Simple method of calculating surface areas and surface averages

K.J. Boyd
Department of Chemistry
University of New Orleans
New Orleans, LA 70148
and
L. Laaksonen
Center for Scientific Computation
Espoo, Finland

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Abstract

A simple method for calculating surface areas and surface averages of contours determined from a three dimensional mesh of points is presented. After a polygonal (triangular) mesh of the desired surface is computed, the area of the best-approximating spherical triangle to the vertices and vertex normals of the mesh is calculated. If the vertex normals are degenerate, the simple planar approximation is used. If the spherical approximation is not satisfactory, as measured by the difference in the radii from each vertex, a new point is calculated based on the circumcenter of the triangle. This process yields three triangles, whose areas are calculated as above. The method is implemented via the gOpenMol molecular graphics program.

1 Introduction

Problems which arise frequently in computational chemistry which require calculation of the area of a contour surface of some calculated property of a molecule (e.g. electron density). These may be simple area calculations, or they may require the averaging of some other property (e.g. electrostatic potential) over the contour surface. For a dense enough contour mesh, these area calculations can be performed by tessellating the contour with closed polygons (usually triangles), and taking the combined area of these polygons as the contour surface area. Property averages then require calculation of the value of the property to be averaged at some characteristic point in or near the corresponding triangle.

The calculation of the mesh may be rather expensive, and the criterion for "dense enough" is often unknown before the calculation is performed. Thus it is desirable to move beyond the planar approximation, and at the same time to find a method for inserting additional polygons into the mesh when necessary. In addition, modern graphics acceleration hardware is very adept at culling degenerate polygons (those with multiple occurrences of the same vertex); contour generation algorithms often exploit this ability by not checking for degeneracy.

2 Method

The surface area calculation is straightforward, and is illustrated for a single triangle in Fig. **??**. The vertices of the triangle will intersect the sphere along a chordal circle. The center of this circle is clearly the circumcenter of the triangle. The area of the spherical section over the triangle can be readily calculated from spherical trigonometry if the appropriate radius is known. It remains to find a good approximation to the radius of the sphere.

There is additional information available from the mesh in the form of vertex normals. These normals are not, in general, consistent with any sphere approximation based only on the vertices. The normal to the triangle plane $\vec{n}$ and each of the three vertex normals $\left\{\vec{a}, \vec{b}, \vec{c}\right\}$ must be radial for a consistent sphere to be drawn; this results in an overdetermined system, even for nondegenerate triangles.

We write the best-fit normal $\vec{N}$ in terms of a three-vector $\vec{\Lambda} = \{\lambda, \mu, \nu\}$ and the vertex normals:

$$\vec{N} = \lambda\vec{a} + \mu\vec{b} + \nu\vec{c}$$

. If the three vertices of the triangle lay on a sphere with the vertex normals oriented radially, the central normal (to which $\vec{N}$ is an approximation) makes equal angles with all three vertex normals. If the vertices lay on a sphere in a plane normal to the central normal, then $\vec{N} = \vec{n}$. In addition, we require that $\vec{N}$ be normalized.

In terms of the elements of $\vec{\Lambda}$, this yields three equations and one constraint.

$$f_0(\vec{\Lambda}; \vec{n}, \vec{a}, \vec{b}, \vec{c}) = \lambda^2 + 2\lambda\mu(\vec{a} \cdot \vec{b}) + 2\lambda\nu(\vec{a} \cdot \vec{c}) + \mu^2 + 2\mu\nu(\vec{b} \cdot \vec{c}) + \nu^2 - 1 \qquad (1)$$

$$f_1(\vec{\Lambda}; \vec{n}, \vec{a}, \vec{b}, \vec{c}) = \lambda(\vec{n} \cdot \vec{c}) + \mu(\vec{n} \cdot \vec{c}) + \nu(\vec{n} \cdot \vec{c}) - 1 \qquad (2)$$

$$f_2(\vec{\Lambda}; \vec{n}, \vec{a}, \vec{b}, \vec{c}) = \frac{\lambda(\vec{a} \cdot \vec{b}) + \mu + \nu(\vec{b} \cdot \vec{c})}{\lambda + \mu(\vec{a} \cdot \vec{b}) + \nu(\vec{a} \cdot \vec{c})} - 1 \qquad (3)$$

$$f_3(\vec{\Lambda}; \vec{n}, \vec{a}, \vec{b}, \vec{c}) = \frac{\lambda(\vec{a} \cdot \vec{c}) + \mu(\vec{b} \cdot \vec{c}) + \nu}{\lambda + \mu(\vec{a} \cdot \vec{b}) + \nu(\vec{a} \cdot \vec{c})} - 1 \qquad (4)$$

which each have optimal value 0. The first equation is a true constraint equation. A solution to Eqs. (1-4) is determined by a Gauss-Newton method similar to that described by Gullikson, Xx, and Wedin, based on the modified QR factorization. This method allows the other three equations to be weighted to lend precedence to either the vertex normals or the triangle normal. We briefly explore such weighting in Section **??**; normally these equations are equally weighted.

If the vertex normal triple is degenerate (which includes the case of degenerate triangles, but is more general), this will be manifested by the Jacobian for Eqs. (1-4) being rank-deficient. Rather than attempt regularization, we recognize that this condition has no good solution, and either generate a new mesh point from the circumcenter or revert to a planar approximation.

Once $\vec{N}$ has been determined, the radius and apex of the best-fit spherical triangle are calculated. The radius for each vertex and the height of the apex for each vertex are determined as illustrated in Fig. **??**. The average radius $\bar{R}$ is calculated. The apex calculation can also be done by finding the point along the vector parallel to $\vec{N}$ passing through the circumcenter of the planar triangle which lies on the contour. This latter method is advantageous when calculating average values of properties; otherwise we use the average of the apices calculated using the geometric construction of Fig. **??**. Once the apex has been determined, the triangle is translated so that the center of the sphere lies at the origin. This simplifies the rest of the calculation because the normals must be radial. The surface area of the spherical triangle is then calculated. First the values $\cos\alpha$, $\cos\beta$, and $\cos\gamma$ are calculated from the dot products of the normals. The angles A, B, and C can then be calculated via

$$
\cos A = \frac{\cos\alpha - \cos\beta\cos\gamma}{\sin\beta\sin\gamma}
$$
$$
\cos B = \frac{\cos\beta\sin\gamma - \sin\beta\cos\gamma\cos A}{\sin\alpha}
$$
$$
\cos C = \frac{\sin\alpha\cot\beta - \sin C\cot B}{\cos\alpha}
$$

We calculate the sines directly from cosines as $\sin\theta = \sqrt{1 - \cos^2\theta}$; this choice forces the angles to lie in $[0,\pi]$. The area of the spherical triangle is then $\bar{R}^2(A + B + C - \pi)$.

2.1 Inserting Mesh Points

If the spherical approximation is inadequate (either by degenerate normals or by large differences in the radii calculated at the three vertices, we increase the mesh by a point related to the circumcenter. We start with the approximate normal at the circumcenter $\vec{N}$. In the case of degenerate normals, we take $\vec{N} = \vec{n}$. We then locate, using a finite differencing Newton method, the point along the vector parallel to $\vec{N}$ passing through the circumcenter which lies on the contour. This point and the three original vertices define three triangles, which are treated as above. This process is continued recursively until an adequate spherical approximant is found. If the planar area of the triangle is below some predetermined threshold, or the number of subdivisions reaches some limit, we take the planar area approximation for that triangle.

2.2 Calculating average quantities

To calculate an average quantity, we evaluate the quantity to be averaged at the apex of the spherical triangle. The average quantity is then calculated by

$$\bar{Q} \;\; = \;\; \frac{\sum_t \sigma(t) q(t)}{\sum_t \sigma(t)}$$

where $\bar{Q}$ is the average quantity being sought, $\sigma(t)$ is the surface area of the tth triangle, and $q(t)$ is the function value calculated for the triangle. In the lowest-order approximation, $q(t)$ is equal to the quantity evaluated at the apex of the approximating spherical triangle, four-point Gaussian cubature can be used over the whole triangle to give a better approximation.

3 Examples

The routine has been tested on several example problems.

3.1 Surface area of a molecule

Defining the surface area of an isolated molecule is difficult as the extent of the electron orbitals is nominally infinite; an arbitrary electron density cutoff is necessary. We have used the routine on several small molecules and several electron density cutoffs; some examples are shown in Fig. **??**, and the results summarized in Table **??**. We have included results taken with several grid densities; higher grid densities lead to denser initial triangulations of the surface. The routine performs rather well, allowing coarser meshes to be refined on the fly. This offers a significant time savings over calculating finer meshes.

3.2 Average electrostatic potential

We have used the routine to calculate the average electrostatic potentials over the surface areas shown in Fig. **??**. The results for single point and four-point Gauss cubature are shown in Table **??**. Again, the advantage of self refinement is apparent, as electrostatic potential calculation is expensive. We evaluate the potential only at the points needed for the averaging. This defines a thin shell of electrostatic potential values around the contour, which represents about 4% of the total number of grid points.

3.3 Accessible surface area

Calculating the solvent-accessible surface area is a common problem in biochemistry. However, empirical potential formulas can be easily used to calculate a grid of potentials for the solvent-molecule complex. The problem then reduces to finding the surface area of a potential contour (typically an energy between the minimum and 0). We illustrate this for the system....

3.4 Accessible surface area of a single residue

Often, it is desirable to find the surface area associated with a single residue or set of residues on a protein.

4 Influence of user-determined parameters

There are a number of preselected thresholds in the routine. In this section, we explore the influence of some of them.

4.1 Area cutoff

4.2 Function weighting

4.3 Maximal radial variation

4.4 Maximal recursion depth

5 Conclusion

References

[1] Useless placeholder.