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THE CALCULATION OF THE TOPOLOGICAL DEGREE BY QUADRATURE*

T. O'NEIL† AND J. W. THOMAS‡

Abstract. The topological degree of a function on R^n , a useful tool in applied mathematics, is computed by applying Gauss–Legendre quadrature to Kronecker's integral definition. An error analysis is developed from the Sarma–Eberlein measure of goodness.

1. Introduction. In recent years many new applications of the topological degree of a mapping have been introduced. Most of these applications depend on, or can be reduced to, the calculation of the topological degree of a function defined on R^n . Examples of applications in which the topological degree of functions defined on R^n is needed include ordinary differential equations (see, for example, [17], [7] or [8]), and bifurcation theory. (See, for example, [17].) Examples of results that allow the calculation of the topological degree on a Banach space to be reduced to the calculation of the degree of a function defined on R^n (where n will usually be small) can be found in [7, p. 217] or [20]. An additional application of the numerical calculation of the topological degree is that of locating zeros of functions defined on R^n . This application is discussed by the authors in [12].

In [2] J. Cronin-Scanlon gives an analytical method for calculating the degree of a homogeneous polynomial. This method is, however, completely restricted to homogeneous polynomials. In [5] P. J. Erdelsky gives a numerical scheme for calculating the Brouwer degree in R^2 .

In this paper we develop a numerical scheme that will enable us to calculate the topological degree of a function defined on R^n . We develop this result by using Kronecker's definition of degree (or what he called the characteristic of a function, see [9] and [10]). This method for calculating the degree and the necessary preliminaries are given in § 2.

In § 3 we give an error analysis for the numerical scheme of § 2 based on the Sarma–Eberlein measure of goodness S_E . Finally, in § 4 we give some numerical results.

The authors would like to thank A. Stroud for his advice concerning the error analysis in § 3.

2. Calculation of the topological degree. We begin this section with Kronecker's definition of the degree of a function. For a discussion of the relationships between this definition of degree and the definitions based on algebraic topology or analysis see [1].

DEFINITION 1. If $f = (f_1, \dots, f_n) \in C^1(\bar{B}_r)$ and if $0 \notin f(\partial B_r)$, then the topological degree of f relative to the point 0 and the set B_r is

$$d(f, B_r, 0) = \frac{1}{K_{n-1}} \int_{\partial B_r} \frac{\det(f, \partial f/\partial s, \dots, \partial f/\partial s_{n-1})}{\|f\|^n} \partial s_1 \cdots \partial s_{n-1}.$$

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where B_r is the open ball $\{(x_1, \dots, x_n) : \|(x_1, x_2, \dots, x_n)\| < r\}$,

$$\det \left(f, \frac{\partial f}{\partial s_1}, \dots, \frac{\partial f}{\partial s_{n-1}} \right) = \det \begin{vmatrix} f_1 & \dots & f_n \\ \partial f_1 / \partial s_1 & \dots & \partial f_n / \partial s_1 \\ \vdots & & \vdots \\ \partial f_1 / \partial s_{n-1} & \dots & \partial f_n / \partial s_{n-1} \end{vmatrix},$$

K_{n-1} is the surface of \bar{B}_1 (the closure of B_1), and $\|\cdot\|$ denotes the usual Euclidean norm.

The above definition is defined only for functions in $C^1(\bar{B}_r)$. However, it is not hard to see that the usual techniques (translating the function, translating the set, using Sard's theorem, and taking a limit of functions, see [1]) can be used to prove the following theorem.

THEOREM 1. *Suppose $f \in C(\bar{D})$, $p \in R^n$, D is an arbitrary bounded open set contained in R^n , and $p \notin f(\partial D)$. Then the degree of f relative to the point p and the set D , $d(f, D, p)$, can be calculated using the Kronecker integral.*

Since the Kronecker integral definition of degree is equivalent to the "usual" definitions, it will have all the properties of the usual topological degree. For a good discussion of these properties see [1].

To evaluate the Kronecker integral we proceed as follows. Let $\lambda : R^{n-1} \rightarrow R^n$ be defined by

$$(1) \quad \lambda(\theta_1, \dots, \theta_{n-1}) = (r \cos \theta_1 \cos \theta_2 \cdots \cos \theta_{n-1}, \\ r \sin \theta_1 \cos \theta_2 \cdots \cos \theta_{n-1}, \dots, r \sin \theta_{n-2} \\ \cdot \cos \theta_{n-1}, r \sin \theta_{n-1}),$$

where $|\theta_1| \leq \pi$; $|\theta_i| \leq \pi/2$, $i = 2, \dots, n-1$. Then λ describes the surface of B_r . We define $g : R^{n-1} \rightarrow R^1$ by

$$(2) \quad g(\theta_1, \dots, \theta_{n-1}) = \frac{\begin{vmatrix} f_1(\lambda) & \dots & f_n(\lambda) \\ \partial f_1(\lambda) / \partial \theta_1 & \dots & \partial f_n(\lambda) / \partial \theta_1 \\ \vdots & & \vdots \\ \partial f_1(\lambda) / \partial \theta_{n-1} & \dots & \partial f_n(\lambda) / \partial \theta_{n-1} \end{vmatrix}}{(f_1^2(\lambda) + \dots + f_n^2(\lambda))^{n/2}}$$

We then have

$$(3) \quad d(f, B_r, 0) = \frac{1}{K_{n-1}} \int_{-\pi/2}^{\pi/2} \cdots \int_{-\pi/2}^{\pi/2} \int_{-\pi}^{\pi} g(\theta_1, \theta_2, \dots, \theta_{n-1}) d\theta_1 d\theta_2 \cdots d\theta_{n-1},$$

where

$$K_{n-1} = \frac{2\pi^{n/2}}{\Gamma(n/2)}.$$

If $f = (f_1, \dots, f_n)$ where $f_i : R^n \rightarrow R^1$, we say f is analytic if each f_i is real analytic. We wish to restrict our investigation of the integral to the case where f is analytic. Since the set of analytic functions defined on \bar{B}_r is dense in the set of

continuous functions defined on \bar{B}_r , we can find the degree of f when f is just continuous through a limiting process. The reason for this restriction will become apparent in § 3 where the error in our approximation of the integral is discussed. We now look at some of the properties of g . Since the proofs of Lemmas 1–3 are elementary and straightforward we state these lemmas without proof.

LEMMA 1. Suppose $f: \bar{B}_r \rightarrow R^n$ is analytic and $0 \notin f(\partial B_r)$. Then g as defined in (2) is real analytic on the parallelepiped

$$(4) \quad P = \{(\theta_1, \dots, \theta_{n-1}) : |\theta_1| \leq \pi; |\theta_i| \leq \pi/2, \quad i = 2, \dots, n-1\}.$$

LEMMA 2. g as defined by (2) is periodic of period at most 2π in each variable.

LEMMA 3. g as defined in (2) vanishes on all but two faces of the parallelepiped P defined in (4).

We attempted to find a multiple integration scheme which would work for various space dimensions and best utilize all of the properties of g . For instance the trapezoid rule works well on the first argument of g since we are integrating over one period of the variable θ_1 , but converges slowly for the other $n-2$ variables. (See [3].) The error formula for the trapezoid rule is also quite difficult to analyze. Some formulas have been developed for small space dimension (see [6]), but little is known for large dimensional spaces. Following the advice of Stroud [18] mostly because g is analytic, we have chosen to employ a Gauss–Legendre product formula.

We define $g^*: C_k \rightarrow R^1$ by

$$(5) \quad g^*(x_1, x_2, \dots, x_k) = g(\pi x_1, \pi x_2/2, \dots, \pi x_k/2),$$

where $k = n-1$ and

$$(6) \quad C_k = \{(x_1, \dots, x_k) : |x_i| \leq 1; \quad i = 1, \dots, k\}.$$

Now apply a change of variable to (3) to get

$$(7) \quad d(f, B_r, 0) = \frac{\pi^k}{K_{n-1} 2^{k-1}} \int_{-1}^1 \dots \int_{-1}^1 \int_{-1}^1 g^*(x_1, x_2, \dots, x_k) dx_1 dx_2 \dots dx_k.$$

We next state the following theorem concerning the Gauss–Legendre integration formula [9, Thm. 10].

THEOREM 2. Let $w(x)$ be nonnegative on $[a, b]$ and let $f(x)$ be continuous on this segment. Let x_i^N and $w_i^N, i = 1, \dots, N$, be the points and coefficients, respectively, of the N -point Gauss–Legendre formula of degree $2N-1$ for w and $[a, b]$. Then

$$\lim_{N \rightarrow \infty} \sum_{i=1}^N w_i^N f(x_i^N) = \int_a^b w(x) f(x) dx.$$

Since g is continuous, g^* is also continuous and we obtain the following corollary to Theorem 2.

COROLLARY 1. Suppose $f: \bar{B}_r \rightarrow R^n$ is analytic in $\bar{B}_r, 0 \notin f(\partial B_r)$ and g^* is defined by (5). Then g^* is real analytic and

$$(8) \quad d(f, B_r, 0) = \frac{\pi^k}{K_{n-1} 2^{k-1}} \lim_{N \rightarrow \infty} \sum_{i_k=1}^N \dots \sum_{i_1=1}^N w_{i_1}^N \dots w_{i_k}^N g^*(x_{i_1}^N, \dots, x_{i_k}^N),$$

where $k = n-1$ and K_{n-1} is as defined in (3).

The problem of finding the degree of f then becomes one of evaluating g^* at several places. To accomplish this a FORTRAN program was written with the components of λ as defined in (1) and their partial derivatives fixed in the program. The components of f and their partial derivatives are then put into a subprogram and the chain rule is then employed to find the values in the matrix in the numerator of g^* .

This technique has the advantage that only the function defining subprogram must be changed to find the degree of a different function. However, we must write a different program for each space dimension in that λ changes with space dimension. We can, however, reduce the number of programs that have to be written by utilizing the following theorem.

THEOREM 3. *Suppose $f \in C^1(B_r^m)$, where B_r^m denotes the ball of radius r with center at 0_m in R^m , $m \leq n$ and*

$$f^*(x_1, x_2, \dots, x_n) = (f_1(x_1, \dots, x_m), \dots, f_m(x_1, \dots, x_m), x_{m+1}, \dots, x_n).$$

Then

$$d(f^*, B_r^n, 0_n) = d(f, B_r^m, 0_m).$$

Proof. This is an immediate consequence of the product theorem of topological degree and the fact that the identity mapping has degree 1. We have

$$\begin{aligned} d(f^*, B_r^n, 0_n) &= d((f, I_{n-m}), B_r^m \times B_r^{n-m}, (0_m, 0_{n-m})) \\ &= d(f, B_r^m, 0_m) \cdot d(I_{n-m}, B_r^{n-m}, 0_{n-m}) \\ &= d(f, B_r^m, 0_m) \cdot 1 = d(f, B_r^m, 0_m). \end{aligned}$$

We have written programs to evaluate the degree in R^3 , R^6 and R^{10} . If we wish to find the degree of a mapping in a space with dimension different from 3, 6 or 10 but less than 10, we apply Theorem 3. We have written more than one program because of the inefficiency in handling extra variables. In §4 we shall calculate the degree of several functions.

3. Error analysis. We shall not attempt to determine the absolute error in our approximation scheme. Instead we shall use the Sarma–Eberlein measure of goodness S_E and apply Chebyshev's inequality to say that the probability of choosing the wrong integer for the degree of a function using the N^k -point Gauss–Legendre product formula is less than some function of k and N . We shall use an approximation of this function to analyze the error in the numerical integration scheme discussed in §2. The approximation of S_E and some sample values appear in [11].

Let us make a special note of the fact that since the topological degree is integer-valued, our problem of error analysis is at least simplified. If we can reduce our error below $1/2$, we then know that the integer part of our solution is exact. This is a property not enjoyed by most numerical calculations.

To save time and space, we shall now reproduce a minimum of notation on the Sarma–Eberlein measure of goodness S_E . We use the notation and definitions given by Stroud in [18]. (See also [13], [14], [15] and [16].)

We suppose that we wish to calculate the integral of an analytic function g defined on the k -cube C_k as defined in (6) and that our numerical scheme is in the form

$$(9) \quad \sum_{i=1}^K A_i g(\beta_i).$$

Then Sarma (who in [13] generalized Eberlein's ([4]), results from R^1 to R^k) defined normalized error to be

$$(10) \quad E^*(g) = 2^{-k} \left\{ \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 g(x) dx_1 \cdots dx_k - \sum_{i=1}^K A_i g(\beta_i) \right\}$$

and the goodness of fit to be

$$(11) \quad S_E = \left\{ \int_{\pi_k} [E^*(g)]^2 dg \right\}^{1/2}.$$

It should be noted that the expression for (11) is not one of the usual integrals. It is, instead, an integral defined on a space π_k of power series coefficients with $\|g\|_1 = \sum |g_{\alpha_1, \dots, \alpha_k}| < 1$.

Moreover, the value of S_E does not depend on the particular function g (it has been integrated out). For a complete discussion of these ideas see [18].

Nonetheless, S_E is a measure of how good the integration formula is for all g 's. Obviously, the smaller S_E , the better the numerical scheme.

To calculate an exact expression for S_E would be very difficult. In [11] one of the authors uses the first nonzero term in a series expansion of S_E for the N^k point Gauss-Legendre formula as an approximation of S_E . We denote this approximation by $S_E^k(N)$ and state the following theorem from [11].

THEOREM 4. *Suppose k and N are as above. Then*

$$S_E^k(N) = \frac{2^{3N}(N!)^4 k^{1/2}}{(2N + 1)[(2N)!]^2 [3\lambda_{2N}^k]^{1/2}},$$

where

$$\lambda_{2N}^k = \prod_{i=1}^{2N} (c_i^k + 1)(c_i^k + 2),$$

$$c_i^k = (k + i - 1)! / (k - 1)! i!.$$

We next consider in particular the error analysis for the integration formula given in Corollary 1 of § 2. Suppose we wish to find the degree of an analytic map f and let g^* be as was defined by (5). Since g^* is then analytic, the error analysis described above is applicable. Let

$$E(g^*) = \int_{-1}^1 \cdots \int_{-1}^1 g^*(x_1, \dots, x_k) dx_1 \cdots dx_k$$

$$- \sum_{i_1=1}^N \cdots \sum_{i_k=1}^N w_{i_1} \cdots w_{i_k} g^*(x_1, \dots, x_k).$$

The absolute error in our approximation scheme is then given by

$$\frac{\pi^k |E(g^*)|}{2^{k-1} K_{n-1}}$$

and the degree of f is integer-valued. We then want to determine the values of N which will give

$$|E(g^*)| < \frac{1}{2} \cdot \frac{2^{k-1} K_{n-1}}{\pi^k}.$$

We cannot accomplish this: but we shall determine a bound on the probability that

$$|E(g^*)| \geq \frac{2^{k-2} K_{n-1}}{\pi^k}.$$

Let $g = g^*/\|g^*\|_1$ so $g \in \Pi_k$. We have by the linearity of E (the usual expected value) and E^* (equation (10)) that

$$E^*(g) = \frac{E(g)}{2^k} = \frac{E(g^*)}{2^k \|g^*\|_1}.$$

By Chebyshev's inequality,

$$Pr\{|E^*(g)| \geq pS_E\} = Pr\{|E(g^*)| \geq 2^k \|g^*\|_1 pS_E\} \leq p^{-2}.$$

If we choose

$$p = \frac{K_{n-1}}{4\pi^k \|g^*\|_1 S_E},$$

we then have

$$Pr\left\{|E(g^*)| \geq \frac{2^{k-2} K_{n-1}}{\pi^k}\right\} \leq \left[\frac{4\pi^k \|g^*\|_1 S_E}{K_{n-1}}\right]^2.$$

Or in other words, the probability that the N^k -point Gauss-Legendre formula does not give the correct answer is less than or equal to

$$(12) \quad \left[\frac{4\pi^k \|g^*\|_1 S_E}{K_{n-1}}\right]^2.$$

If we use our values of $S_E^k(N)$ from Theorem 4 as an approximation of S_E , we have that the probability that our method gives the wrong answer is less than a number which is approximately equal to

$$(13) \quad \left[\frac{4\pi^k \|g^*\|_1 S_E^k(N)}{K_{n-1}}\right]^2 = \left[\frac{4\pi^k \|g^*\|_1 2^{3N} [N!]^4}{K_{n-1} (2N+1) [(2N)!]^2}\right]^2 \frac{k}{3\lambda_{2N}^k}.$$

It should be pointed out that the radius of the ball B_r , in particular the distance from the boundary of B_r to a zero of f , has an effect on $\|g^*\|_1$ (unless f is homogeneous). The size of $\|g^*\|_1$ in turn changes the rate of convergence of our iterative technique. We can, however, say that regardless of the size of $\|g^*\|_1$ it is

possible to make the probability of error arbitrarily small. To show that the error bound given by (12) approaches zero, we apply Theorem 5.14-1 of [18, p. 191]. To show that error expression given by (13) can also be shown to approach zero, we state the following theorem. (This is the expression of error that is most useful in predicting accuracy of calculation. See § 4.)

THEOREM 5. $S_E^k(N)$ is a strictly monotone decreasing function of N and

$$\lim_{N \rightarrow \infty} S_E^k(N) = 0.$$

We state the above theorem without proof. It is not difficult to prove this theorem using the expression for $S_E^k(N)$ given in Theorem 4. Also, if one examines the values of $S_E^k(N)$ that were calculated in [11], it becomes clear that the probability of a wrong answer gets small quickly as N and k get larger.

4. Numerical results. The degrees of several mappings were calculated using the approximation scheme established in § 2. These calculations were performed on an XDS Sigma 7 computer which carries about 6.5 significant places in single precision. All calculations were carried out in single precision to reduce the time expended. Some roundoff error was experienced at large N , but it was felt that the additional accuracy which could be obtained in double precision was not worth the additional time used in this mode.

Programs were written for R^3 , R^6 and R^{10} . Those in R^3 and R^6 seemed to perform efficiently while the program in R^{10} was very slow. Several examples were run for each program. The examples were run for values of N ranging from 2 to 64. In most cases the correct value (within an error of $\frac{1}{2}$) was attained at $N = 2$ (and stayed at that value for all larger values of N). In all of the examples we obtained the correct answer for $N = 10$ (and again for all values larger than 10).

To see why the convergence is as rapid as it is, we return to our error analysis and equation (13). Because of the complexity of g^* , it is next to impossible to obtain any information about $\|g^*\|_1$. This value is, however, constant with respect to N . If we let $n = 3$ and 6, we see that value in (13) is given by $\pi^2 \|g^*\|_1^2 [S_E^2(N)]^2$ and (16) $\pi^4 \|g^*\|_1^2 [S_E^5(N)]^2$, respectively. Using Theorem 4 we see that $S_E^2(2) = 5.27923 \times 10^{-4}$, $S_E^2(10) = 7.85955 \times 10^{-25}$, $S_E^5(2) = 1.64579 \times 10^{-6}$, and $S_E^5(10) = 1.54689 \times 10^{-60}$. Using these values in the above expressions we see that unless $\|g^*\|_1$ is very large, the probability that we have the wrong answer is very small.

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