, r\} \quad & \kappa, \lambda, \mu, \nu &\in \{i, j, k, q\} \, , \\ \Delta &= \left(D^{xy}_{ijk}\right)^{2} + \left(D^{xz}_{ijk}\right)^{2} + \left(D^{yz}_{ijk}\right)^{2} - \left(D^{xr}_{ijk}\right)^{2} - \left(D^{yr}_{ijk}\right)^{2} - \left(D^{zr}_{ijk}\right)^{2} \end{split}$$

3.4 The *InSphere* predicate

Now let us consider the problem we initially set to solve. All sites are considered to be spheres in our three-dimensional complex space \mathcal{Z} , and are in the form $B_{\lambda} = \{b_{\lambda}, r_{\lambda}\} = \{(x_{\lambda}, y_{\lambda}, z_{\lambda}), r_{\lambda}\}$. Our setup consists of four sites, B_i, B_j, B_k, B_ℓ , and let B_t be the site tangent to all four sites. Given another site B_q , we want to determine the situation of B_q in relation to B_t .

According to our previous discussion, if we apply the inversion transformation to our setup, the procedure would be as follows:

- The first step is to apply the transformation $r_{\nu}^* = r_{\nu} r_{\ell}$, $\nu \in \{i, j, k, \ell\}$, which will transform the sites B_{ν} into the sites B_{ν}^* , $\nu \in \{i, j, k, \ell\}$. Obviously, the radius of the site B_{ℓ} is now 0, hence the site has been reduced to the point $b_{\ell} = \{x_{\ell}, y_{\ell}, z_{\ell}\}$.
- Next we must apply the inversion transformation through the point b_{ℓ} . For every site we now have:

$$u_{\nu} = \frac{x_{\nu}^{*}}{p_{\nu}^{*}}, \qquad v_{\nu} = \frac{y_{\nu}^{*}}{p_{\nu}^{*}}, \qquad w_{\nu} = \frac{z_{\nu}^{*}}{p_{\nu}^{*}}, \qquad \rho_{\nu} = \frac{r_{\nu}^{*}}{p_{\nu}^{*}}$$

$$x_{\nu}^{*} = x_{\nu} - x_{\ell}, \qquad y_{\nu}^{*} = y_{\nu} - y_{\ell}, \qquad z_{\nu}^{*} = z_{\nu} - z_{\ell},$$

$$p_{\nu}^{*} = (x_{\nu}^{*})^{2} + (y_{\nu}^{*})^{2} + (z_{\nu}^{*})^{2} - (r_{\nu}^{*})^{2}, \qquad \nu \in \{i, j, k\}.$$

Note that if the quadritangent sphere B_q were present, it would be transformed into a plane by the inversion. The point b_ℓ , on the other hand, is situated at infinity, related to our remaining objects. We are now working in the space \mathcal{W} , and our sites will be mapped onto the sites $W_{\nu} = \{(u_{\nu}, v_{\nu}, w_{\nu}), \rho_{\nu}\}, \ \nu \in \{i, j, k\}.$

• We proceed to find the plane $\Pi := au + bv + cw + d = 0$ tangent to the sites W_i, W_j, W_k . As we previously showed, the coefficients a, b, c and d are found to be

$$a_{ijk} = \frac{-D_{ijk}^{uw}D_{ijk}^{w\rho} - D_{ijk}^{uv}D_{ijk}^{v\rho} + D_{ijk}^{vw}\sqrt{\Delta}}{\left(D_{ijk}^{vw}\right)^{2} + \left(D_{ijk}^{uw}\right)^{2} + \left(D_{ijk}^{uv}\right)^{2}}$$

$$b_{ijk} = \frac{D_{ijk}^{uv}D_{ijk}^{u\rho} - D_{ijk}^{vw}D_{ijk}^{w\rho} - D_{ijk}^{uw}\sqrt{\Delta}}{\left(D_{ijk}^{vw}\right)^{2} + \left(D_{ijk}^{uw}\right)^{2} + \left(D_{ijk}^{uv}\right)^{2}}$$

$$c_{ijk} = \frac{D_{ijk}^{vw}D_{ijk}^{v\rho} + D_{ijk}^{uw}D_{ijk}^{u\rho} + D_{ijk}^{uv}\sqrt{\Delta}}{\left(D_{ijk}^{vw}\right)^{2} + \left(D_{ijk}^{uw}\right)^{2} + \left(D_{ijk}^{uv}\right)^{2}}$$

$$d_{ijk} = \frac{D_{ijk}^{vw\rho}D_{ijk}^{vw} + D_{ijk}^{uw\rho}D_{ijk}^{uw} + D_{ijk}^{uv\rho}D_{ijk}^{uv} - D_{ijk}^{uvw}\sqrt{\Delta}}{\left(D_{ijk}^{vw}\right)^{2} + \left(D_{ijk}^{uw}\right)^{2} + \left(D_{ijk}^{uv}\right)^{2}}$$

where

$$D_{\lambda\mu\nu}^{k\ell m} = \begin{vmatrix} k_{\lambda} & \ell_{\lambda} & m_{\lambda} \\ k_{\mu} & \ell_{\mu} & m_{\mu} \\ k_{\nu} & \ell_{\nu} & m_{\nu} \end{vmatrix} \quad , \qquad \qquad D_{\lambda\mu\nu}^{k\ell} = \begin{vmatrix} k_{\lambda} & \ell_{\lambda} & 1 \\ k_{\mu} & \ell_{\mu} & 1 \\ k_{\nu} & \ell_{\nu} & 1 \end{vmatrix} \quad ,$$

$$k, \ell, m \in \{u, v, w\},$$
 $\lambda, \mu, \nu \in \{i, j, k\}$

and

$$\Delta = \left(D_{ijk}^{uv}\right)^2 + \left(D_{ijk}^{uw}\right)^2 + \left(D_{ijk}^{vw}\right)^2 - \left(D_{ijk}^{u\rho}\right)^2 - \left(D_{ijk}^{v\rho}\right)^2 - \left(D_{ijk}^{w\rho}\right)^2.$$

• Now, to find the sign of the distance of the query site B_q from the quadritangent plane, we can apply the inversion transformation previously described, thus ending up with the inverted site W_q . It is now sufficient to calculate the sign of the distance of the site W_q from the tritangent plane Π . As previously shown, our quest boils down to determining the sign of the quantity

$$\mathbf{Q} = D_{ijkq}^{uv\rho} D_{ijk}^{uv} + D_{ijkq}^{uw\rho} D_{ijk}^{uw} + D_{ijkq}^{vw\rho} D_{ijk}^{vw} - D_{ijkq}^{uvw} \sqrt{\Delta},$$

where

$$D_{\kappa\lambda\mu\nu}^{k\ell mn} = \begin{vmatrix} k_{\kappa} & \ell_{\kappa} & m_{\kappa} & n_{\kappa} \\ k_{\lambda} & \ell_{\lambda} & m_{\lambda} & n_{\lambda} \\ k_{\mu} & \ell_{\mu} & m_{\mu} & n_{\mu} \\ k_{\nu} & \ell_{\nu} & m_{\nu} & n_{\nu} \end{vmatrix} , \qquad D_{\kappa\lambda\mu\nu}^{k\ell m} = \begin{vmatrix} k_{\kappa} & \ell_{\kappa} & m_{\kappa} & 1 \\ k_{\lambda} & \ell_{\lambda} & m_{\lambda} & 1 \\ k_{\mu} & \ell_{\mu} & m_{\mu} & 1 \\ k_{\nu} & \ell_{\nu} & m_{\nu} & 1 \end{vmatrix} ,$$

$$k, \ell, m, n \in \{u, v, w, \rho\} , \qquad \kappa, \lambda, \mu, \nu \in \{i, j, k, q\}$$

and the other quantities remain as previously defined.

Note that all the expressions are now expressed in terms of the space \mathcal{W} . In the previous section we used x, y, z and r (which belong to the space \mathcal{Z}) to simplify our calculations, but we must be careful with our variables. What we would like, is to express our results in terms of our initial variables, so that we need not apply the inversion transformation. We seek an expression as fast and simple as possible.

It is easily seen that the following holds:

$$D_{ijk}^{uv} = \begin{vmatrix} u_i & v_i & 1 \\ u_j & v_j & 1 \\ u_k & v_k & 1 \end{vmatrix} = \begin{vmatrix} \frac{x_i}{p_i^*} & \frac{y_i}{p_i^*} & 1 \\ \frac{x_j^*}{p_j^*} & \frac{y_j^*}{p_j^*} & 1 \\ \frac{x_k^*}{p_k^*} & \frac{y_k^*}{p_k^*} & 1 \end{vmatrix} = \frac{1}{p_i^* p_j^* p_k^*} \begin{vmatrix} x_i^* & y_i^* & p_i^* \\ x_j^* & y_j^* & p_j^* \\ x_k^* & y_k^* & p_k^* \end{vmatrix},$$

$$D_{ijk}^{uvw} = \begin{vmatrix} u_i & v_i & w_i \\ u_j & v_j & w_j \\ u_k & v_k & w_k \end{vmatrix} = \begin{vmatrix} \frac{x_i^*}{p_i^*} & \frac{y_i^*}{p_i^*} & \frac{z_i^*}{p_i^*} \\ \frac{x_k^*}{p_k^*} & \frac{y_j^*}{p_j^*} & \frac{z_j^*}{p_j^*} \\ \frac{x_k^*}{p_k^*} & \frac{y_k^*}{p_k^*} & \frac{z_k^*}{p_k^*} \end{vmatrix} = \frac{1}{p_i^* p_j^* p_k^*} \begin{vmatrix} x_i^* & y_i^* & z_i^* \\ x_j^* & y_j^* & z_j^* \\ x_k^* & y_k^* & z_k^* & p_k^* \end{vmatrix}.$$

Hence we define the quantity

$$\begin{vmatrix} k_\lambda^* & \ell_\lambda^* & m_\lambda^* \\ k_\mu^* & \ell_\mu^* & m_\mu^* \\ k_\nu^* & \ell_\nu^* & m_\nu^* \end{vmatrix} = E_{\lambda\mu\nu}^{k\ell m},$$

and it holds that

$$D_{\lambda\mu\nu}^{\pi\theta} = \frac{1}{p_i^* p_j^* p_k^*} E_{\lambda\mu\nu}^{k\ell p}, \qquad D_{\lambda\mu\nu}^{\pi\theta\eta} = \frac{1}{p_i^* p_j^* p_k^*} E_{\lambda\mu\nu}^{k\ell m}$$

$$\pi_{\nu} = k_{\nu}^* / p_{\nu}^*, \qquad \theta_{\nu} = \ell_{\nu}^* / p_{\nu}^*, \qquad \eta_{\nu} = m_{\nu}^* / p_{\nu}^*,$$

$$\pi, \theta, \eta \in \{u, v, w, \rho\}, \qquad k, \ell, m \in \{x, y, z, r\}, \qquad \lambda, \mu, \nu \in \{i, j, k, q\}.$$

It is easily verified that Δ can be easily transformed into an expression of out initial coordinates:

$$\Delta = \left(D_{ijk}^{uv}\right)^{2} + \left(D_{ijk}^{uw}\right)^{2} + \left(D_{ijk}^{vw}\right)^{2} - \left(D_{ijk}^{u\rho}\right)^{2} - \left(D_{ijk}^{v\rho}\right)^{2} - \left(D_{ijk}^{w\rho}\right)^{2} \Rightarrow$$

$$\Gamma' = \left[\frac{1}{p_{i}^{*}p_{i}^{*}p_{k}^{*}}\right]^{2} \left[\left(E_{ijk}^{xyp}\right)^{2} + \left(E_{ijk}^{xzp}\right)^{2} + \left(E_{ijk}^{yzp}\right)^{2} - \left(E_{ijk}^{xrp}\right)^{2} - \left(E_{ijk}^{yrp}\right)^{2} - \left(E_{ijk}^{zrp}\right)^{2} \right]$$

We consider the expression

$$\Gamma = \left[p_i^* p_j^* p_k^* \right]^2 \Gamma' = \left(E_{ijk}^{xyp} \right)^2 + \left(E_{ijk}^{xzp} \right)^2 + \left(E_{ijk}^{yzp} \right)^2 - \left(E_{ijk}^{xrp} \right)^2 - \left(E_{ijk}^{yrp} \right)^2 - \left(E_{ijk}^{xrp} \right)^2$$

which will prove useful in porting \mathbf{Q} into out initial coordinates. Now we observe that the relations between the quantities D and E holds again in four dimensions:

$$D_{\lambda\mu\nu\xi}^{\pi\theta\eta} = \frac{1}{p_i^* p_j^* p_k^* p_q^*} E_{\lambda\mu\nu\xi}^{k\ell mp}, \qquad D_{\lambda\mu\nu\xi}^{\pi\theta\eta\sigma} = \frac{1}{p_i^* p_j^* p_k^* p_q^*} E_{\lambda\mu\nu\xi}^{k\ell mn},$$

$$\pi_{\nu} = k_{\nu}^* / p_{\nu}^*, \qquad \theta_{\nu} = \ell_{\nu}^* / p_{\nu}^*, \qquad \eta_{\nu} = m_{\nu}^* / p_{\nu}^*, \qquad \sigma_{\nu} = n_{\nu}^* / p_{\nu}^*,$$

$$\pi, \theta, \eta, \sigma \in \{u, v, w, \rho\}, \qquad k, \ell, m, n \in \{x, y, z, r\}, \qquad \lambda, \mu, \nu, \xi \in \{i, j, k, q\}.$$

We can now express the solutions we have found for the coefficients of the plane in terms of the initial coordinates:

$$a_{ijk} = \frac{-E_{ijk}^{xzp} E_{ijk}^{zrp} - E_{ijk}^{xyp} E_{ijk}^{yrp} + E_{ijk}^{yzp} \sqrt{\Gamma}}{\left(E_{ijk}^{yzp}\right)^{2} + \left(E_{ijk}^{xzp}\right)^{2} + \left(E_{ijk}^{xyp}\right)^{2}}$$

$$b_{ijk} = \frac{E_{ijk}^{xyp} E_{ijk}^{xrp} - E_{ijk}^{yzp} E_{ijk}^{zrp} - E_{ijk}^{xzp} \sqrt{\Gamma}}{\left(E_{ijk}^{yzp}\right)^{2} + \left(E_{ijk}^{xzp}\right)^{2} + \left(E_{ijk}^{xyp}\right)^{2}}$$

$$c_{ijk} = \frac{E_{ijk}^{yzp} E_{ijk}^{yrp} + E_{ijk}^{xzp} E_{ijk}^{xrp} + E_{ijk}^{xyp} \sqrt{\Gamma}}{\left(E_{ijk}^{yzp}\right)^{2} + \left(E_{ijk}^{xzp}\right)^{2} + \left(E_{ijk}^{xyp}\right)^{2}}$$

$$d_{ijk} = \frac{E_{ijk}^{yzr} E_{ijk}^{yzp} + E_{ijk}^{xzr} E_{ijk}^{xzp} + E_{ijk}^{xyp} E_{ijk}^{xyp} - E_{ijk}^{xyz} \sqrt{\Gamma}}{\left(E_{ijk}^{yzp}\right)^{2} + \left(E_{ijk}^{xzp}\right)^{2} + \left(E_{ijk}^{xyp}\right)^{2}}$$

If we apply the Inversion transformation to the plane with the above coefficients, we end up with the equation of a sphere, as we expect:

$$\left(x - x_{\ell} + \frac{a_{ijk}}{2d_{ijk}}\right) + \left(y - y_{\ell} + \frac{b_{ijk}}{2d_{ijk}}\right) + \left(z - z_{\ell} + \frac{c_{ijk}}{2d_{ijk}}\right) = \frac{1}{4d_{ijk}^2}$$

We conclude that the sphere tangent to our initial four spheres has its center situated at

$$b_t = \left(x_{\ell} - \frac{a_{ijk}}{2d_{ijk}}, \quad y_{\ell} - \frac{b_{ijk}}{2d_{ijk}}, \quad z_{\ell} - \frac{c_{ijk}}{2d_{ijk}}\right)$$

and its radius is equal to $r_t = \frac{1}{2d_{ijk}} - r_\ell$, where recall that $B_\ell = \{(x_\ell, y_\ell, z_\ell), r_\ell\}$ is the site through which we apply the inversion.

We can now proceed and transform the quantity **Q**:

$$\mathbf{Q} = D_{ijkq}^{uv\rho} D_{ijk}^{uv} + D_{ijkq}^{uw\rho} D_{ijk}^{uw} + D_{ijkq}^{vw\rho} D_{ijk}^{vw} - D_{ijkq}^{uvw} \sqrt{\Delta} \iff$$

$$\mathbf{Q} = \frac{1}{\left(p_i^* p_j^* p_k^*\right)^2 p_q^*} \left[E_{ijkq}^{xyrp} E_{ijk}^{xyp} + E_{ijkq}^{xzrp} E_{ijk}^{xzp} + E_{ijkq}^{yzrp} E_{ijk}^{yzp} - E_{ijkq}^{xyzp} \sqrt{\Gamma} \right]$$

Since the quantity $\frac{1}{\left(p_i^* p_j^* p_k^*\right)^2 p_q^*}$ is constantly positive in the non-degenerate case, we are left with the expression

$$\mathbf{Q}'' = E_{ijkq}^{xyrp} E_{ijk}^{xyp} + E_{ijkq}^{xzrp} E_{ijk}^{xzp} + E_{ijkq}^{yzrp} E_{ijk}^{yzp} - E_{ijkq}^{xyzp} \sqrt{\Gamma}$$

We observe that the expression can be viewed in the form

$$\mathbf{Q}'' = Y_0 + Y_1 \sqrt{\Gamma}$$

where

$$Y_0 = E_{ijkq}^{xyrp} E_{ijk}^{xyp} + E_{ijkq}^{xzrp} E_{ijk}^{xzp} + E_{ijkq}^{yzrp} E_{ijk}^{yzp}$$

$$Y_1 = -E_{ijkq}^{xyzp}$$

We have already seen in Chapter 2 that the sign of quantities in the above form can be determined in the following way:

$$\operatorname{sign}(Y_0 + Y_1 \sqrt{\Gamma}) = \begin{cases} \operatorname{sign}(Y_0) &, \text{ if } \Gamma = 0\\ \operatorname{sign}(Y_1) &, \text{ if } Y_0 = 0\\ \operatorname{sign}(Y_0) &, \text{ if } Y_1 = 0\\ \operatorname{sign}(Y_0) &, \text{ if } \operatorname{sign}(Y_0) = \operatorname{sign}(Y_1)\\ \operatorname{sign}(Y_0) & \operatorname{sign}(Y_0^2 - Y_1^2 \Gamma) &, \text{ otherwise} \end{cases}$$

If we denote the degree of an algebraic expression by the operator deg(X), we can easily see that

$$\deg\left(E_{\lambda\mu\nu}^{k\ell m}\right) = 3, \quad \deg\left(E_{\lambda\mu\nu}^{k\ell p}\right) = 4, \quad \deg\left(E_{\lambda\mu\nu\xi}^{k\ell m n}\right) = 4, \quad \deg\left(E_{\lambda\mu\nu\xi}^{k\ell m p}\right) = 5$$

$$\lambda, \mu, \nu, \xi \in \{i, j, k, q\}, \qquad k, \ell, m, n \in \{x, y, z, q\}.$$

It is obvious that

$$deg(\Gamma) = 8$$
, $deg(Y_0) = 9$, $deg(Y_1) = 5$.

To determine the sign of the quantity \mathbf{Q}'' , we may need to compute the sign of the quantity $Y_0^2-Y_1^2\Gamma$. At a first glance, the algebraic degree of the expression $Y_0^2-Y_1^2\Gamma$ is 18. However, it can be shown that $Y_0^2-Y_1^2\Gamma$ can be factorized as follows:

$$\begin{split} Y_{0}^{2} - Y_{1}^{2}\Gamma &= \left[E_{ijkq}^{xyrp}E_{ijk}^{xyp} + E_{ijkq}^{xzrp}E_{ijk}^{xzp} + E_{ijkq}^{yzrp}E_{ijk}^{yzp}\right]^{2} \\ &- \left(E_{ijk}^{xyzp}\right)^{2} \left[\left(E_{ijk}^{xyp}\right)^{2} + \left(E_{ijk}^{xzp}\right)^{2} - \left(E_{ijk}^{yzp}\right)^{2} - \left(E_{ijk}^{xrp}\right)^{2} - \left(E_{ijk}^{xrp}\right)^{2} - \left(E_{ijk}^{xrp}\right)^{2} \right] \\ &= \left[\left(E_{ijk}^{xyp}\right)^{2} + \left(E_{ijk}^{xzp}\right)^{2} + \left(E_{ijk}^{yzp}\right)^{2}\right] \left[\left(E_{ijkq}^{xyrp}\right)^{2} + \left(E_{ijkq}^{xzrp}\right)^{2} + \left(E_{ijkq}^{xyzp}\right)^{2} - \left(E_{ijkq}^{xyzp}\right)^{2}\right]. \end{split}$$

The quantity $(E_{ijk}^{xyp})^2 + (E_{ijk}^{xzp})^2 + (E_{ijk}^{yzp})^2$ cannot be zero, since this would amount to Y_0 being zero, and this case has already been taken into account. We can therefore conclude that the sign of the above quantity is strictly positive. Hence, the *InSphere* predicate can be answered by computing the sign of the quantities Γ , Y_0 , Y_1 and \mathcal{Q} , where:

$$Q = \left(E_{ijkq}^{xyrp}\right)^2 + \left(E_{ijkq}^{xzrp}\right)^2 + \left(E_{ijkq}^{yzrp}\right)^2 - \left(E_{ijkq}^{xyzp}\right)^2.$$

The algebraic degree of the quantity Q is 10. We, thus, arrive at our main theorem in this work:

Theorem 1. The InSphere predicate can be evaluated by determining the sign of quantities of algebraic degree at most 10 (in the input quantities).

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