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Locating Three-Dimensional Roots by a Bisection Method*

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The evaluation of roots of equations is a problem of perennial interest. Bisection methods have advantages since the volume in which the root is known to be located can be steadily decreased. This method depends on the existence of a criterion for determining whether a root exists within a given volume. Here topological degree theory is exploited to provide this criterion. Only three-dimensional volumes are considered here. The result is of some use in locating roots and in illustrating the theory. The classification of roots as X-points or O-points and the generalization to three dimensions are also discussed.

1. INTRODUCTION

Bisection methods for finding roots of equations have certain distinct advantages, particularly in their stability. They depend on a simple test whose result can guarantee that a root will lie within a given region. Then, further search for the precise location of the root can be limited. This region can be subdivided, each subregion tested for inclusion of a root, and the search can be further restricted. This method will certainly converge if the test for the existence of the root is precise.

In one dimension, the test consists of evaluating the function whose roots are desired at the boundary of the region in question. That is, if we desire roots of the equation $f(x)=0$ in the interval $a<x<b$, we can evaluate $f(a)$ and $f(b)$. Then, there is at least one such root if the calculated $f(a)$ and $f(b)$ have opposite signs. Here, we assume that $f(x)$ is continuous and bounded and that $f(a)$ and $f(b)$ have been evaluated with sufficient accuracy that their signs are known to a high degree of certainty. Further, if $f(b)>f(a)$, then the number of roots at points where $f(x)$ has a positive slope exceeds by one the number of roots at points at which $f(x)$ has a negative slope.

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This test for roots can be generalized to higher-dimensional systems. For definiteness, consider three independent components of the magnetic field that are functions of three coordinates, $B_x(x, y, z)$, $B_y(x, y, z)$, and $B_z(x, y, z)$. It is desired to find those points where all three components vanish simultaneously, that is, where the field has a null point.

We need a test to see if there is a null within a prescribed volume of the configuration space (x, y, z). This can be accomplished as follows. First, the field is evaluated over the surface of this volume. Then, a three-dimensional magnetic field space (B_x, B_y, B_z) can be introduced, in which the field at a given position can be plotted according to the values of its components. The total of all the fields evaluated on the surface of the chosen volume forms a closed surface, a balloon, in the magnetic field space. For each point in the configuration space (x, y, z), there is a point in magnetic field space (B_x, B_y, B_z); that is, there is a mapping back and forth between the two spaces. The interior of the magnetic field balloon maps to the configuration volume. A null point in configuration space is a point that maps to the origin of the magnetic field space. If the former contains the origin, $\mathbf{B}=0$, this maps back to the configuration volume, which therefore contains a null point.

The solid angle subtended by the balloon in magnetic field space, as seen from the origin, determines whether the balloon encloses the origin. This is evaluated as follows. First, the boundary of the region in configuration space is divided into triangular finite elements, also called simplexes, and the field is evaluated at the vertices of the triangles. The field over each triangle is estimated by linear interpolation. Thus, each triangle in configuration space maps to a triangle in magnetic field space. Seen from the origin, $\mathbf{B}=0$, each of these magnetic-field-space triangles subtends some solid angle that carries a sign, plus or minus, depending on the direction of the field relative to the normal to the configuration-space triangles. The solid angle subtended by the balloon is the sum of the solid angles subtended by each triangle. The result must be an integer multiple of 4π. This

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integer is known as the topological degree. Note that an accurate evaluation of this integer can be achieved if the field direction at each point on the surface is estimated to the correct hemisphere. If the topological degree is nonvanishing, there is at least one null point within the volume of interest.

Of course, roots of equations are of very general interest. The particular need that motivated this work arose from a series of papers that emphasized the role of magnetic nulls [1, 2] in plasmas and vorticity nulls [3] in fluid dynamics. To exploit this insight, it is necessary to evaluate such roots in numerical models. A particular concern in this regard is the problem of locating nulls in simulation output, where the field values are given only at grid points. For such situations, it is useful to have a mathematical theory that provides convincing evidence that there are, or are not, nulls within a given grid element. Such a theory is described in Section 2. For some of us, it is useful to implement a theory numerically, to gain a better understanding. This is described in Section 3. Section 4 contains a short discussion of some practical aspects of this method, and Section 5 contains some comparison to other work. The Appendix contains a discussion of the classification of null points, as illuminated by topological degree theory.

2. TOPOLOGICAL DEGREE

What is needed is a way of determining whether a given volume contains a null. The mathematics that underlies the method that is used here is called topological degree theory. This section contains some discussion of this theory, but not in a mathematically satisfactory way. From among many possible references that contain further details, one [4] is suggested here as a place to start.

An essential element of topological degree theory is the linear behavior of the field in the vicinity of each of its nulls. If the null is at the point $x_i = x_{i0}$, $i = 1, 2, 3$, then the field in the neighborhood is given by

$$B_i = \sum_j (\nabla \mathbf{B})_{ij} (x_j - x_{j0}) + \cdots, \tag{1}$$

where

$$(\nabla \mathbf{B})_{ij} = \partial B_i / \partial x_j |_{x_j = x_{j0}}, \tag{2}$$

is a 3×3 matrix of constants.

The topological degree, D, of the field in the particular volume under consideration is given by

$$D = \sum_{\text{nulls}} \text{sign}[\text{determinant } (\nabla \mathbf{B})]. \tag{3}$$

We treat only the case in which all the nulls are isolated so that none of the eigenvalues of $\nabla \mathbf{B}$ vanish. Thus, the determinant is nonvanishing. The topological degree is strongly conserved. Nulls can appear in a given volume only by crossing the boundary, or by the production of pairs with opposite signs of the determinant. The implications of this theory for the classification of nulls are discussed in the Appendix. Note that the topological degree does not provide a count of the null points, but only yields the difference between the number of nulls of positive and negative degree.

The topological degree is additive. That is, the degree of a field in a large volume is the sum of the degrees of each of the smaller volumes of which it is composed.

The quantity D for a given volume can be evaluated from a knowledge of the field on the boundary of the volume. It is this property that we exploit here. If the field on the surface of the boundary is plotted in magnetic field space, D is the number of times the origin is enclosed by the resulting surface. This is described in more detail in Section 3. Thus, D can be evaluated either through Eq. (3) or from the field on the boundary of the region. The equivalence of these two methods can be shown as follows. They are both additive in the sense described above, and they agree for small volumes that either contain, or do not contain, a null point.

3. EVALUATION OF THE TOPOLOGICAL DEGREE

In evaluating the topological degree, it is most convenient to work with a rectangular parallelopiped in configuration space, which will be called a box. For once thing, it is easy to divide a box into subvolumes that are also boxes and proceed to the evaluation of the null. The topological degree of the field in the box is evaluated to determine whether the field vanishes somewhere inside.

To accomplish this, in the particular implementation described here, the field is evaluated at the eight corners of the box. Each of the six sides of the box is divided into two triangles, and the field over each triangle is, in principle, estimated by linear interpolation from its value at the vertices. Thus, in magnetic-field-space we construct a dodecahedron with triangular faces. To see if this dodecahedron encloses the origin, $\mathbf{B} = 0$, we project it onto a unit sphere centered on the origin and calculate the area of the resulting configuration.

The first step is to calculate the area of an individual triangle projected onto the unit sphere, that is, the solid angle subtended by three magnetic field vectors, which we will denote by $\mathbf{B}_1$, $\mathbf{B}_2$, and $\mathbf{B}_3$. The three vertices in configuration space are ordered in a right-handed sense around the outward normal. The area of a spherical triangle is [5]

$$A = 4\tan^{-1}\{[\tan(\theta_1+\theta_2+\theta_3)/4 \times \tan(\theta_1+\theta_2-\theta_3)/4 \times \tan(\theta_2+\theta_3-\theta_1)/4 \times \tan(\theta_3+\theta_1-\theta_2)/4]^{1/2}\}, \quad (4)$$

where the side of a triangle, θ_1, is given by

$$\cos\theta_1 = (\mathbf{B}_2\cdot\mathbf{B}_3)/|\mathbf{B}_2|\,|\mathbf{B}_3|, \quad (5)$$

and similarly for θ_2 and θ_3. When the triple cross product $\mathbf{B}_1\cdot\mathbf{B}_2\times\mathbf{B}_3$ is negative, the area of the triangle is taken to be negative.

To calculate the total area, the area of the 12 triangles is summed. The number of times the projected dodecahedron covers the unit sphere, including a sign, is the area divided by 4π. This number is the topological degree and is the desired quantity. It is possible in principle for the topological degree to be greater than 1, or less than -1, in which case there is more than one null in the box. However, in the implementation described here with only 12 triangles to cover the surface, it is very likely that linear interpolation is invalid on at least one face if the magnitude of the topological degree is greater than one.

Two problems can arise. When the fields at two vertices of a triangle are nearly antiparallel, small errors in calculation can lead to large errors in the area. This can happen when a null point is close to the edge of a triangle. The second problem arises when the area of a triangle is very large. When a triangle covers nearly a hemisphere, small errors of evaluation, or departures from the linearly interpolated field, may lead to an incorrect sign of the area. This happens when the null point in configuration space is close to the side of the box that is being searched. In both of these cases, the size of the box is increased and its center slightly relocated, so that it more securely encloses the null, if there is one.

In addition to the topological degree, a secant calculation is implemented. The field is evaluated at the four vertices of a right tetrahedron in configuration space. Call $\mathbf{B}_0$ the field at the square corner, $\mathbf{B}_x$ the field at a point displaced a distance δx along the x axis, etc. This gives precisely the right amount of information to estimate the field everywhere by linear interpolation. Within this approximation, the value of x at the location of the null is

$$x = x_0 + \frac{\mathbf{B}_0\cdot(\mathbf{B}_y\times\mathbf{B}_z)\,\delta x}{\begin{pmatrix}\mathbf{B}_0\cdot\mathbf{B}_y\times\mathbf{B}_z+\mathbf{B}_0\cdot\mathbf{B}_z\times\mathbf{B}_x\\ +\mathbf{B}_0\cdot\mathbf{B}_x\times\mathbf{B}_y-\mathbf{B}_x\cdot\mathbf{B}_y\times\mathbf{B}_z\end{pmatrix}}. \quad (6)$$

The values of the y and z coordinates of the null can be found by cyclic variation.

The secant method is frequently of limited value. In the implementation that is discussed here, this information is sent to the terminal, so that it can be utilized or discarded by the user.

4. IMPLEMENTATION AND USAGE

Here certain details of the implementation and usage are described.

The independent variables, x, y, z, need not be orthogonal coordinates, nor do the quantities denoted by $\mathbf{B}$ need to form a vector. It is, however, sometimes useful to think of the box as rectangular, even when there is no significance in its actual shape.

It is desirable that the triangles in magnetic-field-space should all be as close to the same size as possible. One way in which this is approached is to scale the x, y, and z components of the magnetic field separately so that the dodecahedron that is evaluated in the previous section is just inscribed within a unit cube. Further, if the unit cube does not enclose the origin, no further calculations are performed. That is, if one or more components of the field has the same sign at all eight vertices, then we predict that there is no null inside the box.

The size of the box used in the initial evaluation should be chosen carefully. If it is distinctly larger than the scale of variation of the field, the approximations of linear interpolation over each of the triangles will be inaccurate, even compared with the weak requirements of the theory. On the other hand, if the box is too small many evaluations will be required before the null is even caught inside a box. The minimum number of evaluations required scales as the cube of the ratio of the system size to the scale of variation of the field. Any information that can be used to reduce this number should be exploited. The present implementation has been written to be interactive, to maximize the flexibility.

If more triangles are used to cover the surface of the box, the box could be made larger without loss of accuracy. For example, a vertex could be added at the center of each face and 24 triangles employed. It would help if the labeling system were organized so that each triangle could be taken in order inside a DO loop.

There is a scale size for which the method described here is most useful. As discussed in the previous paragraph, when the box is too large, the evaluation may be inaccurate. On the other hand, when the boxes are small and the root has been isolated, then the secant method is accurate and efficient. Thus, only a rather small number of bisections of the box are called for before the secant method is preferred.

5. CONCLUSIONS

Much of the previous work using topological degree theory to construct bisection methods for evaluating roots of systems of equations has striven for the generality of working in a space with an arbitrary number of dimensions. The restrictions of this paper to the case of three dimensions results in a different balance between various desired properties of the method. Such considerations are discussed in this section.

Recall that the only result that we are seeking is whether a polyhedron in magnetic field space encloses the origin. It is sometimes possible to move the vertices of this polyhedron, that is, to modify the magnetic field at each of the eight vertices of the box in configuration space, in ways that simplify the calculation but do not change the relation between the polvhedron and the origin in magnetic space. One such operation is to take all the magnetic field vectors that lie in a given octant and transform them to the corner of the cube that lies in that octant. That is, each field component is assigned a value ± 1. Then, all the triangles in the magnetic field space fall into a few types, and their areas can be easily evaluated. This gives accurate results if a sufficient number of triangles is employed to cover the boundary [6, 7]. However, the method used here is to be preferred when the number of dimensions in the space is sufficiently small that the accurate evaluation of the area of triangles (or simplexes) is not unduly onerous. Also, when dealing with numerical simulation output where the field is only evaluated at grid points, it may not be practical to obtain independent field evaluations at other than grid points. That is, it may not be possible to improve the accuracy by subdividing triangles. Then it is most important to make the best use of the available information and to evaluate the areas of the triangles accurately.

A modification of the previous method is to orient the box in configuration space to minimize the errors involved in moving the magnetic field vectors to the corners of a cube [8, 9]. The comments above apply here also. In conclusion, an illustrative routine has been written for the evaluation of three-dimensional roots by a bisection method.

APPENDIX: THE CLASSIFICATION OF NULL POINTS

The theory that has been exploited here to determine the existence of null points of a magnetic field also says something about the classification of null points. Places where the field vanishes differ in the nature of the field lines in their immediate neighborhood. In the linear approximation, these depend on the matrix $\nabla \mathbf{B}$ defined in Eq. (2). In particular, the eigenvalues of $\nabla \mathbf{B}$ are decisive in determining the shape of the field lines. For example, if some eigenvalues are complex then field lines spiral into or out of the null, depending on sign of the real part of the eigenvalues. Thus, the nulls can be classified according to the signs of the real parts of their eigenvalues and according to the vanishing or non-vanishing of their imaginary parts.

However, the topological degree theory shows that the sign of the product of the eigenvalues, that is, the sign of the determinant of $\nabla \mathbf{B}$, is a more fundamental property of the null than are the individual eigenvalues. A single isolated null point puts a sort of kink in the field that has a global effect that can be precisely measured at a distance from the null. That is why the test described in Sections 2 and 3 is useful. The nature of this kink depends on the sign of the product of the eigenvalues of $\nabla \mathbf{B}$. In contrast, the individual eigenvalues have only a local effect. Thus it is reasonable to base the primary classification of nulls on the product of the eigenvalues.

In one dimension, the sign of the determinant of $\nabla \mathbf{B}$ is the slope of $f(x)$ at the null point, in the example in the Introduction. In two and three dimensions, it is convenient to restrict consideration to the case in which the field is divergence-free, so that the trace of the matrix $\nabla \mathbf{B}$ vanishes. This is a case of considerable interest.

Consider next the two-dimensional divergence-free case. If the trace of $\nabla \mathbf{B}$ vanishes and its determinant is positive, then its two eigenvalues must be purely imaginary. In this case, the neighboring field lines lie on closed loops surrounding the null, which is thus classified as an O-point. The other possibility, for which the product of the eigenvalues is negative, has one positive and one negative real eigenvalue. Such nulls are called X-points from the configuration the neighboring field lines. Thus, topological degree theory distinguishes between X- and O-points in two dimensions.

In the three-dimensional divergence-free case, either two eigenvalues have negative real parts, and the third one is positive, or the signs are all reversed. In the first case, which was called an A-null by Cowley [10], the product of the eigenvalues is positive. On the other hand, the poduct of the eigenvalues is negative for B-nulls. Thus, in three dimensions, topological theory distinguishes between A-nulls and B-nulls.

It is widely known that in two dimensions the difference between the number of O-points and the number of X-points is strongly conserved. If a field evolves in such a way that an additional O-point is formed, then there must also be an additional X-point. It is usual to fasten on the shape of the neighboring field, and thus on the reality of the eigenvalues, as the crucial property distinguishing between X- and O-points. However, topological degree theory shows that the essential distinction between X- and O-points that generalizes to three or more dimensions lies in the sign of the product of the eigenvalues. In particular, an A-null is a generalized O-point and a B-null is a generalized X-point. It is the difference between the number of A-nulls and the number of B-nulls that is conserved.

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