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INCLUSION–EXCLUSION–BONFERRONI IDENTITIES AND INEQUALITIES FOR DISCRETE TUBE-LIKE PROBLEMS VIA EULER CHARACTERISTICS

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Improvements to the classical inclusion–exclusion identity are developed. There are two main results: an abstract combinatoric result and a concrete geometric result. In the abstract result conditions are given which guarantee the existence of a depth $d + 1$ identity or inequality for the indicator function of a union of a finite collection of events, that is, an expression which is a linear combination of indicator functions of at most $(d + 1)$-fold intersections of the events. Such an identity or inequality can be integrated with respect to any probability measure to yield a probability identity or inequality. Connections are given to previous work on Bonferroni-type inequalities. The concrete result says that there is a depth $d + 1$ identity for the union of finitely many balls in d-dimensional Euclidean space. With a single correction term this result also holds in the d-dimensional sphere. These results form the basis for a discrete theory of tubes, which up to now has been continuous in nature. The spherical result is used to give a simulation method for finding critical probabilities for multiple-comparisons procedures, and a computer program implementing the method is described. Numerical results are presented which demonstrate that in the tails of the distribution probability estimates based on the method tend to exhibit less variability than estimates based on naive simulation.

1. Introduction. This paper touches on several areas of mathematics, statistics and elementary probability theory. The main results are somewhat technical in proof but easily stated. Consider a finite collection of measurable subsets $\{A_i\}_{i=1}^n$. The classical inclusion–exclusion identity is

$$I\left(\bigcup_{i=1}^n A_i\right) = \sum_{1\le i\le n} I(A_i) - \sum_{1\le i<j\le n} I(A_i \cap A_j) + \cdots + (-1)^{n-1} I(A_1 \cap \cdots \cap A_n),$$

where $I(A)$ denotes the indicator function of the event A. The *depth* of the identity is n, that is, the most complicated intersection is n-fold. A probabilistic identity is obtained by integrating the identity with respect to a probability measure μ. In this paper we are principally interested in identities (and

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associated inequalities) of depth $m < n$:

$$I\left(\bigcup_{i=1}^{n} A_i\right) = \sum_{i_0} I(A_{i_0}) - \sum_{i_0, i_1} I(A_{i_0} \cap A_{i_1}) \tag{1.1}$$
$$+ \cdots + (-1)^{m-1} \sum_{i_0, \dots, i_{m-1}} I(A_{i_0} \cap \cdots \cap A_{i_{m-1}}),$$

where the rth sum is over a restricted set of r-tuples of (ordered) indices.

There are two aspects to the main results: abstract results in Section 2 (Theorems 2.1 and 2.2) which are combinatoric in nature and concrete results (Theorems 3.1 and 4.1) which are more geometric. Theorem 2.1 gives a condition for equality and inequality in a formula of the form (1.1) in terms of the Euler characteristic of certain simplicial complexes and subsimplicial complexes associated with the index sets being summed over. These results are used to extend the theory of *Bonferroni inequalities* as considered by Tomescu (1986). This result is generalized in Theorem 2.2 in a manner which is used in Section 4. Connections, in a combinatorial sense, between the *inclusion–exclusion principle* and the Euler characteristic have previously been established by Rota (1971). The connection developed here is different, in that the geometry of Voronoi diagrams plays a fundamental role. Theorems 3.1 and 4.1 apply the combinatoric results to the situation when the A_i are disks of equal radius, and the dimension of the (Euclidean or spherical) space is d. Integration with respect to the uniform measure gives a statement about the volume of the union of the disks. A key result is that there is always a depth $r + 1$ identity (1.1) for the indicator function of a union of disks, where r denotes the dimension of the affine subspace spanned by the centers of the disks. Since $r \le d$ the depth can always be reduced to $d + 1$.

Excellent intuition, fortunately, is obtained by taking the A_i to be the disks of equal radius in $d = 2$ dimensions. Readers who are used to *covering problems* will share some of the authors' frustrations in handling large collections of overlapping disks. The fact that not all patterns of intersection are obtainable by mapping set-theoretic problems into disks in the plane was apparently known to Venn (1880) [see also Pakula (1989)]. Here is an example to illustrate our Theorem 3.1. Consider five disks of radius 3, $A_1, \dots, A_5$ with centers at P_1: $(0,0)$, P_2: $(1,1)$, P_3: $(-2,1)$, P_4: $(-1,-2)$, P_5: $(1,-2)$, respectively (see Figure 1). Then

$$\begin{aligned} I\left(\bigcup_{i=1}^{5} A_i\right) &= I(A_1) + I(A_2) + I(A_3) + I(A_4) + I(A_5) \\ &\quad - I(A_1 \cap A_2) - I(A_1 \cap A_3) - I(A_1 \cap A_4) - I(A_1 \cap A_5) \\ &\quad - I(A_2 \cap A_3) - I(A_3 \cap A_4) - I(A_4 \cap A_5) - I(A_5 \cap A_2) \\ &\quad + I(A_1 \cap A_2 \cap A_3) + I(A_1 \cap A_3 \cap A_4) \\ &\quad + I(A_1 \cap A_4 \cap A_5) + I(A_1 \cap A_2 \cap A_5). \end{aligned}$$

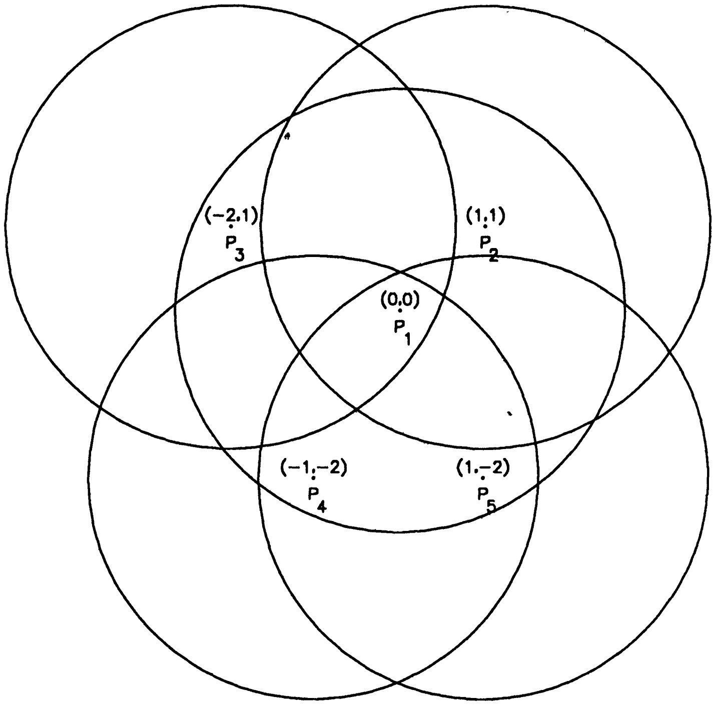

FIG. 1. *Five circles of equal radius in the plane.*

The depth here is 3. For circles in two dimensions we need never use depth greater than 3.

To illustrate how the terms of the identity are determined for the example just described, consider the Voronoi diagram corresponding to the points $P_1, \ldots, P_5$, that is, break up the plane into regions V_i, $i = 1, \ldots, 5$, where V_i consists of those points which are closer to P_i than to any of the other points P_j (see Figure 2). Now form the line segments P_1P_2, P_1P_3, P_1P_4, P_1P_5, P_2P_3, P_3P_4, P_4P_5 and P_5P_2, connecting pairs of points for which the corresponding Voronoi sets share a common boundary, and shade the triangles $P_1P_2P_3$, $P_1P_3P_4$, $P_1P_4P_5$ and $P_1P_2P_5$, corresponding to 3-tuples for which the corresponding V_i share a common point. We obtain a simple *simplicial complex* known as the *Delauney complex* corresponding to the points (see Figure 3).

Note that the Delauney complex is a convex polytope and has Euler characteristic

$$\chi = 5(\text{points}) - 8(\text{edges}) + 4(\text{triangles}) = 1.$$

There is a further result which forms the basis for the main result (Theorem 3.1). Pick any point P (not necessarily one of the P_i) and some radius $r > 0$ and take all points P_i and edges and triangles in the Delauney complex whose elements are within r of P. These form a subcomplex of the Delauney complex

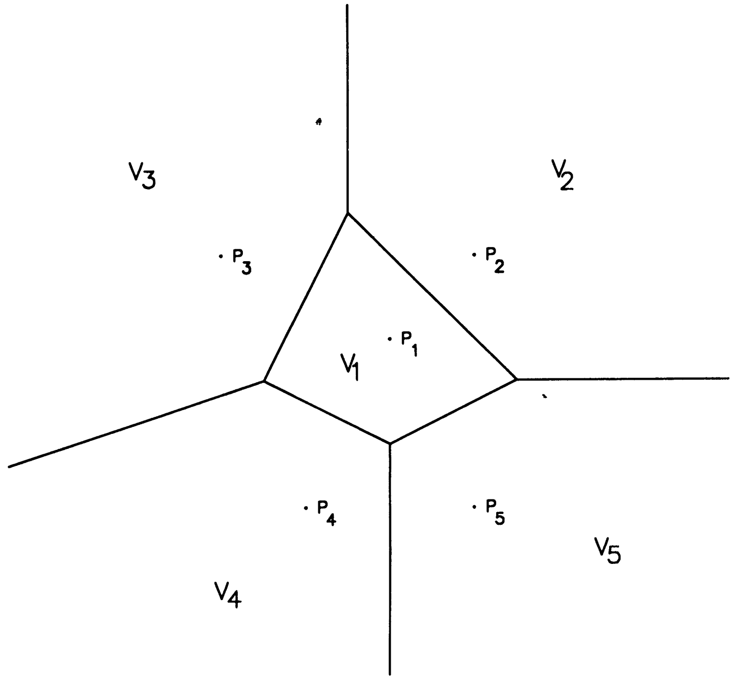

FIG. 2. *Voronoi diagram corresponding to the centers of the circles in Figure* 1.

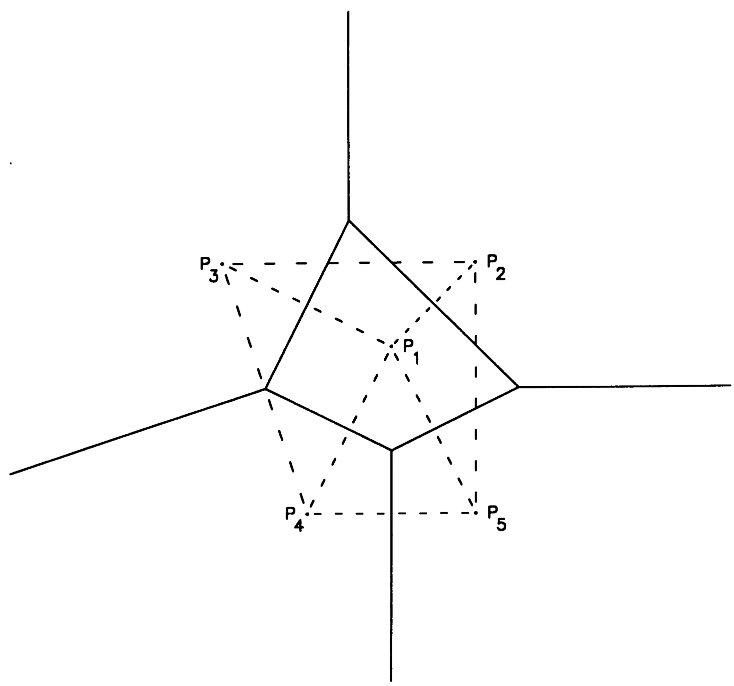

FIG. 3. *The associated Delauney simplicial complex.*

TABLE 1
Subcomplexes of the Delauney complex corresponding to $P = (\frac{1}{2}, \frac{1}{3})$ and varying radii $r \geq 0$

r range	Points	Edges	Triangles	$\Delta\chi$
$[0, \frac{13}{36})$				0
$[\frac{13}{36}, \frac{25}{36})$	P_1			1
$[\frac{25}{36}, \frac{205}{36})$	P_2	P_1P_2		$1 - 1 = 0$
$[\frac{205}{36}, \frac{241}{36})$	P_5	P_1P_2, P_2P_5	$P_1P_2P_5$	$1 - 2 + 1 = 0$
$[\frac{241}{36}, \frac{277}{36})$	P_3	P_1P_3, P_2P_3	$P_1P_2P_3$	$1 - 2 + 1 = 0$
$[\frac{277}{36}, +\infty)$	P_4	P_1P_4, P_3P_4, P_4P_5	$P_1P_3P_4, P_1P_4P_5$	$1 - 3 + 2 = 0$

whose Euler characteristic is unity (assuming r is large enough so that the subcomplex is nonempty). For example, if we take $P = (\frac{1}{2}, \frac{1}{3})$, the points ordered from closest to P to furthest from P are given by P_1, P_2, P_5, P_3 and P_4. As r increases from 0 to $+\infty$, we obtain the subcomplexes listed in Table 1. For $r \in (\frac{13}{36}, \frac{25}{36})$ the subcomplex consists of a single point P_1. For $r \in [\frac{25}{36}, \frac{205}{36})$ we attach the point P_2 and the edge P_1P_2 to the single point P_1. In general, the subcomplex corresponding to a given radius $r > 0$ is the union of all the terms in rows of Table 1, including the relevant row for that radius. Each time r passes a critical level, we modify the subcomplex by adding the points, edges and triangles in the corresponding row of the table. The resulting change in the Euler characteristic is given in Table 1. Note that each row after the first contributes zero to the Euler characteristic. This same phenomenon occurs for any starting point P.

The key to understanding this result is the following *dual* observation. Start with the Voronoi set V_1 corresponding to P_1. This set is star-shaped with respect to P. Now add the sets V_i according to the ordering of the points. Each of the sets $V_1 \cup V_2$, $V_1 \cup V_2 \cup V_5$, $V_1 \cup V_2 \cup V_5 \cup V_3$ and $V_1 \cup V_2 \cup V_5 \cup V_3 \cup V_4$ (see Figure 4) is also star-shaped with respect to P.

The word *tube* is in the title of the paper because a union of overlapping disks is a region consisting of the points closest to the set comprising the centers of the disks, where the distance to a closed set S is defined as

$$d(x, S) = \inf_{y \in S} d(x, y).$$

The set of centers can be considered as the *axis* of the tube. There are close connections between our work and the differential geometric results of Hotelling (1939) and Weyl (1939) on the volumes of tubes, which have been given prominence in the statistical community by several recent papers including Naiman (1986), Naiman (1989), Johansen and Johnstone (1990), Johnstone and Siegmund (1989) and Knowles and Siegmund (1989). In the differential geometric setting, the axis S is a line, curve or a more general surface, that is, d-dimensional submanifold. Hotelling ($d = 1$) and Weyl ($d > 1$) used differential geometric methods to express the volume of the tubular neighborhood of S as an iterated integral over the submanifold, giving d iterates. These results have been extensively refined and connections with

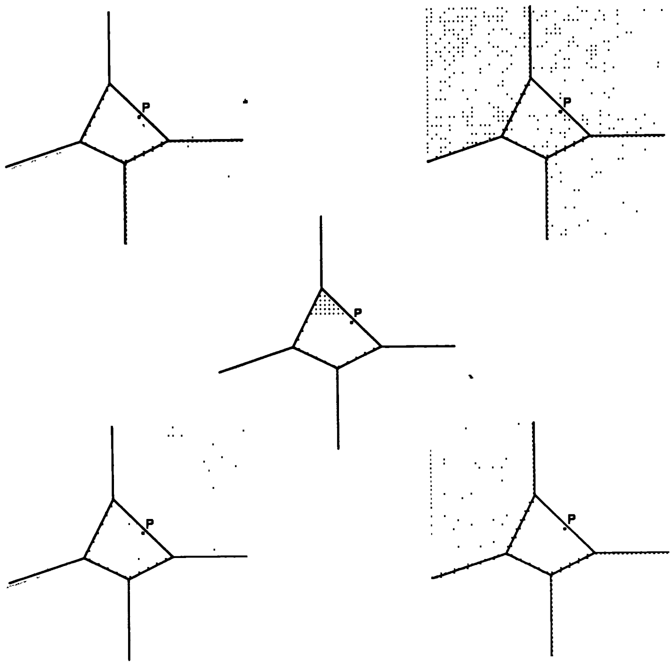

FIG. 4. *Certain unions of Voronoi sets are star-shaped.*

several other areas of geometry have been established. Griffiths (1978) and Gray (1989) mention the importance of Weyl's formula in the early development of the generalized Gauss–Bonnet theorem, and connections with integral geometry and Crofton's formula. Connections with integral geometry and algebraic geometry have also been investigated by Chern (1966), Shifrin (1981) and Langevin and Shifrin (1982). There have also been several attempts by differential geometers to generalize the Hotelling–Weyl formulas to other spaces. See Gray (1989) for an extensive bibliography.

The direct attack on the discrete case in the present paper has, perhaps, been overlooked and the authors feel it reveals a more fundamental result which underpins the continuous cases, by a suitable limiting argument. The main result (Theorem 3.1) is based on a property of Voronoi diagrams that has gone heretofore unnoticed. This is despite the fact that several authors, including Coxeter, Few and Rogers (1959) and more recently Edelsbrunner and Seidel (1986), have used Voronoi diagrams to study the configurations of disks of equal radius in Euclidean space, while others, see, for example, Avis, Bhattacharya and Imai (1988), use the Voronoi diagram to partition the union of balls into star-shaped sets by intersecting the union with each Voronoi set corresponding to the center of a ball. This, of course, leads to a different identity from (1.1), one that involves star-shaped sets which cannot be constructed using set operations on the balls alone. The identity (1.1) has the added advantage that the most complicated multiple-comparisons problem from the class of problems described in Section 5 decomposes into problems in which the number of confidence intervals is at most the dimension of the parameter space (see Remark 5.1).

The work of Groemer (1975), continuing the earlier work of Hadwiger (1955) [see also the expository paper of McMullen and Schneider (1983)], is similar in style to that of this paper. In Groemer (1975), Euler characteristics associated with linear combinations of indicator functions of unions of convex sets are also considered. A key difference between that work and ours is that the Euler characteristic for us is associated with various subsimplicial complexes of a given complex and Groemer assigns a (possibly different) Euler characteristic to the function itself. A careful reading of Groemer's work does not reveal the solution of the present problem. To summarize, we hope to pave the way for discrete tube theory to be alongside and reveal some of the underlying structure of the continuous tube theory.

The original and continuing motivation for us has been the theory of multiple comparisons. It is a standard method, originating with Hotelling, to convert a confidence statement or rejection–acceptance statement for a set of Studentized variables to a statement about the probability content of certain regions on the surface of a sphere with respect to the uniform measure. In important cases we need to evaluate the content of the union of spherical caps of equal radius. Fortunately, on the surface of the sphere the theory also holds. The result then is that one need not consider overlapping disks below "depth" $m = d + 1$, where d is the dimension of the surface of the sphere, provided that no point is common to all of the disks.

The layout of the rest of the paper is as follows. Section 2 discusses simple discrete tubes and tubes on trees as a lead into the abstract version of the result. Section 3 contains the proof of the main concrete theorem for disks in Euclidean space with some associated topological theory which is also used in Section 4. A description of a simulation approach for finding volumes of discrete tubes is also given. Section 4 discusses the analogues of the results in Section 3 for spherical space, which is the domain we are more interested in for statistical applications. Section 5 describes a computer implementation of the basic identity to evaluate critical constants for multiple-comparisons procedures via simulation, and examples are given there to illustrate how simulation based on the use of the identity can result in tremendous improvements in efficiency, especially for very small values of the error probability.

2. Abstract discrete tubes. Let $A_1, \dots, A_n$ be a finite collection of measurable subsets of a probability space with measure μ. Define

$$S_k = \sum_{1 \le i_1 < \cdots < i_k \le n} I(A_{i_1} \cap \cdots \cap A_{i_k})$$

for $1 \le k \le n$. The Bonferroni bounds are

$$\sum_{k=1}^{2r} (-1)^{k-1} S_k \le I\left(\bigcup_{i=1}^{n} A_i\right) \le \sum_{k=1}^{2r-1} (-1)^{k-1} S_k$$

for $r = 1, 2, \ldots$. For example, when $r = 1$,

$$(2.1)\quad \sum_{1\le i\le n} I(A_i) - \sum_{1\le i<j\le n} I(A_i \cap A_j) \le I\left(\bigcup_{i=1}^n A_i\right) \le \sum_{1\le i\le n} I(A_i),$$

which, when integrated, gives the form in which the bounds are most used in practice.

Worsley (1982, 1985) with results generalized by Tomescu (1986) discusses the improvement to the bounds (2.1). Writing

$$S_2^* = \sum_{2\le i\le n} I(A_{i-1} \cap A_i),$$

$$S_3^* = \sum_{1\le i<j\le n} I(A_{i-1} \cap A_i \cap A_j),$$

this improvement is written as

$$(2.2)\quad S_1 - S_2 + S_3^* \le I\left(\bigcup_{i=1}^n A_i\right) \le S_1 - S_2^*.$$

Two important features of this inequality should be stressed.

1. S_2^* and S_3^* are sums over restricted subsets of the sets of indices $\{(i-1, i)\}$ and $\{(i-1, i, j)\colon i < j\}$.
2. Equality is obtained for collections $\{A_i\}$ with special properties.

We are interested here in *equality* statements, for example,

$$(2.3)\quad I\left(\bigcup_{i=1}^n A_i\right) = \sum_{1\le i\le n} I(A_i) - \sum_{2\le i\le n} I(A_{i-1} \cap A_i).$$

DEFINITION 2.1. A collection of sets $\{A_i\}_{i=1}^n$ is called a *simple tube* if

$$A_i \cap A_j = \bigcap_{k=i}^{j} A_k$$

for any pair (i, j) with $1 \le i < j \le n$. By convention, the empty set $\varnothing$ is contained in each A_i. We may state the condition equivalently as

$$A_i \cap A_j \subseteq A_k, \qquad k = i+1, \ldots, j-1.$$

It is instructive to draw Venn diagrams of equally sized disks whose centers lie on a curve in the plane to show the tube-like nature of the condition. It can be seen that if the curve turns too sharply, then the simple tube condition is violated.

LEMMA 2.1. *If $\{A_i\}_{i=1}^n$ is a simple tube, then* (i) $I(\bigcup_{i=1}^n A_i) = S_1 - S_2^*$ *and* (ii) $S_1 - S_2 + S_3^* = S_1 - S_2^*$, *that is, each inequality in* (2.2) *becomes an equality.*

PROOF. (i) For *any* collection $\{A_i\}$ we may write

$$\bigcup_{i=1}^{n} A_i = \bigcup_{i=1}^{n-1}\left\{A_i \Big\backslash \bigcup_{j=i+1}^{n} A_j\right\} \cup A_n = \bigcup_{i=1}^{n-1}\left\{A_i \Big\backslash \bigcup_{j=i+1}^{n} (A_i \cap A_j)\right\} \cup A_n.$$

But from the tube property

$$\bigcup_{j=i+1}^{n} A_i \cap A_j = A_i \cap A_{i+1}$$

so that

$$\bigcup_{i=1}^{n} A_i = \bigcup_{i=1}^{n-1} \{A_i - (A_i \cap A_{i+1})\} \cup A_n.$$

But by the disjointedness of the sets on the right

$$I\left(\bigcup_{i=1}^{n} A_i\right) = \sum_{i=1}^{n-1} I(A_i - (A_i \cap A_{i+1})) + I(A_n)$$

$$= \sum_{i=1}^{n} I(A_i) - \sum_{i=2}^{n} I(A_{i-1} \cap A_i).$$

(ii) From the tube property

$$A_{i-1} \cap A_i \cap A_j = A_{i-1} \cap A_j$$

so we obtain

$$S_2 - S_3^* = \sum_{1 \le i < j \le n} I(A_i \cap A_j) - \sum_{2 \le i < j \le n} I(A_{i-1} \cap A_j)$$

$$= \sum_{i=2}^{n} I(A_{i-1} \cap A_i) = S_2^*. \qquad \square$$

It is helpful to convert the simple tube property to a statement about the linear graph $G = (V, E)$ with vertices $V = \{i\colon i = 1, \dots, n\}$ and edges $E = \{(i-1, i)\colon i = 2, \dots, n\}$. Consider a simple binary stochastic process created by the indicator functions of the sets A_i. Thus $X_i = I(A_i)$. The simple tube condition implies that

$$\{X_i = 1\} \cap \{X_j = 1\} \Rightarrow \{X_k = 1, i \le k \le j\}.$$

It is clear then that the behavior of the X_i process can be decomposed into disjoint events C_k for each of which some connected linear subgraph $G_k = (V_k, E_k)$ has all $X_j = 1$ for $j \in V_k$ and $X_j = 0$ for $j \notin V_k$. Each of the events C_k corresponds to a special elementary event of the form

$$C_k = \bigcap_{i \in V_k} A_i \cap \bigcap_{i \notin V_k} A_i^c.$$

For four sets, for example, the table of possible events is:

G_k	Event, C_k	X_1	X_2	X_3	X_4
$\{1\}$	$A_1 \cap A_2^c \cap A_3^c \cap A_4^c$	1	0	0	0
$\{2\}$	$A_1^c \cap A_2 \cap A_3^c \cap A_4^c$	0	1	0	0
$\{3\}$	$A_1^c \cap A_2^c \cap A_3 \cap A_4^c$	0	0	1	0
$\{4\}$	$A_1^c \cap A_2^c \cap A_3^c \cap A_4$	0	0	0	1
$\{1,2\}$	$A_1 \cap A_2 \cap A_3^c \cap A_4^c$	1	1	0	0
$\{2,3\}$	$A_1^c \cap A_2 \cap A_3 \cap A_4^c$	0	1	1	0
$\{3,4\}$	$A_1^c \cap A_2^c \cap A_3 \cap A_4$	0	0	1	1
$\{1,2,3\}$	$A_1 \cap A_2 \cap A_3 \cap A_4^c$	1	1	1	0
$\{2,3,4\}$	$A_1^c \cap A_2 \cap A_3 \cap A_4$	0	1	1	1
$\{1,2,3,4\}$	$A_1 \cap A_2 \cap A_3 \cap A_4$	1	1	1	1.

We can now give an alternative proof of the identity (2.3) [Lemma 2.1(i)] for simple tubes. Since the C_k are disjoint and $\bigcup_{i=1}^n A_i \subseteq \bigcup_k C_k$,

$$\begin{aligned}
&\sum_{1\le i\le n} I(A_i) - \sum_{2\le i\le n} I(A_{i-1}\cap A_i)\\
&\quad = \sum_{1\le i\le n}\sum_k I(A_i\cap C_k) - \sum_{2\le i\le n}\sum_k I(A_{i-1}\cap A_i\cap C_k)\\
&\quad = \sum_k \left\{\sum_{1\le i\le n} I(A_i\cap C_k) - \sum_{2\le i\le n} I(A_{i-1}\cap A_i\cap C_k)\right\}\\
&\quad = \sum_k \left\{\sum_{i\in V_k} I(C_k) - \sum_{(i,j)\in E_k} I(C_k)\right\}\\
&\quad = \sum_k I(C_k)\{|V_k| - |E_k|\}.
\end{aligned}$$

Since each G_k is connected and linear $|V_k| - |E_k| = 1$ so that the expression reduces to $\sum_k I(C_k)$. Now since the C_k are disjoint and exhaust $\bigcup_{1\le i\le n} A_i$, we have

$$I\Big(\bigcup_{1\le i\le n} A_i\Big) = \sum_k I\Big(\bigcap_{i\in V_k} A_i \cap \bigcap_{i\notin V_k} A_i^c\Big) = \sum_k I(C_k),$$

completing the proof. □

With little alteration the result can be extended to *trees*, a tree being a connected graph which consists of no cycles.

DEFINITION 2.2. A *generalized simple tube* is a collection $\{A_i\}_{i=1}^n$, where the indices form the vertices of a tree $G = (V, E)$ and

$$A_i \cap A_j \subseteq A_k$$

for any k on the path from i to j.

For such a collection, clearly there is a decomposition

$$I\left(\bigcup_{i=1}^{n} A_i\right) = \sum_k I(C_k),$$

where

$$C_k = \bigcap_{i \in V_k} A_i \cap \bigcap_{i \notin V_k} A_k^c,$$

and where the $G_k = (V_k, E_k)$ are connected subtrees of G. The general result is the following.

LEMMA 2.2. *For a generalized simple tube* $\{A_i\}$ *with tree* G,

$$I\left(\bigcup_{i=1}^{n} A_i\right) = \sum_{i \in V} I(A_i) - \sum_{(i,j) \in E} I(A_i \cap A_j).$$

PROOF. This is identical to the above proof of (2.2) with the observation that $|V_k| - |E_k| = 1$ when $G_k = (V_k, E_k)$ is a tree. □

The reader should now be aware that the counting operation in $|V_k| - |E_k| = 1$ is the key. The quantity $|V_k| - |E_k|$ is the Euler characteristic of the tree, which is always unity.

We now generalize to *simplicial complexes*.

DEFINITION 2.3. An *abstract simplicial complex* $\mathscr{K}$ is defined as a collection of subsets F of a finite set $\{0, 1, \dots, n\}$ with the property that if $F \in \mathscr{K}$, then every subset of F is in $\mathscr{K}$. The subsets F are called *faces* of the simplicial complex.

The one-element faces of an abstract simplicial complex $\mathscr{K}$ are called vertices of $\mathscr{K}$ or zero-dimensional faces, the two-element faces are called *edges* or one-dimensional faces and the three-element faces are called *triangles* or two-dimensional faces. More generally, the k-element faces are called $(k-1)$-dimensional *simplices*. We denote the set of q-dimensional faces of $\mathscr{K}$ by $\mathscr{K}_q$. The maximum dimension of a face in $\mathscr{K}$ is called the *dimension* of $\mathscr{K}$. The *Euler characteristic* of a d-dimensional simplicial complex $\mathscr{K}$ is then defined as

$$\chi(\mathscr{K}) = \sum_{q=0}^{d} (-1)^q |\mathscr{K}_q|,$$

where $|\mathscr{K}_q|$ denotes the order (cardinality) of $\mathscr{K}_q$. For a simplicial complex $\mathscr{K}$ with vertices $1, \dots, n$ and a subset of its vertices J, there is a subsimplicial complex $\mathscr{K}(J)$ defined as the collection of faces of $\mathscr{K}$ all of whose vertices are elements of J.

DEFINITION 2.4. A collection of sets $\{A_i\}_{i=1}^n$ together with a d-dimensional simplicial complex $\mathscr{K}$ with vertices $1, \dots, n$ is called an *abstract tube* of dimension d if the subsimplicial complex $\mathscr{K}(J)$ has Euler characteristic unity whenever $J \subseteq \{1, \dots, n\}$ is a nonempty index set such that $A(J) \stackrel{\text{def}}{=} \bigcap_{i \in J} A_i \cap \bigcap_{i \notin J} A_i^c \neq \varnothing$.

As a consequence of the definition $\bigcup_{i=1}^n A_i$ can be partitioned into nonempty events each of which corresponds to a subsimplicial complex of $\mathscr{K}$ with Euler characteristic 1. This generalizes the notion of an abstract simple tube. For the latter, the associated tree is a one-dimensional simplicial complex, and the simple tube property guarantees that whenever $\bigcap_{i \in J} A_i \cap \bigcap_{i \notin J} A_i^c \neq \varnothing$, the (sub)simplicial complex $\mathscr{K}(J)$ is itself a tree, hence has Euler characteristic unity. A large class of examples of more complicated abstract tubes are provided in Sections 3 and 4.

A general result is the following. An even more general result is given in Theorem 2.2.

THEOREM 2.1. *Let the collection of sets $\{A_i\}_{i=1}^n$ and simplicial complex $\mathscr{K}$ form an abstract tube of dimension d. Then the following inclusion–exclusion identity of depth $d+1$ holds*:

$$I\left(\bigcup_{i=1}^n A_i\right) = \sum_{r=0}^d (-1)^r \sum_{F \in \mathscr{K}_r} I\left(\bigcap_{i \in F} A_i\right). \tag{2.4}$$

Conversely, if (2.4) *holds for some simplicial complex $\mathscr{K}$, then the collection of sets together with $\mathscr{K}$ forms an abstract tube.*

PROOF. The basic idea is to show that a point in $A(J)$ is counted exactly once in the expression on the right-hand side for each nonempty index set J, and use the fact that the sets $A(J)$ for J nonempty partition the union of the A_i. Since $\sum_{J \neq \varnothing} I(A(J)) \equiv 1$ we can multiply the right-hand side of (2.4) by $I(A(J))$ and sum over $J \neq \varnothing$ to express it as

$$\sum_{J \neq \varnothing} \sum_{r=0}^d (-1)^r \sum_{F \in \mathscr{K}_r} I\left(\bigcap_{i \in F} A_i \cap A(J)\right).$$

Note that

$$I\left(A_{i_0} \cap \cdots \cap A_{i_r} \cap A(J)\right) = \begin{cases} I(A(J)), & \text{if } \{i_0, \dots, i_r\} \subseteq J, \\ 0, & \text{otherwise,} \end{cases}$$

so that using the discrete tube property the above becomes

$$\begin{aligned} &\sum_{J \neq \varnothing} \sum_{r=0}^d (-1)^r |\mathscr{K}_r(J)| I(A(J)) \\ &\quad = \sum_{J \neq \varnothing} I(A(J)) \chi(\mathscr{K}(J)) = \sum_{J \neq \varnothing} I(A(J)) = I\left(\bigcup_{i=1}^n A_i\right). \end{aligned}$$

For the converse, if $A(J) \neq \varnothing$, then for $x \in A(J)$ if we evaluate (2.4) at x we obtain $1 = \chi(\mathscr{K}(J))$. □

By changing the condition in Definition 2.4 to $\chi(\mathscr{K}(J)) \geq 1$, or $\chi(\mathscr{K}(J)) \leq 1$, we obtain respectively upper and lower bounds for $I(\bigcup_{i=1}^{n} A_i)$ since the next to last equality in the proof of the theorem becomes $\geq$ or $\leq$ respectively. This result explains several improvements in, or versions of, the Bonferroni inequality. The theorem of Worsley (1982) is precisely the special case of a *tree* and takes the form

$$P\Big(\bigcup_i A_i\Big) \leq \sum_{i \in V} P(A_i) - \sum_{(i,j) \in E} P(A_i \cap A_j),$$

when $G = (V, E)$ is a spanning tree for the index set $\{i\}$. Let $\mathscr{K}$ be such a tree. Then we can partition $\bigcup_{i=1}^{n} A_i$ into events C_k which correspond to a connected subtree or the union of connected subtrees. For each such C_k, $\chi(C_k) \geq 1$. In fact, $\chi(C_k)$ is the number of disconnected trees. The inequality in the right-hand side of (2.2) is a special case.

Consider the left-hand side of (2.2). We let $\mathscr{K}$ be the simplicial complex comprising $\{i\}$, $i = 1, \dots, n$, $\{i, j\}$, $i = 1, \dots, n$, $j = i + 1, \dots, n$, and $\{i - 1, i, j\}$, $i = 2, \dots, n$, $j = i + 1, \dots, n$. A little investigation shows that the disjoint events C_k into which $\bigcup_{i=1}^{n} A_i$ can be partitioned all have $\chi \leq 1$. For example let $n = 5$ and suppose A_1, A_3 and A_4 occur but not A_2 and A_5. Then the corresponding (sub)simplicial complex of $\mathscr{K}$ is given by

$$\{1, 3, 4, \{1, 3\}, \{1, 4\}, \{3, 4\}\},$$

and this has $\chi = 0 \leq 1$.

The more general results of Tomescu (1984) fall into this category but we do not develop this connection here. The principle, though, is clear. Lay down a complex $\mathscr{K}$ such that the subcomplexes "triggered" by the A_i (i.e., the i for which $X_i = 1$) have χ all ≤ 1, $= 1$ or ≥ 1.

Observe that in the proof of Theorem 2.1 even if we cannot make any assumptions about the Euler characteristic of $\mathscr{K}(J)$, we obtain an identity. This identity is used in Section 4 to prove Theorem 4.1. For future reference we record this result as the following theorem.

THEOREM 2.2. *Let $\{A_i\}_{i=1}^{n}$ be a collection of sets and let $\mathscr{K}$ be a d-dimensional simplicial complex with vertices $1, \dots, n$. Then*

$$\sum_{r=0}^{d} (-1)^r \sum_{F \in \mathscr{K}_r} I\Big(\bigcap_{i \in F} A_i\Big) = \sum_{\varnothing \neq J \subseteq \{1, \dots, n\}} \chi(\mathscr{K}(J)) I\Big(\bigcap_{i \in J} A_i \cap \bigcap_{i \notin J} A_i^c\Big).$$

3. Unions of balls of equal radius. The main result of this section is that any collection of balls of arbitrary radius in d-dimensional Euclidean space forms an abstract tube of dimension d, so there is a depth $d + 1$ inclusion–exclusion identity for the indicator function of their union. Section 4 describes analogues of these results for the sphere.

In Section 2, we used abstract simplicial complexes because we only needed to represent combinatorial information. In this section, it becomes important to view a simplicial complex as a topological space and exploit its topological properties.

Let $\{x_i\}_{i=1}^n$ be a finite set of points on $\mathscr{R}^d$. It is assumed that the points are in *general position* in the sense that no subcollection of $d+1$ points lie in a $(d-1)$-dimensional affine subspace and no $x \in \mathscr{R}^d$ is equidistant from more than $d+1$ of the points x_i. This is equivalent to saying that

$$\det\begin{pmatrix} 1 & \cdots & 1 \\ x_{j_0} & \cdots & x_{j_d} \end{pmatrix} \neq 0 \tag{3.1}$$

for all distinct $j_0, \dots, j_d$ and

$$\det\begin{pmatrix} 1 & \cdots & 1 \\ x_{j_0} & \cdots & x_{j_{d+1}} \\ \|x_{j_0}\|^2 & \cdots & \|x_{j_{d+1}}\|^2 \end{pmatrix} \neq 0 \tag{3.2}$$

for all distinct $j_0, \dots, j_{d+1}$. Since the set of ordered sequences $\{x_i\}_{i=1}^n$ which fail to be in general position has Lebesgue measure 0 in $\mathscr{R}^{dn}$, a given set of points can always be moved to general position by an arbitrarily small perturbation, if necessary. This observation is used to prove the analogue to Theorem 3.1 for the case when the general position assumption is violated (see Remarks 3.4 and 3.5).

Associated with the given points is the familiar *Voronoi subdivision* of $\mathscr{R}^d$ into regions consisting of points closest in Euclidean distance to each point x_i (see Figure 2). Formally, for each pair of the given points, define the half-space

$$S(x_i, x_j) = \{x \in \mathscr{R}^d : d(x, x_i) \le d(x, x_j)\},$$

where $d(\ ,\ )$ denotes Euclidean distance, and define the ith Voronoi region

$$V_i = \left\{x \in \mathscr{R}^d : d(x, x_i) = \inf_{j=1,\dots,n} d(x, x_j)\right\} = \bigcap_{j=1}^n S(x_i, x_j).$$

The collection $\{V_i: i = 1, \dots, n\}$ forms a *covering* of $\mathscr{R}^d$ by nonempty closed convex polyhedra whose interiors V_i^0 are nonempty and fail to intersect. Since the points x_i are in general position, any collection of more than $d+1$ of the sets V_i has empty intersection.

Any finite covering $\{X_i,\ i = 1, \dots, n\}$ of a topological space X may be used to define a simplicial complex which is referred to by combinatorial topologists as the *nerve of the covering*. This is the simplicial complex having a single vertex $\{i\}$ corresponding to each X_i, and a face $\{j_1, \dots, j_q\}$ whenever $\bigcap_{i=1}^q X_{j_i} \neq \varnothing$. Let $\mathscr{N}$ denote the nerve of the covering $\{V_i\}_{i=1}^n$. This simplicial complex is also referred to as the *Delauney complex*. Because of the general position assumption, this simplicial complex has dimension at most d. We use notation analogous to that in Section 2. In particular, $\mathscr{N}_q$ denotes the set of q-dimensional faces of $\mathscr{N}$.

Let $B_d(x, r)$ denote the open ball in $\mathscr{R}^d$ centered at x and having radius $r > 0$. The main result of this section is the following theorem.

THEOREM 3.1. *The collection of balls* $\{B_d(x_i, r)\}_{i=1}^n$ *together with the simplicial complex* $\mathscr{N}$ *forms an abstract tube of dimension* d, *and the following identity holds*:

$$I\left(\bigcup_{i=1}^{n} B_d(x_i, r)\right) = \sum_{q=0}^{d} (-1)^q \sum_{F \in \mathscr{N}_q} I\left(\bigcap_{i \in F} B_d(x_i, r)\right) \tag{3.3}$$

for any $r > 0$.

Note that the sets in the formula are intersections of at most $d + 1$ balls while the traditional inclusion–exclusion formula would require up to n-fold intersections. Note also that as r increases the $B_d(x_i, r)$ become larger so that the faces F for which $\bigcap_{i \in F} B_d(x_i, r) \neq \varnothing$ become more numerous and the tube depth becomes greater. The basic nerve $\mathscr{N}$, however, remains fixed.

Before giving the proof we need the following definition.

DEFINITION 3.1. A subset $V \subset \mathscr{R}^d$ is said to be *star-shaped* with respect to a point $x \in \mathscr{R}^d$ if V contains the line segment $\overline{xy}$ connecting x and y for each $y \in V$.

REMARK 3.1. The following statements are easily verified. Any convex set is star-shaped with respect to each of its points; however, a set can be star-shaped with respect to one of its points without being convex. The intersection or union of a collection star-shaped sets with respect to the same point is star-shaped with respect to that point.

The basic result upon which the proof of Theorem 3.1 rests is the following lemma. Even though we do not make use of it, we include the converse because it is of interest in its own right since it characterizes the Voronoi decomposition.

LEMMA 3.1. *If* $x \in \mathscr{R}^d$ *and* $r > 0$, *then* $\bigcup\{V_i: d(x, x_i) < r\}$ *is either empty or star-shaped with respect to* x. *Conversely, if closed sets* $W_i \subseteq \mathscr{R}^d$ *with* W_i^0 *nonintersecting have the property that for every* $x \in \mathscr{R}^d$ *and* $r > 0$ *the set* $\bigcup\{W_i: d(x, x_i) < r\}$ *is empty or star-shaped with respect to* x, *then* $W_i = V_i$ *for* $i = 1, \ldots, n$.

PROOF. To prove the first statement, without loss of generality label the x_i so that $d(x, x_1) \leq \cdots \leq d(x, x_n)$ and let $m = m(x)$ be the largest index such that $d(x, x_m) < r$. Note that the *half-space*

$$S(x_i, x_k) = \{x \in \mathscr{R}^d: d(x, x_i) \leq d(x, x_k)\}$$

for $i \le k$ contains x so it is star-shaped with respect to x. Now,

$$\begin{aligned}\bigcup \{V_i: d(x, x_i) < r\} &= \bigcup_{i=1}^{m} V_i \\ &= \bigcup_{i=1}^{m} \{y \in \mathscr{R}^d: d(y, x_i) \le d(y, x_k),\ k = 1, \dots, n\} \\ &= \bigcup_{i=1}^{m} \{y \in \mathscr{R}^d: d(y, x_i) \le d(y, x_k),\ k = m+1, \dots, n\} \\ &= \bigcup_{i=1}^{m} \bigcap_{k=m+1}^{n} S(x_i, x_k),\end{aligned}$$

which contains x. The result follows from Remark 3.1.

For the second statement, suppose $x \in V_m^0$. If $r = d(x, x_m) + \varepsilon$, then $\{i: d(x, x_i) < r\} = \{m\}$ for sufficiently small values of $\varepsilon > 0$ so $\bigcup\{W_i: d(x, x_i) < r\} = W_m$ is star-shaped with respect to x. It follows that $x \in W_m$ so we have shown $V_m^0 \subseteq W_m$. Since W_m is closed $V_m \subseteq W_m$. On the other hand, to show $W_m \subseteq V_m$ it suffices to show $W_m^0 \subseteq V_m$, so suppose $x \in W_m^0 - V_m$. Let $\varepsilon > 0$ be small enough so that $B_d(x, \varepsilon) \subseteq W_m^0$. Since the V_i cover $\mathscr{R}^d$, we have $x \in V_i \subseteq W_i$ for some i. It follows that there exists $y \in B_d(x, \varepsilon) \cap W_i^0$ and so $y \in W_i^0 \cap W_m^0$, which is impossible. □

The following proof of Theorem 3.1 is due to one of the referees. Our original proof is sketched below because we feel that while the first proof is considerably more concise, to us it is somewhat less intuitive than our proof, which uses a standard result and some basic machinery from algebraic topology.

We will need the following facts which are due to Hadwiger (1955) and which may be found in Sections 1 and 2 of McMullen and Schneider (1983). Let $\mathscr{P}^d$ denote the set of compact convex polytopes in $\mathscr{R}^d$, and let $U(\mathscr{P}^d)$ denote the set of all finite unions of sets in $\mathscr{P}^d$. There exists a unique function which assigns an integer (called the Euler characteristic) to each element of $U(\mathscr{P}^d)$ and having the following properties:

$$\chi(P) = \begin{cases} 1, & \varnothing \ne P \in \mathscr{P}^d, \\ 0, & P = \varnothing, \end{cases} \tag{3.4}$$

and

$$\chi(P \cup Q) + \chi(P \cap Q) = \chi(P) + \chi(Q) \quad \text{for all } P, Q \in U(\mathscr{P}^d). \tag{3.5}$$

By induction, the inclusion–exclusion principle

$$\chi\left(\bigcup_{i=1}^{n} P_i\right) = \sum_{u=1}^{n} (-1)^{u-1} \sum_{i_1 < \cdots < i_u} \chi(P_{i_1} \cap \cdots \cap P_{i_u})$$

follows from (3.4) and (3.5).

LEMMA 3.2. *If $P \in U(\mathscr{P}^d)$ is star-shaped with respect to some point, then $\chi(P) = 1$.*

PROOF. Assume $P \in U(\mathscr{P}^d)$ is star-shaped with respect to the point x and let $P = \bigcup_{i=1}^m P_i$, where $P_i \in \mathscr{P}^d$. Let $\bar{P}_i$ denote the convex hull of P_i and x. Then $P = \bigcup_{i=1}^m \bar{P}_i$ and

$$\chi(P) = \sum_{u=1}^{m} (-1)^{u-1} \sum_{i_1 < \cdots < i_u} \chi\left(\bar{P}_{i_1} \cap \cdots \cap \bar{P}_{i_u}\right)$$

$$= \sum_{u=1}^{m} (-1)^{u-1} \sum_{i_1 < \cdots < i_u} 1 = 1. \qquad \square$$

PROOF OF THEOREM 3.1. We proceed to verify the abstract tube property (see Definition 2.4). Let $\varnothing \neq J \subseteq \{1, \dots, n\}$ and suppose $\bigcap_{i \in J} B_d(x_i, r) \cap \bigcap_{i \notin J} B_d(x_i, r)^c \neq \varnothing$. We must show $\chi(\mathscr{N}(J)) = 1$.

Fix $x \in \bigcap_{i \in J} B_d(x_i, r) \cap \bigcap_{i \notin J} B_d(x_i, r)^c$. Let C be any polytope in $\mathscr{P}^d$ containing x and all of the vertices of the Voronoi decomposition $\{V_i,\ i = 1, \dots, n\}$ in its interior, and put $\bar{V}_i = V_i \cap C$, so that $\bar{V}_i \in \mathscr{P}^d$. We have $J = \{i\colon d(x, x_i) < r\}$. Since $J \neq \varnothing$, $Q = \bigcup_{i \in J} \bar{V}_i$ is star-shaped by Lemma 3.1, so that $\chi(Q) = 1$, by Lemma 3.2. Using the inclusion–exclusion principle,

$$\chi(Q) = \sum_{u=1}^{|J|} (-1)^{u-1} \sum_{i_1 < \cdots < i_u} \chi\left(\bar{V}_{i_1} \cap \cdots \cap \bar{V}_{i_u}\right)$$

(where, of course, the summands with $u > d + 1$ are 0). Now $\chi(\bar{V}_{i_1} \cap \cdots \cap \bar{V}_{i_u}) = 1$ if and only if $V_{i_1} \cap \cdots \cap V_{i_u} \neq \varnothing$, since each vertex of V_i is a vertex of $\bar{V}_i$, and this holds if and only if $\{i_1, \dots, i_u\}$ belongs to $\mathscr{N}(J)$. Hence

$$1 = \chi(Q) = \sum_{u=1}^{|J|} (-1)^{u-1} |\mathscr{N}_{u-1}(J)| = \chi(\mathscr{N}(J)). \qquad \square$$

Our original proof proceeds along the following lines. We must show $\chi(\mathscr{N}(J)) = 1$, where J is defined in the proof above. Observe that $\mathscr{N}(J)$ is the nerve of the cover $\{V_i,\ i \in J\}$ of the space $\bigcup_{i \in J} V_i$. Now each subcollection of sets in the cover either has an empty intersection or forms a convex set and is therefore contractible. A cover with this property is referred to as *good*. A basic result from algebraic topology [see Segal (1968)] states that the nerve of a good open cover has the same homotopy type as the space covered. There is a technical problem with applying this result in that the V_i are not open. Nevertheless, it is possible to *thicken* the sets V_i a bit to make them open and retain the goodness of the cover as well as the star-shapedness of the unions in Lemma 3.1. Consequently, the nerve $\mathscr{N}(J)$ has the same homotopy type as a star-shaped set. Since the Euler characteristic is a homotopy invariant, $\chi(\mathscr{N}(J)) = 1$.

REMARK 3.2. The identity of Theorem 3.1 is the same for all tube radii r and can be integrated with respect to an arbitrary measure. The most important case to consider for applications is Lebesgue measure μ_d which leads to a statement about volumes.

By Theorem 3.1 the volume of a discrete tube can be expressed as a linear combination of volumes of sets of the form $A_J(r) = \bigcap_{i \in J} B_d(x_i, r)$, where $|J| \le d + 1$. Whenever the set $A_J(r)$ is nonempty, it is convex. For fixed J there is a simple algorithm for finding a point c_J which is common to all of the nonempty $A_J(r)$, whose description is as follows. For every nonempty $I \subseteq J$ there is a unique d_I lying in the affine hull of $\{x_i,\ i \in I\}$, such that $\|x_i - d_I\| = r_I$, for all $i \in I$ and for some $r_I \ge 0$, which can be found by linear algebra. Let $\mathscr{F}$ denote the collection of index sets $I \subseteq J$ for which $\sup_{i \in J}\|x_i - d_I\| \le r_I$. This set is nonempty because $J \in \mathscr{F}$. Then $c_J = d_I$, where I gives a minimum value for r_I among $I \in \mathscr{F}$.

For a given $v \in S^{d-1}$, the unit sphere in $\mathscr{R}^d$, let $\gamma_J(v)$ denote the Euclidean distance from c_J to the boundary of the set to be measured, that is,

$$\gamma_J(v) = \sup\left\{ s \ge 0; c_J + sv \in \bigcap_{i=1}^{m} B_d(x_{j_i}, r) \right\}.$$

Then a simple argument leads to the following expression, which we have found useful for simulations:

$$\mu_d\left(\bigcap_{i \in J} B_d(x_i, r) \right) = V_d \int_{S^{d-1}} \gamma_J(v)^d \, d\nu_{d-1}(v),$$

where ν_{d-1} denotes the uniform measure in S^{d-1}, and V_d denotes the volume of the unit ball in $\mathscr{R}^d$, so that $V_0 = 1$, $V_1 = 2$ and $V_{d+2} = [2\pi/(d+2)]V_d$.

REMARK 3.3. Under the general position assumption, distinct indices $j_0, \dots, j_d$ define a d-dimensional simplex in $\mathscr{N}$ if and only if the unique sphere passing through $x_{j_0}, \dots, x_{j_d}$ fails to contain any of the remaining x_i's in the ball it bounds. This sphere is easily seen to be the set of points x for which

$$\det\begin{pmatrix} 1 & \cdots & 1 & 1 \\ x_{j_0} & \cdots & x_{j_d} & x \\ \|x_{j_0}\|^2 & \cdots & \|x_{j_d}\|^2 & \|x\|^2 \end{pmatrix} = 0.$$

It is easy to verify that the algebraic version of the simplex condition states that

$$\det\begin{pmatrix} 1 & \cdots & 1 & 1 \\ x_{j_0} & \cdots & x_{j_d} & x_i \\ \|x_{j_0}\|^2 & \cdots & \|x_{j_d}\|^2 & \|x_i\|^2 \end{pmatrix} \det\begin{pmatrix} 1 & \cdots & 1 \\ x_{j_0} & \cdots & x_{j_d} \end{pmatrix} > 0 \tag{3.6}$$

for all $i \notin \{j_0, \dots, j_d\}$.

We finish this section with remarks which strengthen the conclusion of Theorem 3.1.

REMARK 3.4. Even if the general position assumption for the centers of the balls is violated, the proof of Theorem 3.1 shows that collection of balls together with the nerve of the Voronoi cover still forms an abstract tube, except that in this case the dimension of this nerve can be greater than d. In Remark 3.5 we show there is a way to reduce this dimension to at most d. Nevertheless, even if the dimension exceeds d for the nerve of the Voronoi cover, we obtain an identity

$$I\left(\bigcup_{i=1}^{n} B_d(x_i, r)\right) = \sum_{(j_0,\ldots,j_m)\in\mathcal{N}} (-1)^m I\left(\bigcap_{i=0}^{m} B(x_{j_i})\right), \tag{3.7}$$

where the terms on the right-hand side can involve intersections of more than $d+1$ balls. For example, consider the extreme case when the x_i are all equidistant from the origin, so that all of the Voronoi sets contain the origin. Then the nerve of the Voronoi cover consists of every subset of indices so the identity reduces to the familiar inclusion–exclusion formula.

REMARK 3.5. When the dimension of $\mathcal{N}$ is greater than d, we can find modify $\mathcal{N}$ to define a d-dimensional simplicial complex $\mathcal{N}'$ which gives a depth $d+1$ identity for the indicator function of the union of balls which holds except possibly on the union of the boundaries of the balls. In particular, the identity is valid almost everywhere with respect to Lebesgue measure. The argument proceeds as follows. We can assume $n \geq d+2$ since otherwise the problem is trivial. Suppose the identity (3.7) has depth m, where $m > d+1$. This means that (3.1) or (3.2) fails to hold for some indices. For given indices $j_0, \ldots, j_d$ the set of distinct points for which (3.1) fails forms the solution set to a polynomial equation in $\mathscr{R}^{nd}$, and similarly, so is the set of distinct points for which (3.2) fails for given $j_0, \ldots, j_{d+1}$. The set M of points which are not in general position is a union of finitely many such sets, so there exists a smooth curve $\phi\colon [0,1] \to \mathscr{R}^{nd}$ such that:

(i) $\phi(0) = (x_1, \ldots, x_n)$,
(ii) $\phi(t) = (\phi(t)_1, \ldots, \phi(t)_n) \notin M$ for all $t > 0$.

As t varies throughout $(0,1]$, by (ii), none of the determinants in (3.6) vanishes; consequently, they undergo no sign changes. It follows from Remark 3.4 that the nerve $\mathcal{N}'$ of the Voronoi cover corresponding to the points $\{\phi(t)_i,\ i = 1, \ldots, n\}$ remains unchanged, and since the points are in general position the dimension of this nerve is at most d. By Theorem 3.1 the identity (3.3) holds with $\mathcal{N}$ replaced by $\mathcal{N}'$, and x_i replaced by $\phi(t)_i$, for any $t > 0$. Taking the limit as $t \to 0$ gives the identity

$$I\left(\bigcup_{i=1}^{n} B_d(x_i, r)\right) = \sum_{q=0}^{d} (-1)^q \sum_{F\in\mathcal{N}'_q} I\left(\bigcap_{i\in F} B_d(x_i, r)\right),$$

which holds except possibly for points in $\bigcup_{i=1}^{n} \partial B_d(x_i, r)$.

REMARK 3.6. If the subspace L spanned by $x_1, \ldots, x_n$ has dimension d', then d in Theorem 3.1 may be replaced by d' while the balls $B_d(x_i, r)$ remain in $\mathscr{R}^d$. This can be established easily by conditioning on (intersecting with) affine subspaces parallel to L. The intersection reduces to a problem with d replaced by d' and r by $r' \leq r$.

REMARK 3.7. The collection of possibly unequal size balls $\{B_d(x_i, r_i)\}_{i=1}^n$ forms an abstract tube of dimension d. The proof, which is quite similar to the proof of Theorem 3.1, uses the decomposition analogous to the Voronoi decomposition of $\mathscr{R}^d$ into regions

$$V_i^* = \{y \in \mathscr{R}^d : d(y, x_i)/r_i \leq d(y, x_k)/r_k,\ k = 1, \dots, n\}.$$

4. The spherical case. Theorem 3.1 has an analogue for the spherical case which is proven by similar techniques. Rather than give all of the details, most of which are analogous to the Euclidean case, we mention some of the key features which are different for the spherical case.

For points $u, v \in \mathscr{S}^d$, the unit sphere in $\mathscr{R}^{d+1}$, let $\rho(u, v) = \cos^{-1}\langle u, v\rangle$ denote the angular distance between u and v and define the spherical disk

$$D_d(u, r) = \{v \in \mathscr{S}^d : \rho(u, v) \leq r\}.$$

As in the Euclidean case we fix points $\{u_i\}_{i=1}^n \subseteq \mathscr{S}^d$ in *general position*, meaning that no subset of $d+1$ of the points lies in a d-dimensional subspace, and no point in $\mathscr{S}^d$ is equidistant from more than $d+1$ of the points. This amounts to the statement that none of the determinants

$$\det(x_{j_0} \ \cdots \ x_{j_d}), \qquad \det\begin{pmatrix} 1 & \cdots & 1 \\ x_{j_0} & \cdots & x_{j_{d+1}} \end{pmatrix}$$

vanishes for distinct indices $j_0, \dots, j_{d+1}$. The corresponding Voronoi regions $V_i \subseteq \mathscr{S}^d$ are defined as before and are easily seen to be *spherical convex polyhedra* in the sense they are intersections of finite collections of *half-spheres* (instead of half-spaces). The nerve of this covering of the sphere will be denoted by $\mathscr{N}$.

The analogue of Theorem 3.1 is the following theorem.

THEOREM 4.1. *We have*

$$I\left(\bigcup_{i=1}^n D_d(u_i, r)\right) + (-1)^d I\left(\bigcap_{i=1}^n D_d(u_i, r)\right) = \sum_{q=0}^{d} (-1)^q \sum_{F \in \mathscr{N}_q} I\left(\bigcap_{i \in F} D_d(u_i, r)\right) \tag{4.1}$$

for $0 \leq r \leq \pi/2$.

COROLLARY 4.1. *If* $\bigcap_{i=1}^n D_d(u_i, r) = \varnothing$, *then the collection of sets* $\{D_d(u_i, r)\}$ *together with* $\mathscr{N}$ *forms an abstract tube of dimension d and*

$$I\left(\bigcup_{i=1}^n D_d(u_i, r)\right) = \sum_{q=0}^{d} (-1)^q \sum_{F \in \mathscr{N}_q} I\left(\bigcap_{i \in F} D_d(u_i, r)\right)$$

for $0 \leq r \leq \pi$.

In many applications of interest in multiple comparisons, the assumption in Corollary 4.1 will be satisfied because the points u_i are paired with their antipodes. Note that when $\bigcap_{i=1}^{n} D_d(u_i, r) \neq \varnothing$ there is an extra n-fold intersection term which can be quite difficult to evaluate. In these situations some other methods will be needed to bound this term.

In order to prove Theorem 4.1 it is necessary to introduce terminology analogous to that used in the Euclidean case. In particular, it becomes necessary to clarify what we mean by a star-shaped subset of the sphere. Recall in the sphere given any two points which are not antipodes there is a unique *geodesic arc* which connects them. If the points are antipodes there are infinitely many geodesic arcs connecting them. We are thus led to introduce the following definition.

DEFINITION 4.1. A set $V \subset \mathscr{S}^d$ is said to be *star-shaped* with respect to $u \in V$ if for every $y \in V$, V contains *every* geodesic arc connecting u to y.

Under this definition, spherical convex sets (intersections of half-spheres) are star-shaped so we have the following analogue to Lemma 3.1 which is proved in the same manner.

LEMMA 4.1. *If* $u \in \mathscr{S}^d$ *and* $0 \leq r \leq \pi$, *then* $\bigcup\{V_i: \rho(u, u_i) < r\}$ *is either empty or star-shaped with respect to* u.

The proof of Theorem 4.1 proceeds along the same lines as the proof of Theorem 3.1. Let $\mathscr{Q}_d$ denote the set of spherical convex polyhedra in $\mathscr{S}^d$ and let $U(\mathscr{Q}_d)$ denote the set of finite unions of sets in $\mathscr{Q}_d$. The spherical analogue of the Euler characteristic used in Section 3 is the following. There is a unique integer-valued function χ on $U(\mathscr{Q}_d)$ which assigns the value 0 to the empty set, 1 to every nonempty element of $\mathscr{Q}_d$, and satisfies the additivity property (3.5).

A critical difference between the Euclidean case and the spherical case is that a subset of $\mathscr{S}^d$ can be star-shaped without having Euler characteristic 1. In fact, the sphere itself is star-shaped, but its Euler characteristic is easily seen to be $1 + (-1)^d$. Fortunately, this is the only pathological case, and we have the following analogue to Lemma 3.2.

LEMMA 4.2. *If* $Q \in U(\mathscr{Q}_d)$ *is star-shaped, then*

$$\chi(Q) = \begin{cases} 1, & \text{if } Q \neq \mathscr{S}^d, \\ 1 + (-1)^d, & \text{if } Q = \mathscr{S}^d. \end{cases}$$

PROOF. If Q is star-shaped with respect to x and $Q \neq \mathscr{S}^d$, then $-x \notin Q$. The same technique used in the proof of Lemma 3.2 shows that $\chi(Q) = 1$. On the other hand, by choosing a particular covering of $\mathscr{S}^d$ with spherical convex polyhedra it follows from the additivity property that $\chi(\mathscr{S}^d) = 1 + (-1)^d$. □

PROOF OF THEOREM 4.1. If J is a proper nonempty subset of $\{1, \dots, n\}$, then, as in the proof of Theorem 3.1, by Lemmas 4.1 and 4.2 and the inclusion–exclusion property

$$1 = \chi\left(\bigcup_{i \in J} V_i\right) = \chi(\mathscr{N}(J)).$$

On the other hand, if $J = \{1, \dots, n\}$ we obtain

$$1 + (-1)^d = \chi(\mathscr{S}^d) = \chi\left(\bigcup_{i=1}^{n} V_i\right) = \chi(\mathscr{N}(J)).$$

It follows that the right-hand side of the identity given in Theorem 2.2 coincides with the left-hand side of the identity in the statement of the theorem. □

Finally, we summarize the changes to Remarks 3.2–3.7 that lead to corresponding results in the spherical case.

The uniform probability measure of each set $\bigcap_{i \in J} D_d(u_i, r)$ can be evaluated as follows, whenever $|J| \le d + 1$. There exists a point $c_J \in \mathscr{S}^d$ which lies in every nonempty intersection $\bigcap_{i \in J} D_d(u_i, r)$ (as r varies). It is easily checked that this point is the unit vector in the direction of the point x that minimizes $\|x\|$ subject to the condition $\langle u_i, x \rangle \ge 1$, for all $i \in J$, and this can be found by a simple algorithm. Define $\mathscr{S}^{d-1}(c_J) = \{v \in \mathscr{S}^d \colon \langle v, c_J \rangle = 0\}$, which forms a $d - 1$-dimensional subsphere of $\mathscr{S}^d$, and for given $v \in \mathscr{S}^{d-1}(c_J)$ let $\rho_J(v)$ denote the angular distance from c_J to the boundary of $\bigcap_{i \in J} D_d(u_i, r)$ along a great circle in the direction v. Then

$$\begin{aligned} &\nu_d\left(\bigcap_{i \in J} D_d(u_i, r)\right) \\ (4.2)\qquad &= \int_{\mathscr{S}^{d-1}(c_J)} \int_0^{\rho(v)} \sin^{d-1}(t)\, dt\, d\nu_{d-1}(v) \Big/ \mathscr{B}(d/2, 1/2), \end{aligned}$$

where ν_{d-1} denotes the uniform probability measure on $\mathscr{S}^{d-1}(c_J)$.

The condition for when indices $j_0, \dots, j_d$ define a simplex of $\mathscr{N}$ has the same geometric description as in the Euclidean case, while the algebraic condition becomes

$$\det\begin{pmatrix} 1 & \cdots & 1 & 1 \\ x_{j_0} & \cdots & x_{j_d} & x_i \end{pmatrix} \det(x_{j_0} \quad \cdots \quad x_{j_d}) > 0$$

for all $i \ne j_0, \dots, j_d$.

When the general position assumption is violated, the identity (4.1) remains valid except that the sum on the right-hand side is up to the dimension of $\mathscr{N}$. It is always possible to find a simplicial complex $\mathscr{N}'$ whose dimension is at most d, which, when substituted for $\mathscr{N}$ in (4.1) gives an identity which holds everywhere except possibly at points on the boundary of the sets $D_d(u_i, r)$. If the points u_i lie on a subspace of dimension d', there is an identity (4.1) for which the simplicial complex on the right-hand side has dimension at most d'.

As in the Euclidean case, there is an analogous result in which the disks can have unequal radii.

5. Applications to multiple comparisons. We restrict attention to multiple comparisons. In Section 5.1 we give a straightforward account of the use of Theorem 4.1 to arbitrary multiple-comparisons problems. In Section 5.2 we briefly describe the full computer implementation and in Section 5.3 we show its versatility and efficiency for some standard and nonstandard problems.

5.1. *Geometry of simultaneous confidence intervals.* The basic setting we focus on is the following familiar one. Let B be a random p-vector having a standard multivariate normal distribution: $B \sim N_p(0, I_p)$, and let s^2 be an independent χ_q^2/q random variable. Typically, $B = (\hat{\beta} - \beta)/\sigma$, where β denotes the unknown parameter vector in a regression model whose design has been orthogonalized, $\hat{\beta}$ denotes its least squares estimator and $s^2 = \hat{\sigma}^2/\sigma^2$. Let $x_i^t B$, $i = 1, \dots, m$, be m linear combinations of B. The statements whose probabilities we are interested in evaluating represent failure of coverage for certain Scheffé-type [see Scheffé (1953, 1959)] simultaneous confidence intervals, and take the form

$$x_i^t B > c\|x_i\| s \quad \text{for some } i = 1, \dots, m. \tag{5.1}$$

Write $a_i = x_i/\|x_i\|$, $U = B/\|B\|$ so that the a_i are fixed unit p-vectors and U has a uniform distribution in $\mathscr{S}^{p-1}$. Statement (5.1) can be written as

$$a_i^t U > cs/\|B\| \quad \text{for some } i = 1, \dots, m, \tag{5.2}$$

or

$$U \in \bigcup_{i=1}^{m} D_{p-1}(a_i, \omega), \tag{5.3}$$

where $\omega = \cos^{-1}(c/R)$ and $R \sim \sqrt{pF_{p,q}}$ independent of U. [Here we define $\cos^{-1}(x) = 0$ for $x > 1$.]

Conditioning on R (and hence ω), we can compute the probability of (5.3) using the results of Section 4. The union $\bigcup_{i=1}^{m} D_{p-1}(a_i, \omega)$ has a depth p identity so long as $\bigcap_{i=1}^{m} D_{p-1}(a_i, \omega)$ is empty. For two-sided confidence procedures we obtain each vector $-x_i$ among the vectors x_i, so that each $-a_i$ appears among the a_i. Thus $\bigcap_{i=1}^{m} D_{p-1}(a_i, \omega) = \varnothing$ since the angular radius ω does not exceed $\pi/2$ (since $c/R \geq 0$). The full probability of (5.1) is

$$E_R\left[P\left(U \in \bigcup_{i=1}^{m} D_{p-1}(a_i, \omega)\right)\middle| R\right]. \tag{5.4}$$

REMARK 5.1. It is of interest to note that when we substitute the basic identity into (5.4), use the linearity of the conditional expectation and then take expectations over R, we express the error probability in the original multiple-comparisons problem as a linear combination of error probabilities for a collection of smaller problems in each of which the number of points a_i is at most the dimension of the parameter space.

5.2. *Implementation.* The multiple-comparisons application has been fully implemented as a computer program written in C. The program is described briefly as follows.

(i) *Input.* The program accepts the matrix of unit vectors $A = [a_1^t, \dots, a_n^t]^t$ (see Section 5.1) together with the two dimension parameters p (parameters) and q (residuals). There are options to make the rows of A into unit vectors if they are not upon input and to symmetrize by expanding A to include all $-a_i^t$ for each a_i appearing in A without its antipode.

(ii) *Rank reduction.* In many examples, A is not full rank so that the input dimension p can be reduced to some $p' < p$. This is carried out using a singular value decomposition. This automatic dimension reduction is useful in complex problems.

(iii) *Perturbation.* It is necessary to place the points in general position before carrying out the Voronoi reduction. This is effected by adding small independent uniform random deviates in $(-\delta, \delta)$ to each entry of the matrix A, where δ is an additional input. There is also an option to select the direction of the perturbation. Then the rows of A are renormalized and the result is used to carry out the Voronoi reduction. The original matrix is used for the final probability calculations.

(iv) *Voronoi reduction.* First the simplex condition of Section 4 is checked for every subset of size p' of the a_i. The theory says that every face of the Delauney simplicial complex (the nerve of the Voronoi covering) corresponding to the a_i (in the sphere $\mathscr{S}^{p'-1}$) is a subface of one of these *minimal* simplices, so after listing these simplices, a test is carried out for each subset of size 1 through $p' - 1$ of the rows of A to discover if it is to be included in the full Delauney complex.

(v) *Centers.* For each face of each dimension in the Delauney complex (with corresponding index set J), the point c_J (see Section 4 and Remark 3.2) is determined using the unperturbed points a_i.

(vi) *Integration in the sphere.* The conditional probability in (5.4) is expanded as a sum of terms of the form

$$\pm P\left(U \in \bigcap_{j=1}^{m} D_{p'-1}(a_{i_j}, \omega) \middle| R\right),$$

with each term corresponding to a face of the simplicial complex found in (iv). Each is evaluated using simulation and the expression (4.2) as a spherical integral. Each integral is evaluated using a sample of random directions. These directions are obtained from a sample of unit vectors in $\mathscr{S}^{p'-1}$. This sample can be used to construct a sample of unit vectors in each subsphere $\mathscr{S}^{p'-1}(c_J)$ by removing each projection of each vector onto the ray through c_J. This allows for the possibility of using the same sample of unit vectors for *all* of the spherical integrals, which leads to more computational efficiency. At the same time, this leads to greater storage requirements. The values of R used are generated separately [see (vii)].

(vii) *Integration in the angle*. The expectation $E_R(\cdot)$ step is performed by using the following idea. The event (5.2) can be written as

$$c/R \leq 1 \quad \text{and} \quad \cos^{-1}(a_i^t U) \leq \cos^{-1}(c/R) = \omega, \qquad i = 1, \dots, m,$$

where $R = \|B\|/s = \sqrt{pF_{p,q}}$. The full probability then becomes

$$(5.5) \qquad P\left(U \in \bigcup_{i=1}^{m} D_{p-1}(a_i, \omega) \middle| R \geq c \right) P(R \geq c).$$

The last probability is evaluated using a fast routine for the $F_{p,q}$ tails and pseudorandom angles ω are generated according to the conditional distribution of $\cos^{-1}(c/R)$ given $R \geq c$ are generated by rejection. The angles are used in the sphere integration in (vi).

(viii) *Consolidation, output*. A typical goal is to find the critical constant c so that the coverage probability (5.4) takes some prescribed value. Several programming decisions described above were made with this goal in mind. For example, since the result of Steps (iv) and (v) is the same for all values of c, those steps are carried out before values of c are specified. The sample of random directions in (vi) can be used for every value of c in some specified range. However, for generating the random angles in (vii), the sampled distribution depends on c, so the following method is utilized to save computation time. The program accepts as input a minimum $c_{\min}$ and maximum value $c_{\max}$ of c and the number of (evenly spaced) intermediate values to use. Once a sample of values of R (with $R \geq c_{\min}$) is used to generate random angles for $c = c_{\min}$, for each new value of $c > c_{\min}$, the subsample of values for which $R > c$ is used to give a corresponding sample, and the second probability in (5.5) is determined easily. The program outputs a probability estimate along with the resulting sample size for the random angles. As long as the resulting sample size remains positive, the simulated probability constitutes an unbiased estimator. Once a value of c has been found, the user has the option of obtaining a more accurate estimate of the associated coverage probability by repeated simulation with larger sample sizes.

The results of the simulations can be compared with the naive simulation which merely uses the original statements (5.1) and normal and χ_q^2 variates. Although full evaluation must await further research, preliminary analyses of speed and accuracy indicate (i) very close agreement with naive simulation verifying the general efficacy of the method, (ii) for roughly the same computation time, a considerable increase in accuracy over naive simulation in the tails (large c) and (iii) a rich understanding of the contributions of disk intersections of particular depths.

5.3. *Examples.* For each example a little work is needed to prepare the matrix A for input, and for many standard examples, the program carries out this step automatically. The authors are in a position to compute the critical value c for any size α, for multiple-comparisons procedures of reasonable dimension (less than 10), using the technology described in this paper. Rather than present tables for particular problems, we outline a handful of examples to merely indicate the versatility.

EXAMPLE 1 (Tukey–Kramer Studentized range). For the one-way layout with p cells and n_i observations in the ith cell, a problem which has received considerable attention in the literature is that of bounding all pairwise differences between cell means θ_i, based on independent estimates $\hat{\theta}_i \sim N(\theta_i, \sigma^2/n_i)$ and $\hat{\sigma}^2 \sim \sigma^2\chi^2_\nu$. In this context, the program finds critical values for the quantity

$$T = \max_{i,j}\left|\frac{\left(\hat{\theta}_i - \theta_i\right) - \left(\hat{\theta}_j - \theta_j\right)}{\hat{\sigma}\sqrt{\dfrac{1}{n_i} + \dfrac{1}{n_j}}}\right|,$$

so that $B = (\sqrt{n_1}(\hat{\theta}_1 - \theta_1), \dots, \sqrt{n_p}(\hat{\theta}_p - \theta_p))^t$ and the linear combinations are of the form $(0, \dots, 0, 1/\sqrt{n_i}, 0, \dots, 0, -1/\sqrt{n_j}, 0, \dots, 0)$. The dimension p is reduced to $p - 1$ in the rank reduction [Step (ii)]. Typically, $q = \Sigma_i n_i - p$ (residual degrees of freedom) but the program allows this value to be arbitrary. As in Dunnett (1980), we take $a_i^2 = 1/n_i$ and we allow a_i to be arbitrary.

For unbalanced designs, using $c = q_{p,\nu}^{(\alpha)}/\sqrt{2}$, where $q_{p,\nu}^{\alpha}$ denotes the critical point from the Studentized range distribution, was conjectured by Tukey (1953) to give rise to a conservative procedure and this conjecture was finally resolved by Hayter (1984). Dunnett (1980) carried out an extensive simulation study to determine the degree of conservatism of the procedure, using an approach close to what we have called naive simulation.

We present as a preliminary example one of the cases from Dunnett (1980). Take $p = 4$ and $(a_1, a_2, a_3, a_4) = (1, 1, 1, 1), (10, 1, 1, 1)$ and $q = 5$. The simulation values are presented in Table 2. We have taken a critical value c as close as possible to achieving $\alpha = 0.05$ and then determined the approximate rejec-

TABLE 2
Studentized range critical values

(a_1, a_2, a_3, a_4)	**Voronoi**	**Naive**	**Dunnett**
(1, 1, 1, 1)	0.049144	0.048150	0.0513
(10, 1, 1, 1)	0.042332	0.042050	0.0431
Difference	0.006812	0.006100	0.0082

tion probability α by simulation. Following Dunnett, the critical constants are compared for the balanced and the unbalanced procedures. The sample sizes are taken to be 10,000 (each for angles and directions) for the Voronoi procedure and 100,000 for the naive simulation. (Dunnett quotes a sample size of 10,000.) Our simulation study indicates (i) close agreement between simulated α values using the Voronoi and naive simulation methods and (ii) consistency with Dunnett's figures, which corroborated Tukey's conjecture.

Note that positive differences between α values is indicative of the conservatism of the Studentized range procedure in the unbalanced case. Also, since Dunnett uses a different value for c, only the difference in α values should be comparable.

The two methods can be compared in terms of computing speed, accuracy and memory utilization. The memory utilization requirements tend to be far more substantial for the Voronoi method than for the naive method because (i) simplices and their corresponding center points need to be stored and (ii) we stored the samples of unit vectors and angular radii for re-use. For the calculations below we used a Sun Sparcstation 1, with the storage capacity which allowed for double precision arrays of size one million.

To investigate speed and accuracy, we picked a few examples and chose the following simulation experiment. For each value of the critical constant c, the naive simulation method is carried out with a sample size of 10,000 for nine independent trials. The average and the interquartile range of the nine estimates ($\hat{\alpha}_N$) are determined, as well as the average computing time per trial. Then a single test trial is carried out using the Voronoi method with a sample size of 1000. This is used to determine the approximate sample size for which the Voronoi method achieves the same computing time per trial as the naive method. Then nine independent probability estimates ($\hat{\alpha}_V$) are obtained using the Voronoi method. The average and interquartile ranges are determined for the Voronoi method and the naive method, as well as the average computing time per trial. In all cases the actual computing times (based on the scaled sample sizes) were close enough as to be taken as identical.

It is important to emphasize that the Voronoi reduction step is not taken into account when comparing computing times. Arguably, our comparison is biased in favor of the Voronoi method when one is interested in finding the coverage probability for a single value of c. However, we are interested in determining coverage probabilities for a whole range of possible values of the constant c, so that we can choose c to obtain a prescribed level for the procedure. Since the Voronoi step need only be carried out once for several values of c, asymptotically, as the number of values of c goes to ∞, the time spent on this step becomes negligible compared to the time spent on the simulation.

The results are summarized in Figure 5. We considered three different ANOVA models with $(3,4,5)$, $(3,4,5,6)$ and $(3,4,5,6,7)$ observations per cell. For each model considered, the error degrees of freedom is the total number of observations minus the number of cells. The graph gives the log of the ratio of interquartile ranges (LRIQR) for the Voronoi method estimates and the naive

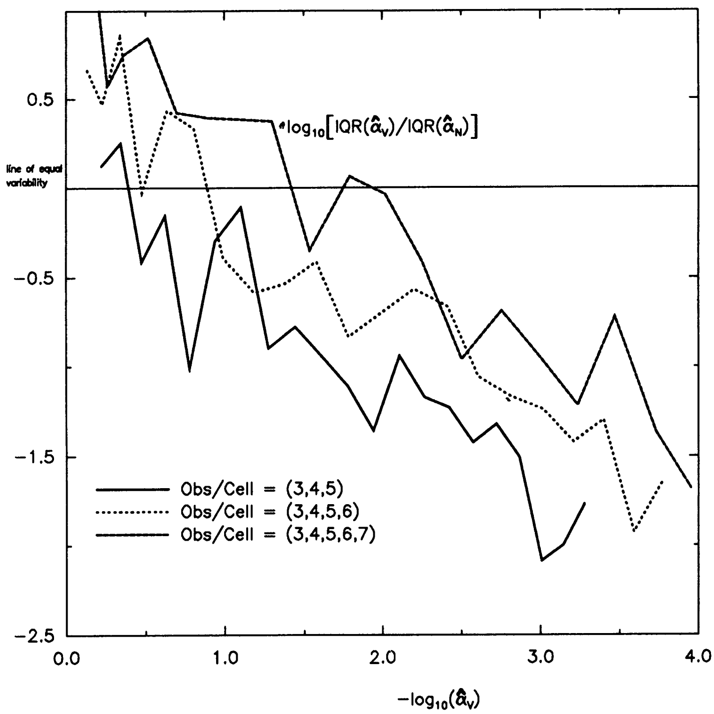

FIG. 5. *Relative variability of probability estimates: confidence intervals for pairwise differences of cell means (one-way ANOVA).*

estimates, for a range of values of c, versus the average of the estimates of the error probabilities $\hat{\alpha}_V$.

Note that in each case, as the error probability decreases (as c increases) the Voronoi estimate shows less and less variability relative to the naive estimate, and for sufficiently small values of α the variability of the Voronoi estimates is below that of the naive estimates, represented by the fact that the graph of the LRIQR curve falls below the horizontal line where the LRIQR equals 0. We see that for values of α less than about 0.1 or 0.01, the Voronoi estimates improve upon the naive estimates. For small values of α this improvement can be quite substantial. For $\alpha \approx 10^{-2.5} \approx 0.0032$ the Voronoi method gives estimates with $1/10$ of the interquartile range of that of the naive method. The most dramatic improvement occurs for small numbers of cells. This is typical behavior for other examples we have been able to study.

EXAMPLE 2 (Simple slippage). For the same models as in Example 1, instead of finding confidence intervals for all pairwise differences we may wish to decide if one of the cell means differs significantly from the others, the so-called *slippage problem*. For this purpose, one may construct confidence

TABLE 3
Estimated error probabilities for the simple slippage procedure with three cells and $c = 2.75$[a]

(Observation / cell) / m	m = 1	m = 2	m = 3	m = ∞
3 3 3	(0.074150)	(0.037157)	(0.029026)	(0.016428)
1 1 7	0.001423	0.000881	0.000756	0.000480
1 2 6	0.002292	0.001415	0.001186	0.000703
1 3 5	0.003277	0.002009	0.001655	0.000954
1 4 4	0.003619	0.002205	0.001819	0.001043
2 2 5	0.000538	0.000373	0.000309	0.000188
2 3 4	0.000428	0.000295	0.000240	0.000143

[a]Actual estimate for row other than the first is the corresponding term in the first row minus the entry.

intervals for all differences

$$\theta_i - \frac{1}{m-1}\sum_{j\neq i}\theta_j.$$

Thus quantiles are to be determined for

$$T = \max_i \frac{\left|(\hat{\theta}_i - \theta_i) - \frac{1}{p-1}\Sigma_{j\neq i}(\hat{\theta}_j - \theta_j)\right|}{\hat{\sigma}\sqrt{\frac{1}{n_i} + \frac{1}{(p-1)^2}\Sigma_{j\neq i}\frac{1}{n_j}}}.$$

We compare again the balanced case with the unbalanced case demonstrating conservativeness, for some cases, of the procedure which uses the critical points for the balanced cases, and we show how the Voronoi method leads to more efficient estimates in the tails of the distribution.

First, we restrict attention to a model with $p = 3$ and $p = 4$ cells, and we compare error probabilities for procedures with $c = 2.75$ for varying numbers of observations per cell. The results are summarized in Tables 3 and 4. The leftmost columns in Tables 3 and 4 give the relative numbers of observations in each cell, which are to be multiplied by m to give the actual number of observations in each cell. In each case, to make the example as realistic as possible, the number of degrees of freedom equals the total number of observations minus the number of cells. The first row of the tables give estimates of error probabilities while the remaining rows are differences between estimated error probabilities and the estimates for the balanced case (the first row). For each entry the estimate is based on the Voronoi method with a sample size of 10,000. Note in each of the rows besides the first the difference is positive, which is consistent with the conjecture that using tables for the balanced case leads to a conservative procedure.

Again it is of interest to compare the Voronoi method with the naive simulation method, in the manner as was carried out for the Tukey–Kramer problem. Figure 6 gives a graph of the relative variability of the Voronoi

TABLE 4
Estimated error probabilities for the simple slippage procedure with four cells and $c = 2.75^a$

(Observation / cell) / m	$m = 1$	$m = 2$	$m = 3$	$m = \infty$
3 3 3 3	(0.078658)	(0.043742)	(0.035163)	(0.022593)
1 1 1 9	0.000166	0.000281	0.000145	0.000151
1 1 2 8	0.000733	0.000544	0.000375	0.000251
1 1 3 7	0.001355	0.000825	0.000600	0.000356
1 1 4 6	0.001736	0.000993	0.000729	0.000417
1 1 5 5	0.001868	0.001049	0.000765	0.000438
1 1 3 7	0.000791	0.000617	0.000442	0.000298
1 2 3 6	0.001192	0.000798	0.000610	0.000398
1 2 4 5	0.001418	0.000895	0.000692	0.000443
1 3 3 5	0.001424	0.000988	0.000741	0.000492
1 3 4 4	0.001551	0.001038	0.000786	0.000520
2 2 2 6	0.000064	0.000146	0.000096	0.000076
2 2 3 5	0.000141	0.000132	0.000126	0.000082
2 2 4 4	0.000210	0.000137	0.000143	0.000091
2 3 3 4	0.000089	0.000108	0.000078	0.000049

[a]Actual estimate for row other than the first is the corresponding term in the first row minus the entry.

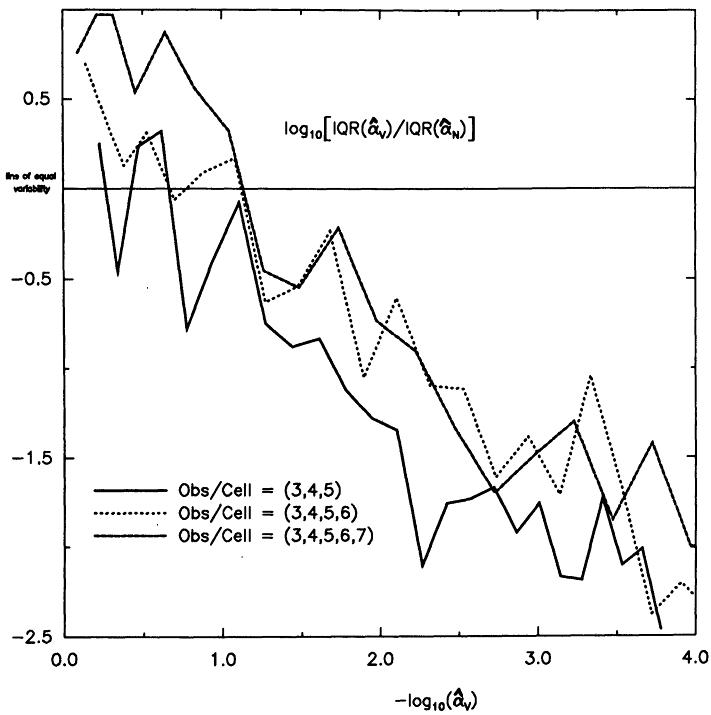

FIG. 6. *Relative variability of probability estimates: confidence intervals for all simple slippage contrasts.*

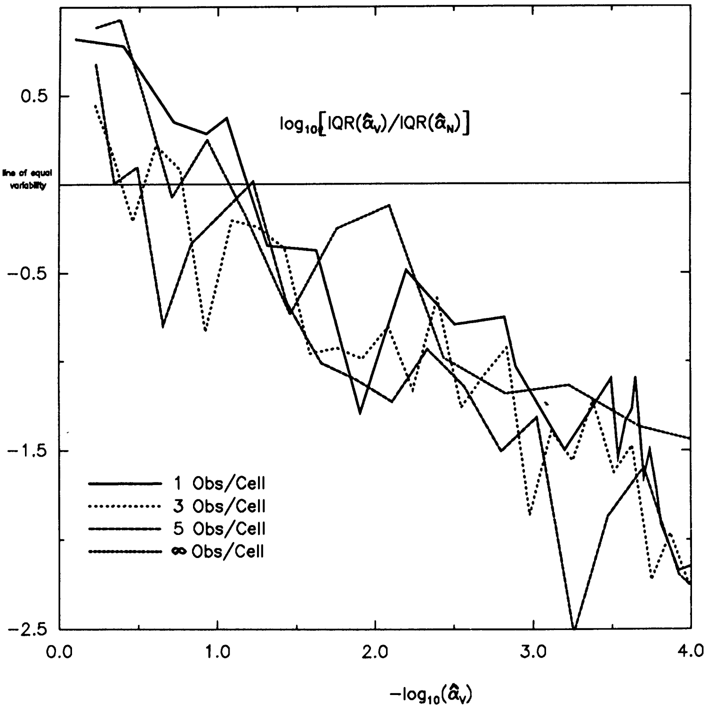

FIG. 7. *Relative variability of probability estimates: confidence intervals for all pairwise differences of cell means* (2×2 *table*).

method estimates to that of the naive method estimates for three different designs. Note the same qualitative features described for Figure 5 are present, and the improvement of the Voronoi method is even more dramatic. Here we see that for $\alpha < 0.1$ the Voronoi method is more efficient.

EXAMPLE 3 (Pairwise differences in two-way layouts). To obtain an example with a little more structure, we consider the problem of bounding all pairwise differences of cell means in a balanced additive (no interactions) two-way layout with r rows and c columns and m observations per cell. The standardized cell estimates in standard notation are $\hat{\theta}_{ij} = \overline{Y}_{i..} + \overline{Y}_{.j.} - \overline{Y}_{...}$, where the Y_{ijk} are independent $N(0, \sigma^2)$. Here we determine the quantiles of the distribution of

$$T = \max_{(i,j)\neq(u,v)} \frac{\left|\left(\hat{\theta}_{ij} - \theta_{ij}\right) - \left(\hat{\theta}_{ij} - \theta_{ij}\right)\right|}{\hat{\sigma} d_{ijuv}},$$

where d_{ijuv} is the appropriate standardization constant.

We looked at $(r, c) = (2, 2)$ (Figure 7) and $(2, 3)$ (Figure 8) and $m = 1, 3, 5, \infty$ and compared the variability of estimates using naive simulations to the

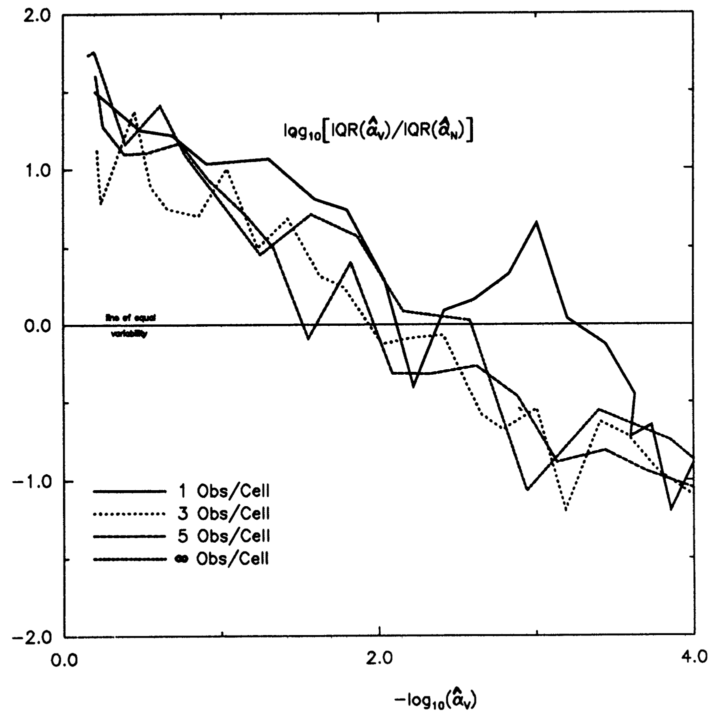

FIG. 8. *Relative variability of probability estimates: confidence intervals for all pairwise differences of cell means* (2 × 3 *table*).

Voronoi method, as for the previous examples. For the 2 × 2 case (Figure 7), and for all of the values of m we looked at, the Voronoi method is more efficient than the naive method when $\alpha < 10^{-1.3} \approx 0.05$, and the graph is remarkably similar to the one in Figure 5. The 2 × 3 case (Figure 8) seems to require smaller values of α (≈ 0.003) before the Voronoi method improves on the naive method, and the case of one observation per cell (two degrees of freedom for the error) seems to require α less than about 0.001. Again, it is possible to improve the accuracy by a factor of 10 in a practical range of α values. Unfortunately, larger problems (e.g., the 2 × 4 case) are not feasible for extensive study given our currently available computing resources, but we expect the conclusions for these problems to be similar.

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