Conic tangency equations and Apollonius problems in biochemistry and pharmacology

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Abstract

The Apollonius Circle Problem dates to Greek antiquity, circa 250 B.C. Given three circles in the plane, find or construct a circle tangent to all three. This was generalized by replacing some circles with straight lines. Viéte [Canon mathematicus seu Ad triangula cum adpendicibus, Lutetiae: Apud Ioannem Mettayer, Mathematicis typographum regium, sub signo D. Ioannis, regione Collegij Laodicensis, p. 1579] solved the problem using circle inversions before 1580. Two generations later, Descartes considered a special case in which all four circles are mutually tangent to each other (i.e. pairwise). In this paper, we consider the general case in two and three dimensions, and further generalizations with ellipsoids and lines. We believe, we are the first to explicitly find the polynomial equations for the parameters of the solution sphere in these generalized cases. Doing so is quite a challenge for the best computer algebra systems. We report later some comparative times using various computer algebra systems on some of these problems. We also consider conic tangency equations for general conics in two and three dimensions.

Apollonius problems are of interest in their own right. However, the motivation for this work came originally from medical research, specifically the problem of computing the medial axis of the space around a molecule: obtaining the position and radius of a sphere which touches four known spheres or ellipsoids.
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1. Introduction

Perhaps the best introduction to the Apollonius Circle Problem is in Courant and Robbins ([7], pp. 125 and 161). They describe the circle inversion technique, among other approaches to the general and special problems. Many people worked on the Apollonius Circle questions in the 20th century, including Boyd [3], Coxeter [6], Kasner and Supnick [11], and Pedoe [15]. Frederick Soddy, a Nobel Prize winner in

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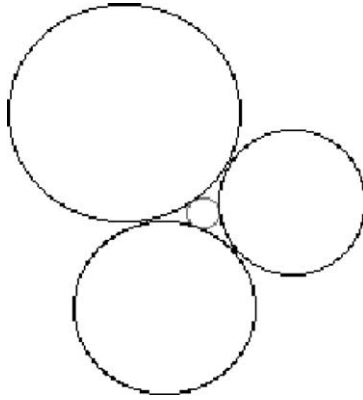*E-mail address:* rlewis@fordham.edu (R.H. Lewis).

Fig. 1. Special case, two dimensions, where all circles are mutually tangent; solution circle: innermost.

chemistry in 1921, expressed a solution to the special case as a theorem in the form of a poem, "The Kiss Precise," which was published in the journal *Nature* [18]. Soddy proved that for four mutually tangent circles the curvatures are related by

$$2(\kappa_1^2 + \kappa_2^2 + \kappa_3^2 + \kappa_4^2) = (\kappa_1 + \kappa_2 + \kappa_3 + \kappa_4)^2$$

(which was known to Descartes) and similarly for $n + 2$ mutually tangent n-spheres in $(n + 1)$-space:

$$n \left(\sum_{i=1}^{n+2} \kappa_i^2 \right) = \left(\sum_{i=1}^{n+2} \kappa_i \right)^2$$

Recently, Lagarias et al. [13] have written a paper describing packings of such circles/spheres in hyperbolic n-space and other geometries. Roanes-Lozano and Roanes-Macias [17] have a different approach to some of the questions we ask here (see Figs. 1 and 2).
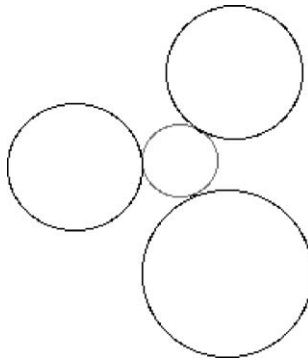

Fig. 2. General case, two dimensions, solution circle is tangent to the original three, which are arbitrarily placed. In general there are eight solutions, based on each of the originals being inside or outside the solution.
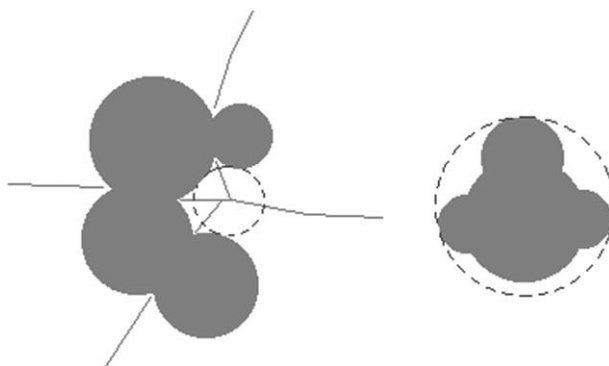
Fig. 3. Left: medial axis (lines) for a very simple two-dimensional molecule (gray atoms) with one medial disc shown (dashed circle). Right: the diameter of the enclosing (dashed) circle around this molecule quickly confirms that it is too big to fit into the pocket in the molecule on the left.

2. Biochemical motivation

Apollonius problems are of interest in their own right. However, the motivation for this work came originally from medical research, specifically the problem of computing the medial axis of the space around a molecule: obtaining the position and radius of a sphere which touches four known spheres or ellipsoids (Fig. 3).

All life forms depend on interactions between molecules. X-ray crystallography and nuclear magnetic resonance (NMR) yield the three-dimensional structure of many large and important proteins. The coordinates of atoms within these molecules are now available from public databases and can be visualized on computer displays.

Within these molecules there are receptor sites, where a correctly shaped and correctly charged hormone or drug (often referred to as a "ligand") can attach, distorting the overall shape of the receptor molecule to cause some important action within the cell. This is similar to the concept of the correct key fitting into a lock. However, in biochemistry, the "lock" often changes shape slightly to accommodate the key. Moreover, there are often several slightly differently shaped keys that fit the lock, some binding to the receptor strongly and others binding weakly.

For instance, the shape of the blood's haemoglobin molecule means an oxygen molecule binds weakly to it, so the oxygen can be released where needed, whereas carbon monoxide, being a slightly different shape, binds very strongly to the same site on haemoglobin. This can be fatal.

2.1. Automated docking algorithms

Identifying which naturally occurring ligand molecules fit into which receptor is a very important task in biochemistry and pharmacology. Moreover, in *rational drug design* the aim is often to design drugs which better fit the receptor than the natural hormone, so blocking the action of the natural hormone. The design of the ACE inhibitor used to reduce blood pressure is a good example of this.

The use of computer algorithms to select a potential drug from thousands of known ligands for a particular receptor is receiving much research interest by several groups. Some aims for such an algorithm include

- helping to identify potential binding sites in proteins,
- estimating if a ligand can reach the binding site,
- predicting the ligand's most suitable orientation in the site,
- determining how good a fit the ligand would be, compared to other known ligands.

Software such as DOCK 4.0 [8] is being used by pharmaceutical companies. For larger molecules, methods have been investigated such as Ackermann et al. [1] which use a numerical best-fit estimate.

2.2. *The medial axis*

We present here another approach, the "medial axis". The medial axis is defined as the locus of the center of a maximal disc (in two-dimensional), or sphere (in three-dimensional) as it rolls around the interior or exterior of an object. It is effectively a skeleton of the original object, and has been found helpful in computer aided engineering for meshing, simplifying and dimensionally reducing components.

In the medial axis of a molecule the medial edges or surfaces are equidistant from the atoms which the sphere touches, and the radius of the medial sphere varies to be maximal (Fig. 3). This is different from the Conelly surfaces, where a probe sphere of constant size is used. As the images below demonstrate, the medial axis approach leads to the Apollonius type questions of spheres touching other spheres, ellipsoids, or lines.

3. Mathematical approach

We are interested in the general Apollonius problem, a solution circle (or sphere) to be tangent to the original ones, which are arbitrarily placed. We want to "know" the solution symbolically and algebraically. That is, for the radius and for each coordinate of the center, we want an equation expressing it in terms of the symbolic parameters of the three (four) given circles, ellipses, or lines (spheres, ellipsoids). Ideally, the equation will be of low degree so that if numerical values are plugged in for the symbolic parameters of the given shapes, a relatively simple one variable equation will result. We will see later that in some cases we can attain this ideal, but in others we compromise by assuming that the lines or ellipsoids are in certain important but special orientations.

We begin with a system of polynomial equations

$$f_1(x, y, z, a, b, \ldots) = 0$$
$$f_2(x, y, z, a, b, \ldots) = 0$$
$$f_3(x, y, z, a, b, \ldots) = 0$$
$$\ldots$$

expressing the intersection and tangency conditions. Suppose that x, y, and z are the desired variables of the solution circle (sphere) and that $a, b, \ldots$ are the parameters of the given figures. For each of x, y, z in turn we want to derive from the system $\{f_i\}$ a single equation, the *resultant*, containing only it and the parameters $a, b, \ldots$ To accomplish this elimination, we use either Gröbner Bases or methods from the theory of resultants. Gröbner Bases are fairly well known (see for instance [2]), but here is a brief description: from a set of polynomials, for example, the $\{f_i\}$ above, we generate an *ideal* by

taking all sums of products of other polynomials with the elements in the set. Then analagous to the basis of a vector space, a certain set of polynomials that are "better" generators than the original $\{f_i\}$ can be produced. If this Gröbner Basis is chosen carefully, it will contain the desired resultant. Resultant methods are less well known, especially the apparent method of choice, the Bezout–Cayley–Dixon–KSY method [4,12,14], which we describe in subsequent sections.

We shall compare solutions done with computer algebra systems Maple 6, Mathematica, CoCoA 4.0 [5], and Fermat 2.6.4 [9].

4. The Cayley–Dixon–Bezout–KSY resultant method

Here is a brief description. More details are in [12].

To decide if there is a common root of n polynomial equations in $n-1$ variables $x, y, z, \ldots$ and k parameters $a, b, \ldots$

$$f_1(x, y, z, \ldots, a, b, \ldots) = 0$$
$$f_2(x, y, z, \ldots, a, b, \ldots) = 0$$
$$f_3(x, y, z, \ldots, a, b, \ldots) = 0$$
$$\ldots$$

- Create the Cayley–Dixon matrix, $n \times n$, by substituting some new variables $t_1, \ldots, t_{n-1}$ into the equations in a certain way.
- Compute $cd =$ determinant of the Cayley–Dixon matrix (a function of the new variables, variables, and parameters).
- Form a second matrix by extracting the coefficients of cd relative to the variables and new variables. This matrix can be large; its size depends on the degrees of the polynomials f_i.
- Ideally, let $dx =$ the determinant of the second matrix. If the system has a common solution, then $dx = 0$. dx involves only the parameters.
- Problem: the second matrix need not be square, or might have det $= 0$ identically. Then the method appears to fail.
- However, we may continue [12,4]: find *any* maximal rank submatrix; let *ksy* be its determinant. Existence of a common solution implies *ksy* $= 0$.
- *ksy* $= 0$ is a sufficient equation, but one must be aware of *spurious factors*, i.e. the true resultant is usually a small factor of *ksy*. Indeed, finding the small factor without actually computing *ksy* is very desirable.

5. Two-dimensional Apollonius results

Problem 1. Three circles given, find a fourth tangent to all three.

First step: Given one circle A with center (ax, ay) and radius ar find equation(s) that a second "solution" circle S, (sx, sy, sr) must satisfy to be tangent. We could begin by letting (x, y) be the point of intersection. Then (x, y) is on the first circle iff $(x-ax)^2+(y-ay)^2 = ar^2$, and on the second iff $(x-sx)^2+(y-sy)^2 =$
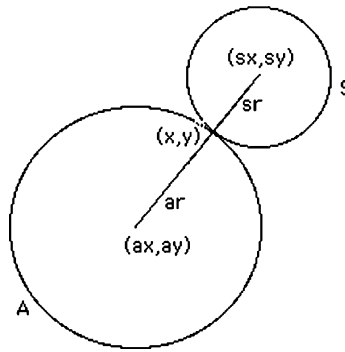
Fig. 4. Two tangent circles.

sr^2 (see Fig. 4). Using derivatives, tangency gives a third equation, so we may eliminate x, y. This *first step* gives the equation that the six parameters must satisfy for tangency.

However, the desired *first step* equation is geometrically obvious without going through the process in the previous paragraph: from Fig. 4, the point of tangency is on the line connecting the centers. Each center is on the circle with the other's center and the sum of the two radii. Thus, the equation we want, is obviously

$$(sx - ax)^2 + (sy - ay)^2 = (sr + ar)^2$$

So, given three circles A, B, and C, the solution circle parameters *sx*, *sy*, *sr* must satisfy three equations:

$$(sx - ax)^2 + (sy - ay)^2 = (sr + ar)^2$$
$$(sx - bx)^2 + (sy - by)^2 = (sr + br)^2$$
$$(sx - cx)^2 + (sy - cy)^2 = (sr + cr)^2$$

These are the equations for the case of interest to us, when each of the original circles is outside the solution circle. Other possibilities involve changing some pluses to minuses above.

Second step (*the solution*): There are several ways to proceed. As pointed out in [7], one may expand the previous equations and subtract to eliminate square terms, then solve for some variables and substitute back. Then too, one may simplify the equations by assuming that one of the circles, say A, is centered at the origin, as this is simply a translation, and furthermore that $ar = 1$, as this is just a change of scale. However, for consistency and comparison of later more difficult cases, let us proceed with the fully symbolic, Dixon–KSY method without substituting any constants. We used the computer algebra system, Fermat 2.6.4 [9] running on a Macintosh Blue and White G3 at 400 MHz. Think of the above as three equations in the "variables" *sx* and *sr* and the "parameters" *sy* plus the nine *a*, *b*, *c* parameters. Eliminate *sx*, *sr* and obtain the resultant in *sy*, i.e. the equation *sy* must satisfy in terms of the original data. It takes about 3MB of RAM, 0.6 s. The answer, an irreducible polynomial, has 593 terms, is degree two in *sy*. Similar results obtain for *sx* and *sr*.

Problem 2. Three ellipses given, find a circle tangent to all three.
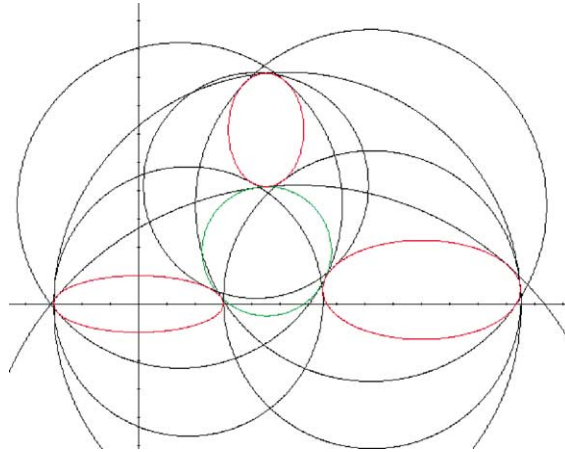
Fig. 5. All eight solution circles (black and green) tangent to three given ellipses (red).

Five given ellipses in black.
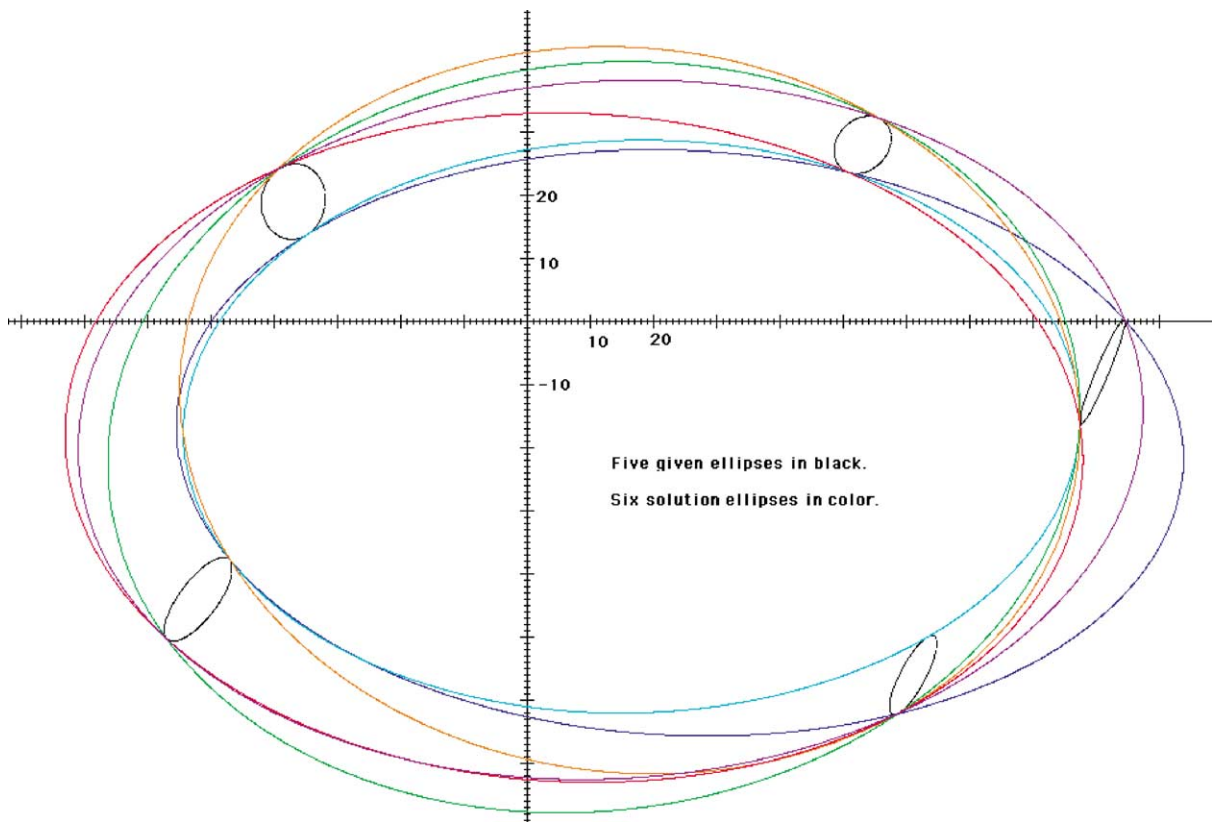
Six solution ellipses in color.

Fig. 8. Six solution conics tangent to five given ellipses.

Again, the question is of interest in its own right mathematically. Biochemically, it may be useful to model atoms by ellipses instead of circles. We assume the ellipses are all parallel to the axes (see Section 7.1).

Write the equation of ellipse A and circle S, then the tangency equations:

$$a_2^2(x - ax)^2 + a_1^2(y - ay)^2 = a_1^2 a_2^2$$

$$(x - sx)^2 + (y - sy)^2 = sr^2$$

$$a_1^2(y - ay)(x - sx) - a_2^2(x - ax)(y - sy) = 0$$

First step: Just as in Problem 1, we must eliminate x, y from the above. But it is not so easy now! The point of tangency need not lie on the line connecting the centers.

Using again Fermat/Dixon/Mac G3, the elimination is completed using 2.1 s and about 3MB RAM. The irreducible answer has 696 terms in the parameters ax, ay, a_1, a_2, sx, sy, sr. Recall that this first step was trivial in the three circles case and fit easily on one line.

Second step: For a fully symbolic solution, we would now produce three such 696 term polynomials, one for each of three given ellipses A, B, C. Then we would get an equation for, say, sr by eliminating sx and sy. However, already in the Dixon–KSY algorithm at the early step of computing cd, the determinant of the Cayley–Dixon matrix, Fermat exhausted all 700MB of RAM on the machine. Therefore, instead of a fully symbolic solution, we made up numerical examples of three ellipses, with all parameters integer. Each of the three equations now had only the three variables sr, sx, sy, between 36 and 92 terms. We applied Dixon–KSY to get the equation for sr. The second matrix was 88×88, with each entry a polynomial over the integers in sr only. The rank was 72. The determinant computation (by one method) took 92 min, and the final answer had 169 terms.

However, more realistic examples will probably have parameters that are decimals or "floats", not integers, with some error tolerance. So, alternatively, we forgoed the Dixon–KSY method in the previous paragraph. We took the three equations in sr, sx, sy with 36–92 terms and solved numerically with a multivariate Newton's method. This converges in a few seconds. One example is shown in Fig. 5, with all eight solution circles.

6. Three-dimensional Apollonius results

Problem 3. Four spheres given, find a sphere tangent to all.

Analogous to the circles in two-dimensional space:

$$(sx - ax)^2 + (sy - ay)^2 + (sz - az)^2 = (sr + ar)^2$$

$$(sx - bx)^2 + (sy - by)^2 + (sz - bz)^2 = (sr + br)^2$$

$$(sx - cx)^2 + (sy - cy)^2 + (sz - cz)^2 = (sr + cr)^2$$

$$(sx - dx)^2 + (sy - dy)^2 + (sz - dz)^2 = (sr + dr)^2$$

By elimination, get an equation for sr in terms of the a, b, c, d variables, etc. The answer has 18,366 terms and is quadratic in sr.

Several people used their favorite CAS to work on this problem. Cejtin [10] used a Gröbner Basis library written in Scheme. He used an elimination-ordering. To get the equation for *sr* took just over 1 h and about 50MB of RAM. Doing it for the special case where *ax*, *ay* and *az* are all $= 0$ took 46 s and used a bit under 8MB of RAM. Solving for *sx* took 1.75 h CPU time and used 60MB RAM. In the $ax = ay = az = 0$ special case it took 300 s CPU time and used under 13MB of RAM. All of these times are on an 400 MHz Pentium II machine.

Coauthor Stephen Bridgett ran Mathematica with the simplified version of the equations (i.e. $ax = ay = az = 0$) with the *Solve* command. Computing *sy* took 4.6 h and 41MB RAM. It could not do the full problem.

Israel [16] ran Maple 6 *with* (*Gröebner*) on a Sun SPARC Solaris. Maple gave up after 42 min, using 647MB RAM. On the simplified problem $ax = ay = az = 0$ it completed in 14 min using 574MB RAM.

Coauthor Lewis tried the full problem with CoCoA 4.0 on the same Macintosh as above. Using Gröbner bases and the *Elim* command, the full problem was solved for *sr* in 95 min and 29MB RAM.

Coauthor Lewis tried the full problem with Fermat/Dixon/Mac G3. Computing *sr* took 1.7 s and 5MB of RAM. Parameters *sx*, *sy*, and *sz* took essentially the same amounts of time and space. This is with Fermat 2.6.4, released in January 2002. These times are approximately a 6-fold improvement over the earlier version of Fermat, and a 10-fold improvement in space. Note that even the times from an earlier version of Fermat (10 s) are two orders of magnitude faster than any competitor above.

Problem 4. Four ellipsoids given, find a sphere tangent to all.

Similar to two-dimensional case of three ellipses. Define the ellipsoid by semi-axes a_1, a_2, a_3, center (ax, ay, az). (So, the ellipsoid is parallel to the axes. But see Section 7.1.) Let (x, y, z) be the point of common tangency with a sphere *sx*, *sy*, *sz*, *sr*. As before, the first step is to get two equations saying (x, y, z) is on the ellipsoid and sphere, and two more from partial derivatives. Try to eliminate (x, y, z). As before, we could consider first plugging in $ax = ay = az = 0$ (the reduced case).

Bridgett and Cejtin both reported complete failure after many hours, even with the reduced case. Fermat/Dixon solves the reduced case rather easily, 130 s using 113MB of RAM. As a challenge, Lewis had Fermat/Dixon solve the full case. It took about 400MB of RAM and 438 min. Determinant *cd* had 1.8 million terms, and the final answer 80,372 terms.

Recall that this is all just step one.

Next, as with the ellipse case in two dimensions, we made up an example and ran a multivariate Newton's method. This finished rather easily and yields, for example, Fig. 6.

Problem 5. Four lines given, find a sphere tangent to all.

A line *b* is defined by a point on the line (bx, by, bz) and a vector (through the origin) parallel to the line (bxn, byn, bzn) (see Fig. 7).

First step: Four equations that a point (x, y, z) must satisfy if it lies on the sphere *sx*, *sy*, *sz*, *r* and the line *b* and is the point of tangency of the line to the sphere:

$$(x - sx)^2 + (y - sy)^2 + (z - sz)^2 - r^2 = 0$$

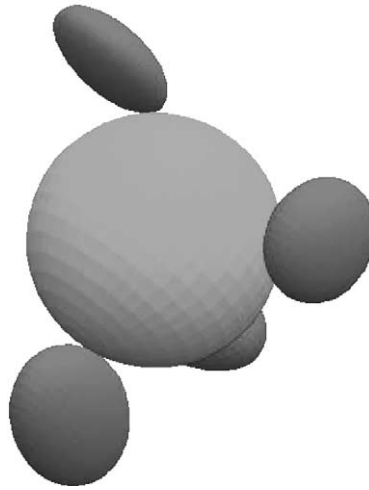$$bxn(x - sx) + byn(y - sy) + bzn(z - sz) = 0$$

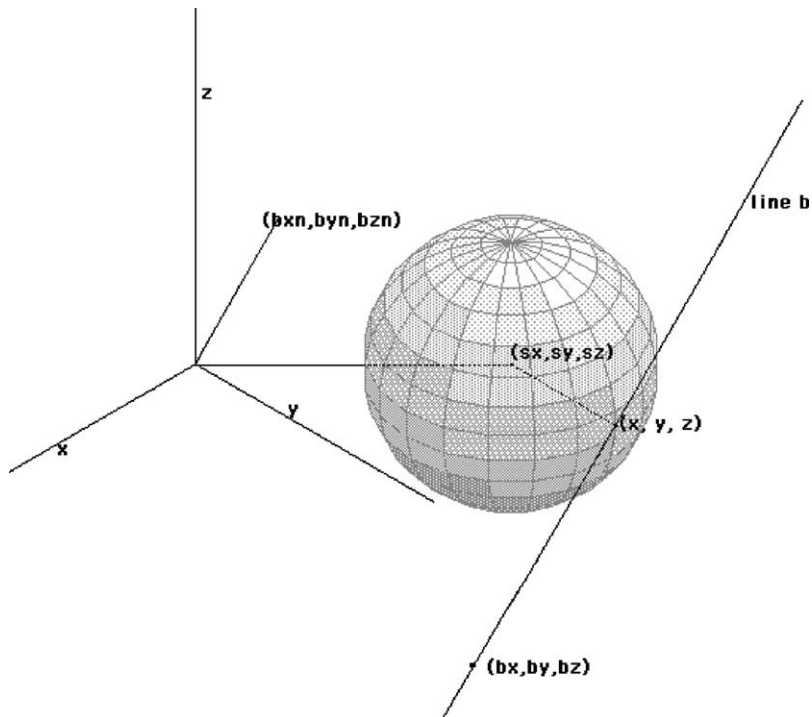Fig. 6. Solution sphere tangent to four given ellipsoids.

Fig. 7. Parameterization of line tangent to sphere in three-dimensional space.

$$byn(z - bz) - bzn(y - by) = 0$$

$$bxn(z - bz) - bzn(x - bx) = 0$$

The first equation says (x, y, z) is on the sphere. The second equation says that the vector $(x - sx, y - sy, z - sz)$ is perpendicular to the line b. The third and fourth come from the fact that the cross-product of the vectors $(x - bx, y - by, z - bz)$ and (bxn, byn, bzn) is 0.

We applied Dixon–KSY to that system, easily eliminating (x, y, z) and got the resultant *bres*:

$$
\begin{aligned}
&(-bzn^2 - byn^2 - bxn^2)r^2 + (byn^2 + bxn^2)sz^2 + (((-2byn)bzn)sy + ((-2bxn)bzn)sx \\
&\quad + ((2by)byn + (2bx)bxn)bzn + (-2bz)byn^2 + (-2bz)bxn^2)sz + (bzn^2 + bxn^2)sy^2 \\
&\quad + (((-2bxn)byn)sx + (-2by)bzn^2 + ((2bz)byn)bzn + ((2bx)bxn)byn + (-2by)bxn^2)sy \\
&\quad + (bzn^2 + byn^2)sx^2 + ((-2bx)bzn^2 + ((2bz)bxn)bzn + (-2bx)byn^2 + ((2by)bxn)byn)sx \\
&\quad + (by^2 + bx^2)bzn^2 + (((-2by)bz)byn + ((-2bx)bz)bxn)bzn + (bz^2 + bx^2)byn^2 \\
&\quad + (((-2bx)by)bxn)byn + (bz^2 + by^2)bxn^2
\end{aligned}
$$

Second step: Now we need four lines a, b, c, d each with an equation like the above, *ares*, *bres*, *cres*, *dres*. For a full symbolic solution, we want four resultants, in which one of each variable sx, sy, sz, r is retained, along with all the parameters $bxn, byn, bzn, bx, by, \ldots, ax, ay, axn, \ldots, cx, \ldots$ Theoretically, we could feed all four equations into the Dixon–KSY method to get the four equations one by one. This seemed to be hopeless, given the 750MB of RAM available. We added the reasonable assumption that the first line a is the x-axis, $ax = ay = az = 0$, $axn = 1$, $ayn = 0$, $azn = 0$. But this was still too large a problem. We therefore considered in addition several special cases of actual biochemical interest.

Case 1. $bx = by = 0$, $cz = dz = 0$, $bzn = 0$. Line b passes through a point on the z-axis, is in a plane parallel to the xy-plane. Assume also line c and line d pass through xy-plane. Fermat/Dixon completed it. The answer for sx has 394,477 terms and occupies a text file of 9.5MB.

Case 2. Three lines touch at a point, so $ax = ay = az = 0$, $bx = by = bz = 0$, $cx = cy = cz = 0$. The fourth line is oriented parallel to the x-axis but could be located anywhere, so $dx = 0$, $dzn = dyn = 0$, $dxn = 1$.

The second matrix in the Dixon method was 5×5. The determinant took 140 s to compute and had 607,704 terms. It took 20 mins to compute its content, which had six terms. Dividing the content yields the answer for sy. In total this took 168MB RAM. The answer for sy has 282,741 terms and occupies a text file of 5.8MB.

Problem 6. Four planes given, find a sphere tangent to all.

This is solvable by elementary geometry or vector algebra.

7. General conic tangency problems

Although not necessarily arising from biochemical considerations, it is reasonable at this point to try to solve the equations resulting from tangency of general conics.

7.1. Tangency of general conics in two dimensions

Consider two conics called G and S. With symbolic parameters their equations are

$$ag\,x^2 + bg\,xy + cg\,y^2 + dg\,x + eg\,y + fg = 0,$$
$$as\,x^2 + bs\,xy + cs\,y^2 + ds\,x + es\,y + fs = 0$$

Requiring that they be tangent adds the equation

$$(2ag\,x + dg + bg\,y)(bs\,x + 2\,cs\,y + es) - (2as\,x + ds + bs\,y)(bg\,x + 2\,cg\,y + eg) = 0$$

As before, the first step is to eliminate x and y from these three equations, keeping all symbolic coefficients. Using the same Macintosh computer as before, Lewis found that Maple 6 was unable to get an answer in 10 h, that CoCoA 4.0 computed the answer (3210 terms) in about 5 min (Gröbner Bases, *Elim* command), and Fermat/Dixon got the answer in 11 s. Both systems used under 10MB of RAM.

Second step: Continuing symbolically when each equation has 3210 terms seems hopeless, so we will try a numerical example.

The web page http://krum.rz.uni-mannheim.de/cabench/ca-challenge.html contains several computer algebra challenge problems, the second of which is exactly of this type: to find a conic that touches the five given conics:

$$11689x^2 - 9600xy + 2169y^2 - 2204198x + 908304y + 103910536 = 0$$

$$11281x^2 - 10800xy + 4036y^2 - 1981082x + 1110832y + 91469653 = 0$$

$$221x^2 - 264xy + 144y^2 + 11368x - 1056y + 269456 = 0$$

$$17425x^2 - 7560xy + 17056y^2 - 1635370x - 554456y + 50763289 = 0$$

$$58825x^2 - 6160xy + 41764y^2 + 4470090x - 1814952y + 98454609 = 0$$

Proceeding as in earlier problems, we ran a multivariate Newton's method and found six solutions in about half an hour real time. All the conics are ellipses. The solutions are pictured in Fig. 8.

7.2. Tangency of general conics in three dimensions

The equation of the general conic in three dimensions is

$$a_1x^2 + a_2y^2 + a_3z^2 + a_4xy + a_5xz + a_6yz + a_7x + a_8y + a_9z + a_{10} = 0.$$

Proceeding as in two dimensions, for step one we would take two such equations, derive two more equations of tangency using partial derivatives, and try to eliminate x, y, z from the four equations. This seems to be beyond the limitations of current algorithms and hardware, even if one of the equations is rotated to eliminate the three cross-terms.

We want some reasonable simplifying assumptions. Let us assume first that one of the conics is a sphere centered at the origin by translation. The four equations are

$$a_1x^2 + a_2y^2 + a_3z^2 + a_4xy + a_5xz + a_6yz + a_7x + a_8y + a_9z + a_{10} = 0$$
$$x^2 + y^2 + z^2 + ds = 0$$

$$x(2a_3 z + a_5 x + a_6 y + a_9) - z(2a_1 x + a_4 y + a_5 z + a_7) = 0$$

$$y(2a_3 z + a_5 x + a_6 y + a_9) - z(2a_2 y + a_4 x + a_6 z + a_8) = 0$$

We then rotate the other conic to eliminate the cross-terms a_4, a_5, and a_6. Fermat/Dixon solves this problem in 1.3 min; the answer has 2525 terms. CoCoA 4.0 was unable to get an answer in 10 h. Next, since rotations involve square roots and are somewhat problematical, let us try to put back the cross-terms. With a_4 present and $a_5 = a_6 = 0$, Fermat/Dixon finds the solution (6508 terms) in 9.2 min using 24MB of RAM. With a_4 and a_5 present and $a_6 = 0$, we make the further reasonable assumption that $a_{10} \neq 0$ (since the sphere contains the origin), so we divide through and assume that $a_{10} = 1$. Then Fermat/Dixon finds the solution (14,373 terms) in 97 min using 58MB of RAM. Leaving a_{10} as a symbolic parameter, Fermat/Dixon finds the solution (14,373 terms) in 345 min using 68MB of RAM. The degree of the resultant in each parameter is either 10 or 6 and the largest coefficient is 10,752.

We did not attempt to go on to step two in this case with numerical examples.

8. Summary

We were able to find equations for two- and three-dimensional problems of the Apollonius type, i.e. finding circles or spheres tangent to some given circles, ellipses, spheres, ellipsoids, or lines. We found that the Bezout–Dixon–KSY resultant is definitely the method of choice. For several problems our solutions are fully symbolic, for others we had to add simplifying assumptions to get an answer within RAM constraints. These problems arise from the biochemistry and pharmacology of molecules fitting against molecules.

We also explored the tangency problem of general conics in two and three dimensions. The problem in two dimensions is solved in complete generality, but in three dimensions we must add simplifying assumptions. Our large polynomial solutions may be downloaded from Robert H. Lewis by writing to the given e-mail address.

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