

Statistics for Spatial Data

Statistics for Spatial Data

Revised Edition

NOEL A. C. CRESSIE

Iowa State University



A Wiley-Interscience Publication

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To Yoko, Amie, and Sean

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Preface

The purpose of this book is to present Statistics for spatial data to scientists and engineers. (Notice that Statistics is capitalized to distinguish it from its other meaning: a collection of numbers that summarize a complex phenomenon—such as baseball or cricket.) In the last 10 years, much interest has been generated in the area, but its exposure in the literature has been uneven. This book attempts to take that literature and extend it, correct it, and unify it. What appears to be a gathering of unconnected subject areas can be annealed into a cohesive approach to the analysis of spatial data. Chapter 1 provides an overview of the approach and of the enormous diversity of problems involving spatial data, from the microscopic to the astronomic.

The book attempts to give a somewhat complete coverage of each of three parts, dealing with *geostatistical data*, *lattice data*, and *point patterns*. Thus, the subject areas are classified according to the type of observations encountered, reflecting my belief that the roots of statistical science are in data. Statistical models, then, try to make sense out of the data, albeit imperfectly. Design, inference, and diagnostics are natural consequences of the data–model symbiosis, and all play an important role in Statistics for spatial data.

This book grew from lecture notes for a one-semester, 3-credit Statistics graduate course that I conduct at Iowa State University. In 45 lectures, each of 50-minutes duration, I cover the following topics:

Part I (Geostatistical Data): All of Chapter 2 except Section 2.5. All of Chapter 3 except Sections 3.3 and 3.6.

Part II (Lattice Data): Chapter 6. Chapter 7, Sections 7.2, 7.3, and 7.6.

Part III (Point Patterns): Chapter 8, Sections 8.1, 8.2, 8.4, 8.5.1, 8.5.2, 8.5.3. Chapter 9, Section 9.1.

Prerequisites for the Statistics graduate course are one semester of Masters-level statistical inference and one semester of Masters-level linear models. While giving the course and preparing the book, I have benefitted from useful reference books in the area. Reading lists for the course have included Matern (1960), Bartlett (1975), Journel and Huijbregts (1978), Cliff and Ord (1981), Ripley (1981), and Upton and Fingleton (1985).

It is my hope that this book can be read in varying depths by people with varying mathematical and statistical backgrounds. However, there are sections in the book, on random processes, point processes, and random sets, that are beyond a Masters-level student and closer to the frontiers of theoretical research (these sections are denoted by an asterisk). Equally, there are sections that concentrate purely on an application and do not add to the theoretical development of the subject (these sections are denoted by a dagger). These applications-oriented sections of the book should appeal to a large number of scientists and engineers, with at least the background of a service course in Statistics (or equivalent). For this reason, most chapters begin with an application, which is meant to be an invitation to read on. The emphasis on applications has led to considerable use of graphs and illustrations.

There are some features of the book that I believe will enhance its value as a textbook and as a reference book. An attempt has been made at completeness, in terms of the topics covered, and uniformity, in terms of the depth to which they are covered, except for Chapters 5 and 9. These two chapters contain material that is either of personal interest or is speculative in nature. The reader will notice frequent referencing to a diverse literature; one of the interesting features of Statistics for spatial data is that a large proportion of it is appearing *outside* Statistics journals. The referencing allows me to pick up apparently different streams of thought and tie them together. Equally importantly, I have tried to give credit where it is due. The linear reader will also notice a certain amount of repetition between chapters (and, to a lesser extent, between sections). This is deliberate and is meant to help the sporadic reader who wants to understand the essence of a topic but who has not read all the previous pages.

We should not forget our roots. All data sets for the various spatial statistical analyses are given in the book, as well as some background to the problems being studied. Further, each of the three parts has a section devoted to sources of spatial data, both real and simulated.

No exercises are given at the end of sections; the depth of coverage within a section should allow practice exercises to suggest themselves to an instructor teaching from the book. Software is not given. (A geostatistics package, *Toolkit*, by Geostokos, London, was used for the kriging presented in Chapter 3.) Currently, those of us who work in the area tend to custom-build our own software, which is usually not very portable. Statistics for spatial data will truly realize its enormous potential when a comprehensive software package is developed.

This is a big book. I had thought of splitting it into smaller volumes; however, the present format emphasizes the subject's unity. This may be the last time spatial Statistics will be squeezed between two covers. A healthy exponential growth of the literature is apparent from the bibliography.

The future of the subject is in solving problems for spatiotemporal data; some sections are devoted to it, but a proper treatment needs another book. Statistics for spatial and temporal data would provide dynamic models for phenomena distributed through space and evolving in time. Onward into the next decade!

NOEL CRESSIE

Ames, Iowa
December 1, 1990

Acknowledgments

As a boy, knowing “why,” “how,” and “when” was not enough for me. With encouragement from my parents, a keen interest in the “where” question eventually led me to summer jobs with mining companies in Western Australia (while an undergraduate) and three years of doctoral work at Princeton University. There, I had the good fortune to be taught by Geof Watson, John Tukey, and, in my last year, Julian Besag. Geof gave me an appreciation for all things spatial and geometric, John showed me how to make my data speak (sometimes, even sing) to me, and Julian introduced me to the mysteries of Markov random fields (and English hockey). More recently, in his role as a series editor for Wiley and as an aficionado of Statistics for spatial data, Geof Watson has been of immense help with his comments and his support.

The influence of Georges Matheron of the École Nationale Supérieure des Mines de Paris in Part I and Chapter 9 is obvious; his work has been truly pioneering. I was fortunate to spend a post-doctoral period of five months at his center in Fontainebleau, France, in 1975.

My coauthors on spatial articles provided valuable impetus to my research in the subject and my colleagues throughout the world have (through their letters, their telephone calls, their questions at seminars, their anonymous referees’ reports, and their comments in hallways) helped shape my current opinions on Statistics in general and on Statistics for spatial data in particular. Along with those mentioned in the paragraphs above, I would like to thank Peter Diggle for early suggestions on topics that a course on spatial statistics might cover, Dale Zimmerman for comments on Chapter 5, Subhash Lele for comments on parts of Chapters 6 and 7, and Daryl Daley for comments on Chapter 8.

The task of taking a diverse and uneven literature on spatial Statistics and extending it, correcting it, and unifying it has not been an easy one. The editors at Wiley have been very understanding of my desire for a complete and uniformly comprehensive product. Bea Shube provided ideas and encouragement in the early stages of this project. In the last three years, helpful advice has come from Kate Roach, and, for a brief period before her, from Maggie Irwin. My department head at Iowa State University, Dean Isaacson,

has been equally understanding and in various ways helped to make an impossible task possible.

The writing of this book started in the second half of 1985 while I was an ASA/NSF/Census Fellow at the U.S. Bureau of the Census. Based on an experimental course called Spatial Statistics that I conducted at Iowa State University in 1984, I gave a series of seven seminars at the Census Bureau and distributed material that later became Chapter 6. The rest of the book (over 90%) was written at Iowa State, partially supported by the Department of Statistics and by the National Science Foundation. A special mention should be made of the superb journal and book collection of the Parks Library at Iowa State; it is one of the great resources of the University, and has helped me achieve a coverage that would otherwise have been impossible.

We are very fortunate, in our Department of Statistics, to be surrounded by intelligent and motivated graduate students. I have now offered my course on Spatial Statistics four times; it has helped me attract good students with a keen interest in the subject. As research assistants and as candidates for graduate degrees, they have been involved in various aspects of this book. The contributions of three of them deserve special mention and thanks. Stephen Rathbun wrote a preliminary draft of Sections 8.3, 8.5 through 8.9, and 7.4, and commented on subsequent drafts of Chapter 8. Carol Gotway wrote a preliminary draft of Sections 3.6 and 5.1, Martín Grondona wrote a preliminary draft of Sections 5.6 and 5.7, and Gotway and Grondona gave comments on Part I. All three were involved in the production of the figures. My thanks also go to Renkuan Guo, Jeff Helterbrand, Fred Hulting, and Jay Ver Hoef, who contributed in various ways to the preliminary through penultimate and final drafts.

This manuscript was turned into immaculate type by Sharon Shepard; by comparing what I gave her and what she gave me, it is clear that Sharon was able to work near miracles. Jeanette LaGrange, Rose Ann Anderson, and Jan Franklin also provided valuable secretarial assistance.

A trace of my space–time line would show a trip to Tokyo, Japan, in 1987. There I met Yoko. She could rightly claim that Western marriage vows say nothing about writing a book. Yet somehow she understood. We are fortunate to have been able to create two new space–time lines in our household, Amie and Sean. It was difficult for them to understand, and even harder for me to persevere. My deepest gratitude goes to all of them for their love and patience.

I am glad I started exploring Statistics for spatial data, because I have learned a great deal. Some of the territory is now well charted. Other parts are only passable by those who are sure-footed, and by not looking down. Much more of it I can only glimpse and tell you what I see. It is an exciting area that deserves a place in every statistical scientist's repertoire; I hope you will agree.

N. A. C. C.

Statistics for Spatial Data

CHAPTER 1

Statistics for Spatial Data

*Perhaps, it may turn out a Sang;
Perhaps, turn out a Sermon.*

ROBERT BURNS

Statistics, the science of uncertainty, attempts to model order in disorder. It is not surprising that students (and their teachers) find the subject enigmatic. However, as life experiences and scientific experiences accumulate, Statistics is usually recognized as an extremely powerful research tool. Even when the disorder is discovered to have a perfectly rational explanation at one scale, there is very often a smaller scale where the data do not fit the theory *exactly*, and the need arises to investigate the new, residual uncertainty.

Scientists and engineers have attempted to measure the level of disorder through, among other things, a quantity called *entropy*; see Jaynes (1957) and his subsequent writings (Rosenkrantz, 1983). Suppose there are $i = 1, \dots, k$ possible states of nature that occur at random according to a probability distribution $(p_1, p_2, \dots, p_k)$, where $0 \leq p_i \leq 1$, $i = 1, \dots, k$, and $p_1 + p_2 + \dots + p_k = 1$. Shannon (1948) defined entropy as

$$E \equiv - \sum_{i=1}^k p_i \cdot \log p_i,$$

where $x \cdot \log x \equiv 0$, for $x = 0$. When the state of nature i has a numerical interpretation, the mean $\mu \equiv \sum_{i=1}^k i \cdot p_i$ could be thought of as the center of the distribution and the variance $\sigma^2 \equiv \sum_{i=1}^k (i - \mu)^2 p_i$ as the amount of variability in the distribution. It is σ^2 that statisticians mostly use to quantify disorder, but not surprisingly E and σ^2 are closely related (see, e.g., Mukherjee and Ratnaparkhi, 1986).

There is a very interesting entropy inequality that can be proved. Consider the initial probability distribution $\mathbf{p}' \equiv (p_1, \dots, p_k)$ evolving into a subsequent probability distribution $\mathbf{p}'A$, where A is a $k \times k$ matrix of nonnegative

elements each of whose rows sums to 1. Write $A = (a_{ij})$; then a_{ij} can be interpreted as the *conditional* probability that the subsequent state of nature is j given that the initial state of nature was i , and A is called a transition matrix. When states of nature evolve through repeated application of a stochastic mechanism described by the matrix A , the result is called a Markov chain (see, e.g., Isaacson and Madsen, 1976; Section 6.3). The entropy inequality is

$$E(\lambda^{(1)} : \mu^{(1)}) \geq E(\lambda^{(0)} : \mu^{(0)}),$$

where $E(\lambda^{(l)} : \mu^{(l)}) \equiv -\sum_{j=1}^k \lambda_j^{(l)} \cdot \log(\lambda_j^{(l)} / \mu_j^{(l)})$, $l = 0, 1$. Initially, $\lambda_j^{(0)} = p_j$ and $\mu_j^{(0)} = 1$, $j = 1, \dots, k$, so that $E(\lambda^{(0)} : \mu^{(0)})$ is simply $E = -\sum_{j=1}^k p_j \cdot \log p_j$. The subsequent measures are $\lambda_j^{(1)} = \sum_{i=1}^k a_{ij} \lambda_i^{(0)} = \sum_{i=1}^k a_{ij} p_i$ and $\mu_j^{(1)} = \sum_{i=1}^k a_{ij} \mu_i^{(0)} = \sum_{i=1}^k a_{ij}$, $j = 1, \dots, k$, depending on the transition matrix A .

A physical interpretation of this inequality might be that the universe tends to seek levels of entropy that are higher in relation to previous levels. Technology attempts to slow the *increase* in entropy by constraining evolving systems, but there are convincing arguments given that it will never decrease total entropy (e.g., Brooks and Wiley, 1988, Chapter 2). In short, Statistics is important because disorder is here to stay.

Independent-and-Identically Distributed-Data Model

Beginning classes in Statistics (and many of the more advanced ones) always assume that observations on a phenomenon are taken under identical conditions and that each observation is taken independently of any other. The data then form a random sample [i.e., are independent and identically distributed (i.i.d.)]; standard statistical techniques can be applied to build a statistical model and to estimate the model's parameters (see, e.g., Hogg and Craig, 1978). For example, Heyl and Cook (1936) describe experiments performed between May 1934 and July 1935 to determine the acceleration of gravity in a laboratory of the National Bureau of Standards, Washington, D.C. The method used was that of the reversible pendulum; various configurations of pendulum tube diameter and type of knife edge were used. One particular configuration, taken late May/early June 1934, yielded (*after* appropriate adjustments for flexure and clock rate were made)

$$76, 82, 83, 54, 35, 46, 87, 68,$$

expressed as deviations from $980,000 \times 10^{-3}$ cm/sec², in units of 10^{-3} cm/sec² (Heyl and Cook, 1936, Table 12). That these data can be modeled as arising from a random sample is probably a fair assumption, but a later experiment performed under a different configuration yielded deviations (again after appropriate adjustments)

$$76, 76, 78, 79, 72, 68, 75, 78,$$

in units of 10^{-3} cm/sec² (Heyl and Cook, 1936, Table 8). Again these could be modeled as a random sample, but because each experiment attempted to measure the same physical constant, the data should obviously be *combined* in some way. Is it fair to model the preceding 16 numbers as observations from a random sample?

Inhomogeneous-Data Model

Lack of homogeneity in data is usually accounted for in statistical models by a nonconstant-mean assumption; often the mean is assumed to be a linear combination of several explanatory variables. However, even after these large-scale variations are accounted for, there are often reasons to suspect inhomogeneous small-scale variations.

Cressie (1982) assumes the data from the experiment (to determine the acceleration of gravity) just described to be independent realizations from statistical distributions whose means are constant but whose *variances differ* (sometimes called heteroskedasticity) markedly, depending on the configurations of pendulum tube diameter and type of knife edge. Standard one-sample theory no longer applies, but it is still possible to construct a confidence interval for the common mean, based on a weighted *t*-like statistic.

The preceding example shows a relaxation of the identical-distribution assumption. Relaxation of the independence assumption is a further obvious way to generalize statistical models, but are these more general models of any scientific value? In the pages to follow, I hope to convince the reader that the answer to this question is very definitely “Yes.”

Dependent-Data Model

Independence is a very convenient assumption that makes much of mathematical–statistical theory tractable. However, models that involve statistical dependence are often more realistic; two classes of models that have commonly been used involve intraclass-correlation structures and serial-correlation structures. These offer little scope for spatial data, where dependence is present in all directions and becomes weaker as data locations become more dispersed.

We have not yet been able to escape the three-dimensional world in which we live, nor the unidirectional flow of time through which we live. The notion that data close together, in time or space, are likely to be correlated (i.e., cannot be modeled as statistically independent) is a natural one and has been used successfully by statisticians to model physical and social phenomena. Purely temporal models, or time series models as they have come to be known (e.g., Box and Jenkins, 1970), are usually based on identically distributed observations that are dependent and occur at equally spaced time points. The unidirectional flow of time underlies the construction of these models.

Spatial models are a more recent addition to the Statistics literature. Geology, soil science, image processing, epidemiology, crop science, ecology,

forestry, astronomy, atmospheric science, or simply any discipline that works with data collected from different spatial locations, need to develop (not necessarily statistical) models that indicate when there is dependence between measurements at different locations. However, the models need to be more flexible than their temporal counterparts, because past, present, and future have no analogy in space, and furthermore it is simply not reasonable to assume that spatial locations of data occur regularly, as do most time series models.

When dealing with data where (space–time) dependencies are likely, two approaches can be contrasted. Departures from the independence paradigm could be modeled, or statistical procedures could be constructed that would be robust to these departures. Throughout this book I shall consider mostly the modeling approach.

The Weather

It is useful to consider an example that has both the temporal and spatial component in it. The weather is a universal topic of conversation (some would say it is a resort of the desperate), and among its various facets that of rainfall is paramount. To the more than one million inhabitants of South Australia, the driest state in the driest continent, drought can be devastating. In a series of papers, Cornish, with others (1936, 1954, 1958, 1961, 1976), looked at temporal and spatial aspects of 26 rainfall recording stations in South Australia, shown in Figure 1.1. Data analyzed were monthly rainfall amounts at 26 locations that had been recording for a period of 30 years or more. Thus, at any one location, the data form a typically lengthy time series (e.g., for Adelaide, the capital city of South Australia, there were 1248 monthly observations available), and at any one time point, the data are spatial and not more than 26 in number; over time and space they form a collection of approximately 20,000 observations. More recently, meteorological space–time data sets have been collected for the purposes of studying the effects of atmospheric pollution, in particular *acid rain* (see e.g., Peters and Bonelli, 1982). Daily data collection over a number of years at various locations throughout say the northeast United States, yields a massive data set. But most of it is temporal so that, spatially speaking, the data are still rather sparse. Nevertheless, spatial prediction is just as important as temporal prediction, because people living in those cities and rural districts without monitoring stations have the same right to know how little or how much their water or their air is polluted. (Section 4.6 discusses some of the issues surrounding acid rain and analyzes a spatial data set.)

Scope and Purpose

The topics covered in this book are almost exclusively related to data analysis and statistical modeling of spatial data; the basic components are spatial locations $\{s_1, \dots, s_n\}$ and data $\{Z(s_1), \dots, Z(s_n)\}$ observed at those locations. Usually the data are assumed random and sometimes the locations are

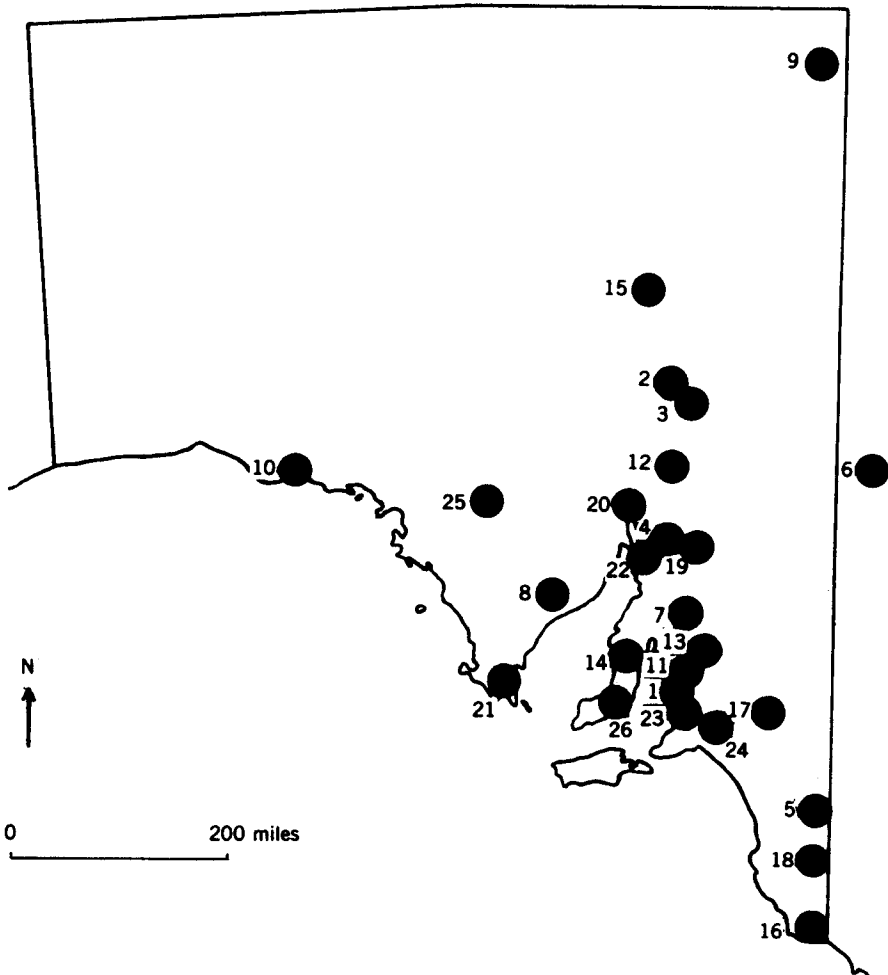


Figure 1.1 Map of South Australia showing 26 rainfall recording locations: Adelaide (1), Beltana (2), Blinman (3), Booleroo Centre (4), Bordertown (5), Broken Hill (6), Clare (7), Cleve (8), Cordillo Downs (9), Fowler's Bay (10), Gawler (11), Hawker (12), Kapunda (13), Maitland (14), Marree (15), Mount Gambier (16), Murray Bridge (17), Naracoorte (18), Peterborough (19), Port Augusta (20), Port Lincoln (21), Port Pirie (22), Stirling West (23), Strathalbyn (24), Yardea (25), Yorketown (26).

assumed random. Moreover, once the locations are given, the possibility of mistaken or imprecise positioning is generally not modeled. Some modifications to this paradigm are occasionally considered; for example, see Sections 4.4, 4.5, and 6.1.

Issues regarding the measurement, storage, and retrieval of spatial information are extremely important, although that is not the emphasis in this book. A geographic information system (GIS) is a collection of computer

software tools that facilitate, through georeferencing, the integration of spatial, nonspatial, qualitative, and quantitative data into a data base that can be managed under one system environment (e.g., Burrough, 1986). Much of the research in GIS has been concerned with computational geometry, spatial discretization, spatial languages and user interfaces, systems designs and architectures for data integration, spatial data handling approaches for alternative system architectures (such as parallel processing and neural networks), and so forth. Satellites are amassing huge amounts of data, a small fraction of which is being analyzed. This embarrassment of riches must be controlled by being selective; selectivity can be guided by the types of problems solved and the models that will be needed to solve them. Geographic information systems have only recently begun to incorporate model-based spatial analyses into their information-processing subsystems; it is hoped that this book will provide ideas for further initiatives.

Another topic that receives little attention in this book is the definition of “distance” between two sites at known locations. Mostly, I represent the two sites as vectors $\mathbf{s} = (s_1, \dots, s_d)$ and $\mathbf{u} = (u_1, \dots, u_d)$ in Euclidean space $\mathbb{R}^d$ and use the Euclidean distance, $\|\mathbf{s} - \mathbf{u}\| \equiv \{\sum_{i=1}^d (s_i - u_i)^2\}^{1/2}$, although in Section 4.6 great-arc distances are chosen instead. In any particular problem, other distances may be more appropriate, such as road miles or a measure that combines, say, travel expense, convenience, and time. These alternative metrics lead naturally to questions of *clustering* (e.g., Mardia et al., 1979, Chapter 13). For example, which regions are “close” on a “map” drawn according to the new metric? Based only on pairwise “distances” between sites, multidimensional scaling (e.g., Kruskal and Wish, 1977; Mardia et al., 1979, Chapter 14) constructs a geometric configuration of the site “locations.” A danger in the uncritical use of clustering methods for spatial data analysis is that important spatial contiguities may be violated; Legendre (1987) advocates constraining the clustering to respect these contiguities.

My principal purpose for writing this book is to make statistical theory and methods for spatial data available to scientists and engineers. I believe that the full potential of Statistics is seen in its application to substantive problems, and I have tried to reinforce this in the applications I have given throughout the book. I hope that readers will find ideas and information here that will be useful in their own areas of scientific endeavor, although I do recognize that there are large parts that may be inaccessible to all but the most theoretically inclined. Such sections have been marked with an asterisk to warn the nonstatistician to obtain help in reading them. By way of balance, those sections that are truly oriented toward applications have been marked with a dagger.

The book is divided into three parts, dealing with spatial processes indexed over continuous space (a topic sometimes referred to as geostatistics), spatial processes indexed over lattices in space (the spatial analogue of time series), and spatial point processes (including marked point processes and

random set processes). These are convenient subareas that do not exhaust all of the statistical models one might use to analyze spatial data. The next section gives some background on spatial problems and defines the general model considered in this book.

1.1 SPATIAL DATA AND SPATIAL MODELS

The first manifestations of statistics for spatial data appear to have arisen in the form of data maps. For example, Halley (1686) superimposed, onto a map of land forms, directions of trade winds and monsoons between and near the tropics, and attempted to assign them a physical cause.

Spatial models appeared much later. For example, Student (1907) was concerned with the distribution of particles throughout a liquid. Instead of analyzing their spatial positions he aggregated the data into counts of particles per unit area: A hemocytometer of area 1 mm^2 , divided into 400 squares, was used to count yeast cells. Student found that the distribution of the number of cells per square followed a Poisson distribution. (Daley and Vere-Jones, 1988, p. 8, can be consulted for a brief history of counting problems.)

R. A. Fisher was clearly aware of spatial dependence in agricultural field experiments, because he went to such great lengths to remove it (see Fisher, 1935, Chapter IV). In the 1920s and 1930s, at Rothamsted Experimental Station in England, he established the principles of randomization, blocking, and replication. As well as controlling for unwanted bias, randomization also neutralizes (but does not remove) the effect of spatial correlation (Yates, 1938; Section 5.6.2). However, it should be realized that randomization does *not* neutralize the spatial correlation at spatial scales larger or smaller than the plot dimensions.

Fairfield Smith (1938) was concerned with choosing plot dimensions so that any increase in plot size would yield little decrease in error variance. Although his analysis was empirical, the very formulation of the problem recognizes the presence of spatial correlation in field experiments. Models for such phenomena did not begin to appear until much later (Whittle, 1954).

Nearest-neighbor methods for analyzing agricultural field trials attempt to take spatial dependence into account, indirectly, by using residuals from neighboring plots as covariates, or by differencing (Papadakis, 1937; Bartlett, 1938, 1978; Wilkinson et al., 1983; Besag and Kempton, 1986). A review of these methods is given in Section 5.7.1.

Presently, Statistics can be found in any quantitative discipline, giving rise to rich variations on the theme that was played at Rothamsted 60 years ago. In areas such as geology, ecology, and environmental science, it is not often possible (nor always appropriate) to randomize, block, and replicate the data. There is a need for new statistical models and approaches that address new questions arising from old and new technologies. Many of the resulting

problems, such as resource assessment, environmental monitoring (e.g., for global warming), and medical imaging, are spatial in nature.

The General Spatial Model

Statistics, in all its guises from exploratory data analysis to asymptotic distribution theory of parameter estimators, relies on a more or less vague stochastic model. I shall present such a model for spatial data, which has a very simple structure that is flexible enough to handle an extremely large class of problems (including the ubiquitous i.i.d. case). The data may be continuous or discrete, they may be spatial aggregations or observations at points in space, their spatial locations may be regular or irregular, and those locations may be from a spatial continuum or a discrete set. At the very least, the stochastic model is used to summarize extant data or to predict unobserved data. It may or may not explain why a particular phenomenon occurs, and so should be distinguished from the more commonly accepted use of the word “model.” To many scientists, a model must have causative dynamic components, but that is not necessarily the case in this book.

Let $s \in \mathbb{R}^d$ be a generic data location in d -dimensional Euclidean space and suppose that the potential datum $Z(s)$ at spatial location s is a random quantity. Now let s vary over index set $D \subset \mathbb{R}^d$ so as to generate the multivariate random field (or random process)

$$\{Z(s): s \in D\}; \quad (1.1.1)$$

a realization of (1.1.1) is denoted $\{z(s): s \in D\}$. This “superpopulation” model for spatial data is used exclusively throughout the book, although brief discussion of a design-based approach (whose randomness is derived from sampling the deterministic process $\{z(s): s \in D\}$) is given in Section 2.3.

Usually, D is assumed to be a *fixed* (i.e., nonrandom) subset of $\mathbb{R}^d$ (see, e.g., Vanmarcke, 1983), but I shall assume more generally that D is a *random set*. Formally speaking, a random set is a measurable mapping from a probability space onto a measure space of (usually closed) subsets of $\mathbb{R}^d$ (see Section 9.3 for more details). Less formally speaking, I shall assume that D as well as Z may vary from realization to realization, giving another source of randomness to the problem. This simple structure allows me to talk about problems with continuous spatial index, problems with lattice index, spatial point patterns, and more, all under the same umbrella. Thus, the three seemingly distinct parts of this book alluded to earlier treat special cases of (1.1.1), where the index set D could be a random set. Specifically:

Part I (Chapters 2 through 5): Geostatistical data. D is a fixed subset of $\mathbb{R}^d$ that contains a d -dimensional rectangle of positive volume; $Z(s)$ is a random vector at location $s \in D$.

Part II (Chapters 6 and 7): Lattice data. D is a fixed (regular or irregular) collection of countably many points of $\mathbb{R}^d$ (this can be generalized to

where D is a graph in $\mathbb{R}^d$; see Section 6.1); $\mathbf{Z}(s)$ is a random vector at location $s \in D$.

Part III (Chapter 8): Point patterns. D is a point process in $\mathbb{R}^d$ or a subset of $\mathbb{R}^d$; $\mathbf{Z}(s)$ is a random vector at location $s \in D$. In its most general form this generates a *marked spatial point process*; when no $\mathbf{Z}$ is specified the usual spatial point process is obtained [or one could think of scalar $Z(s) \equiv 1$, for all $s \in D$].

Part III (Chapter 9): Objects. D is a point process in $\mathbb{R}^d$; $\mathbf{Z}(s)$ is *itself* a random set. This yields processes such as the Boolean model (Section 9.4) and a related cell-growth process (Section 9.7).

The flexibility of (1.1.1) is now apparent, and although it is clear that D and $\mathbf{Z}(s)$ could be even more general random quantities, the fact that D is a subset of $\mathbb{R}^d$ allows (1.1.1) to be called a *spatial process*. It is even possible to think of the ubiquitous i.i.d. (possibly multivariate) model as a 0-dimensional spatial process, because any spatial index is unimportant. I have not mentioned how the D process and the $\mathbf{Z}$ process might covary. For most of this book, one or the other is fixed so the question does not arise. When both are random, they are usually assumed to be independent, or one process is analyzed conditionally upon the observed values of the other. Spatial modeling occurs then within the $\mathbf{Z}$ process (Parts I and II), within the D process, or within both processes (Part III), and typically involves modeling the large- and the small-scale variations in terms of a finite number of parameters.

I prefer to keep (multivariate) *time-series* processes separate from spatial processes by using the index t and denoting them as

$$\{\mathbf{Z}(t): -\infty < t < \infty\}. \quad (1.1.2)$$

The unidirectional flow of time sometimes forces one to distinguish between (1.1.2) and (1.1.1) in $\mathbb{R}^1$ (see Section 6.3).

A *space-time process* will be denoted as

$$\{\mathbf{Z}(s; t): s \in D(t), t \in T\}, \quad (1.1.3)$$

where each of $\mathbf{Z}$, D , and T is possibly random. This is as general a process as will be considered in this book.

Description, Indication, and Estimation

As disciplines in Statistics mature, their statistical analyses advance through three stages of development that I describe as *description*, *indication*, and *estimation*. For the first, the goal is to summarize the data (perhaps to suggest models). For the second, estimates of model parameters are obtained from the data, but no measures of precision are available. For the third, enough distribution theory is at hand to allow (approximate) inference on the model parameters; for example, the bias and variance of an estimator can be

calculated and estimated. Statistics for spatial data is still a young discipline, showing increasing signs of maturity. I hope this book will contribute to, and be an influence on, its formative years.

1.2 INTRODUCTORY EXAMPLES

In this section, I shall present examples where data are spatial in nature. Some data sets are new and some have already appeared in the literature, although they may not have been analyzed spatially. It is not my intention to present spatial statistical analyses in this section, but rather to illustrate the range of problems that can be addressed. For some of these data, more complete analyses are carried out later in the book.

As described in Section 1.1, spatial data can be thought of as resulting from observations on the stochastic process

$$\{Z(s): s \in D\}, \quad (1.2.1)$$

where D is possibly a random set in $\mathbb{R}^d$. I shall present some special cases that are typical of spatial statistical problems one might encounter.

1.2.1 Geostatistical Data

Geostatistics (Matheron, 1962, 1963a, 1963b) emerged in the early 1980s as a hybrid discipline of mining engineering, geology, mathematics, and statistics. Its strength over more classical approaches to ore-reserve estimation is that it recognizes spatial variability at both the large scale *and* the small scale, or in statistical parlance it models both spatial trend *and* spatial correlation. Trend-surface methods (e.g., Whitten, 1970) include only large-scale variation, assuming independent errors. Watson (1972) compares the two approaches and points out that most geological problems have a small-scale variation, typically exhibiting strong positive correlation between data at nearby spatial locations. One of the most important problems in geostatistics is to predict the ore grade in a mining block from observed samples. Matheron (1963b) has called this process of prediction *kriging* (see Chapter 3).

Exploration data on coal ash (Gomez and Hazen, 1970, Tables 19 and 20) for the Robena Mine Property in Greene County, Pennsylvania, are an example of regularly spaced data in $\mathbb{R}^2$, although some locations have not been sampled or their observations are missing. Section 2.2 performs a spatial exploratory data analysis on these mining data, and kriging is carried out in Section 3.4.

The geostatistical method has found favor among soil scientists who seek to map soil properties of a field from a small number of soil samples at known locations throughout the field. For example, soil pH in water, soil

electrical conductivity, exchangeable potassium in the soil, soil–water tension, and soil–water infiltration are some of the variables that could be sampled. Water erosion is of great concern to agriculturalists, because rich topsoil can be carried away in runoff water. Some forms of tillage result in greater soil–water infiltration than others, and the study described in Section 4.3 investigates this question. The greater the infiltration, the less the runoff, resulting in less soil erosion and less stream pollution by pesticides and fertilizers. Also, greater infiltration implies better soil structure that is more conducive to crop growth. In Cressie and Horton (1987) and Section 4.3, it is explained how double-ring infiltrometers were placed at regular locations in a field that had received four tillage treatments. From these data the spatial relationships can be characterized, treatments compared, and kriging maps drawn.

There are many published sources for case studies using geostatistics, although the original data are usually not given for confidentiality reasons (original data for both of the examples just introduced are available in Sections 2.2 and 4.3, respectively). The books by David (1977, 1988), Journel and Huijbregts (1978), and Clark (1979) are all devoted to applications in the mining industry. Application of geostatistics in other areas abound; for example, in rainfall precipitation (e.g., Ord and Rees, 1979), atmospheric science (e.g., Thiebaut and Pedder, 1987), soil mapping (e.g., Burgess and Webster, 1980), and predicting groundwater contaminant concentrations (e.g., Istok and Cooper, 1988). For further applications, see the various sections of Chapter 4 that contain analyses of data sets from hydrology, soil science, public health, uniformity trials, and acid rain.

Geostatistical-type problems are distinguished most clearly from lattice- and point-pattern-type problems by the ability of the spatial index s to vary *continuously* over a subset of $\mathbb{R}^d$. That is not to say that methods from one class of problems cannot be borrowed from methods usually associated with another class; see, for example, Sections 4.4 and 7.6, where the same public-health data set is analyzed using two approaches.

1.2.2 Lattice Data

A *lattice* of locations evokes an idea of regularly spaced points in $\mathbb{R}^d$, linked to nearest neighbors, second-nearest neighbors, and so on. In this book these will be referred to as *regular* lattices, allowing for the possibility of *irregular lattices*, whose relative displacements do not follow a predictable pattern and whose linkages are not always obvious from their geometry. Of all the possible spatial structures that (1.2.1) can generate, a data set whose spatial locations are a regular lattice in $\mathbb{R}^d$ is the closest analogue to a time series observed at equally spaced time points.

Remote sensing from satellites offers an efficient means of data gathering. For example, it allows information to be gathered rapidly on weather patterns, mineral distribution, and crop acreage without having to conduct

lengthy and labor-intensive traditional surveys. Satellites orbit the earth and receive data in the form of electromagnetic reflectance waves at a number of frequencies, including those in the visible part of the spectrum. By various sampling and integration methods (see Section 7.4 for more details), the earth's surface is divided into small rectangles (e.g., 56 m $\times$ 56 m) called *pixels* (short for picture elements). An agricultural scene of interest (around, say, 34,000 km²) has certain proportions devoted to wheat, corn, soybeans, and so forth that need to be estimated. These various crops have their own reflectance properties that, together with noise, are remotely sensed. Thus the data are received as a regular lattice in $\mathbb{R}^2$ (neglecting the earth's curvature) and are identified with the centers of their respective pixels. (This is analogous to temporal problems where economic time-series data, such as yearly export earnings, are aggregated over the whole year but are identified with single, equally spaced points on the time axis.) There is a large overlap between remote-sensing techniques and (low-level) medical-imaging techniques; although the spatial scales are vastly different, the form of the data and the questions being asked are often similar. Statistical models for such data need to express the fact that observations nearby (in time or space) tend to be alike; see Section 7.4.

Sometimes it might be expected that nearby observations tend to be dissimilar. Competition between plants for light and soil nutrients could lead to large healthy plants being surrounded by less sturdy ones. Mead (1967) analyzes data on cabbages and investigates this competition effect.

In contrast to geostatistical problems, data from lattice problems may be exhaustive of the phenomenon. Of course, sampling may also occur; for example, suppose only a small window of the full data set is available.

There have been various published studies based on lattice data (although such studies have not always exploited the spatial component) that include Mercer and Hall (1911) (see also Sections 4.5 and 7.1), Batchelor and Reed (1918), Cochran (1936), Bartlett (1974), Cliff and Ord (1981), Ripley (1981), Symons et al. (1983) (see also Sections 4.4, 6.2, and 7.6), and Cressie and Chan (1989).

1.2.3 Point Patterns

Point patterns arise when the important variable to be analyzed is the location of “events.” Most often the first question to be answered is whether the pattern is exhibiting complete spatial randomness, clustering, or regularity. For example, consider the locations of longleaf pines in a natural forest in southern Georgia (given in Section 8.2). What is the biological significance of clustering of these trees? The variable, diameter at breast height, is also recorded along with the tree's location. Do large (small) trees cluster and how do large and small trees interact? The size variable is usually called a *mark variable*, and the whole process is then called a *marked spatial point process*.

But the mark variable does not have to be a real variable; it could, for example, be a set. The process then consists of $\{Z(s_i): s_i \in D\}$, D a spatial point process and $Z(s_i)$ a *random set* (Section 9.3) located at $s_i \in D$. Data from this process are often observed as a realization of

$$X = \cup \{Z(s_i): s_i \in D\}, \quad (1.2.2)$$

which is referred to as a (generalized) Boolean model (Serra, 1980) or a mosaic process (Diggle, 1981b). The data are often images, and their assimilation to a model like (1.2.2) requires higher levels of image analysis than the methods considered in Section 7.4 of Part II. The goal is to estimate parameters of the random set *and* the point process; see Cressie and Laslett (1987) and Section 9.5 where an artificially generated Boolean model of random parallelograms is analyzed. Diggle (1981b) analyzes the incidence of heather according to a Boolean model; see also Section 9.5. A model for tumor growth that iterates the Boolean model through successive stages is developed in Section 9.7. Pictures of cell islands growing *in vitro* are presented and analyzed in a manner that takes *shape* as well as size into account.

Published studies involving analyses of spatial point patterns can be found *inter alia* in Pielou (1959, 1977), Matern (1960), Getis and Boots (1978), Marquiss et al. (1978), Ripley (1981), Diggle (1983), and Upton and Fingleton (1985). Of course, there is a large overlap of methods for patterns occurring in space and for those occurring in time; the reader interested in *temporal* methods is referred to Cox and Lewis (1966), the articles in Lewis (1972) (in particular the review by Daley and Vere-Jones, 1972), Cox and Isham (1980), and Daley and Vere-Jones (1988). A second-moment measure of spatial point patterns is adapted for the temporal animal-behavior data in Section 8.4.

1.3 STATISTICS FOR SPATIAL DATA: WHY?

Some simple spatial models will be given to show the effect of correlation on estimation, prediction, and design. The models allow closed-form expressions to be calculated, from which discussion of more general issues can be initiated.

Estimation

Consider the following simple statistical model, taught in all beginning Statistics service courses. Suppose $Z(1), \dots, Z(n)$ are independent and identically distributed (i.i.d.) from a Gaussian (i.e., normal) distribution with unknown mean μ and known variance σ_0^2 . The minimum-variance unbiased

estimator of μ is

$$\bar{Z} \equiv \sum_{i=1}^n Z(i)/n, \quad (1.3.1)$$

and inference on μ is straightforward: The estimator $\bar{Z}$ is Gaussian with mean μ and variance σ_0^2/n . Thus, a two-sided 95% confidence interval for μ is

$$(\bar{Z} - (1.96)\sigma_0/\sqrt{n}, \bar{Z} + (1.96)\sigma_0/\sqrt{n}). \quad (1.3.2)$$

Instead of independent data, now suppose the data are positively correlated with a correlation that decreases as the separation between data increases:

$$\text{cov}(Z(i), Z(j)) = \sigma_0^2 \cdot \rho^{|i-j|}, \quad i, j = 1, \dots, n, 0 < \rho < 1. \quad (1.3.3)$$

It is well known that such a correlation function results from a first-order autoregressive process $Z(i) = \rho Z(i-1) + \epsilon(i)$, $i \geq 1$, where $\epsilon(i)$ is part of an i.i.d. sequence of Gaussian random variables with zero mean and variance $\sigma_0^2(1 - \rho^2)$ and is independent of $Z(i-1)$; see, e.g., Fuller (1976, Section 2.3). However, that is *not* the generating mechanism I have in mind; here, $Z \equiv (Z(1), \dots, Z(n))'$ are *spatial* data in $\mathbb{R}^1$ from which prediction of $Z(0)$ or $Z(3/2)$ is just as appropriate as that of $Z(n+1)$.

Now,

$$\begin{aligned} \text{var}(\bar{Z}) &= n^{-2} \left\{ \sum_{i=1}^n \sum_{j=1}^n \text{cov}(Z(i), Z(j)) \right\} \\ &= \{\sigma_0^2/n\} \left[1 + 2\{\rho/(1-\rho)\}\{1 - (1/n)\} \right. \\ &\quad \left. - 2\{\rho/(1-\rho)\}^2(1 - \rho^{n-1})/n \right]. \end{aligned} \quad (1.3.4)$$

For $n = 10$ and $\rho = 0.26$, $\text{var}(\bar{Z}) = \{\sigma_0^2/10\}[1.608]$, and a two-sided 95% confidence interval for μ is

$$(\bar{Z} - (2.485)\sigma_0/\sqrt{10}, \bar{Z} + (2.485)\sigma_0/\sqrt{10}).$$

Thus, failure to realize the presence of positive correlation in the data leads to a confidence interval (1.3.2) that is *too narrow*; for $n = 10$ and $\rho = 0.26$, the actual coverage probability of (1.3.2) is 87.8%, not 95%. [If $-1 < \rho < 0$, (1.3.2) would be too wide, but because positive spatial dependence is seen more often, these introductory remarks concentrate on situations where ρ is positive.]

Some intuitive understanding of the effect of spatial correlation can be obtained from (1.3.4). Write it as

$$\text{var}(\bar{Z}) = \sigma_0^2/n', \quad (1.3.5)$$

where

$$n' \equiv n / \left\{ 1 + 2\{\rho/(1-\rho)\}\{1 - (1/n)\} - 2\{\rho/(1-\rho)\}^2(1 - \rho^{n-1})/n \right\} \quad (1.3.6)$$

can be interpreted as the *equivalent number of independent observations* (see Section 4.6.2). If $n = 10$ and $\rho = 0.26$, then $n' = 6.2$; that is, 6 independent observations achieve approximately the same precision as 10 correlated observations [correlated according to (1.3.3) with $\rho = 0.26$]. For large n , $n' \approx n/[(1+\rho)/(1-\rho)]$, showing that correlation has an effect on inferences even in large samples.

Spatial models, more complicated than (1.3.3), show the same general behavior. Haining (1988) considers constant-mean Gaussian models in $\mathbb{R}^2$ that are conditionally specified autoregressions (Section 6.6), and simultaneously specified autoregressions and moving averages (Section 6.7.1), each with an unknown variance parameter σ^2 . He compares the variance of $\bar{Z}$ assuming independence, with the variance of $\bar{Z}$ assuming positive dependence; he also compares the latter with the variance of the maximum likelihood estimator $\hat{\mu}$ of the constant mean μ . In general, classical inference based on $\bar{Z}$ and $\hat{\sigma}^2/n$ is misleading; for positive spatial dependence, $\widehat{\text{var}}(\bar{Z})$ and $\widehat{\text{var}}(\hat{\mu})$ are typically much larger than $\hat{\sigma}^2/n$.

Grenander (1954) demonstrates that, for a class of time-series models that includes (1.3.3), $\bar{Z}$ and the maximum likelihood estimator

$$\hat{\mu} = \left\{ Z(1) + (1-\rho) \sum_{i=2}^{n-1} Z(i) + Z(n) \right\} / \{n - (n-2)\rho\}$$

(which is also the minimum variance unbiased estimator) have the same asymptotic (100%) efficiency as $n \rightarrow \infty$. Does this contradict the preceding calculations? No, because there, inference for μ was based on $\bar{Z}$ and σ_0^2/n , and was found to be invalid. Grenander's result allows one to conclude that inference based on $\bar{Z}$ and σ_0^2/n' [n' is given by Eq. (1.3.6)] is not only valid but is also asymptotically *efficient*. General models for which this happens are given by Grenander and Rosenblatt (1984, Section 7.4), and they include stationary autoregressive time series.

Prediction

Suppose now that an unknown observation $Z(n+1)$ is to be *predicted* from data $\mathbf{Z} \equiv (Z(1), \dots, Z(n))'$, where it is assumed $Z(1), \dots, Z(n), Z(n+1)$ are jointly Gaussian, identically distributed with unknown mean μ and known variance σ_0^2 , and *independent*. From Section 3.2, the predictor $p(\mathbf{Z}; n+1)$ that satisfies the unbiasedness condition $E(p(\mathbf{Z}; n+1)) = \mu$ and minimizes

the mean-squared prediction error

$$E(Z(n+1) - p(\mathbf{Z}; n+1))^2 \quad (1.3.7)$$

is

$$p_0(\mathbf{Z}; n+1) = \bar{Z}, \quad (1.3.8)$$

the sample mean. The minimized mean-squared prediction error is

$$ms_0 = \sigma_0^2 \{1 + (1/n)\}. \quad (1.3.9)$$

When the independence assumption is replaced with (1.3.3), the unbiased predictor that minimizes the mean-squared prediction error (1.3.7) is

$$\begin{aligned} p_\rho(\mathbf{Z}; n+1) \\ = \rho Z(n) + (1-\rho) \frac{\{Z(1) + (1-\rho)\sum_{i=2}^{n-1} Z(i) + Z(n)\}}{\{n - (n-2)\rho\}}; \end{aligned} \quad (1.3.10)$$

see Section 3.2. Abbreviate (1.3.10) to $p_\rho(\mathbf{Z})$. Notice that $\rho = 0$ in (1.3.10) yields (1.3.8). If $\bar{Z}$ is used instead of (1.3.10), the mean-squared prediction error is

$$\begin{aligned} E(Z(n+1) - \bar{Z})^2 \\ = \sigma_0^2 \left\{ 1 + (1/n) \left[1 + 2\{\rho/(1-\rho)\} \{\rho^n - (1/n)\} \right. \right. \\ \left. \left. - 2\{\rho/(1-\rho)\}^2 (1 - \rho^{n-1})/n \right] \right\}. \end{aligned} \quad (1.3.11)$$

For $n = 10$ and $\rho = 0.26$, (1.3.11) is $\sigma_0^2\{1.09051\}$. Compare this to (1.3.9), which is $\sigma_0^2\{1.1\}$: The difference is not large. Indeed, when spatial correlations decay geometrically with distance, classical prediction intervals are often approximately *valid*. However, they can be highly *inefficient*.

Assuming the dependence model given by (1.3.3), the minimized mean-squared prediction error is obtained by calculating (1.3.7) with optimal predictor (1.3.10). That is,

$$ms_\rho = \sigma_0^2 \left[1 - \rho^2 + \{(1-\rho)^2(1+\rho)/(n - (n-2)\rho)\} \right]; \quad (1.3.12)$$

see Section 3.2. Notice that $\rho = 0$ in (1.3.12) yields (1.3.9).

For $n = 10$ and $\rho = 0.26$, (1.3.12) is $\sigma_0^2\{1.01952\}$. Thus a 95% prediction interval for $Z(n+1)$, based on the optimal predictor (1.3.10), is

$$\left(p_\rho(\mathbf{Z}) - (1.96)\sigma_0\{1.01952\}^{1/2}, p_\rho(\mathbf{Z}) + (1.96)\sigma_0\{1.01952\}^{1/2} \right). \quad (1.3.13)$$

This should be compared to the *wider* 95% prediction interval for $Z(n+1)$ based on $\bar{Z}$:

$$(\bar{Z} - (1.96)\sigma_0\{1.09051\}^{1/2}, \bar{Z} + (1.96)\sigma_0\{1.09051\}^{1/2}). \quad (1.3.14)$$

For large n , the squared ratio of the prediction-interval width from using $p_\rho(\mathbf{Z})$ to that from using $\bar{Z}$ is approximately $1 - \rho^2$, which is a measure of the (asymptotic) efficiency of inference based on $\bar{Z}$ versus inference based on the optimal predictor $p_\rho(\mathbf{Z})$. Thus, for $\rho = 0.26$ the efficiency measure is 93% and for $\rho = 0.5$ it is 75%.

Experimental Design

Another example of the importance of exploiting spatial correlation is in the area of experimental design. Suppose that experimental units are laid out in a $t \times b$ array made up of b blocks (columns), each with t units in them. Units that are most alike are put in the same block so that all of the gross heterogeneity occurs between blocks. Suppose further that t treatments are to be compared as follows. A response variable is measured after applying the treatments to experimental units in such a way that each treatment appears exactly once in each block. A design (i.e., an allocation of treatments to units) of the type just described is known as a *complete block design*.

In papermaking, toward the end of the process when the paper is still a continuous sheet in a roll (that is typically 10 ft wide and 3×10^4 ft long), the sheet is *calendered*. A calender is a stack of two or more hard smooth rollers through which the paper is passed, whose purpose is to reduce the caliper of the sheet (so making it more dense) and increase the smoothness of the sheet. In calendering, high compressive stresses are used to make a more compact, thinner sheet with a smoother surface. In terms of basic smoothness and thickness, most of the variation is across the width of the paper roll. Therefore, any experiment on calender treatments (e.g., number and degree of smoothness of calender rolls, temperature of the sheet) has to take this into account, as well as the possible spatial correlation running the length of the sheet.

A well designed calendering experiment in the laboratory should split the sheet into several narrower sheets (e.g., each of width 2 ft), allowing these to form the blocks of the experiments. Within the blocks, pages closer together will tend to be more alike (in terms of gloss or caliper) than those further apart, and this can be modeled with (one-dimensional) spatial correlation. Therefore, when a calender treatment is applied to a “page,” its location within the block should be useful information for performing an efficient analysis.

Let the response on the i th unit of the j th block be $Y_{ij(k)}$, $i = 1, \dots, t$, $j = 1, \dots, b$, $k = 1, \dots, t$, where k denotes the treatment assigned (according to the design) to that unit. Assume an additive model

$$Y_{ij(k)} = \mu + \alpha_k + \beta_j + \delta(i, j), \quad (1.3.15)$$

where $\delta(\cdot, \cdot)$ is a Gaussian error process with zero mean. Further, assume independence of the δ s between blocks but spatial dependence (1.3.3) down blocks. That is,

$$\text{cov}(\delta(i, j), \delta(i', j')) = \begin{cases} 0, & j \neq j', \\ \sigma^2 \rho^{|i-i'|}, & j = j', \end{cases} \tag{1.3.16}$$

where $|\rho| < 1$.

A goal of experimental design is to find the allocation of treatments to units that will give the most precise estimates of (estimable) treatment effects, $\tau_k \equiv \alpha_k - (\sum_{l=1}^t \alpha_l / t)$, $k = 1, \dots, t$. Specifically, one might minimize

$$A \equiv \sum_{1 \leq k < l \leq t} \text{var}(\hat{\tau}_k - \hat{\tau}_l) / \binom{t}{2}, \tag{1.3.17}$$

where $\{\hat{\tau}_k: k = 1, \dots, t\}$ are the generalized-least-squares estimators of the treatment effects (see Section 5.6.2). Gill and Shukla (1985a) find that *first-order nearest-neighbor (NN) balanced* designs, whose end units satisfy further balance conditions, are optimal designs. First-order NN balanced means that the number of times two treatments appear adjacent in a block is constant for every possible pair of treatments. For example, consider $t = 10$ and $b = 5$; then Table 1.1 shows an assignment of treatments $0, 1, \dots, 9$ within the five blocks that is a first-order NN balanced design.

Let A_O , A_N , and A_R denote the value of (1.3.17) for, respectively, the optimal design, the design in Table 1.1, and a randomized complete block design. Table 1.2 shows relative efficiencies (to two decimal places) for different values of ρ in (1.3.16).

Table 1.1 Example of a First-Order NN Balanced Complete Block Design

Blocks				
1	2	3	4	5
1	2	0	3	9
2	3	1	4	0
0	1	9	2	8
3	4	2	5	1
9	0	8	1	7
4	5	3	6	2
8	9	7	0	6
5	6	4	7	3
7	8	6	9	5
6	7	5	8	4

Source: Grondona and Cressie (1992).

Table 1.2 Relative Efficiencies of the First-Order NN Balanced Design Given in Table 1.1 (A_O/A_N), and a Randomized Complete Block Design (A_O/A_R)

	ρ						
	-0.75	-0.50	-0.25	0	0.25	0.50	0.75
A_O/A_N	1.00	1.00	1.00	1.00	1.00	1.00	1.00
A_O/A_R	0.33	0.67	0.92	1.00	0.87	0.63	0.36

Source: Grondona and Cressie (1992).

Optimal designs may not exist; first-order NN balanced designs are relatively easier to construct and appear to be (almost) as efficient as the optimal designs. Further, from Table 1.2, randomized complete block designs can be grossly inefficient when $|\rho| \geq 0.5$. More general spatial correlation structures are considered in Grondona and Cressie (1992) and Section 5.6.2; the same efficiency patterns emerge.

There is often a big difference between what scientists and engineers *should* do to obtain statistical optimality and what they do in practice. Randomized complete block designs may be inefficient, but they are very, very easy to construct. In Section 5.7, it is shown how to recover some of the lost efficiency after the inefficient (nonspatial) design is used. My preference is for a spatial modeling approach, such as the one described in Section 5.7.2 and in Grondona and Cressie (1991): The strategy there is to estimate and model the spatial correlation from (median-polish) residuals, and then to use generalized-least-squares estimates of the treatment effects $\{\tau_k: k = 1, \dots, t\}$. An artificial experiment is constructed by adding treatment effects (according to a randomized complete block design) to spatially correlated uniformity data; the spatial analysis yields gains in efficiency of over 30%.

In many applications of Statistics to problems that are inherently spatial, data are observational rather than the result of a controlled experiment. Thus, the opportunity to randomize, block, and replicate is often not available. In these circumstances, the model fitted to the data may implicitly assume that some uncontrolled-for effects or interactions are zero. Hopefully, such assumptions are based on prior knowledge of the phenomenon and not on mathematical convenience. Wiens et al. (1986) report an interesting seven-year study of territorial locations, territorial sizes, and breeding densities within bird-breeding areas in central Oregon. They manipulated the habitat composition and structure by removing 75%, 50%, 25%, and 0% of the shrubs from 625-m² blocks in a checkerboard design. A nearby, unaltered area served as the control. In spite of the elaborate experiment, the authors expressed concern about uncontrollable factors such as site tenacity by breeding adults and about the appropriateness of the spatial scale on which the manipulation was conducted. In fact, these same concerns are relevant to *all* designed experiments; it is simply a question of degree.

Linear Models with Spatially Dependent Error

Suppose the spatial data $Z(s_1), \dots, Z(s_n)$, observed at spatial locations $\{s_1, \dots, s_n\}$, are modeled as a collection of random variables, generated by the random process

$$Z(s) = \sum_{l=1}^q \beta_l x_l(s) + \delta(s), \quad s \in D \subset \mathbb{R}^d, \quad (1.3.18)$$

where $\{x_l(\cdot): l = 1, \dots, q\}$ is a collection of q nonrandom explanatory variables that may or may not depend on spatial location and $\delta(\cdot)$ is a zero-mean finite-variance error process that may or may not be spatially correlated.

For example, the model with constant mean μ and covariances given by (1.3.3) is a special case of (1.3.18) in $\mathbb{R}^1$, with just one explanatory variable $x_1(\cdot) \equiv 1$, $\beta_1 \equiv \mu$, and $\text{cov}(\delta(u), \delta(v)) = \sigma_0^2 \cdot \rho^{|u-v|}$, $u, v \in \mathbb{R}^1$. Also, the complete-block-design model (1.3.15) and (1.3.16) is a special case of (1.3.18) in $\mathbb{R}^2$, where explanatory variables are $x_1(\cdot) \equiv 1$, $x_{k+1}(i, j) = 1$ if the (i, j) th plot receives the k th treatment and zero otherwise ($k = 1, \dots, t$), and $x_{l+t+1}(i, j) = 1$ if $j = l$ and zero otherwise ($l = 1, \dots, b$). The error process has anisotropic spatial correlation given by (1.3.16), specifying correlation within blocks but not between blocks.

It is helpful to write the observations as $\mathbf{Z} \equiv (Z(s_1), \dots, Z(s_n))'$ and the model given by (1.3.18) in matrix and vector notation. That is,

$$\mathbf{Z} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\delta}, \quad (1.3.19)$$

where $\mathbf{X}$ is an $n \times q$ matrix whose (i, j) th element is $x_j(s_i)$, $\boldsymbol{\beta} \equiv (\beta_1, \dots, \beta_q)'$, and $\boldsymbol{\delta} \equiv (\delta(s_1), \dots, \delta(s_n))'$.

Often (although not always), the parameters of greatest interest are the “large-scale-variation” parameters $\boldsymbol{\beta}$. For the moment, assume that any “small-scale-variation” parameters associated with the error process $\delta(\cdot)$ are known. That is, one can obtain

$$\text{var}(\boldsymbol{\delta}) = \boldsymbol{\Sigma}, \quad (1.3.20)$$

where $\boldsymbol{\Sigma}$ is a known $n \times n$, symmetric, nonnegative-definite matrix.

To keep the exposition simple, in all that is to follow, I shall assume that the regression coefficients $\boldsymbol{\beta}$ are estimable, $\boldsymbol{\Sigma}$ is invertible, and matrix inverses exist whenever I need them. Generalizations of this simple paradigm can be found, for example, in Searle (1971), Section 5.8.

Suppose the goal is efficient *estimation* of $\boldsymbol{\beta}$. [Efficient *prediction* of an unknown $Z(s_0)$ is another possible goal; see Chapter 3.] The best linear unbiased estimator of $\boldsymbol{\beta}$ is also the *generalized-least-squares* (g.l.s.) estimator

(Aitken, 1935), that is, the value of β that minimizes

$$(\mathbf{Z} - \mathbf{X}\beta)' \Sigma^{-1} (\mathbf{Z} - \mathbf{X}\beta). \quad (1.3.21)$$

It is

$$\hat{\beta}_{\text{gls}} = (\mathbf{X}' \Sigma^{-1} \mathbf{X})^{-1} \mathbf{X}' \Sigma^{-1} \mathbf{Z}, \quad (1.3.22)$$

which is also the maximum likelihood estimator if $\delta(\cdot)$ is a Gaussian process. The variance matrix of (1.3.22) is

$$\text{var}(\hat{\beta}_{\text{gls}}) = (\mathbf{X}' \Sigma^{-1} \mathbf{X})^{-1}. \quad (1.3.23)$$

When $\Sigma = \sigma^2 I$, which it is under classical (nonspatial) assumptions of i.i.d. errors, (1.3.21) reduces to $(\mathbf{Z} - \mathbf{X}\beta)'(\mathbf{Z} - \mathbf{X}\beta)/\sigma^2$. Then the appropriate minimizer is

$$\hat{\beta}_{\text{ols}} = (\mathbf{X}' \mathbf{X})^{-1} \mathbf{X}' \mathbf{Z}, \quad (1.3.24)$$

which is the *ordinary-least-squares* (o.l.s.) estimator of β . However, when $\Sigma \neq \sigma^2 I$ [e.g., Σ has entries given by (1.3.16)], the o.l.s. estimator is often inefficient. Specifically,

$$\text{var}(\hat{\beta}_{\text{ols}}) = (\mathbf{X}' \mathbf{X})^{-1} (\mathbf{X}' \Sigma \mathbf{X}) (\mathbf{X}' \mathbf{X})^{-1} \quad (1.3.25)$$

and the difference $\text{var}(\hat{\beta}_{\text{ols}}) - \text{var}(\hat{\beta}_{\text{gls}})$ is nonnegative-definite (e.g., Searle, 1971, Section 3.3). Notice that when $\Sigma = \sigma^2 I$, the difference is 0.

Because the o.l.s. estimator (1.3.24) does not require knowledge of Σ , considerable research effort has been devoted to finding conditions on $\mathbf{X}$ and Σ for which o.l.s. and g.l.s. are equally efficient or for which o.l.s. and g.l.s. estimators are the same. Zyskind (1967) derives eight equivalent necessary and sufficient conditions for the latter to happen; for example, one such condition is $\mathbf{X}(\mathbf{X}' \mathbf{X})^{-1} \mathbf{X}' \Sigma = \Sigma \mathbf{X}(\mathbf{X}' \mathbf{X})^{-1} \mathbf{X}'$, which occurs if and only if Σ is of the form $a^2 I + P_1 A P_1 + P_2 B P_2$, where $P_1 = \mathbf{X}(\mathbf{X}' \mathbf{X})^{-1} \mathbf{X}'$ and $P_2 = I - P_1$.

However, care should be taken. Just because o.l.s. and g.l.s. yield the same estimators, it cannot be assumed that all inference can proceed as if $\Sigma = \sigma^2 I$. Indeed, under Zyskind's conditions, $\text{var}(\hat{\beta}_{\text{ols}}) = \text{var}(\hat{\beta}_{\text{gls}}) = (\mathbf{X}' \Sigma^{-1} \mathbf{X})^{-1}$, which depends on Σ . Therefore, from a total-inference point of view, results on the equivalence of o.l.s. and g.l.s. are not all that helpful. Moreover, except for a few special cases, spatial linear models like (1.3.18) generally give rise to matrices $\mathbf{X}$ and Σ that do *not* satisfy Zyskind's conditions. [Kramer and Donneringer, 1987, give one of these special cases when $\delta(\cdot)$ is a spatial autoregressive process of the type described in Section 6.7.2. Curiously, they show that o.l.s. can be as *efficient* as g.l.s. when the spatial-

dependence parameter in $\delta(\cdot)$ tends to its largest possible value.] The generally poor performance of classical statistical-inference procedures in the presence of spatial dependence (see, e.g., the simple examples above; Cliff and Ord, 1981, Chapter 7; Dow et al., 1982; Anselin and Griffith, 1988) and the ubiquity of such spatial dependence, demonstrate why Statistics for spatial data should be part of every statistician's repertoire.

Valid Spatial Models

In reality, Σ is unknown; typically it will depend on parameters θ obtained from a spatial parametric covariance model $C(\mathbf{u}, \mathbf{v}; \theta) \equiv \text{cov}(\delta(\mathbf{u}), \delta(\mathbf{v}))$, $\mathbf{u}, \mathbf{v} \in D \subset \mathbb{R}^d$. For example, assuming homoskedasticity, one parameter will certainly be $\sigma^2 \equiv \text{var}(\delta(\mathbf{u}))$. Let $\Sigma(\theta)$ denote the $n \times n$ variance matrix $\text{var}(\mathbf{Z})$ whose (i, j) th element is $C(\mathbf{s}_i, \mathbf{s}_j; \theta)$.

Choice of an appropriate model can be a difficult task because one must take care to use valid models; that is, use only those θ for which $\sum_{i=1}^m \sum_{j=1}^m a_i C(\mathbf{u}_i, \mathbf{u}_j; \theta) a_j \geq 0$, for any m , any sequence of real numbers $\{a_i: i = 1, \dots, m\}$, and any sequence of spatial locations $\{\mathbf{u}_i: i = 1, \dots, m\}$. For example, a valid covariance model in $\mathbb{R}^1$ is $C(\mathbf{s}_i, \mathbf{s}_j; \theta) = C_T(|\mathbf{s}_i - \mathbf{s}_j|; \theta)$, the "tent" covariogram

$$C_T(h; \theta) \equiv \begin{cases} \sigma^2 \left(1 - \frac{|h|}{\theta}\right), & 0 \leq |h| \leq \theta, \\ 0, & |h| > \theta. \end{cases}$$

However, in $\mathbb{R}^2$, $C(\mathbf{s}_i, \mathbf{s}_j; \theta) \equiv C_T(\|\mathbf{s}_i - \mathbf{s}_j\|; \theta)$ is *not* a valid model; see Section 2.5.1 for a counterexample. On the other hand, if the spatial model for data $\mathbf{Z} = (Z(\mathbf{s}_1), \dots, Z(\mathbf{s}_n))'$ has sufficient measurement error so that $\Sigma(\theta)$ is diagonally dominant, that is, if

$$C(\mathbf{s}_i, \mathbf{s}_i; \theta) \geq \sum_{\substack{j=1 \\ j \neq i}}^n |C(\mathbf{s}_i, \mathbf{s}_j; \theta)|, \quad i = 1, \dots, n,$$

then $\Sigma(\theta)$ is always nonnegative-definite (Varga, 1962, p. 22ff) and hence a valid model is obtained. In the preceding simple examples, the models (1.3.3) and (1.3.16) are valid provided the parameter $\rho \in (-1, 1)$.

Questions of validity of the various spatial models presented in this book will be dealt with as they arise. It is important to ensure that the parameter space Θ of θ consists only of valid models, and that an estimate $\hat{\theta}$ of θ belongs to Θ .

Estimated Generalized Least Squares

Assume that the spatial dependence parameter θ is contained in a known parameter space Θ , any member of which yields a valid spatial model. Any estimator $\hat{\theta}$ will be assumed to belong to Θ , with probability 1.

Estimated generalized-least-squares (e.g.l.s.) estimators are obtained by substituting $\Sigma(\hat{\theta})$ for $\Sigma(\theta)$ in (1.3.22):

$$\hat{\beta}_{\text{egls}} = \left(X' \Sigma(\hat{\theta})^{-1} X \right)^{-1} X' \Sigma(\hat{\theta})^{-1} Z, \quad (1.3.26)$$

where $\hat{\theta}$ is an estimator of the small-scale-variation parameters θ .

Prediction of an unknown $Z(s_0)$ proceeds in a similar way, often by assuming that the estimated value $\hat{\theta}$ is the true value (Chapter 3). The consequences of this assumption are investigated in Section 5.3.

Two different approaches are often employed to obtain $\hat{\theta}$. If the probability density (or mass) function of Z is completely specified as $f(z; \beta, \theta)$, then the likelihood

$$l(\beta, \theta) \equiv f(Z; \beta, \theta)$$

can be maximized with respect to β and θ to yield estimators $\hat{\beta}$ and $\hat{\theta}$. Then (1.3.26) is the maximum likelihood (m.l.) estimator of $\hat{\beta}_{\text{gls}}$. Sections 7.2 and 7.3 deal mainly with this approach.

A second possibility is to obtain an initial estimate of β (e.g., $\hat{\beta}_{\text{ols}}$), construct residuals

$$R \equiv Z - X \hat{\beta}_{\text{ols}}, \quad (1.3.27)$$

and, using these residuals as a proxy for δ , estimate θ free from the presence of β . This method is often employed in a semiparametric setting where the joint distribution of Z is not specified, but the mean $X\beta$ and the variance $\Sigma(\theta)$ are specified. Then, $\hat{\theta}$ can be obtained from an approximate method-of-moments approach based on R (Section 2.6.2). From $\hat{\theta}$ and (1.3.26), $\hat{\beta}_{\text{egls}}$ is obtained. One then has the option of substituting this estimate back into (1.3.27) to obtain a new R , a new $\hat{\theta}$, and a new $\hat{\beta}_{\text{egls}}$, and so forth. Terminating at this second step yields a two-stage estimation procedure.

The example considered throughout this section [Z Gaussian with covariances defined by (1.3.3)] satisfies the conditions of Mardia and Marshall's (1984) theorem given in Section 7.3.1. Hence, for $\theta = (\sigma^2, \rho)$ and $\hat{\theta}$ its m.l. estimator, $\hat{\beta}_{\text{egls}}$ given by (1.3.26) is asymptotically Gaussian with mean β and variance matrix $(X' \Sigma(\theta)^{-1} X)^{-1}$ and is asymptotically independent from $\hat{\theta}$. However, for small sample sizes, the m.l. estimators of the small-scale-variation parameters are notoriously biased. A review of results for the model (1.3.3) can be found in Dielman and Pfaffenberger (1989), together with small-sample simulations and recommendations.

The exact variance of $\hat{\beta}_{\text{egls}}$ is difficult to compute because Z appears in (1.3.26) nonlinearly. Preliminary tests on θ (see Section 7.3.1) are often employed to determine whether g.l.s. (actually, e.g.l.s.) will be used in preference to o.l.s. Intuitively, as sample size increases, e.g.l.s. will be indistinguishable from g.l.s., provided $\hat{\theta}$ is a consistent estimator of θ .

Williams (1975) can be consulted for results that formalize this intuition. In finite samples, terms of smaller orders of magnitude can improve the asymptotic distribution of $\hat{\beta}_{\text{egls}}$ (e.g., Rothenberg, 1984; Grubb and Magee, 1988). Asymptotics in spatial problems can be of the infill type (Sections 2.6 and 5.8) or of the increasing-domain type (Section 7.3). Statisticians and probabilists are most familiar with the latter; indeed, all of the asymptotic results mentioned in this section are for increasing domains.

Some interesting finite-sample results that establish inequalities between $E(\widehat{\text{var}}(\mathbf{c}'\hat{\beta}_{\text{gls}}))$, $\text{var}(\mathbf{c}'\hat{\beta}_{\text{gls}})$, and $\text{var}(\mathbf{c}'\hat{\beta}_{\text{egls}})$ are proved by Harville (1985) and Eaton (1985). For example, Harville shows that if $\hat{\theta}$ is an even, translation-invariant estimator, and the data are Gaussian, then

$$\text{var}(\mathbf{c}'\hat{\beta}_{\text{gls}}) \leq \text{var}(\mathbf{c}'\hat{\beta}_{\text{egls}}), \quad (1.3.28)$$

for all $\mathbf{c} \in \mathbb{R}^q$. Using a matrix form of Jensen's inequality, Eaton shows that if $E(\Sigma(\hat{\theta})) = \Sigma(\theta)$, then

$$E(\widehat{\text{var}}(\mathbf{c}'\hat{\beta}_{\text{gls}})) \leq \text{var}(\mathbf{c}'\hat{\beta}_{\text{gls}}), \quad (1.3.29)$$

where $\widehat{\text{var}}(\mathbf{c}'\hat{\beta}_{\text{gls}})$ is $\mathbf{c}'(X'\Sigma(\hat{\theta})^{-1}X)^{-1}\mathbf{c}$, the often used estimator of $\text{var}(\mathbf{c}'\hat{\beta}_{\text{gls}})$; see (1.3.23). Although for $\hat{\theta}$ a consistent estimator of θ the three quantities in (1.3.28) and (1.3.29) are asymptotically indistinguishable, the inequalities show that, as an estimator of $\text{var}(\mathbf{c}'\hat{\beta}_{\text{egls}})$, $\widehat{\text{var}}(\mathbf{c}'\hat{\beta}_{\text{gls}})$ has potentially two sources of negative bias. Harville and Jeske (1992) investigate estimators of $\text{var}(\mathbf{c}'\hat{\beta}_{\text{egls}})$ that attempt to correct for this bias.

Spatial Data Analysis and Modeling: A Summary

- All data have a more-or-less precise spatial and temporal label associated with them. A purely spatial model usually has no causative component in it; such models are useful when a space–time process has reached temporal equilibrium (e.g., ore deposition), or when short-term causal effects are aggregated over a fixed time period (e.g., final presidential election returns from the states of the United States).
- Whether the spatial labels are thought to be an important part of the modeling and analysis of the data is a concern that should be addressed problem by problem.
- Data that are close together in space (and time) are often more alike than those that are far apart. A spatial model incorporates this spatial variation into the generating mechanism, in contrast to a nonspatial model.
- It is almost always true that the classical, nonspatial model is a special case of a spatial model, and so the spatial model is more general (space–time models are even more general).

- Whether one chooses to model the spatial variation through the (nonstochastic) mean structure (called large-scale variation throughout the book) or the stochastic-dependence structure (called small-scale variation) depends on the underlying scientific problem, and can sometimes be simply a trade-off between model fit and parsimony of model description. What is one person's (spatial) covariance structure may be another person's mean structure.
- Explanatory variables (suggested by the problem under investigation) should be included in the mean structure first, and great care should be taken to find all of them. A missed variable that is itself varying spatially will contribute to the spatial dependence, as can a misspecification of the functional relationship between the independent and explanatory variables. As a consequence, a model that includes a spatial-dependence component pays a low-cost premium that insures against misspecification of the mean structure (e.g., Dubin, 1988).
- Having allowed for explanatory variables, models with spatial dependence typically have a more parsimonious description than classical trend-surface models. They also have more stable spatial extrapolation properties and yield more efficient estimators of explanatory-variable effects.

Some Final Remarks

The simple examples presented in this chapter serve to illustrate a general principle in all of Statistics, namely that inferences can depend crucially on assumptions. In situations such as for spatial or temporal data, where it is often more realistic to abandon the independence assumption, classical inferences can be very misleading. Stephan (1934) saw this very clearly in problems dealing with social data; he wrote

...Data of geographic units are tied together, like bunches of grapes, not separate, like balls in an urn. Of course, mere contiguity in time and space does not of itself indicate lack of independence between units in a relevant variable or attribute, but in dealing with social data, we know that by virtue of their very *social* character, persons, groups and their characteristics are interrelated and not independent. Sampling error formulas may yet be developed which are applicable to these data, but until then the older formulas must be used with great caution. Likewise, other statistical measures must be carefully scrutinized when applied to these data

In the last 40 years, considerable attention has been devoted to concerns of the type expressed by Stephan; see Section 5.6.1 for a brief review.

Among the exact sciences, it is often believed that the only source of variability is measurement error, which is usually modeled as a white-noise random process. In my opinion, this viewpoint is far too simplistic, and could lead to important small-scale (spatial or nonspatial) effects being missed.

Problems in the earth sciences, ecology, soil science, hydrology, and so on can provide the statistician with a considerable challenge. Often studies are observational rather than designed, and there is no replication because there is just one unit: the earth! Nevertheless, explanations for various phenomena can be conjectured and their consistency across time or space can be assessed. But, what is the source of random variation in the spatial models (and temporal models, for that matter) proposed? A standard tactic in science is that when there are infinitely many possible data values from which to choose, those possibilities are dealt with statistically. With no data, but with experience in the way, say, oilfields of a particular type behave, one might assume that a spatial model with trend and additive stationary error would be appropriate.

Suppose that you are confronted with a spatial data set and a scientific or engineering problem to solve. After some *descriptive* analyses of the data, the set of potential models can hopefully be narrowed to just a few. An *indication* of a model's parameters can be obtained by applying an estimation criterion, such as maximum likelihood, maximum pseudolikelihood, method-of-moments, and so forth. Whether these fitted parameters are significant is determined by statistical-inferential methods. *Estimation* of a model's parameters involves both indication and, at least, measures of the estimator's variation. In either case (indication or estimation), it is important to check the fit of the model (because no model is exactly true) using *diagnostic* statistics and plots.

The approach taken in this book is to broaden the classical models and methods to those that recognize the presence and importance of spatial information. The success of these spatial models and methods will be judged by their powers of organization, explanation, and prediction. Much has been accomplished in the last 20 years, and a vigorous future (in modeling, simulation, estimation, computation, inference, asymptotics, diagnostics, etc.) for the subject is assured.

A rereading of Section 1.1 would be helpful at this point, but for those who are ready to jump in, a brief synopsis is given as follows. Chapters 2, 3, and 4 deal with geostatistical data, and Chapter 5 is a collection of special topics of interest to me (Part I). Chapters 6 and 7 deal with lattice data (Part II). Chapters 8 and 9 deal with, respectively, point patterns and objects based on point patterns (Part III).

We shall not cease from exploration
And the end of all our exploring
Will be to arrive where we started
And know the place for the first time. (T. S. Eliot)

PART III

Spatial Patterns

CHAPTER 9

Modeling Objects

The three- or four-dimensional world in which we live is full of objects to be measured and summarized. Very often a parsimonious finite collection of measurements is enough for scientific investigation into an object's genesis and evolution. At the other extreme, images of an object viewed from many different angles are a rich source of data that can overwhelm the scientist or engineer with its complexity.

There is a growing need to describe and model objects through their form as well as their size, yet still retain parsimony in their description and modeling. These considerations are important when deciding the type of data to collect in the first place. Thus, the question of whether data or models come first is not always clear, although new models (modified in the light of data analyses) almost always give rise to new ideas about data collection.

In this chapter, the data will be recordings of objects, often images on a photographic plate or a television screen. Such visual images may be analyzed *per se* or they may be converted into numerical data by defining discrete picture elements (pixels); each pixel is recorded according to its gray level or its (color) frequency and intensity. A further conversion to a two-phase image might be made by recording black or 1 if the gray level of a pixel is above a certain threshold or of a certain color, and white or 0 everywhere else. In the sections that follow, I shall concentrate mainly on 0-1 images and the mathematical sets that are used to model them. (Section 7.4 also addresses the problem of analyzing spatial data defined on pixels. However, it is a low-level type of image analysis where the goal, typically, is not characterization of the form of objects. Rather, one is usually most interested in prediction and classification of various collections of pixels.) Not all of the set models are random, but one that is, the *Boolean model*, provides useful descriptions of objects analyzed in this chapter. Other set models are mentioned briefly in Sections 9.1 and 9.3.

Stereology

How to sample high-dimensional objects so that the loss of information is small, but also so that informative measurements are taken in lower (more

manageable) dimensions, is the subject of *stereology*. This very important area deserves the treatment of a whole book; instead, I shall take just a few paragraphs and refer the interested reader to a number of very accessible references.

A set in three dimensions consists of volumes, surfaces, curves, and points. Various quantities could be measured in an attempt to characterize the set; for example, one could measure the specific volume, the specific surface area, or the specific length (the word “specific” here refers to the measurement per unit of volume under consideration). One could also consider the set’s connectivity number, curvature, convexity measure, and so forth (e.g., Serra, 1982). Based on data from a one- or two-dimensional probe of the object, it is desired to estimate any or all of these quantities.

Sampling considerations are paramount in stereology. Some procedures are able to take images of the object in a highly regularized manner, such as slices at a fixed spacing (in much the same way a wire egg slicer cuts up a boiled egg). The sampling need not be destructive. The important subject of *tomography* came from an idea to use an x-ray machine to measure the transmission across all lines traversing a solid object, calculate the Fourier transform, and then invert it. This has generated considerable mathematical and statistical discussion; see, for example, Shepp and Kruskal (1979), Herman (1980), and Vardi et al. (1985). A more recent development, which is similar in concept but uses a combination of radio frequency waves and high energy magnetic field strengths, is magnetic resonance imaging (MRI). It is a powerful diagnostic tool that allows noninvasive evaluation of brain tumors, herniated discs in the spine, knee injuries to ligamentous structures, and so forth.

Other sampling designs define random probes; indication and estimation then proceed based on this randomness (e.g., Davy and Miles, 1977). If the object is modeled as a random set, stereological methods can be developed from the probability measure of the set model; see Davy (1978).

Much of the ingenuity and creativity of stereologists has been directed toward reducing or removing estimation bias, with too little attention given to variances of estimators (and estimators of those variances). For more details and recent developments in stereology, the reader should consult Coleman (1979), Weibel (1980), Ambartzumian (1982), Sterio (1984), Jensen et al. (1985), Gundersen (1986), Jensen (1987), and Stoyan et al. (1987, Chapter 11).

Chapter Summary

Section 9.1 presents a number of set models of naturally occurring objects. One of them, the Boolean model, receives particular attention in this chapter. An exploratory analysis of a simulated Boolean model is given in Section 9.2. The mathematical foundations for random set models are laid in Section 9.3, and Section 9.4 discusses the properties of the Boolean model. Sections 9.5 and 9.6 continue this discussion into parameter estimation and

inference, respectively. Finally, in Section 9.7, a conditional Boolean model is fitted to successive images of *in vitro* cancerous growth.

9.1 SET MODELS

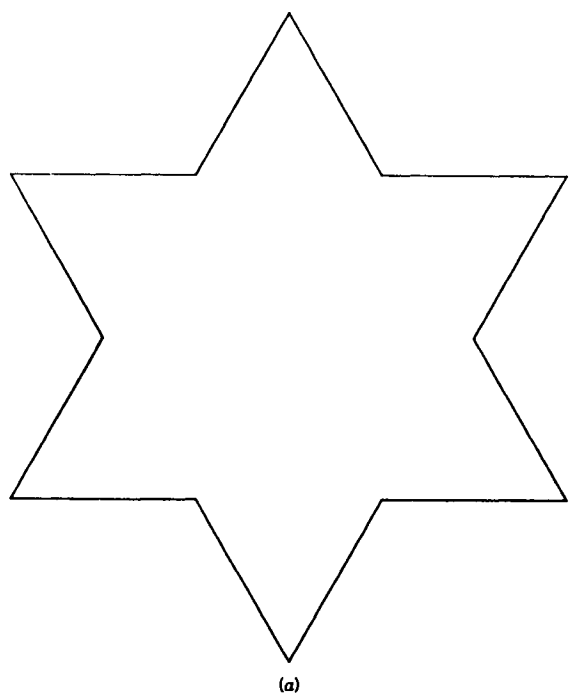
Consider the data at hand to be a large finite number of vector-valued variables, each one indexed by the spatial location of its pixel (picture element). In this chapter, the vector-valued variable will be assumed real-valued (in fact, usually 0-1). Thus, a random set might be viewed as a 0-1 random function. However, the usual random-function techniques handle the geometry of the random set rather crudely. New (nonlinear) operations are needed to probe and sort complicated sets; mathematical morphology (Matheron, 1975; Serra, 1982) systematizes this approach.

It will be assumed that the resolution of the object's image is so good that it is equivalent to consider the data as being defined in Euclidean space. The problems of loss of information in going from continuous space to discrete space and the reconstruction of continuous images from discrete ones are considered by Switzer (1975) and Serra (1982, Part 2). The sets given in this section are mathematical constructs, defined in $\mathbb{R}^d$. Some knowledge of Euclidean topology will be assumed, to the level of knowing the definitions of open, closed, compact, and convex sets (see, e.g., Royden, 1968). Certain classes of sets are often used to model objects, and some of these are presented in the following text.

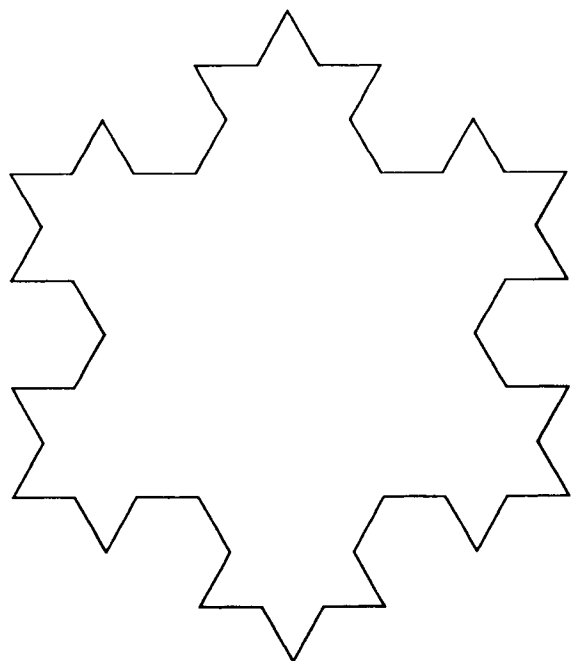
9.1.1 Fractal Sets

"Fractal" (from Latin, *fractus*, meaning irregular or fragmented) is a word coined by B. Mandelbrot (see, e.g., Mandelbrot, 1982) to describe sets with abrupt and tortuous edges. Mandelbrot argues that fractals are very good models of many natural phenomena, for example, coastlines with their sharpness and convolutedness, or fine particles observed under an electron microscope. What is needed is some way of characterizing these irregular boundaries. (Although it must be said that, depending on the question being addressed, a set model with smooth boundaries may suffice.)

Most of the applications of mathematics use Euclidean geometry, but suppose instead the boundary of the object is modeled by a curve that has no tangents. Mandelbrot (1982) quantifies these non-Euclidean curves using an irregularity index he calls the *fractal dimension*, which is larger than the usual Euclidean dimension. For example, a six-pointed star in $\mathbb{R}^2$ has a boundary of dimension equal to 1, but by successively adding smaller and smaller triangular spikes to each side of the star a compact set in $\mathbb{R}^2$ is created whose *boundary* has fractal dimension D equal to $(\log 4)/(\log 3) = 1.2618$. Mandelbrot (1982, pp. 36, 37) calls this compact set a triadic Koch island, whose early stages of construction are given in Figure 9.1.



(a)



(b)

Figure 9.1 Triadic Koch island. (a), (b), and (c) show the initial stages of construction of its boundary.

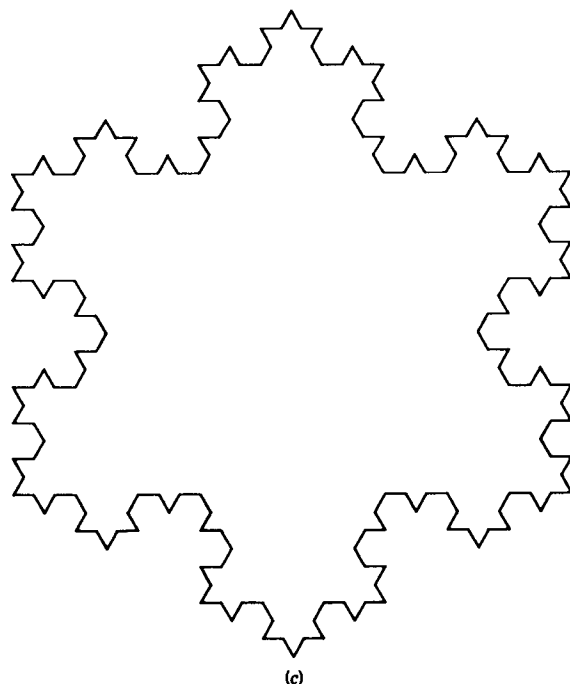


Figure 9.1 (continued)

Fractal Dimension

How is the fractal dimension D obtained? Taylor (1986) has a rigorous definition, but I shall take a more intuitive approach here. Suppose your task is to measure the length of a closed boundary in $\mathbb{R}^2$ and you are given a pair of calipers of *fixed* width ν , say, to do it. Starting at some arbitrary point on the boundary, the caliper allows you to step around the boundary $l(\nu)$ times (disregarding the last incomplete step). Then the length of the boundary using the “yardstick” ν is $\nu \cdot l(\nu)$. Now vary ν , letting it become smaller and smaller. Define the fractal dimension as

$$D \equiv - \lim_{\nu \rightarrow 0} \frac{\log l(\nu)}{\log \nu}. \quad (9.1.1)$$

It is clear now why the previously mentioned triadic Koch island has a boundary with fractal dimension $D = (\log 4)/(\log 3)$ (see Mandelbrot, 1982, p. 36).

In $\mathbb{R}^d$, suppose a compact set X has boundary such that it takes $l(\nu)$ $(d-1)$ -dimensional cubes of side ν to cover it. Then the fractal dimension D is as defined in (9.1.1). Thus, $l(\nu) \simeq c \cdot \nu^{-D}$, or the measure of the boundary is approximately $c \cdot \nu^{d-1-D}$.

Estimation of the fractal dimension D has often been obtained from a log-log plot of $\{(\log \nu_i, \log l(\nu_i)): i = 1, \dots, n\}$. By choosing a range of ν values and fitting a straight line through the resulting set of n points and the origin, the estimated fractal dimension is the negative slope of the line [see (9.1.1)]. In $\mathbb{R}^d$, $d \geq 3$, a direct application of this cube-counting method can be very unstable; Dubuc et al. (1989) develop a more reliable variation method in $\mathbb{R}^3$. The fractal dimension might also be estimated from the relationship of volume to surface measure: The volume of X , in units of ν^d , is proportional to $(l(\nu))^{d/D}$ (Mandelbrot, 1977, p. 72). In words, volume $\propto$ (surface measure) $^{d/D}$; for example, in $\mathbb{R}^2$, area $\propto$ (perimeter) $^{2/D}$ or perimeter $\propto$ (area) $^{D/2}$. For further details on the estimation of fractal dimension, see Cutler and Dawson (1990), Ramsay and Yuan (1990), and Theiler (1990).

Self-Similarity

Fractal sets may be self-similar (i.e., a small part of the boundary magnified resembles a larger part of the boundary), but are not necessarily so. For example, for the triadic Koch island it is only necessary to use different shaped triangular spikes at each step to obtain a fractal that is not self-similar. Hutchinson (1981) explores the notions of self-similarity and fractals from a theoretical point of view.

Consider the geostatistical problem treated in Part I of this book. A finite number of observations $\{Z(s_i): i = 1, \dots, n\}$ are taken from $\{Z(s): s \in D\}$, a potentially uncountable number. Some geophysical questions need to be answered at a scale smaller than the smallest spacing, $\min\{\|s_i - s_j\|: 1 \leq i < j \leq n\}$. Assuming a fractal structure for the possible trajectories $\{z(s): s \in D\}$, more specifically a *self-similar* fractal structure, knowledge gained from the data at the observed spatial scales can be extrapolated down to the unobserved scales. Because this self-similar fractal structure can only be verified at the scale of observation, it is only a *hope* that similar structure is manifested at the microscale. Until more experience is gained with its applicability, caution should be exercised. Section 5.5 discusses further the fractal properties of random-field trajectories.

Fractal Set Models of Natural Phenomena

Small volumes surrounded by enormous surface areas are frequently the rule in our bodies: To enrich the blood with oxygen, our lungs require a surface area that is approximately the size of two basketball courts. Every cell in our body receives nutrients from an intricate branching network of blood vessels. In these and other examples, the volumes involved are just a small percentage of total body volume, indicating that fractals can be the result of evolution toward efficiency of natural processes.

Mandelbrot (1982) describes how fractal sets might model sponges, tree branching, surfaces of the brain and lung, rivers, watersheds, the vascular system, coastlines, and so on (see also Frontier, 1987; Goodchild and Mark,

1987; Tarboton et al., 1988). His general approach has been one of parsimonious description of a phenomenon rather than explanation of its genesis. However, by summarizing these sets using their fractal dimension, a phenomenon whose genesis is highly complex could be monitored for *changes*.

Random Fractals

Random fractals are usually obtained by considering the trajectories of stochastic processes. For example, a Brownian trail in two dimensions (obtained from the locus of points visited by two-dimensional Brownian motion) has fractal dimension $D = 2$, because eventually almost every trajectory will fill the plane (i.e., will visit every point in $\mathbb{R}^2$). The trajectories of a temporal stochastic process considered as functions of time may have a fractal dimension. Mandelbrot and Van Ness (1968) detail how a fractional Brownian motion can be constructed, where $\text{var}(X(t + \Delta t) - X(t))$ is proportional to $|\Delta t|^{2H}$, $0 < H \leq 1$. The case $H = 1/2$ refers to the usual Brownian motion, whose trajectories have a fractal dimension of 1.5, larger than its topological dimension of 1. In general, the trajectories have a fractal dimension $2 - H$. For $H > 1/2$, fractional Brownian motion no longer has independent increments and displays long-range dependence (or persistence). Mandelbrot (1982) uses higher-dimensional versions of random functions to produce attractive pictures of computer-generated planetscapes; see Section 5.5 for further discussion. Taylor (1986) can be consulted for the appropriate measure theory associated with these types of random fractals.

For random fractals analogous to, but more general than, the deterministic triadic Koch island, the interested reader should consult Falconer (1986). His construction of random fractals is more direct, as he does not use the path properties of stochastic processes.

Finally, it should be pointed out that, for many purposes, modeling an object or process with abrupt and tortuous surfaces is not necessary; for example, Switzer (1976) investigates geometrical measures of the *smoothness* of random functions. If inferences are to be made on only one spatial scale, fractal set models are probably not appropriate. They are very useful, however, when considering phenomena at scales that span orders of magnitude.

9.1.2 Fuzzy Sets

Scientific investigations always have some elements of uncertainty, ambiguity, and vagueness. I think it is fair to say that the more the investigation involves quantification of and by human beings, the more uncertain the data become. For example, the medical assessment of side effects of a drug may be based on patients' responses like "drowsy," "nauseous," and "lousy."

Probability theory is one way of dealing with uncertainty. From the classical axioms that define a probability space $(\Omega, \mathcal{A}, P)$, an elegant theory

can be built (e.g., Chung, 1968) that is the underpinning of all the Statistics in this book. Relatively recently, Zadeh (1965) has introduced a different approach, namely, the modeling of uncertainty by fuzzy sets. Its premise is that all data are imprecise, even *after* they have been observed. The uncertainty in Probability and Statistics usually refers to future data; those that have been observed have a precise value.

To quantify data that are vague, Zadeh defined a membership function $\mu_A(\cdot)$, where $0 \leq \mu_A(\cdot) \leq 1$ and A is a set in $\mathbb{R}^d$. If $\mu_A(s)$ is near zero, then s is probably not in the set A , whereas if $\mu_A(s)$ is near 1, s is probably in the set A . For example, suppose a newly manufactured mechanical part is within specification if its diameter s is between 2.9 and 3.0 cm. Let

$$A \equiv \{s: 2.9 \leq s \leq 3.0\}.$$

A quality-control inspector observes many such parts every day, but has to be selective about the ones that will be taken off the production line to be measured. A perfect inspector is one whose candidate defective parts are all defective and who leaves no defective parts on the production line. In reality, mistakes are made. Therefore, it seems sensible to think of each quality control inspector as having a membership function; the “closer” it is to the ideal

$$\mu_A^*(s) = \begin{cases} 1, & \text{if } s \in A, \\ 0, & \text{elsewhere,} \end{cases}$$

the better the inspector.

The example just given quantifies a subjective reaction to objective data, and there are obvious ways that membership functions could be estimated using techniques developed in bioassay (see, e.g., Finney, 1971). However, a subjective reaction to subjective data, such as might occur in medical diagnosis, brings forth very challenging problems of modeling. Nevertheless, attempts have been made to use fuzzy sets to quantify the diagnostic process *inter alia* by Sanchez (1979), Fordon and Bezdek (1979), and Esogbue and Elder (1980). Shafer's (1976) belief function and its calculus bears a striking resemblance to fuzzy set theory; some discussion of this is given in Shafer (1987).

Definition of a Fuzzy Set

A fuzzy set in $\mathbb{R}^d$ is defined abstractly as $\{(s, \mu(s)): s \in \mathbb{R}^d\}$, where $0 \leq \mu(\cdot) \leq 1$. To distinguish a fuzzy set from a usual set in $\mathbb{R}^d$, denote fuzzy sets by $\tilde{A}$, $\tilde{B}$, and so on. By analogy with the usual set theory, the (fuzzy) union, (fuzzy) intersection, and (fuzzy) complement of fuzzy sets $\tilde{A}_i \equiv \{(s, \mu_i(s)):$

$\mathbf{s} \in \mathbb{R}^d$, $i = 1, 2$, are defined as

$$\begin{aligned}\tilde{A}_1 \cup \tilde{A}_2 &\equiv \{(\mathbf{s}, \max(\mu_1(\mathbf{s}), \mu_2(\mathbf{s}))) : \mathbf{s} \in \mathbb{R}^d\}, \\ \tilde{A}_1 \cap \tilde{A}_2 &\equiv \{(\mathbf{s}, \min(\mu_1(\mathbf{s}), \mu_2(\mathbf{s}))) : \mathbf{s} \in \mathbb{R}^d\}, \\ \tilde{A}_1^c &\equiv \{(\mathbf{s}, 1 - \mu_1(\mathbf{s})) : \mathbf{s} \in \mathbb{R}^d\},\end{aligned}$$

respectively. A simple illustration of fuzzy sets in $\mathbb{R}^1$ and the union operation is given in Figure 9.2. However, notice that

$$\tilde{A}_1^c \cup \tilde{A}_1 \neq \{(\mathbf{s}, 1) : \mathbf{s} \in \mathbb{R}^d\},$$

although other properties, such as DeMorgan's laws,

$$\begin{aligned}(\tilde{A}_1 \cup \tilde{A}_2)^c &= \tilde{A}_1^c \cap \tilde{A}_2^c \\ (\tilde{A}_1 \cap \tilde{A}_2)^c &= \tilde{A}_1^c \cup \tilde{A}_2^c,\end{aligned}$$

are satisfied. There are alternative definitions to these fuzzy set operations, and the interested reader can consult Kaufman (1975) for more details.

Almost any branch of set theory can be “fuzzified,” usually in a number of different ways. This has led to a large literature, most of which has paid little real attention to potential applications in psychology, linguistics, speech recognition, artificial intelligence, and so on.

Gray-Tone Functions as Fuzzy Sets

Image data that are received as gray tones are very precise, but could be thought of as fuzzy sets. Suppose the intensity is compressed so that 0 denotes white, 1 denotes black, and various grays correspond to values between 0 and 1. Denote this gray-tone function as $\mu(\cdot)$. Then $\{(\mathbf{s}, \mu(\mathbf{s})) : \mathbf{s} \in \mathbb{R}^2\}$ is a surface in $\mathbb{R}^3$ that can be constructed from the image. It can also be thought of as a fuzzy set, and many of the fuzzy operations make sense from an image analysis point of view. Serra (1982, Chapter 12) analyzes image data using several such operations, although his work was developed independently. With the explosion of mathematical results in fuzzy set theory, it would be profitable to catalogue them from this image-analysis viewpoint; Bandemer and Roth (1987) develop a fuzzy exploratory data analysis in this way.

Probability Measures of Fuzzy Sets

The probability of a fuzzy event was defined initially by Zadeh (1968). First, a fuzzy event is a fuzzy set $\tilde{A}$ in $\mathbb{R}^d$, whose membership function

$$\mu : \mathbb{R}^d \rightarrow [0, 1]$$

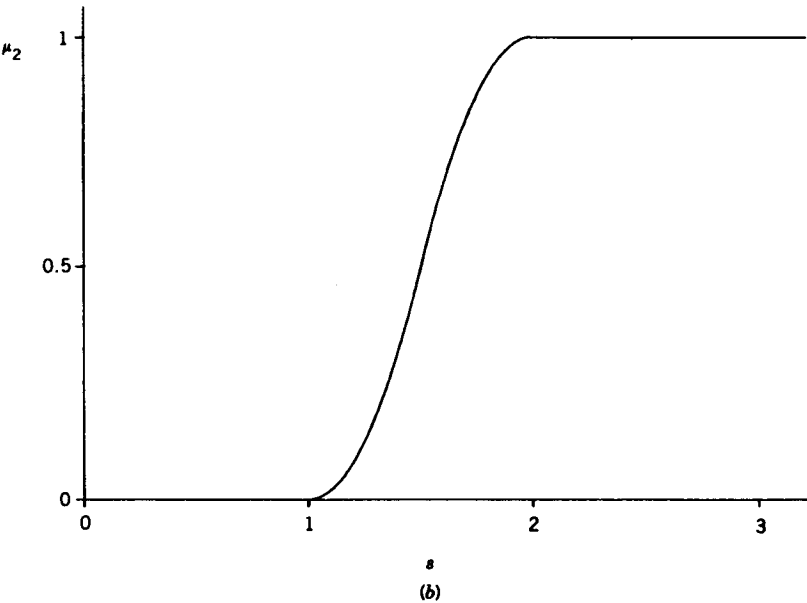
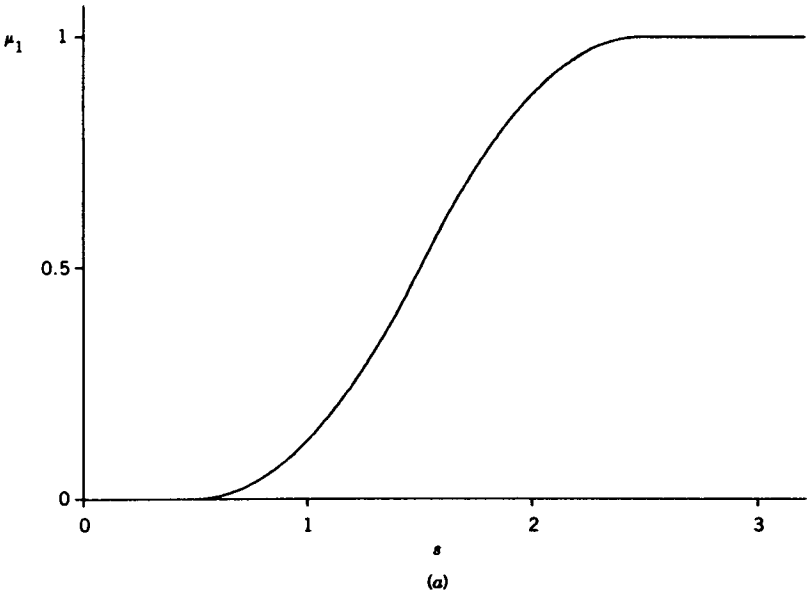


Figure 9.2 (a) The fuzzy set $\tilde{A}_1$, with membership function μ_1 . (b) The fuzzy set $\tilde{A}_2$, with membership function μ_2 .

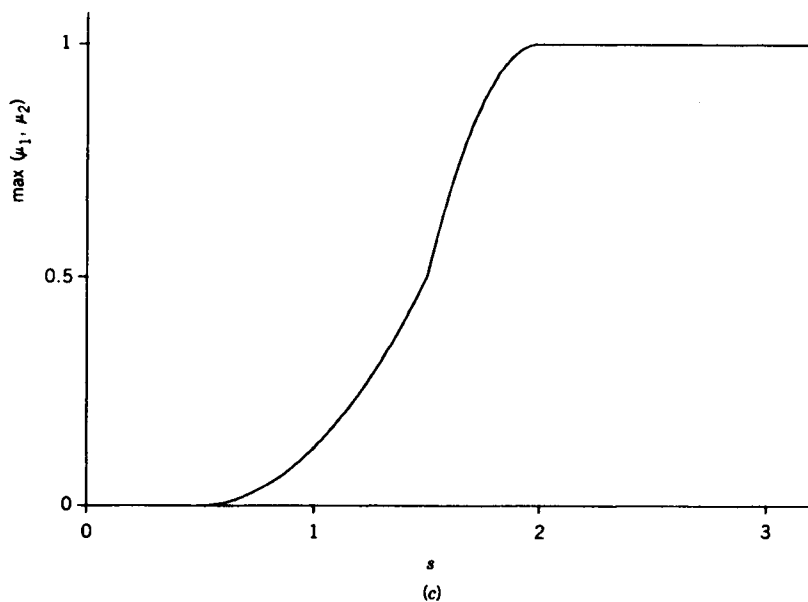


Figure 9.2 (c) The fuzzy union of $\tilde{A}_1$ and $\tilde{A}_2$, with membership function $\max(\mu_1, \mu_2)$.

is measurable (i.e., μ -inverse images of Borel subsets of $[0, 1]$ are Borel subsets of $\mathbb{R}^d$). Second, suppose that P is a probability measure on the Borel subsets of $\mathbb{R}^d$. Finally, the *probability* $\tilde{P}(\tilde{A})$ of a fuzzy event $\tilde{A}$ is defined by

$$\tilde{P}(\tilde{A}) \equiv \int_{\mathbb{R}^d} \mu(s) P(ds). \quad (9.1.2)$$

Another way to think of (9.1.2) is as the *expectation* of the membership function. Notice that

$$\tilde{P}(\tilde{A}^c) = 1 - \tilde{P}(\tilde{A}),$$

along with many other familiar probability equalities and inequalities (Zadeh, 1968). However, it is *not* necessarily true that $\tilde{P}(\tilde{A}^c \cap \tilde{B}) = \tilde{P}(\tilde{B}) - \tilde{P}(\tilde{A} \cap \tilde{B})$, which has an effect on the way fuzzy set *independence* should be defined. Buoncrisiani (1983) shows that Zadeh's (1968) definition of independence of $\tilde{A}$ and $\tilde{B}$, namely,

$$\tilde{P}(\tilde{A} \cap \tilde{B}) = \tilde{P}(\tilde{A}) \cdot \tilde{P}(\tilde{B}),$$

needs modification and offers instead

$$\tilde{P}(\tilde{A}|\tilde{B}) = \tilde{P}(\tilde{A});$$

the fuzzy conditional probability $\tilde{P}(\tilde{A}|\tilde{B})$ is defined by

$$\tilde{P}(\tilde{A}|\tilde{B}) \equiv \frac{\tilde{P}(\tilde{A} \cap \tilde{B})}{\tilde{P}(\tilde{A} \cap \tilde{B}) + \tilde{P}(\tilde{A}^c \cap \tilde{B})}.$$

Random Fuzzy Sets

The most obvious way to generate a well defined random fuzzy set is through a stochastic process $\{Z(s): s \in \mathbb{R}^d\}$, where $0 \leq Z(\cdot) \leq 1$. Then, intuitively,

$$\tilde{A}_Z \equiv \{(s, Z(s)): s \in \mathbb{R}^d\}$$

is a random fuzzy set [although it takes a little work to obtain the right σ algebra in the image space (Zadeh, 1968, p. 424)]; see also Feron (1976).

It appears that random fuzzy sets are more general, in that one can define a whole sequence of random sets through the level sets

$$A_Z(u) \equiv \{s: Z(s) \geq u\}, \quad 0 \leq u \leq 1.$$

In the rest of this chapter I shall discuss the simpler random sets. Fuzzy sets would provide useful models for the purposes of this chapter if a fuzzy set calculus were developed that has direct application to inference for models of objects.

9.1.3 Random Closed Sets: An Example

Although not as general as a random fuzzy set, the notion of a random closed set (RACS) is sufficiently rich to model highly complex objects, yet often sufficiently simple to allow inferences on model parameters. The general definition of a RACS is given in Section 9.3 as a measurable mapping from a probability space into the set of all closed sets in $\mathbb{R}^d$ equipped with the “hit-or-miss” topology (Matheron, 1971a).

An important and flexible class of random closed sets is the Boolean model. Suppose D is a homogeneous Poisson process in $\mathbb{R}^d$ (see Section 8.3) and Z is a random polygon (random sides and angles) or a random compact set generated by random scaling (e.g., a disk of random radius). Define the displaced random set

$$Z \oplus s \equiv \{z + s: z \in Z\}, \quad s \in \mathbb{R}^d$$

and suppose that $Z_1, Z_2, \dots$ are i.i.d. as Z . Then, the random set

$$X \equiv \cup \{Z(s_i): s_i \in D\}, \quad (9.1.3)$$

where $Z(s_i) \equiv Z_i \oplus s_i$, is known as a Boolean model with “grains” $Z_1, Z_2, \dots$ (independent RACS, each with probability measure the same as that of Z) and “germs” $s_1, s_2, \dots$ (points of the point process D). A simulated realization of X is given in Figure 9.3, where Z is a disk of random radius.

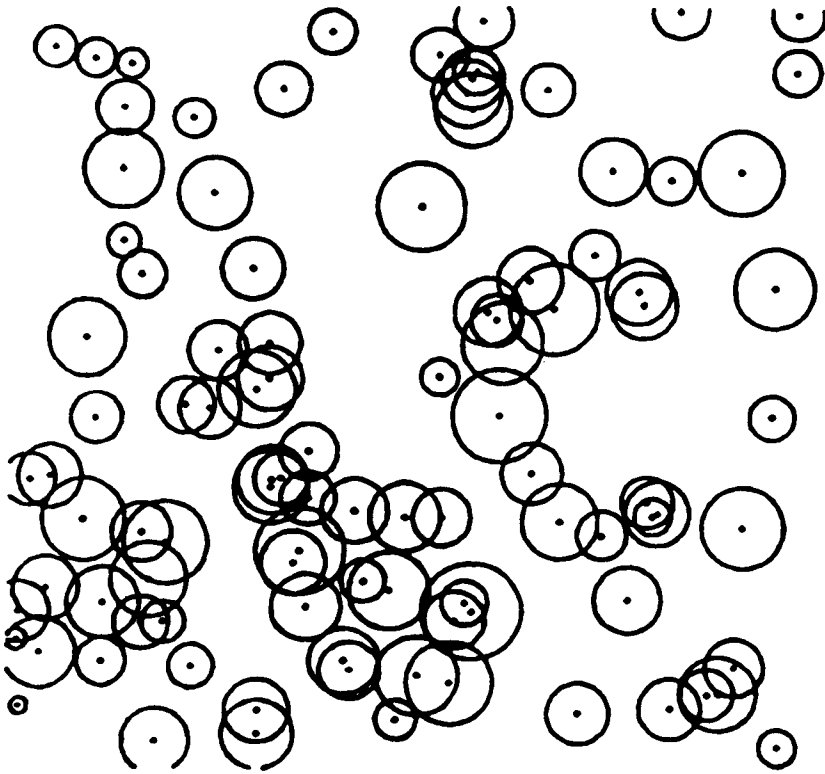


Figure 9.3 The union of the disks shown is a partial realization of a Boolean model in $\mathbb{R}^2$. Germs are points of a homogeneous Poisson process and grains are disks of random radius.

Figure 9.4 is a real data set that could be modeled by the RACS defined in (9.1.3). These data are the result of a cloud-seeding experiment and represent water droplets in a cloud. A glass slide (7.5×2.5 cm) was coated with magnesium oxide and mounted on a small airplane that was flown at a known speed through the cloud under study. The slide was exposed for a fixed time interval, returned to the laboratory, and examined under a microscope. A droplet causes a crater in the magnesium oxide; the microscope is focused on the surface level of the magnesium oxide so that the bright ring is the edge of the crater and the dark center is its out-of-focus center. Figure 9.4 shows only a very small part of the 7.5×2.5 -cm slide; the scale is shown on the figure. After adjustment for the spread of the droplets on impact and for occasional oblique impact, it is sensible to think of the data as representing various sized water droplets scattered randomly over the area of interest. Notice that a big crater could obliterate a small one, so that simple computation of the number of observed craters and their size distribution gives a *biased* summary of the droplet intensity and droplet size distribution. However, an analysis of such data, based on the Boolean model (9.1.3), can compensate for these biases.

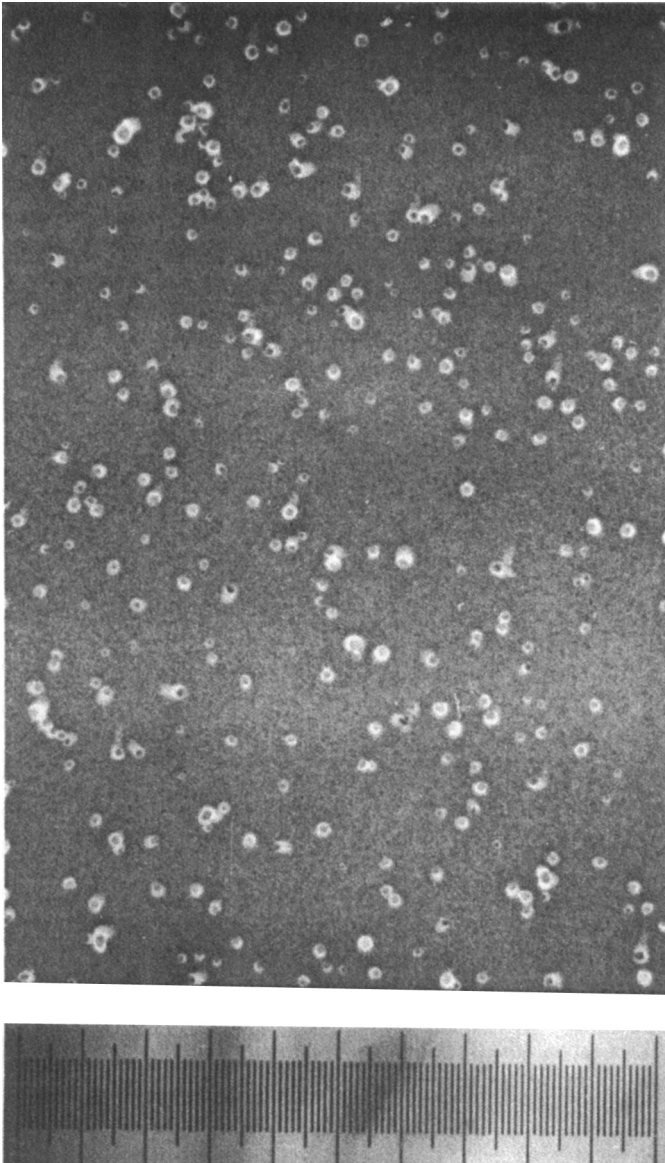


Figure 9.4 Cloud-droplets data. The size and location of a droplet is shown by a bright ring. The overall length of the scale shown is 1 mm. [Source: Dr. S. C. Mossop, Division of Atmospheric Research, CSIRO]

The Boolean model and its variants are considered in some detail in this chapter. Section 9.2 presents a simulated example, definitions and properties are given in Section 9.4, inferential aspects are discussed in Sections 9.5 and 9.6, and in Section 9.7 a conditional Boolean model is used to model tumor growth.

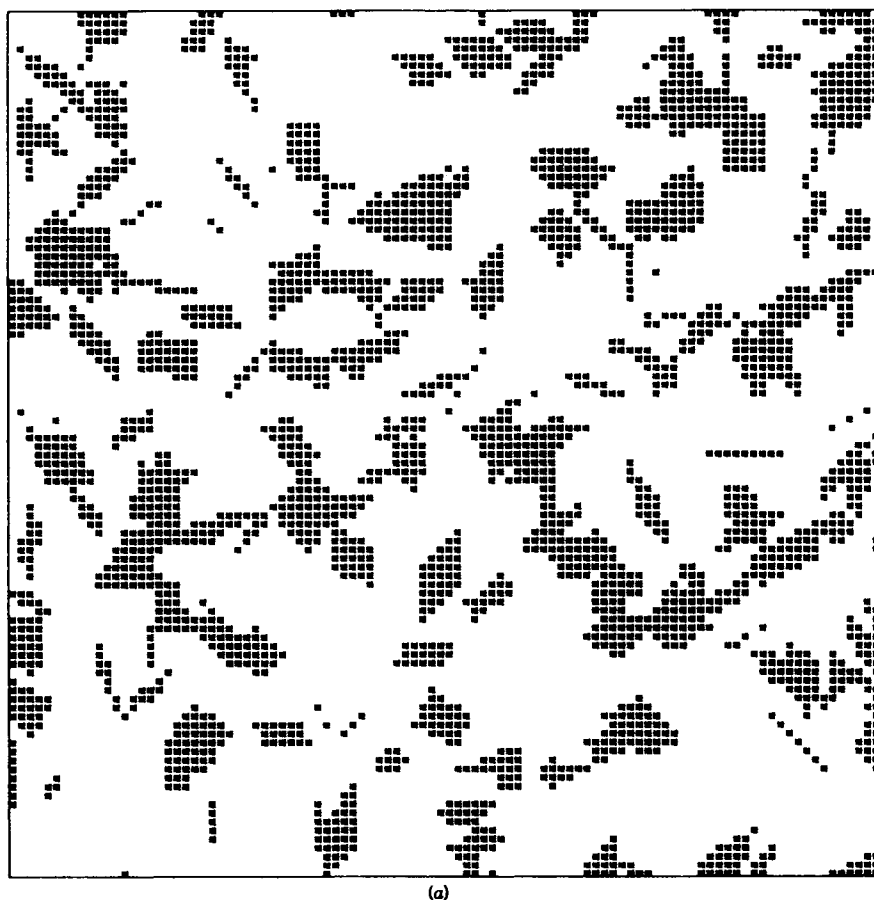


Figure 9.5 (a) A realization of a Boolean model (restricted to a square mask) whose grains are random parallelograms. The realization is discretized into 100×100 pixels. [Source: Cressie and Laslett, 1987] Reprinted with permission from the *SIAM Review*, volume 29, no. 4, pp. 557–574. Copyright 1987 by the Society for Industrial and Applied Mathematics. All rights reserved.

9.2[†] RANDOM PARALLELOGRAMS IN $\mathbb{R}^2$

This section gives a brief exploratory data analysis of simulated data, generated according to the Boolean model defined by (9.1.3). The data are analyzed further in Section 9.5.

Figure 9.5a and b presents two realizations of (9.1.3) restricted to a square mask of 100×100 pixels, where the grains are i.i.d. random compact sets, more specifically, random parallelograms, and the germs are events of a two-dimensional homogeneous Poisson process with intensity $\lambda = 0.02$ per pixel area (see Section 8.3). These data were first presented in Cressie and

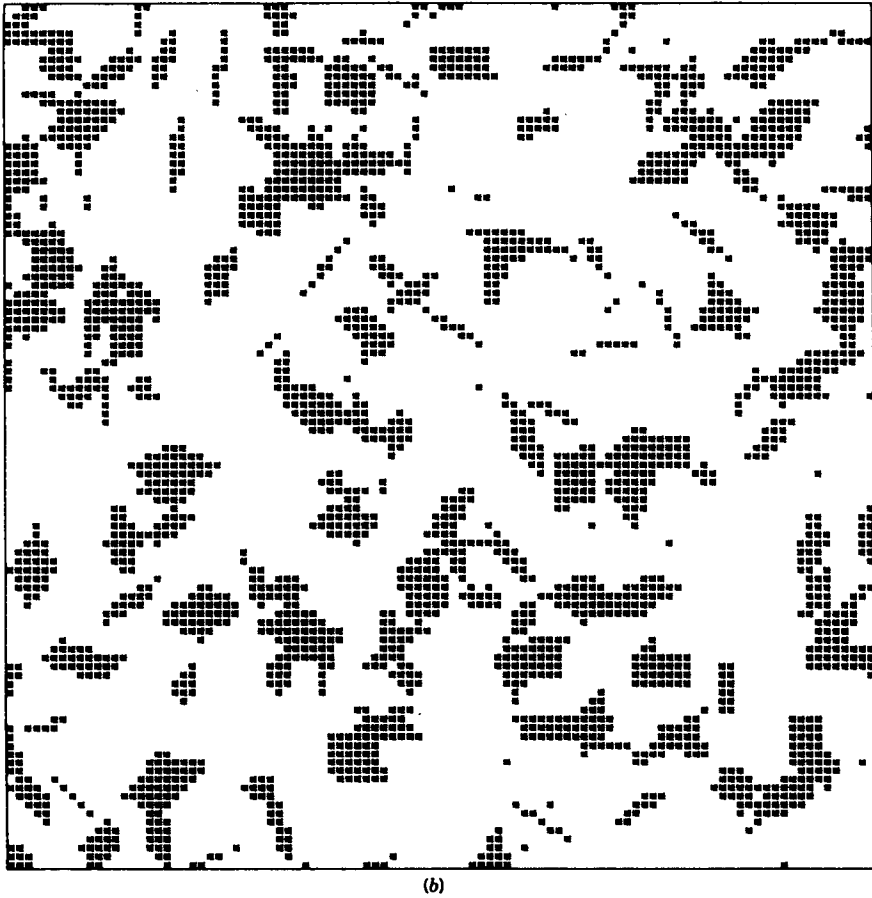


Figure 9.5 (b) Another realization of the same Boolean model, described in (a). [Source: Cressie and Laslett, 1987]

Laslett (1987). The bottom left-hand corner of the random parallelogram was fixed at each point of the realization of the Poisson process. The length of both sides of the parallelogram was uniformly distributed on $[2.5, 7.5]$ and the angle between the adjacent sides was uniform on $[0, \pi)$. Finally, the parallelogram was uniformly oriented on $[0, 2\pi)$. Figure 9.5a and b shows two realizations *after discretization*.

Faced with data of this kind, the statistician struggles. I shall briefly describe some exploratory techniques that are appropriate for Figures 9.5a and b. Section 9.5.1 continues the analysis and fits back a Boolean model. If one wants to consider such data as representative of a phenomenon, that is, as carrying information on interpretable “average” quantities (parameters) associated with the phenomenon, then one must turn to a model. This is true for studying any type of variation, but it is particularly difficult here because

of the dearth of tractable random-set models available; see Section 9.3 for more discussion.

I shall give some summary statistics for the data presented in Figure 9.5a. The most basic one is the specific area, that is, the area of the set per unit of area under consideration. In this case the area under consideration is 10^4 square units. Here

$$\text{specific area} = 0.27050.$$

Notice that $1 - (\text{specific area}) = 0.72950$ is called the *porosity*. The number of distinct contiguous sets and the boundary length could also be calculated, but to anticipate Section 9.5, it turns out that the specific area of a dilated version of Figure 9.5a is of more interest. Define

$$X \oplus tC \equiv \{s + tc: s \in X, c \in C\},$$

where X is the set in Figure 9.5a, C is a solid square of side 2 units with center of gravity centered at the origin, and t is a dilation factor. As t increases, the original set X becomes more and more “bloated”. At each value of t , the specific area of $X \oplus tC$ can be calculated; Table 9.1 gives the values for $t = 0, 1, 2, 3, 4$.

Ripley (1988, Chapter 6) gives a host of other summary statistics that are defined in terms of morphological transformations on X with structuring element tB (where B is often chosen to be a disk). Plotting the area of the transformed X against t gives an exploratory way of summarizing the image data, as well as a tool for fitting (or diagnosing the fit of) a random-set model.

From the summary statistics provided by Table 9.1 and assuming Figure 9.5a was generated by a Boolean model (which it was), it is possible to estimate various parameters of the model. The theoretical details are given in Section 9.4, followed by an analysis of these data in Section 9.5.

Table 9.1 Specific Areas of the Dilated Set $X \oplus tC$, Where X is Given by Figure 9.5a

t	Specific Area
0	0.27050
1	0.55862
2	0.77203
3	0.90052
4	0.96432

9.3* RANDOM CLOSED SETS AND MATHEMATICAL MORPHOLOGY

The statistical and probabilistic theory that ensures the existence of stochastic models and the efficient estimation of their parameters is very well developed for data modeled as independent-and-identically-distributed *random variables*. The interrelationships between any two subcollections are extremely simple, and one only needs to determine the law of any individual to determine the law of the whole. In fact, only the probability of the events “ $\{X \leq x\}$, for all $x \in (-\infty, \infty)$ ” are needed. This theory has been extended for (1) a sample whose variables are vectors, elements of a Banach space, and so forth and (2) a collection of (often real-valued but also vector-valued) random variables whose dependence structure is Markov, (strongly or weakly) stationary, and so forth. Further theoretical and methodological extensions are needed for random sets.

Although the main goal of this chapter is to model (images of) objects, it should be noted that the theory of random sets has much wider potential. For example, Barnett (1986) discusses how economists could benefit by viewing the economy as a random set. Indeed, a sample of n random variables can either be viewed as a set of n points in $\mathbb{R}^1$ or as a vector in $\mathbb{R}^n$. Taking the latter point of view allowed Fisher (1915) and Hotelling (1939) to calculate the distributions of intuitively appealing test statistics. Taking the former point of view, more generally for a random sample of n random vectors in $\mathbb{R}^d$, one can ask questions about the convex hulls of subsets of such points. (Through these, the notion of order statistics can be generalized to higher dimensions or the support of a population distribution can be estimated.) These are addressed *inter alia* by Efron (1965), Fisher (1971), Ripley and Rasson (1977), Eddy and Gale (1981), Moore (1984), Davis et al. (1988), and Brozius (1989). One might also consider each point in $\mathbb{R}^d$ as having a set associated with it and ask questions about the sum of the n sets' indicator functions (Robbins, 1944) or about the coverage of the union of the n sets (see, e.g., Hall, 1988a).

In what is to follow, the main results for modeling and inference for random sets will be reviewed. It will become clear that this subject is still in its infancy, and much remains to be done.

Random Sets and Random Functions

In one sense, a random set is just a special case of a random function (e.g., Adler, 1981) that takes only the values 0 or 1. In fact, if any random function is sliced at some level u and looked at from above, then the boundary of the slice traces out the boundary of a random set. Any analysis of the original random function should be equally possible on these level sets indexed by u , and conversely. Radchenko (1985) considers geometric measures (e.g., length, area, etc.) of level sets of an almost surely continuous random function defined on a metric space X (e.g., $\mathbb{R}^d$) and gives conditions under which these are measurable.

Both random sets and random functions have the concept of covariation; however, beyond this there seems little in common in their analysis [see the discussion later in this section and Adler (1981, p. 71)]. The main reason is that random-function operations, such as convolution and Fourier filtering, are linear, whereas the random-set morphological transformations [i.e., transformations that affect form, such as can be found in Serra (1982, Part 1)] are highly nonlinear.

Recall from Section 2.3 that the variogram of a random function $\{Z(\mathbf{s}): \mathbf{s} \in \mathbb{R}^d\}$ is defined as $\text{var}(Z(\mathbf{s} + \mathbf{h}) - Z(\mathbf{s}))$, which is usually considered to be a function only of the vector $\mathbf{h}$ [known as intrinsic stationarity; see Matheron (1971b) and Section 2.3]. Now suppose that X is a stationary random closed set in $\mathbb{R}^d$ (defined in the following text) and let $Z_X(\cdot)$ denote its indicator function. Then, it is not difficult to prove that $\{Z_X(\mathbf{s}): \mathbf{s} \in \mathbb{R}^d\}$ is a random function satisfying intrinsic stationarity with variogram $2\{p - \Pr(\mathbf{s} \in X, \mathbf{s} + \mathbf{h} \in X)\}$, where $p = \Pr(\mathbf{s} \in X)$. Write $X \oplus \{-\mathbf{h}\}$ for the (random) set X translated to $-\mathbf{h}$. Then the expression for the variogram becomes $2\{p - \Pr(\mathbf{s} \in X \cap X \oplus \{-\mathbf{h}\})\}$. Clearly, $\kappa(\mathbf{h}) \equiv \int \Pr(\mathbf{s} \in X \cap X \oplus \{-\mathbf{h}\}) d\mathbf{s}$ is the probabilistic analogue of the *geometrical covariance* of a (deterministic) set $A \subset \mathbb{R}^d$, defined as $\nu(A \cap A \oplus \{-\mathbf{h}\})$, where $\nu(\cdot)$ denotes Lebesgue measure in $\mathbb{R}^d$. Notice that $\kappa(\mathbf{h})$ contains information about the surface measure of X as $\mathbf{h} \rightarrow \mathbf{0}$: Provided X is almost surely (a.s.) regular (see Serra, 1982, p. 274), then $\{\kappa(\mathbf{h}) - \kappa(\mathbf{0})\}/\|\mathbf{h}\|$ exists; call it $\kappa'_u(\mathbf{0})$, where $\mathbf{u} \equiv \mathbf{h}/\|\mathbf{h}\|$. In $\mathbb{R}^2$,

$$-(1/2) \int_0^{2\pi} \kappa'_u(\mathbf{0}) d\mathbf{u} = E(\text{perimeter of } X). \quad (9.3.1)$$

Now, knowledge gained from the behavior at the origin of the covariance of a random function usually relates to the behavior of its spectrum at very high frequencies. This is exactly what is happening in the relation (9.3.1), where the random function is the indicator function of a random set: The left-hand side can be interpreted simply as covariance behavior near the origin and the right-hand side pertains to the boundary of X where there is high frequency, that is, where the 0-1 random function undergoes its most drastic changes. However, it is at this stage of an image analysis that a random-function approach fails to capture the full geometric complexities of the image. This is clear when $X \cap X \oplus \{-\mathbf{h}\}$ is written in terms of the *erosion* operation $X \ominus \tilde{B} \equiv \bigcap \{X \oplus \{-\mathbf{b}\}: \mathbf{b} \in B\}$. The choice of structuring element $B = \{\mathbf{0}, \mathbf{h}\}$, which yields $X \cap X \oplus \{-\mathbf{h}\}$, is one of *many* that could be made in order to “sort” the random set X . The scope of geometric possibilities expands enormously through varying the structuring element B ; (linear) spectral analysis in random function theory is just one of a number of possibilities. Even more general ways of probing the image are found in the AFATL Image Algebra (Ritter et al., 1990), which provides a common mathematical environment for the development of image-processing algorithms and an image-processing language.

Random Sets Based on Tessellations

A *tessellation* of $\mathbb{R}^d$ is a partition such that the Euclidean space is divided into mutually exclusive subsets whose union is the whole space. For example, random straight lines in $\mathbb{R}^2$ tessellate the space, as does the Dirichlet tessellation or Delauney triangulation (e.g., Diggle, 1983, p. 6) of some arbitrary point process. Moller (1989a) gives an extensive review of random tessellations in $\mathbb{R}^d$.

Each subset of the tessellation with nonzero Lebesgue measure is called a *tile* of the tessellation; tiles (and their boundaries) are random sets. Further randomness could be introduced by coloring each tile; this might be done independently or according to a Markov random field (e.g., Arak and Surgailis, 1989), defined in Section 6.4. Ambartzumian (1982) can be consulted for constructions of random sets based on tessellations. However, the emphasis in this book is principally on random sets based on point processes and Boolean models.

Size and Shape

In what is to follow in this section, and for that matter in this chapter, the principal goal is the mathematical treatment of objects of varying size and shape. I shall take a random-set-model approach; the calculus associated with it has been called *mathematical morphology* by G. Matheron [a short account of which is given in Watson (1975) and in Section 9.3.1]. A more eclectic viewpoint of size and shape can be found in Lord and Wilson's (1984) book, but it has little development of stochastic modeling. I shall now review briefly some of the ways size and shape have been quantified.

Sometimes the data come as points in $\mathbb{R}^d$, and the collection of points is studied for the size and shape it engenders. These *landmarks* are useful in biology for comparing size and shape of specimens; for example, nine landmarks of primate skulls might be external occipital protuberance, posterior-most point of the foramen magnum, anterior-most point of the foramen magnum, deepest point of pituitary fossa, deepest point of ethmoid fossa, deepest point of curvature of nasal bones, terminus of internasal suture, tip of alveolar bone between upper central incisors, and posterior end of the hard palate. The area of biology that considers such problems is known as *morphometrics*: A single form could be characterized by distances or ratios of distances between landmarks. To compare two forms, one can either superimpose them on each other (Siegel and Benson, 1982; Bookstein, 1986), deform one form into the other (Lew and Lewis, 1977), or use the maximal invariant implied by the underlying group structure (Lele, 1991b). Biologists are often interested in studying the association of size and shape in such situations, a subject known as *allometry*. Mosimann (1970) gives a number of mathematical models that might be used in such studies.

Bookstein (1986) introduces a stochastic spatial component by assuming (unrealistically, it seems to me) that the landmarks (in $\mathbb{R}^2$) are independent bivariate Gaussian variates. Kendall (1984, 1989) has a statistical theory of shape based on k not-totally-coincident points in $\mathbb{R}^d$; for example, $k = 3$,

$d = 2$ yields triangles in the plane. Small (1988) compares Kendall's approach with Bookstein's. Watson (1986) considers the shapes of a random sequence of triangles in the plane.

Algorithms for computing triangles based on planar point sets can be found in, for example, Kirkpatrick and Radke (1985). These descriptive summaries are typically devoid of any stochastic interpretation.

For sets in $\mathbb{R}^d$, the subjective notions of size and shape can be quantified by the experimenter's choice of structuring elements that are used to interact with the image. For example, a purely descriptive (and arbitrary) measure of the size of X might be defined as

$$\Lambda_B(X) \equiv \sup\{\lambda: \{\lambda \mathbf{b} + \mathbf{s}: \mathbf{b} \in B\} \subset A, \text{ for some } \mathbf{s}\}.$$

Consider the planar case $d = 2$. When the structuring element B is a unit disk centered at $\mathbf{0}$, $\Lambda_B(X)$ is the maximum inscribed circle within X . When $B = \{\mathbf{s}: \mathbf{s} = \alpha \mathbf{e}; 0 \leq \alpha \leq 1\}$, $\Lambda_B(X)$ is the maximum intercept in the direction $\mathbf{e}$, and when $B = \{\mathbf{0}, \mathbf{e}\}$, $\Lambda_B(X)$ is the maximum distance between two points of X in the direction $\mathbf{e}$. Shape can be investigated using set operations, such as addition, subtraction, opening, closing, and so forth (with various structuring elements), defined in the next section. These have been hard-wired into an optocodigital machine called a texture analyzer (Serra, 1982, p. 24) to avoid tedious programming and to accomplish real-time imaging.

Although summary descriptions of set data can be very insightful, the main goal of this chapter is to introduce various random-set models, along with methods of fitting them to image data. My intention is to progress from description to indication and then to estimation (as described in Section 1.1).

9.3.1* Theory and Methods

A summary of the main definitions and results of random-set theory (Matheron, 1971a, 1975; Kendall, 1974) and mathematical morphology (e.g., Serra, 1982) will be needed. Let E be a locally compact, Hausdorff, and separable space, and define $\mathcal{F}$ to be the set of all closed subsets of E (including the empty set $\emptyset$). For example, let $E = \mathbb{R}^d$. Let $\mathcal{K}$ denote the set of all compact sets and let $\mathcal{K}' \equiv \mathcal{K} \setminus \emptyset$ be the set of all nonempty compact sets. For any set of sets $\mathcal{R}$, $C(\mathcal{R})$ denotes that subset whose sets are convex. For any $A \subset E$, define

$$\mathcal{F}_A \equiv \{F \in \mathcal{F}: F \cap A \neq \emptyset\}, \quad \mathcal{F}^A \equiv \{F \in \mathcal{F}: F \cap A = \emptyset\}. \quad (9.3.2)$$

For any K compact and any $G_1, \dots, G_n$ open, generate sets of the form $\mathcal{F}^K \cap \mathcal{F}_{G_1} \cap \dots \cap \mathcal{F}_{G_n}$. It can be shown that this class of subsets of $\mathcal{F}$ is a *base* for a topology on $\mathcal{F}$ (called the hit-or-miss topology) and that the topological space is compact, Hausdorff, and separable. In fact, it can be shown (Matheron, 1975, p. 28) that all that is needed is hit-or-miss information, either on the set of all compact sets or on the set of all open sets; I shall

return to this point later. Equipped with a topology on $\mathcal{F}$, it is now possible to be rigorous about convergence of a sequence of closed sets. Furthermore, by taking countable unions and intersections of the open sets of the topological space $\mathcal{F}$, a σ algebra Σ on $\mathcal{F}$ is generated.

Definition. A *random closed set* or RACS (which is often just called a random set) is defined as a measurable mapping X from a probability space $(\Omega, \mathcal{A}, \mu)$ into the measure space $(\mathcal{F}, \Sigma)$. Let Pr be the law of X ; that is, the probability induced on Σ by

$$\text{Pr}(\mathcal{V}) \equiv \mu(X^{-1}(\mathcal{V})), \quad \mathcal{V} \in \Sigma. \quad \blacksquare$$

Special cases are random variables, random vectors, simple point processes (e.g., the index set D in Chapter 8), and random subsets of Euclidean space $\mathbb{R}^d$. Matheron's (1975) requirement of a locally compact, Hausdorff, and separable topological space E is weakened by Ross (1986). Zahle (1982, 1988) considers random-set processes in $\mathbb{R}^d$.

Set Operations

Mathematical-morphology preliminaries are now given; more details can be found in Serra (1982) and Giardina and Dougherty (1988). It is important to define the basic set operations in $\mathbb{R}^d$:

Translation.

$$A \oplus \mathbf{h} \equiv \{\mathbf{a} + \mathbf{h} : \mathbf{a} \in A\}. \quad (9.3.3)$$

Minkowski Addition.

$$A_1 \oplus A_2 \equiv \{\mathbf{a}_1 + \mathbf{a}_2 : \mathbf{a}_1 \in A_1, \mathbf{a}_2 \in A_2\} \quad (9.3.4)$$

or

$$A_1 \oplus A_2 \equiv \bigcup \{A_1 \oplus \mathbf{a}_2 : \mathbf{a}_2 \in A_2\};$$

see Minkowski (1903) and Hadwiger (1957).

Scalar Multiplication.

$$\lambda A \equiv \{\lambda \mathbf{a} : \mathbf{a} \in A\}. \quad (9.3.5)$$

Reflection.

$$\check{A} \equiv \{-\mathbf{a} : \mathbf{a} \in A\}. \quad (9.3.6)$$

Complementation.

$$A^c \equiv \{\mathbf{s} \in \mathbb{R}^d : \mathbf{s} \notin A\}. \quad (9.3.7)$$

Subtraction.

$$A_1 \ominus A_2 \equiv (A_1^c \oplus A_2)^c \quad (9.3.8)$$

or

$$A_1 \ominus A_2 \equiv \bigcap \{A_1 \oplus \mathbf{a}_2 : \mathbf{a}_2 \in A_2\};$$

see Hadwiger (1957).

Corrected Subtraction (Erosion).

$$A_1 \ominus A_2 \equiv A_1 \ominus \check{A}_2. \quad (9.3.9)$$

Opening.

$$A_1 \circ A_2 \equiv (A_1 \ominus A_2) \oplus A_2. \quad (9.3.10)$$

Closing.

$$A_1 \bullet A_2 \equiv (A_1 \oplus \check{A}_2) \ominus A_2. \quad (9.3.11)$$

Hausdorff Distance.

$$\rho(A_1, A_2) \equiv \inf\{r : A_1 \subset A_2 \oplus rb(\mathbf{0}, 1) \text{ and } A_2 \subset A_1 \oplus rb(\mathbf{0}, 1)\}, \quad (9.3.12)$$

where $b(\mathbf{0}, 1)$ is the closed ball of radius 1 centered at $\mathbf{0}$.

Volume.

$$\nu(A) \text{ (or } |A|) \equiv \int_A \nu(ds), \quad (9.3.13)$$

where $\nu(\cdot)$ is Lebesgue measure in $\mathbb{R}^d$.

Hit-or-Miss

The hit-or-miss topology is basic to this theory of random sets. It was chosen because it reflects the way image data in $\mathbb{R}^d$ are analyzed; that is, its roots are in applications. Often there is little to be gleaned from an image or pattern in $\mathbb{R}^d$ just by looking at it (although of course it is the first thing to do). Clearly, some sort of systematic probing is needed, which leads to the use of structuring elements B to check whether “ B hits X ” ($B \cap X \neq \emptyset$) or “ B misses X ” ($B \cap X = \emptyset$). Furthermore, suppose $\mathcal{P}(\mathbb{R}^d)$, the set of all subsets of $\mathbb{R}^d$, is equipped with a σ algebra generated by $\mathcal{P}_G = \{P \in \mathcal{P}(\mathbb{R}^d) : P \cap G \neq \emptyset, G \text{ open}\}$. Then the equivalence

$$P \cap G \neq \emptyset \quad \text{if and only if} \quad \bar{P} \cap G \neq \emptyset$$

shows that, in order to study any random set with the σ algebra generated by

$\mathcal{P}_G$, it is equivalent to study its closure using the σ algebra Σ . Thus, the hit-or-miss approach virtually *demands* the study of random *closed* sets. This restriction of the type of sets under study is a strength of the approach, because it reflects the reality of the objects being modeled. For example, no experiment can hope to distinguish between X being a disk of the plane versus X being the set of irrational points in that disk.

Choquet's Theorem and the Hitting Function

It can be shown that all the interesting set transformations (dilation, erosion, opening, closing, convexification, etc.) of a RACS X are themselves RACS. Matheron (1975, p. 28) has demonstrated that, provided the set transformation is upper or lower semicontinuous into $\mathcal{F}$, the transform of the RACS X is also a RACS. Therefore, to analyze set data, all one needs is a "bagful" of random-set models, and the rest is, in principle, straightforward. But it is here where the random-set approach has difficulty fulfilling its potential.

How can the models be specified? What are the important events that make two random sets different? For a partial answer, return to the hit-or-miss topology. If $\Pr(X \in \mathcal{F}^K \cap \mathcal{F}_{G_1} \cap \cdots \cap \mathcal{F}_{G_n})$ can be specified for all compact K and all open $G_1, \dots, G_n$, for all integers n , in a consistent way, then X is well defined. This can be burdensome, but, fortunately, a great reduction of test sets is possible.

For any $K \in \mathcal{K}$, define the *hitting function* T_X as

$$T_X(K) \equiv \Pr(X \in \mathcal{F}_K) = \Pr\{X \cap K \neq \emptyset\}. \quad (9.3.14)$$

Then T_X has the following properties (Matheron, 1975, p. 29):

1. $T_X(\emptyset) = 0$ and $0 \leq T_X \leq 1$.
2. T_X is increasing.
3. T_X satisfies the following recurrence relations. For any $n \geq 0$, let $S_n(B_0; B_1, \dots, B_n)$ denote the probability that X misses B_0 but hits $B_1, \dots, B_n$. Then

$$\begin{aligned} S_0(B_0) &= 1 - T_X(B_0) \geq 0, \\ S_1(B_0; B_1) &= T_X(B_0 \cup B_1) - T_X(B_0) \geq 0, \\ &\vdots \\ S_n(B_0; B_1, \dots, B_n) &= S_{n-1}(B_0; B_1, \dots, B_{n-1}) \\ &\quad - S_{n-1}(B_0 \cup B_n; B_1, \dots, B_{n-1}) \geq 0. \end{aligned}$$

That is, T_X is a Choquet capacity of infinite order. A powerful result, proved independently by Matheron (1971a) and by Kendall (1974), is *Choquet's Theorem* in the context of random-set theory. It says that the converse

of the preceding statement is true. In other words, if a given T on $\mathcal{K}$ is a Choquet capacity of infinite order, then there exists a *necessarily unique* P_T on Σ such that

$$P_T(\mathcal{F}_K) = T(K), \quad \text{for all } K \in \mathcal{K}.$$

Ross (1986) generalizes this result to random sets of a not-necessarily-separable space E .

An immediate example of its use is when the RACS X is a simple point process (i.e., with probability 1, no more than one event is at any location) in $\mathbb{R}^d$, almost surely locally finite. Let $N(A)$ denote the number of points of the process in $A \subset \mathbb{R}^d$. Then Choquet's Theorem says the point process is completely specified from

$$T_X(K) = 1 - \Pr(X \cap K = \emptyset) = 1 - \Pr(N(K) = 0), \quad \text{for all } K \in \mathcal{K}.$$

This observation, that the point process is uniquely determined from $\{\Pr(N(K) = 0): K \in \mathcal{K}\}$, was made by Ripley (1976b, p. 989), and is one of the consequences of the Equivalence Theorem for point processes (Section 8.3.2).

It is tempting to bracket Choquet's Theorem with the result that says that a random variable X is well defined once the probabilities of events $\{X \leq x\}$, for all $x \in (-\infty, \infty)$, are specified in a consistent way. But the results, although similar, are not identical. In fact, Choquet's Theorem for a random variable, where the RACS X is a.s. a one point set in $\mathbb{R}^1$, involves test sets $\{[a, b]: -\infty < a \leq b < \infty\}$. More work is needed to modify the necessary test sets down to $\{(-\infty, x]: -\infty < x < \infty\}$. It is in this domain, namely, finding ways to reduce the hitting-function test sets down from the full complement $\mathcal{K}$, where results are scarce. I believe that this has held back considerably the development of random-set *models*.

If something extra is known about the RACS X , say that all of its Minkowski functionals (e.g., volume, surface area, diameter, etc.) almost surely exist and are finite (see Serra, 1982, Chapter V), then in principle this extra knowledge should reduce the number of test sets needed (Molchanov, 1984). For example, Tr  der and Eddy (1981) considered almost surely compact convex sets and were able to work with events $\{X \subset C\}$, for all $C \in C(\mathcal{K})$. But $\Pr(X \subset C) = \Pr(X \cap C^c = \emptyset) = 1 - \Pr(X \cap C^c \neq \emptyset) = 1 - T_X(C^c)$. Not only are the number of test sets reduced from that of Choquet's Theorem, but also $\{C^c: C \in C(\mathcal{K})\}$ is not even contained in $\mathcal{K}$. Tr  der (1981) has demonstrated the quite general result that just as $\{T_X(K): K \in \mathcal{K}\}$ determines the probability measure of a RACS X , so also does $\Pr(X \subset K)$, for all $K \in \mathcal{K}$; that is, so also does $\{T_X(K^c): K \in \mathcal{K}\}$. This is perhaps not so surprising because K^c is an open set, which in turn can be approximated by a sequence of compact sets, and the compact sets themselves are measure determining. Ripley (1981, Section 9.1) also discusses the problem of choice

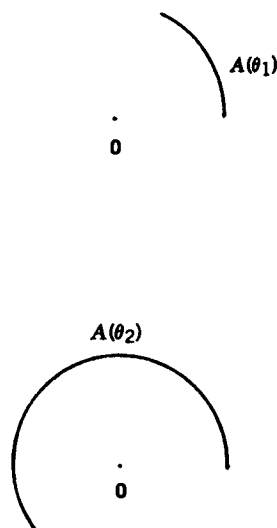


Figure 9.6 Examples of test sets for random rays on the unit disk in $\mathbb{R}^2$. [Source: Cressie and Laslett, 1987]. Reprinted with permission from the *SIAM Review*, volume 29, no. 4, pp. 557–574. Copyright 1987 by the Society for Industrial and Applied Mathematics. All rights reserved.

of test sets. A strong result in this regard is owing to Salinetti and Wets (1986), who prove that $\{T_X(U): U \in \text{set of all finite unions of closed balls in } E\}$ determines the probability measure of a RACS X .

Those who wish to build models depending on sets more regular than those of $\mathcal{X}$ struggle with the test sets of Choquet's Theorem, and even when a reduction is possible it is not always easy to calculate the hitting function. Suppose that the random set X in $\mathbb{R}^2$ is the random ray obtained by taking a random point on the unit circle according to a distribution function given by $F(\theta) = \Pr\{\text{point} \in \text{arc } [0, \theta]\}$ and joining this point to the origin. The test sets are simply the arcs $\{A(\theta): \theta \in [0, 2\pi]\}$, two of which are pictured in Figure 9.6.

Now generate an independent random *vector* W in $\mathbb{R}^2$, according to a distribution function $G(\cdot)$. Then the random set $X \oplus W \equiv \{s + W: s \in X\}$ is well defined and has hitting function $T_{X \oplus W}(K) = \int_{\mathbb{R}^2} T_X(K \oplus \{-w\})G(dw)$, $K \in \mathcal{X}$. In fact, the test sets can again be reduced to arcs, but they are no longer necessarily centered at the origin. Hence $\Pr\{X \cap (A(\theta) \oplus s) \neq \emptyset\}$, for any $s \in \mathbb{R}^2$ and any $\theta \in [0, 2\pi]$, needs to be calculated. This is not a trivial task once the harmony of both X and the test set being centered at the origin is broken.

9.3.2* Inference on Random Closed Sets

Too often, probabilistic research into stochastic modeling is not well counterbalanced with statistical research. Specifically, beyond multivariate analysis and time series, inference techniques for more general stochastic processes

are often rudimentary. This is particularly so for random-set models of objects.

In the fortunate circumstance where a number of objects are observed that could be thought of as independent realizations of the same random set, limit theorems are available. An important set parameter to estimate is the expected value $E(X)$ of the random set X . The expected value of a random set is defined to be the set of expected selections, where a selection is any random vector that almost surely belongs to the random set (Aumann, 1965; Artstein and Vitale, 1975). The natural estimator is

$$\bar{X}_n \equiv (X_1 \oplus X_2 \oplus \cdots \oplus X_n)/n,$$

the Minkowski average of n independent copies $X_1, X_2, \dots, X_n$ of X . Limit theorems for this estimator are necessary for formal inference. Artstein and Vitale (1975), Cressie (1978b), Hess (1979, 1985), Artstein and Hart (1981), and Puri and Ralescu (1983) prove strong laws of large numbers for $\bar{X}_n$ under various conditions. They show that $\bar{X}_n$ converges (with respect to the Hausdorff metric) to the expected *convex hull* of X , with probability 1; Schurger (1983) does likewise for subadditive superstationary X_i s. The result is generalized to convergence of weighted sums of random sets by Taylor and Inoue (1985). Notice that the limiting set is necessarily convex. For example, suppose $\mathbf{a}_i$ and $\mathbf{b}_i$ are random vectors in $\mathbb{R}^d$ and let $X_i = [\mathbf{a}_i, \mathbf{b}_i] \equiv \{\mathbf{s}: \mathbf{s} = \lambda \mathbf{a}_i + (1 - \lambda) \mathbf{b}_i; 0 \leq \lambda \leq 1\}$ be the line segment joining $\mathbf{a}_i$ and $\mathbf{b}_i$. Then $\bar{X}_n$ converges almost surely to a zonoid (by definition, a zonoid is the limit of a sequence of Minkowski sums of line segments), which is convex. A different strong law of large numbers for a possibly nonconvex limiting set is proved by Kovyazin (1986).

Cressie (1979b), Ljasenko (1979), Trader and Eddy (1981), Vitale (1981), Weil (1982), and Artstein (1984) show that, under various conditions, the rate of convergence in the strong law of large numbers is $n^{-1/2}$. Cressie's central limit theorem is geometric in that limiting normalized sets are given, whereas the other authors' theorems are in terms of normalized Hausdorff distances, which lose the geometric subtleties of the limiting process. These latter methods are employed by Giné et al. (1983) to carry over any probability result in a Banach space (law of large numbers, central limit theorem, law of the iterated logarithm, etc.) to Minkowski sums of compact *convex* random sets. The convexity condition is dispensed with in Puri and Ralescu (1985).

To model the limiting random set, one should look for classes of models from among those random sets that are infinitely divisible under Minkowski addition $\oplus$ (Mase, 1979). Giné and Hahn (1985) give a representation for such sets of Lévy–Hincin type.

The limit results referred to in the preceding text are not proved by hitting-function considerations, but rather by direct inspection of the random set $(X_1 \oplus \cdots \oplus X_n)/n$. Norberg's (1984) result, which says that convergence

in distribution of RACS requires convergence of hitting functions only on a certain countable class of bounded Borel sets, does not seem helpful in this regard. The difficulty lies in not having a formula for $T_{X_1 \oplus X_2}$ in terms of T_{X_1} and T_{X_2} .

Analogues to extreme-value limit theorems can be obtained by considering limits of $X_1 \cup \cdots \cup X_n$ or $X_1 \cap \cdots \cap X_n$; that is, replace $\oplus$ with $\cup$ or $\cap$ (Eddy, 1982).

Consider the more general problem of convergence of a sequence of random sets $\{Z_n: n \geq 1\}$ to a limiting random set Z . Assuming $\{Z_n\}$ is a set-valued martingale (defined via the conditional expectation of selections), Hiai and Umegaki (1977), Bagchi (1985), and Papageorgiou (1989) give various convergence results.

The importance of the hitting function justifies its estimation. Suppose $X_1, \dots, X_n$ are independent copies of X , available as data, and define $T_n(K) \equiv \sum_{i=1}^n I(X_i \cap K \neq \emptyset)/n$. Molchanov (1987) considers conditions under which $T_n(K)$ converges to $T_X(K) = \Pr(X \cap K \neq \emptyset)$, uniformly in K . This allows one to obtain, for example, a consistent estimator of $\chi(\mathbf{h})$, the covariogram of the pores of a stationary RACS. Now, $\chi(\mathbf{h}) \equiv 1 - T_X(\{\mathbf{0}, \mathbf{h}\})$. Then

$$\hat{\chi}(\mathbf{h}) \equiv \sum_{i=1}^n I(\mathbf{0} \in X_i^c \cap (X_i^c \oplus \{-\mathbf{h}\}))/n, \quad \mathbf{h} \in \mathbb{R}^d,$$

is a consistent estimator.

One Observation on X

Usually data consist of just one observation; in this case, inference is impossible unless repeatability in space is assumed. The statistical methods used in Chapters 2 through 8 all have some type of stationarity (actually, ergodicity) assumption to ensure their consistency. Without it, any statistical analysis can only claim to be descriptive.

But stationarity puts its own restrictions on X . Matheron (1975) has shown that a nonempty stationary RACS in $\mathbb{R}^d$ is almost surely *unbounded*. Thus, there are various types of phenomena that are not amenable to stochastic modeling and inference.

The rest of this chapter is concerned with one particular class of unbounded sets, namely the Boolean model and its variants (see Section 9.4 for definitions). There are pragmatic reasons for choosing this class; it will be seen that inference on its parameters is possible from just one observation X (Sections 9.5 and 9.6) and it exhibits a great deal of flexibility for modeling objects. Let X be any RACS in $\mathbb{R}^d$ whose realizations are in the extended convex ring $\mathcal{S}^d$. (That is, for any compact convex set C , $X \cap C$ is a finite union of compact convex sets.) Surprisingly, this rather mild regularity condition is enough to ensure that X is a (generalized) Boolean model of convex grains (Weil and Wieacker, 1984, 1988).

9.4 THE BOOLEAN MODEL

In this section I shall present what is arguably the most important random-set model, namely, the Boolean model. Generalizations to other models will be discussed in Section 9.4.2, but it is clear that a fruitful path to truly broad classes of models has yet to be developed.

The basic ideas behind the construction of this model are found in Avrami (1939), Armitage (1949), Solomon (1953), Matern (1960), and Roach (1968). Marcus (1966, 1967) uses the Boolean model to examine the meteoroidal-impact hypothesis for the origin of lunar craters, Dupac (1980) considers the etching of tracks formed by the fission of randomly located uranium atoms in a fission material, Serra (1980) models ore sintering, and Diggle (1981b) uses it to model the incidence of heather (he calls it a random binary mosaic).

Special cases of the Boolean model were given in Sections 9.1.3 and 9.2. The Boolean model X is obtained by locating independent realizations of a *bounded RACS* Z (of which random polygons, disks, and parallelograms are special cases) at each point of a realization of a *homogeneous Poisson process* D in $\mathbb{R}^d$ (Section 8.3) and then taking the union. That is,

$$X \equiv \bigcup \{Z(s_i) : s_i \in D\}, \quad (9.4.1)$$

where $Z(s_i) \equiv Z_i \oplus s_i$, a realization of the (almost surely) bounded RACS Z (i.e., a *grain*) translated to a point s_i (i.e., a *germ*) of the Poisson process D . Thus, there are two sources of randomness in the model: (1) the Poisson process characterized by its intensity parameter λ and (2) the probability law of the bounded random grain Z .

The Hitting Function

The hitting function of the Boolean model X , defined by (9.4.1), can be constructed in several stages.

Consider the *homogeneous* Poisson process D in $\mathbb{R}^d$ with intensity λ , which, according to Section 8.3, is characterized as follows. Let $N(A)$ denote the number of points of the process in any subset $A \subset \mathbb{R}^d$. Then, if $A_1 \cap A_2 = \emptyset$, $N(A_1)$ and $N(A_2)$ are independent Poisson random variables with respective means $\lambda|A_1|$ and $\lambda|A_2|$. Also

$$\Pr\{N(ds) = 0\} = 1 - \lambda \cdot \nu(ds) + o(\nu(ds)),$$

$$\Pr\{N(ds) = 1\} = \lambda \cdot \nu(ds) + o(\nu(ds)),$$

where $\nu(ds)$ is the volume element (Lebesgue measure) of the infinitesimal region ds , located at $s \in \mathbb{R}^d$.

Now the complement of the hitting function of X is

$$Q_X(K) \equiv \Pr(X \cap K = \emptyset) = \Pr(Z(s_i) \cap K = \emptyset, \text{ for all } i).$$

In the infinitesimal region ds , two mutually exclusive events may happen:

1. There is no element of $\{s_1, s_2, \dots\}$ in ds . This occurs with approximate probability $1 - \lambda \cdot \nu(ds)$.
2. There is one element of $\{s_1, s_2, \dots\}$ in ds , but $Z(s_i)$ does not hit K . This occurs with approximate probability $\lambda \cdot \nu(ds) \cdot Q_Z(K \oplus \{-s\})$.

To the order of magnitude ignored, this yields the probability,

$$\begin{aligned} &1 - \lambda(1 - Q_Z(K \oplus \{-s\}))\nu(ds) \\ &= \exp\{-\lambda(1 - Q_Z(K \oplus \{-s\}))\nu(ds)\} + o(\nu(ds)). \end{aligned}$$

Finally, $Q_X(K)$ is obtained by taking the product over all infinitesimal regions:

$$Q_X(K) = \exp\left\{-\lambda \int_{\mathbb{R}^d} (1 - Q_Z(K \oplus \{-s\}))\nu(ds)\right\}. \quad (9.4.2)$$

This formula is fundamental in linking the hitting function of X to the hitting function of Z .

Now define $I_{\check{Z} \oplus K}(\cdot)$ to be the indicator function of $\check{Z} \oplus K \equiv \{-s + k : s \in Z, k \in K\}$; see (9.3.4) and (9.3.6). But

$$|\check{Z} \oplus K| = \int_{\mathbb{R}^d} I_{\check{Z} \oplus K}(s)\nu(ds),$$

and so

$$E(|\check{Z} \oplus K|) = \int E(I_{\check{Z} \oplus K}(s))\nu(ds) = \int T_Z(K \oplus \{-s\})\nu(ds),$$

because $s \in \check{Z} \oplus K$ if and only if $Z \cap (K \oplus \{-s\}) \neq \emptyset$. Hence,

$$E(|\check{Z} \oplus K|) = \int (1 - Q_Z(K \oplus \{-s\}))\nu(ds),$$

where the integrals with respect to s are taken over $\mathbb{R}^d$. Therefore, from (9.4.2),

$$T_X(K) = 1 - Q_X(K) = 1 - \exp\{-\lambda E(|\check{Z} \oplus K|)\}, \quad K \in \mathcal{K}. \quad (9.4.3)$$

The flexibility in choice of K makes (9.4.3) a very useful result; for example, the porosity and covariogram of the pores are derived from it in the next section. When K is a straight line segment, $Q_X(K)$ is the probability that one end of the segment is visible to an observer positioned at the other

end of the segment. Such visibility problems have been discussed by Yadin and Zacks (1985) and, in a more general context, by Wieacker (1986).

9.4.1* Main Properties

In this section, I shall summarize the main properties of the Boolean model, from which it should be clear why it is central among random set models. More details can be found in Serra (1980).

1. *Porosity q .* Porosity is the probability that a point of the space is in the complement of the RACS X (i.e., in the pores). Let $K = \{s\}$. Then $q \equiv Q_X(\{s\}) = \Pr\{s \in X^c\}$; that is, from (9.4.3),

$$q = e^{-\lambda E(|Z|)}.$$

This is a coverage property of the Boolean model; Avrami (1939) is the earliest reference I know of where such problems are addressed in $\mathbb{R}^2$. Hall (1988a) contains a complete discussion of coverage, vacancy, counting, and clumping for the Boolean model.

2. *Covariogram of the Pores $\chi(\mathbf{h})$.* This is defined to be the probability that two points separated by a vector $\mathbf{h}$ are both in the complement of the RACS X . It measures dependence between pores. Let $K = \{s, s + \mathbf{h}\}$ and $\chi(\mathbf{h}) \equiv Q_X(\{s, s + \mathbf{h}\})$. Then, from (9.4.3),

$$\begin{aligned}\chi(\mathbf{h}) &= \Pr\{s, s + \mathbf{h} \in X^c\} \\ &= \exp\{-\lambda E(|Z \cup Z \oplus \{-\mathbf{h}\}|)\} = q^2 e^{\lambda \kappa(\mathbf{h})},\end{aligned}$$

where

$$\kappa(\mathbf{h}) \equiv E(|Z \cap Z \oplus \{-\mathbf{h}\}|) = \int \Pr\{s \in Z \cap Z \oplus \{-\mathbf{h}\}\} \nu(ds),$$

the probabilistic analogue of the geometrical covariance.

3. *Stationarity.* Because $E(|\cdot|)$ in (9.4.3) ignores location, X is clearly stationary.
4. *Stability under Dilation.* From (9.4.3), the RACS $X \oplus L \equiv \{s + \mathbf{l} : s \in X, \mathbf{l} \in L\}$, where L is any deterministic compact set, is also a Boolean model.
5. *Cross Sections are Boolean Models.* This is true because K in (9.4.3) may belong to a subspace of $\mathbb{R}^d$.
6. *Infinite Divisibility with Respect to Union.* A RACS Y is said to be *infinitely divisible with respect to union* if, for any integer $m > 0$, Y is equivalent to $\bigcup_{i=1}^m Y_i$ of m independent stochastically equivalent RACS $\{Y_i : i = 1, \dots, m\}$. The Boolean model has this property, which shows it to be a candidate model for limits of unions of RACS.

7. *The Boolean Model with Convex Grain Z is Semi-Markov.* A RACS Y is said to be *semi-Markov* if for any K, L , and $M \in \mathcal{K}$, and K and M separated by L (i.e., the segment joining any point of K to any point of M hits L), the RACS $Y \cap K$ and $Y \cap M$ are conditionally independent given $Y \cap L = \emptyset$. The Boolean model with convex grains has this property, which shows that its probability law is really determined by local conditions. Widely separated parts of the set are only weakly dependent. In terms of the functional Q , Matheron (1975, p. 132) has shown that if Y is infinitely divisible with respect to union and if, for any K, M , and $K \cup M \in C(\mathcal{K})$ (the space of compact convex sets),

$$Q_Y(K \cup M)Q_Y(K \cap M) = Q_Y(K)Q_Y(M),$$

then Y is semi-Markov.

8. *The Union of Two Independent Boolean Models with Identically Distributed Grains Z is a Boolean Model.* Furthermore, if the Poisson points of a Boolean model are *thinned* so that they now occur with an intensity $\rho \cdot \lambda$ ($0 \leq \rho < 1$), leaving behind a Boolean model whose union is taken with another independent Boolean model of intensity $(1 - \rho) \cdot \lambda$ and the same probability law for its grains, then the resulting random set is a Boolean model identically distributed to the original one.

A Characterization Theorem

Matheron (1975, p. 148) has provided the following important characterization theorem (presented here in $\mathbb{R}^3$). Any RACS in $\mathbb{R}^3$ that is stationary, infinitely divisible with respect to union, and semi-Markov, is equivalent to

$$X_1 \cup X_2 \cup X_3,$$

where X_1, X_2 , and X_3 are stationary and independent, X_1 is a Boolean model with convex grains, X_2 is a union of cylinders with bases that are two-dimensional Boolean models with convex grains (in $\mathbb{R}^2$), and X_3 is a union of cylinders with bases that are one-dimensional Boolean models with convex grains (in $\mathbb{R}^1$). Notice that if the grains in X_2 and X_3 are almost surely points, then the associated cylinders become Poisson lines and Poisson planes, respectively, yielding Poisson-flat processes (studied extensively by Miles, 1969).

9.4.2* Generalizations of the Boolean Model

The choice of mathematical models available to the data analyst is often governed by their tractability rather than their applicability. When the data are sets, this leaning is even more pronounced. Serra (1982, Chapter XIII) has provided users with a menu of models and of examples for which they are

appropriate. By far the most important group is that based on the Boolean model, which I shall present and extend here.

One extension already mentioned in Section 9.4.1 is to the Poisson-flat processes of Miles (1969). There, hyperplanes of infinite extent and random orientation are placed at points of a homogeneous Poisson process in $\mathbb{R}^d$. Another extension is due to Cowan (1989), who assumes only that the point process of germs has constant intensity. The point process may be dependent on the grains $\{Z_i\}$, which are assumed to have smooth boundaries. He obtains mean-value formulas for features seen in an observation window of general size and shape, but his assumptions are too weak to allow calculation of hitting functions.

The most fruitful extension of the Boolean model is the so-called *grain-germ model* (Hanisch, 1980). It removes the Poisson assumption, the independence of the Z_i s, and allows for nonoverlapping of the grains (e.g., Mase, 1986). Let

$$X = \bigcup \{Z_i \oplus s_i : (s_i, Z_i) \in N\}, \quad (9.4.4)$$

where N is a marked point process with mark space $\mathcal{X}$, the set of compact sets. Let Π_N be the induced measure on $(\Phi_{\mathcal{X}}, \mathcal{N}_{\mathcal{X}})$, where $\Phi_{\mathcal{X}}$ is the set of all Radon counting measures ϕ on $\mathbb{R}^d \times \mathcal{X}$ with $\phi(B \times \mathcal{X}) < \infty$ for any bounded Borel set B , and $\mathcal{N}_{\mathcal{X}}$ is the corresponding σ algebra (Section 8.7). Let U be the set of all measurable functions from $\mathbb{R}^d \times \mathcal{X}$ to $[0, 1]$ and $V \equiv \{1 - u : u \in U\}$. The functional $G_N: V \rightarrow [0, 1]$, which is given by

$$G_N(v) = \int_{\Phi_{\mathcal{X}}} \prod_{(s, Z) \in \phi} v(s, Z) \Pi_N(d\phi), \quad v \in V, \quad (9.4.5)$$

is called the probability generating functional of the marked point process N . For X given by (9.4.4), Hanisch is able to relate the complement of the hitting function Q_X to G_N :

For $K \in \mathcal{X}$, let v_K be the mapping given by

$$v_K(s, Z) = 1 - I_{Z \oplus K}(s), \quad s \in \mathbb{R}^d, Z \in \mathcal{X}.$$

Then,

$$Q_X(K) = G_N(v_K), \quad K \in \mathcal{X}. \quad (9.4.6)$$

Special cases of (9.4.4) yield models already studied in the literature:

1. The marked point process N almost surely yields *independent* markings; see Stoyan (1979b) and Mase (1982b).
2. The point process is a Neyman–Scott process where parent events are generated according to a homogeneous Poisson process and offspring

events are generated independently and identically around each initial point; see Neyman and Scott (1958) and Section 8.5.3.

3. The point process is regionally independent, in particular, a (not necessarily homogeneous) Poisson process with intensity function $\{\lambda(s): s \in \mathbb{R}^d\}$. If the *weighted* measure of $\check{Z} \oplus K$ is defined as

$$|\check{Z} \oplus K|_\lambda \equiv \int_{\mathbb{R}^d} I_{\check{Z} \oplus K}(s) \lambda(s) \nu(ds), \quad (9.4.7)$$

then the complement of the hitting function is

$$Q_X(K) = \exp\{-E(|\check{Z} \oplus K|_\lambda)\}. \quad (9.4.8)$$

Hypothesis testing for constant intensity function in the Boolean model is an area of inference that needs investigation.

4. The point process is a homogeneous Poisson process. Serra (1982, p. 484ff) has a detailed discussion of the model and some of its associates. When the mark process is independent of the point process and consists of independent realizations of an almost surely bounded RACS Z , then the Boolean model (9.4.1) is obtained. One interesting extension is to consider a series of independent Boolean models occurring from the infinite past: At each instant of time the Boolean model fills part of the space. At the next instant, some of the pores (and sets) will be covered by a set from the new Boolean model and some of the sets (and pores) will remain exposed. The procedure is continued until the present, so that finally a tessellation of the space results. This is called the *dead-leaves model*, which has been further extended by Jeulin (1989) to sequential-random-function models.
5. The events are not generated by a point process, but are fixed and finite in number in $\mathbb{R}^d$, namely, $\{\mathbf{a}_1, \dots, \mathbf{a}_n\}$. The only source of randomness is from the mark process, assumed to be generated by independent realizations of a bounded RACS Z . Then, from (9.4.5),

$$G_N(v_K) = \prod_{i=1}^n E(v_K(\mathbf{a}_i, Z_i)).$$

Hence,

$$Q_X(K) = \prod_{i=1}^n Q_Z(K \oplus \{-\mathbf{a}_i\}). \quad (9.4.9)$$

6. The point process is homogeneous Poisson, independent from the mark process generated by independent realizations of a bounded RACS Z , with the property that $|Z|$ is *not* random (although in general un-

known). In this case,

$$\log q = -\lambda|Z|,$$

$$\int_{\mathbb{R}^d} \log(\chi(\mathbf{h})/q^2) d\mathbf{h} = \lambda|Z|^2,$$

where the porosity q and the covariogram of the pores $\chi(\mathbf{h})$ are given by properties 1 and 2 of Section 9.4.1 and can be estimated from the set data. Hence λ and $|Z|$ can be estimated by the method-of-moments, although little is known about the efficiency of these estimators; Sections 9.5, 9.6, and 9.7 can be consulted for matters of estimation and inference on data of this type.

7. The point process is homogeneous Poisson, independent of the mark process generated by independent realizations of the RACS $b(\mathbf{0}, R)$, the closed ball of random radius R centered at $\mathbf{0}$. The Poisson-intensity parameter λ and the distribution of R can be estimated from the covariance $\chi(\mathbf{h})$ (Serra, 1980), although little is known about the estimators' statistical properties; see Dupac (1980) and Section 9.6.

9.5 METHODS OF BOOLEAN-MODEL PARAMETER ESTIMATION

Several data sets in the form of images have been presented in this chapter so far. The cloud-droplets data of Figure 9.4 are naturally suited to the fitting of a Boolean model. Of the parameters estimated, cloud physicists are very interested in the droplet size distribution; the mean and variance of the droplet radius give some idea of the efficacy of the cloud-seeding treatment. Cloud droplets are three-dimensional but the data are two-dimensional, representing the cumulative projection of droplets over a region of the cloud. Problems of stereology (i.e., estimating d -dimensional quantities from data taken in lower, more manageable dimensions) were discussed generally in remarks made at the beginning of this chapter. Weil (1987) gives an account of the results available for the (generalized) Boolean model.

Cressie and Laslett (1987) generated a Boolean model in $\mathbb{R}^2$ made up of random parallelograms; they are reproduced in Figure 9.5. An analysis of these data is presented in Section 9.5.1; however, some preliminary formulas are needed before I can proceed.

Steiner's Formula

Consider an almost surely compact convex grain Z , whose probability law is invariant under rotations of Z about $\mathbf{0}$. Then the Boolean model X defined by (9.4.1) is stationary and isotropic. Under these circumstances, and for K compact convex, Steiner's formula (Mack, 1954; Serra, 1982, p. 111) in $\mathbb{R}^2$ yields

$$E\{|\check{Z} \oplus K|\} = E(|Z|) + \frac{1}{2\pi} E(P(Z))P(K) + |K|, \quad (9.5.1)$$

where $P(A)$ denotes the perimeter of the set A . When $Z = b(\mathbf{0}, R)$, the disk centered at $\mathbf{0}$ of random radius R , $E(P(Z))/(2\pi) = E(R)$ and $E(|Z|)/\pi = E(R^2)$. Weil and Wieacker (1984) can be consulted for generalizations of (9.5.1) to generalized Boolean models (presented in Section 9.4.2) in higher dimensions.

With one realization of what is believed to be a Boolean model in $\mathbb{R}^2$, the goal is to make inferences about the random set Z . From (9.4.3) and (9.5.1),

$$Q_X(K) = \exp \left[-\lambda \left\{ |K| + \frac{1}{2\pi} E(P(Z)) P(K) + E(|Z|) \right\} \right], \quad (9.5.2)$$

and hence estimators can be found for λ , $E(P(Z))$, and $E(|Z|)$: For example, let K be $b(\mathbf{0}, t)$, the disk of radius t ; then vary t . Theoretically,

$$-\log Q_X(b(\mathbf{0}, t)) = \lambda \{ \pi t^2 + E(P(Z))t + E(|Z|) \} \quad (9.5.3)$$

$$\equiv \beta_0 + \beta_1 t + \beta_2 t^2, \quad (9.5.4)$$

where $\beta_0 \equiv \lambda E(|Z|)$, $\beta_1 \equiv \lambda E(P(Z))$, and $\beta_2 \equiv \lambda \pi$.

Boolean-Model Parameter Estimators

By scanning the image appropriately, one can obtain an estimate $\hat{Q}_X(b(\mathbf{0}, t))$, for various t , which, when regressed on 1 , t , and t^2 yields estimates $\hat{\beta}_0$, $\hat{\beta}_1$, and $\hat{\beta}_2$. Image analyzers (e.g., Serra, 1982, Part II) are specifically built to do this type of task; however, it is not difficult to use conventional computers to analyze random-set data like Figure 9.5. Cressie and Laslett (1987) compute both ordinary-least-squares and generalized-least-squares estimates of quadratic-regression coefficients for Figure 9.5a. Estimates of set parameters are easily obtained from (9.5.4) through the transformations

$$\hat{\lambda} = \hat{\beta}_2 / \pi,$$

$$\hat{E}(P(Z)) = \hat{\beta}_1 / \hat{\lambda}, \quad (9.5.5)$$

$$\hat{E}(|Z|) = \hat{\beta}_0 / \hat{\lambda}.$$

Alternatively, choice of the three different types of test set, K_0 the origin, K_1 the straight line segment of length l , and K_2 the closed square of side l , yields (in $\mathbb{R}^2$)

$$Q_X(K_0) = \exp \{ -\lambda E(|Z|) \},$$

$$Q_X(K_1) = \exp \left\{ -\lambda \left\{ E(|Z|) + \frac{l}{\pi} E(P(Z)) \right\} \right\}, \quad (9.5.6)$$

$$Q_X(K_2) = \exp \left\{ -\lambda \left\{ E(|Z|) + \frac{2l}{\pi} E(P(Z)) + l^2 \right\} \right\},$$

from which method-of-moments estimators could be obtained. Hall (1985b) and Kellerer (1985) take essentially this approach; however, it leaves no degrees of freedom to assess model adequacy. The same comment applies to the intensity-based method-of-moments estimators given by Stoyan et al. (1987, p. 88).

9.5.1 Analysis of Random-Parallelograms Data

Because the original Boolean model has been discretized onto a square grid, Figure 9.5a was analyzed with $K = tC$, where C is a square of side 2 units centered on $\mathbf{0}$, and $t = 0, 1, 2, 3, 4$ (larger values of t led to $\hat{Q}_X \equiv 0$). Then (9.5.2) gives

$$-\log Q_X(tC) = \lambda E(|Z|) + \{4\lambda E(P(Z))/\pi\}t + 4\lambda t^2. \tag{9.5.7}$$

Consider the estimator

$$\hat{Q}_X(tC) \equiv \sum_{\mathbf{x}_i \in E_t} \{1 - I_{X \oplus tC}(\mathbf{x}_i)\}/N_t, \quad t = 0, \dots, 4, \tag{9.5.8}$$

where N_t is the total number of pixels (at locations $\{\mathbf{x}_i: i = 1, \dots, N_t\}$) in the mask $E_t = E \ominus tC$ [see (9.3.8)] placed over the region of interest E . (In Figure 9.5a and b, E is the bordered region.) Clearly, this is an unbiased estimator of $Q_X(tC)$. Write $\mathbf{Y}' \equiv (-\log \hat{Q}_X(tC): t = 0, \dots, 4)$ and let T be the 5×3 matrix whose t th row is $(1, t, t^2)$, $t = 0, \dots, 4$. Then the usual ordinary-least-squares (o.l.s.) estimator is given by $(T'T)^{-1}T'\mathbf{Y}$, which estimates the coefficients of 1, t , and t^2 without taking into account correlations between the elements of $\mathbf{Y}$. Estimates of higher efficiency can be obtained by taking a generalized-least-squares (g.l.s.) approach. Table 9.2 gives the o.l.s. and g.l.s. estimates for the data of Figure 9.5a.

Table 9.2 Summary Statistics and Final Estimates for the Simulated Boolean Model Data of Figure 9.5a^a

t	$\hat{Q}_X(tC)$	Fitted Quadratic (g.l.s.)	Fitted Quadratic (o.l.s.)
0	0.72950	0.72985	0.72692
1	0.44138	0.44137	0.44430
2	0.22797	0.22678	0.22831
3	0.09948	0.09901	0.09863
4	0.03568	0.03673	0.03582
		Parameter Estimates ^a (g.l.s.)	Parameter Estimates ^a (o.l.s.)
	$\hat{\lambda}$	0.020	0.022
	$\hat{E}(P(Z))$	16.27	14.69
	$\hat{E}(Z)$	15.47	14.71

Source: Cressie and Laslett (1987). Reprinted with permission from the *SIAM Review*, volume 29, no. 4, pp. 557–574. Copyright 1987 by the Society for Industrial and Applied Mathematics. All rights reserved.

^aThe true values of the parameters are $\lambda = 0.02$, $E(P(Z)) = 20.00$, and $E(|Z|) = 15.92$.

Generalized-Least-Squares Estimation

To give the g.l.s. estimator explicitly, some definitions are needed first. From the definition of $\hat{Q}_X(tC)$, given by (9.5.8), it is easily seen that, for the Boolean model,

$$\text{cov}(\hat{Q}_X(tC), \hat{Q}_X(uC)) = \sum_{\mathbf{x}_i \in E_t} \sum_{\mathbf{x}_j \in E_u} C_{t,u}(\mathbf{x}_i - \mathbf{x}_j) / (N_t N_u), \quad (9.5.9)$$

where

$$C_{t,u}(\mathbf{h}) \equiv [\exp\{\lambda E(|(Z \oplus tC) \cap (Z \oplus \{-\mathbf{h}\} \oplus uC)|)\} - 1] \\ \times \exp\{-\lambda E(|Z \oplus tC|) - \lambda E(|Z \oplus uC|)\}. \quad (9.5.10)$$

The first term in this expression for $C_{t,u}(\mathbf{h})$ can be simplified for special cases of the structuring element C . Regardless, the expression for the covariance depends on the unknown parameters; recall that the objective is to estimate these parameters. Instead of trying to minimize a complicated objective function with parameters also in the covariance terms, the approach taken here will be to use the *empirical* covariance function in g.l.s. estimation of the parameters.

The pixels of Figure 9.5 are regularly spaced, and so $C_{t,u}(\mathbf{h})$ can be estimated for $\mathbf{h}$ in horizontal, vertical, and diagonal directions. Let

$$\hat{C}_{t,u}(\mathbf{h}) \equiv \left[\sum_{\mathbf{x}_i, \mathbf{x}_j \in M(\mathbf{h})} \{1 - I_{X \oplus tC}(\mathbf{x}_i)\} \{1 - I_{X \oplus uC}(\mathbf{x}_j)\} \right] / \left[\sum_{\mathbf{x}_i, \mathbf{x}_j \in M(\mathbf{h})} 1 \right] \\ - \hat{Q}_X(tC) \cdot \hat{Q}_X(uC), \quad (9.5.11)$$

where $M(\mathbf{h}) \equiv \{(\mathbf{x}_i, \mathbf{x}_j): \mathbf{x}_i \in E_t, \mathbf{x}_j \in E_u, \mathbf{x}_i - \mathbf{x}_j = \mathbf{h}\}$. Substituting (9.5.11) for $C_{t,u}(\mathbf{h})$ in (9.5.9) yields $\text{cov}(\hat{Q}_X(tC), \hat{Q}_X(uC))$. Write

$$\hat{\Sigma} \equiv (\widehat{\text{cov}}(\hat{Q}_X(tC), \hat{Q}_X(uC)): t = 0, \dots, 4; u = 0, \dots, 4), \quad (9.5.12)$$

which is a 5×5 matrix. The error vector is

$$\delta' \equiv (\hat{Q}_X(tC) - \exp\{-\beta_0 - \beta_1 t - \beta_2 t^2\}: t = 0, \dots, 4). \quad (9.5.13)$$

Cressie and Laslett (1987) proposed a g.l.s. estimator for $\beta_0 = \lambda E(|Z|)$, $\beta_1 = \{4\lambda E(P(Z))/\pi\}$, and $\beta_2 = 4\lambda$ by minimizing $\delta' \hat{\Sigma}^{-1} \delta$ with respect to β_0 , β_1 , and β_2 . This is carried out using a quasi-Newton numerical optimization procedure. (A g.l.s. estimator on the log-transformed scale is discussed in Section 9.6.)

Cressie and Laslett (1987) reported that occasionally $\hat{\Sigma}$ was not positive-definite. Difficulties of this sort are to be expected when empirical covariances are used; for example, a time series $\{z_t: t = 1, \dots, n\}$ has an

(approximately) unbiased empirical covariance function $\{\sum_{i=1}^{n-h}(z_{i+h} - \bar{z})(z_i - \bar{z})/(n-h): h = 1, \dots, n-1\}$, which is not assured of being positive-definite. The usual way around this problem is to fit a positive-definite model to the empirical covariance function. One suggestion made by Diggle (1981b) is to fit a shifted Weibull density to (9.5.11).

9.5.2 Analysis of Heather-Incidence Data

Diggle (1981b) presented an image of the incidence of heather, *Calluna vulgaris*, over a 10×20 -m rectangle at Jadrass, Sweden. Individual heather plants grow from seedlings into roughly hemispherical bushes. As the individual bushes expand, their branches intermingle, but a map of presence or absence of heather does not record the multiplicity of bushes at any particular spatial location; see Figure 9.7.

Diggle (1981b) fits the Boolean model in $\mathbb{R}^2$,

$$X = \bigcup \{Z(s_i): s_i \in D\}, \quad (9.5.14)$$

where $Z(s_i) \equiv Z_i \oplus s_i (i = 1, 2, \dots)$, $Z_1, Z_2, \dots$ are disks centered at $\mathbf{0}$ whose radii $R_1, R_2, \dots$ are i.i.d. as R with density function $f(\cdot)$, and D is a homogeneous Poisson process of intensity λ . Define $H(\cdot)$ to be the distribution function of the distance from an arbitrary point to the nearest point occupied by heather. Then $H(u) = 1 - Q_X(b(\mathbf{0}, u))$, where Q_X is given by (9.4.2), and hence,

$$H(u) = 1 - \exp\left\{-\lambda\pi \int_0^\infty (u+r)^2 f(r) dr\right\}, \quad u \geq 0. \quad (9.5.15)$$

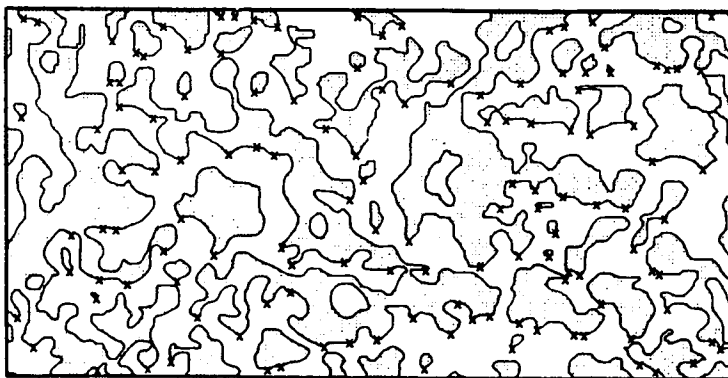


Figure 9.7 Incidence of *Calluna vulgaris* (shaded area) over a 10×20 -m rectangular area at Jadrass, Sweden. Exposed marker points (see Section 9.5.3) are identified with a cross. [Source: Laslett et al., 1985]

Notice that $H(\cdot)$ depends on $f(\cdot)$ only through $E(R)$ and $E(R^2)$. An empirical version $\hat{H}$ of H can be calculated by superimposing a fine grid over the rectangle E in Figure 9.7 and randomly sampling N nodes of the grid. This would yield $U_1, \dots, U_N$ distances to the nearest heather point (a number of U_i s will be zero, should their respective nodes be in the set of heather). Then $\hat{H}(u) = \sum_{i=1}^N I(U_i \leq u)/N$. Some modification can be made for edge effects by only sampling from $E \ominus b(\mathbf{0}, u_{\max})$, where $u_{\max}$ is the largest value of u considered. Diggle proposed to estimate parameters λ , $E(R)$, and $\{\text{var}(R)\}^{1/2}$ by minimizing

$$\int_0^{u_{\max}} (H(u) - \hat{H}(u))^2 du. \quad (9.5.16)$$

He also considers the covariance $\kappa_X(\mathbf{h}) \equiv \Pr(s \in X, s + \mathbf{h} \in X)$ and calculates that, for the Boolean model (9.5.14),

$$\kappa_X(\mathbf{h}) \equiv \kappa_X^\circ(h) = \exp\{-2\pi\lambda E(R^2)\} \left[\exp\left\{\lambda \int_{h/2}^{\infty} V_h(r) f(r) dr\right\} - 1 \right],$$

$$\|\mathbf{h}\| \equiv h \geq 0, \quad (9.5.17)$$

where

$$V_h(r) \equiv 2r^2 \left\{ \cos^{-1}(h/(2r)) - (h/(2r))(1 - h^2/(4r^2))^{1/2} \right\} \quad (9.5.18)$$

is the area of intersection of two disks with common radius r and centers that are a distance h apart. Notice that $\kappa_X(\mathbf{h})$ is related to the porosity q and the covariogram of the pores $\chi(\mathbf{h})$, given in Section 9.4.1, through $\kappa_X(\mathbf{h}) = 1 - 2q + \chi(\mathbf{h})$. The empirical version $\hat{\kappa}_X^\circ(h)$ can be calculated by measuring the area of $X \cap X \ominus \{-\mathbf{h}\}$ for various choices of $\mathbf{h}$. Using $\hat{\kappa}_X^\circ(h)$ as a diagnostic, Diggle (1981b) finds that fitting the parameters by minimizing (9.5.16) is unsatisfactory for the heather-incidence data.

His second approach is to minimize

$$\int_0^{h_{\max}} \{\kappa_X^\circ(h) - \hat{\kappa}_X^\circ(h)\}^2 dh, \quad (9.5.19)$$

where he chooses $h_{\max} = 0.1$ units (here, 1 unit = 10 m). He fits a parametric form, namely, the shifted Weibull distribution, to $f(\cdot)$:

$$f(r) = \begin{cases} 0, & r < \delta, \\ k\rho(r - \delta)^{k-1} \exp\{-\rho(r - \delta)^k\}, & r \geq \delta, \end{cases} \quad (9.5.20)$$

where δ is a shift parameter that removes disks of small radius and $k > 0$. He obtains a good fit of $\kappa_X^\circ(h)$ to $\hat{\kappa}_X^\circ(h)$ and a satisfactory diagnostic

comparison of plots of $H(u)$ with $\hat{H}(u)$. For cross-validation purposes, he splits up the area of Figure 9.7 into two unit areas (each 10×10 m); using (9.5.19) and (9.5.20), he obtains

$$\text{plot 1: } (\hat{\lambda}, \hat{\delta}, \hat{k}, \hat{\rho}) = (221, 0.0281, 0.8471, 144.7),$$

$$\text{plot 2: } (\hat{\lambda}, \hat{\delta}, \hat{k}, \hat{\rho}) = (211, 0.0226, 1.011, 128.4).$$

Without some notion of variation of these parameter estimates, it is impossible to tell how well the estimation procedure is doing. Hall (1985b) analyzes the same data set taking essentially the approach described by (9.5.6). Unfortunately, once again no estimate of variation is available. It would be interesting to see how the approach described in Section 9.5.1 (for the random-parallelgram data) compares to those already tried on the heather-incidence data. This has not been carried out because there is evidence that the Boolean model is unsatisfactory. Diggle (1981b) himself provides some of it by simulating the theoretical model and comparing it to the observed image (given by Figure 9.7). Section 9.5.3 provides further evidence by taking a very different approach (but one for which the Boolean model assumption of homogeneous λ is essential) to estimate λ and finding a large discrepancy.

9.5.3* Intensity Estimation in the Boolean Model

This section is concerned with analyzing data in $\mathbb{R}^2$, using the Boolean model

$$X = \bigcup \{Z(s_i) : s_i \in D\},$$

where $Z(s_i) \equiv Z_i \oplus s_i$ ($i = 1, 2, \dots$), $Z_1, Z_2, \dots$ are independent realizations of an almost surely bounded (not necessarily convex) RACS Z , and D is a homogeneous Poisson process with intensity λ . In particular, it concentrates on estimation of the intensity λ .

Write a generic point s in $\mathbb{R}^2$ as $s = (x, y)'$. Assume that each realization of Z has a uniquely identifiable point on its boundary, referred to as its *marker point*. If $y^* \equiv \inf\{y : s = (x, y)' \in Z\}$, $x^* \equiv \inf\{x : s = (x, y^*)' \in Z\}$, then $s^* \equiv (x^*, y^*)'$ is defined to be the marker point of Z and for Z convex corresponds to its most southwesterly point. Marker points have previously been used to construct edge-corrected estimators in image analysis (Miles, 1974; Gundersen, 1978). Notice that s^* depends on the coordinate system chosen, although final estimates will be little affected by that choice. Further, assume that $|\partial Z| = 0$ almost surely, where ∂Z is the boundary of the random grain Z .

It will be shown that the observed marker points, after suitable transformation, form a planar homogeneous Poisson process with the *same* intensity

as the original Boolean model. Although previous methods of analysis described in Sections 9.5.1 and 9.5.2 have given estimates of the intensity, the following method neatly separates out the spatial-location information. The development follows closely that of Laslett et al. (1985).

A Transformation of the Boolean Model

Consider the Boolean model with grain Z and Poisson points (germs) occurring at constant intensity λ per unit area. It follows that the original germ can be replaced with a more convenient point on the boundary of the grain without changing the stochastic properties of the process. In particular, the marker point can be chosen. Define a marker point s^* to be *exposed* if s^* belongs to $\overline{X^c}$, the closure of the background.

The idea is to remove X from the two-dimensional image, *except* for the exposed marker points, and close up, along the x direction, the gaps in the background left by the departed set X . Now, instead of points in the background having coordinates (x, y) , they will have new coordinates (χ, ψ) . The transformation ξ from (x, y) to (χ, ψ) is defined as follows. Assume, without loss of generality, that $x \geq 0$. For $s = (x, y)' \in \overline{X^c}$, let $L(s) = (0, x] \times \{y\}$. Then define $\chi \equiv |L(s) \cap \overline{X^c}|_1$, where $|\cdot|_1$ is one-dimensional Lebesgue measure, $\psi \equiv y$, and $(\chi, \psi) \equiv \xi(x, y)$. For $s = (x, y)' \notin \overline{X^c}$, let $x_l \equiv \sup\{x' : x' < x, (x', y) \in \overline{X^c}\}$. Then define $\xi(x, y) \equiv \xi(x_l, y)$ and $(\chi, \psi) \equiv \xi(x, y)$.

Let $\Omega \equiv \xi(\overline{X^c} \cap \{(x, y) : x \geq 0\})$ denote the range of ξ . Although the transformation ξ onto Ω is not invertible, the transformation $\underline{\xi} : \overline{X^c} \rightarrow \Omega$ is, and when necessary I shall write $\xi^{-1}(\omega)$ for the location, in $\overline{X^c}$, of ω in Ω . Points and sets in Ω will be denoted by Greek letters and those in $\mathbb{R}^2$ by Latin letters.

The following theorem, owing to G. M. Laslett, can be proved:

Laslett's Theorem If X is a Boolean model with intensity λ and grain Z for which there exists a unique marker point, then the exposed marker points of X (called the *induced point process*) form a homogeneous Poisson process of intensity λ in Ω .

Proof (Laslett et al., 1985). The proof can be accomplished by replacing $\mathbb{R}^2$ with a square grid of points $\{s(i, j) : i = 0, 1, \dots, j = \dots, -1, 0, 1, \dots\}$ of density m per unit area. Based on the same density of points, Ω is replaced with $\{\omega(\eta, \kappa) : \eta = 0, 1, \dots, \kappa = \dots, -1, 0, 1, \dots\}$. As $m \rightarrow \infty$, the effect of this discretization is shown to be negligible.

Suppose that at grid point $s(i, j)$ there are placed independent Bernoulli random variables $Y(i, j)$ such that $\Pr\{Y(i, j) = 1\} = \lambda/m$. As part of the discretization, the Poisson germs in $\mathbb{R}^2$ are replaced with the set $P = \{s(i, j) : Y(i, j) = 1\}$. For each $s(i, j) \in P$, consider the associated grain $Z_{i,j}(s(i, j))$.

For the reasons given in the following text, define the subset $A(i_0, j_0)$ of the square grid by

$$A(i_0, j_0) \equiv \{s(i, j): i \geq 0, j < j_0; \text{ or } 0 \leq i < i_0, j = j_0\}.$$

Let $X(i_0, j_0) \equiv \cup \{Z_{i,j}(s(i, j)): s(i, j) \in P \cap A(i_0, j_0)\}$; that is, take only that part of the discretized model whose marker points are either below the $j = j_0$ line or on the $j = j_0$ line but to the left of i_0 . The particular definition used for marker point determines this choice of A .

Replace $\overline{X_m^c}$ with the set $\overline{X_m^c} \equiv \{s(i, j): s(i, j) \notin X(i, j)\}$. Define $\eta_0 \equiv \#\{s(l, j_0): s(l, j_0) \in \overline{X_m^c}, \text{ and } 0 \leq l \leq i_0\}$ (i.e., η_0 is the number of grid points in the background to the left of i_0 and along the line $j = j_0$); then

$$s(i_0, j_0) = \xi^{-1}(\omega(\eta_0, \kappa_0)),$$

where $\kappa_0 = j_0$. To conclude the discretization, define Bernoulli random variables $\zeta(\eta_0, \kappa_0) \equiv Y(i_0, j_0)$, where $s(i_0, j_0) = \xi^{-1}(\omega(\eta_0, \kappa_0))$. The induced point process is then $\{\zeta(\eta, \kappa)\}$.

Let $N(\Theta)$ be the number of marker points in a set $\Theta \subset \Omega$, where Θ contains μ grid points. It is sufficient to derive $\Pr\{N(\Theta) = 0\}$ for arbitrary sets, because probabilities of other events can be obtained combinatorially from these. For the (η_0, κ_0) th point in Ω , let $\Delta(\eta_0, \kappa_0) \equiv \{\omega(\eta, \kappa): \eta \geq 0, \kappa < \kappa_0; \text{ or } 0 \leq \eta < \eta_0, \kappa = \kappa_0\}$, similar to the preceding definition of $A(x_0, y_0)$ (but here in the transformed space). Define $\Theta(\eta, \kappa) \equiv \Theta \cap \Delta(\eta, \kappa)$. Then

$$\Pr\{N(\Theta) = 0\} = \prod_{\eta, \kappa \in \Theta} \Pr\{\zeta(\eta, \kappa) = 0 | N(\Theta(\eta, \kappa)) = 0\}.$$

This is a spatial generalization of the usual sequential conditioning argument found in time-series analysis. (One of the $\Theta(\eta, \kappa)$ s will be empty, in which case the conditional probability is interpreted as the unconditional $\Pr\{\zeta(\eta, \kappa) = 0\}$.) Because in the transformed space only $\overline{X_m^c}$ has been retained, a point $\omega(\eta, \kappa)$ in Ω can result from any one of $\{s(i, j): i \geq \eta, j = \kappa\}$. Therefore,

$$\begin{aligned} \Pr\{N(\Theta) = 0\} &= \prod_{\eta, \kappa \in \Theta} \sum_{i \geq \eta} \Pr\{Y(i, \kappa) = 0 | N(\Theta(\eta, \kappa)) = 0, \xi^{-1}(\omega(\eta, \kappa)) = s(i, \kappa)\} \\ &\quad \times \Pr\{\xi^{-1}(\omega(\eta, \kappa)) = s(i, \kappa) | N(\Theta(\eta, \kappa)) = 0\}. \end{aligned}$$

The first conditional probability can be simplified because the shapes of the sets A and Δ guarantee that random variables in the conditioning event are independent of the random variable $Y(i, \kappa)$. It is equal to $(1 - \lambda/m)$, not

depending on i . Thus,

$$\begin{aligned} \Pr\{N(\Theta) = 0\} &= \prod_{\eta, \kappa \in \Theta} (1 - \lambda/m) \sum_{i \geq \eta} \Pr\{\xi^{-1}(\omega(\eta, \kappa)) = s(i, \kappa) | N(\Theta(\eta, \kappa)) = 0\} \\ &= (1 - \lambda/m)^\mu. \end{aligned} \quad (9.5.21)$$

To prove the theorem in $\mathbb{R}^2$, let m tend to infinity. Then, up to integerization, $\mu = m|\Theta|$, so that (9.5.21) converges to $\exp\{-\lambda|\Theta|\}$. Furthermore, the expected number of marker points per unit area in $\mathbb{R}^2$ that coincide with boundaries of other associated primary sets is zero, so that these can be ignored in the limit. Finally, by construction, the limiting point process is simple, and so the result follows from the Equivalence Theorem in Section 8.3.2. ■

The converse of the theorem is not true, and counterexamples are readily derived. Consider a random set process in $\mathbb{R}^2$ produced as follows: Let C_i be the square of side 1 unit having $s_i = (x_i, y_i)'$, $i = 1, 2, \dots$, as its top right-hand corner, where $\{s_1, s_2, \dots\}$ are the points of a Poisson process of intensity λ . A new point $s'_i = (x_i + 1/2, y_i + 1/2)'$ is generated if $\{s_j : j \neq i\} \cap C_i = \emptyset$ (i.e., if the square does not intersect with any other Poisson points). Now let $\{s_i\} \cup \{s'_i\}$, $i = 1, 2, \dots$, be southwesterly marker points for associated grains of unit squares. The union of these grains defines a random-set process. The exposed marker points are a subset of $\{s_1, s_2, \dots\}$ and, as can be proved using the aforementioned techniques, form a Poisson process of intensity λ in the transformed space Ω . However, the random set process is not Boolean nor is it equivalent to a Boolean model, as would be the case if every s_i gave rise to an s'_i .

Heather-Incidence Example

Figure 9.7 shows a representation of the incidence of heather. These data (discussed briefly in Section 9.5.2) were analyzed by Diggle (1981b), who suggested that they could be treated as a realization of a Boolean model. The exposed marker points are shown on the same figure. The shaded set is removed and the background closed up toward the left-hand vertical axis. The closed-up marker points and the closed-up background are shown in Figure 9.8.

For convenience of arithmetic and in order to reduce possible edge effects, a rectangular subset of the transformed data was used to estimate the intensity. This region, shown with a solid perimeter in Figure 9.8, is exactly half of one 10×10 -m unit in area (a quarter of the size of the original sample). The finite extent of the data set means that the full range Ω of the transformation is not available and necessitates masking out some of the points in the right-hand part of Figure 9.8. This does not mean that information is necessarily lost, because one could also close up the back-

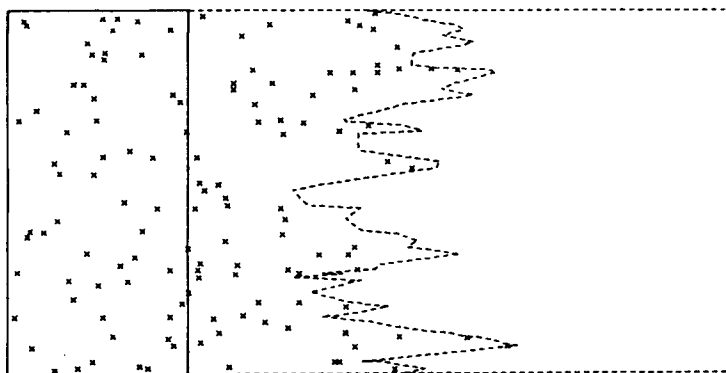


Figure 9.8 Transformed image showing location of marker points, after removal of the heather-incidence set and closing up the background. The rectangle in bold delineates the area used to estimate the intensity. [Source: Laslett et al., 1985]

ground of Figure 9.7 toward the right-hand vertical axis and mask out left-hand marker points in the transformed space.

The half unit area of Figure 9.8 contains 58 marker points, so that the heather intensity is estimated to be $\hat{\lambda} = 116$ plants per unit area, substantially less than Diggle's final estimate of $\hat{\lambda} = 211$ plants per unit area. In discussion, Diggle points out that the data contain fewer patches than do simulations of the model, and the lower estimate reflects this, at least in part. Some of the discrepancy must also be due to the quality of the heather-incidence data, which, in fact, was collected on a square grid; the boundary lines in Figure 9.7 are smooth approximations to the actual heather boundary. The fact that this is a discretized map means that some small or hardly exposed particles may fall between grid points and their marker points missed. This will not be a concern when analogue data are taken from actual pictures. Indeed, exposed marker points could be sampled directly as part of the data collection process.

Some Final Remarks

Because the clustering of points from an inhomogeneous Poisson process is an important alternative, one might ask how the previously defined transformation ξ deals with clustered original marker points. Globally speaking, ξ will distort the relative positions of exposed marker points so that clustering (or regularity) may be lost in the transformed space. However, a test for the Boolean model could be constructed at the local level. For example, choose at random a number of origins and axes within a large realization of the process under investigation. After transformation, tests based on first nearest neighbors, in the immediate vicinity of the randomly chosen origins and axes, are recommended. The advantage of distorting the original space via ξ is that the method can ignore poor resolution areas of the picture. In satellite

imagery, for example, if cloud cover should block part of an image, the cloud is simply “removed” along with the set, and the preceding results still apply.

In summary, an alternative way of estimating the Boolean-model intensity has been proposed that, when applied to the heather-incidence data, disagrees with previous estimates (Diggle, 1981b; Hall, 1985b). The germs for those data are not well fitted by random disks, which will almost certainly influence the associated intensity estimates; both Diggle and Hall assume a random-disk Boolean model. On the contrary, the approach of this section makes no such strong assumption about grain shape (but it does require constant intensity λ). A measure of the variation of the proposed estimator of λ has yet to be developed.

Good diagnostic methods and distribution theory for estimators are needed for inference on any stochastic model. The Boolean model is no exception; limited results are given in the next section.

9.6 INFERENCE FOR THE BOOLEAN MODEL

The estimation technique of Section 9.5.1 could be liberally described as a method-of-moments. The matching of theoretical moments to sample values in order to estimate parameters is well known in statistics for random variables and random vectors, although it is usually used only when other approaches, such as maximum likelihood, have failed. This is because there is no general theory that yields distributional properties of the method-of-moments estimators nor is there any guarantee that they are asymptotically efficient.

Likelihood

What is the likelihood function for the Boolean model $X = \bigcup \{Z(s_i); s_i \in D\}$ defined by (9.4.1)? The random set X can be considered equivalently as a random function

$$\{I_X(s): s \in \mathbb{R}^d\},$$

where I_X denotes the indicator function of the set X ; see Section 9.3. Thus a particular realization consists of 0-1 values throughout $\mathbb{R}^d$, which in practice is discretized onto a regular grid. In fact, define a new process

$$\xi(s) = \begin{cases} 1, & \text{with probability } p, \\ 0, & \text{with probability } 1 - p, \end{cases} \quad s \in \mathbb{Z}^d \cap A, \quad (9.6.1)$$

where $\mathbb{Z}^d$ is the d -dimensional lattice of integers and A is the (rescaled) domain of observation. Rescaling the domain of observation is important because the lattice dimension is scaled to be 1 unit in (9.6.1). Let $|\mathbb{Z}^d \cap A|$ denote the number of lattice points in the domain of observation. In order to

equate Boolean-model parameter λ with its discretized version, put $p \cdot |\mathbb{Z}^d \cap A| = \lambda \cdot \nu(A)$ or

$$p = \lambda \cdot \nu(A) / |\mathbb{Z}^d \cap A|, \quad (9.6.2)$$

where $\nu(\cdot)$ is Lebesgue measure. Because in practice the number of lattice points in the domain of observation is chosen to be greater than the expected number of events of the Poisson point process, $p \in (0, 1)$.

Let Z be an almost surely bounded RACS Z and suppose $\{Z_u: u \in \mathbb{Z}^d \cap A\}$ is a sequence of independent realizations of Z . Define

$$a(s; u) \equiv I_{Z_u}(s - u) \quad (9.6.3)$$

and

$$\eta(s) \equiv \sup\{\xi(u) \cdot a(s; u): u \in \mathbb{Z}^d \cap A\}, \quad s \in \mathbb{Z}^d \cap A. \quad (9.6.4)$$

Then $\eta(\cdot)$ is a discretized version of $I_X(\cdot)$, the indicator function of the Boolean model X , in the domain of observation A . The data are

$$\{\eta(s): s \in \mathbb{Z}^d \cap A\}, \quad (9.6.5)$$

a finite number of 0s and 1s. However, their joint distribution and hence the likelihood cannot be written down in an illuminating way. The sup in (9.6.4) causes the difficulty; see Section 9.4.1, where the marginal distribution of $\eta(s)$ is given by property 1 and the bivariate distribution of $(\eta(s), \eta(s + h))$ is given by properties 1 and 2. Notice that, *in principle*, all the trivariate, quadrivariate, and so on, distributions can be obtained from the recurrence relations that allow the hitting function (9.3.14) to be called a Choquet capacity of infinite order [see property 3 following (9.3.14)], but the calculations are practically prohibitive.

In conclusion, obtaining the likelihood function for (a discretized version of) the Boolean model does not yield tractable results. Moreover, it is not clear that maximum likelihood estimators would be optimal in any sense. In another context, where the parameters of the random set represent set boundaries and the data are i.i.d. uniform vectors over that set in $\mathbb{R}^d$, DeGroot and Eddy (1983) carry out inference based on the likelihood. In the case where the data are exhaustively observed sets (up to the limits of digitization), it seems that more success can be gained from fitting the empirical hitting function to the theoretical hitting function or, more generally, from the method of moments. The properties of the resulting estimators will now be discussed.

Method of Moments

Matching theoretical expressions with empirical expressions and solving for (theoretical) parameters will liberally be called the method-of-moments.

Exact distribution theory for such estimators (as for any other Boolean-model parameter estimators) is unavailable, but some limited results will be presented. Simulations of Boolean models could always be carried out to indicate distributions of statistics under given hypotheses.

Dupac (1980) considers an application of the Boolean model (9.4.1) in $\mathbb{R}^2$ to the analysis of fission tracks. The grains are assumed to be i.i.d. random disks $b(0, R)$, where R is a random variable with probability density function $f(\cdot)$. Assume a large domain of observation, or equivalently that the domain A is a unit square, λ is large, and $E(\pi R^2)$ is small. The aim is to estimate λ , $E(R)$, and $\text{var}(R)$. Dupac equates three theoretical moments of the Boolean model with their empirical counterparts, namely, the porosity given in Section 9.4.1, and the expectation and the variance of the circular clumps. Approximate variances for $\hat{\lambda}$, $\hat{E}(R)$, and $\widehat{\text{var}}(R)$ are obtained, but some of his assumptions have not been satisfactorily verified. The estimators are certainly biased and covariances between them are nonzero. Unfortunately, the order of his approximations does not allow investigation of these quantities.

Tallis and Davis (1984) consider a Boolean model whose grains are random spheres in $\mathbb{R}^3$. Superimposed upon the problem of parameter determination is the stereological problem of having to infer three-dimensional quantities from two-dimensional probes of the object. Assuming that $\log R$ is $\text{Gau}(\mu, \sigma^2)$, method-of-moment estimators for λ , μ , and σ^2 are obtained. With the exception of the estimator of the intensity parameter λ , biases, variances, and covariances of estimators are not given. Method-of-moments estimation when the Boolean model consists of convex grains is discussed, but no attention is given to the statistical properties of the estimators.

Ohser (1980) considers the Boolean model in $\mathbb{R}^d$, where the grains $Z_1, Z_2, \dots$ are i.i.d. compact convex sets in $\mathbb{R}^d$. He shows how, by matching the theoretical and empirical hitting function, parameters λ , $E(W_k(Z))$, $k = 1, \dots, d$, can be estimated in precisely the same way as λ , $E(P(Z))$, and $E(|Z|)$ were estimated in (9.5.5). The quantity $E(W_k(Z))$ is the expectation of the k th Minkowski functional of the random compact convex set Z (Matheron, 1975, p. 78). In $\mathbb{R}^2$, these Minkowski functionals reduce to *perimeter* and *area*, and it is this case that will now be considered in some detail.

Inference in $\mathbb{R}^2$

The data of Figure 9.5 are realizations of a Boolean model in $\mathbb{R}^2$ with random compact convex grain, in particular with random parallelograms. A slightly more general version of (9.5.4) is

$$-\log Q_X(tK_0) = \beta_0 + \beta_1 t + \beta_2 t^2,$$

where $\beta_0 = \lambda E(|Z|)$, $\beta_1 = \lambda E(P(Z))P(K_0)/(2\pi)$, $\beta_2 = \lambda |K_0|$, Q_X is the complement of the hitting function of the Boolean model X , and K_0 is a fixed compact convex set *symmetric* about the origin.

Now, for any compact convex K_0 ,

$$Q_X(tK_0) = \exp(-\lambda E(|\check{Z} \oplus tK_0|)) = Q_{X \oplus t\check{K}_0}(\mathbf{0}), \quad (9.6.6)$$

because $X \oplus t\check{K}_0$ is a Boolean model with grain $Z \oplus t\check{K}_0$. That is, $Q_X(tK_0)$ is simply the *porosity* of $X \oplus t\check{K}_0$. It is now clear how to estimate $Q_X(tK_0)$:

$$\hat{Q}_X(tK_0) = \text{proportion of pixels not in } X \oplus t\check{K}_0; \quad (9.6.7)$$

the exact formula (for K_0 the square C) is given by (9.5.8).

Now write

$$\mathbf{Y} = T\boldsymbol{\beta} + \boldsymbol{\delta}, \quad (9.6.8)$$

where $\mathbf{Y}' \equiv (-\log \hat{Q}_X(tK_0): t = t_1, \dots, t_n)$, T is an $n \times 3$ matrix whose i th row is $(1 \ t_i \ t_i^2)$ and $\boldsymbol{\delta}$ is an $n \times 1$ error vector with $E(\boldsymbol{\delta}) = 0$ and $\text{var}(\boldsymbol{\delta}) = \Sigma$. From the approximation

$$\text{cov}(-\log U_1, -\log U_2) \simeq \{E(U_1)E(U_2)\}^{-1} \cdot \text{cov}(U_1, U_2),$$

the (i, j) th element of Σ is approximately

$$\{Q_X(t_i K_0)Q_X(t_j K_0)\}^{-1} \cdot \text{cov}(\hat{Q}_X(t_i K_0), \hat{Q}_X(t_j K_0)). \quad (9.6.9)$$

Equations (9.5.9) and (9.5.10) (for K_0 the square C) allow evaluation of (9.6.9), which is seen to depend on the unknown parameters of X . Let each term in (9.6.9) be estimated by its empirical version, such as (9.5.8), (9.5.9), and (9.5.11), giving

$$\hat{\Sigma} = \left\{ \left\{ \hat{Q}_X(t_i K_0) \hat{Q}_X(t_j K_0) \right\}^{-1} \cdot \widehat{\text{cov}}(\hat{Q}_X(t_i K_0), \hat{Q}_X(t_j K_0)) \right\}. \quad (9.6.10)$$

Note that $\hat{\Sigma}$ may not be positive-definite; fitting of a “closest” positive-definite matrix to $\hat{\Sigma}$ is advisable in these cases. How this might be done is worthy of further research [Diggle (1981b) suggests fitting a shifted Weibull to the empirical Boolean-model covariance (9.5.11)].

Parameter Estimates, Bias Estimates, and Variance Estimates

A (estimated) generalized-least-squares estimator of the coefficients $\boldsymbol{\beta}$ in the linear equation (9.6.8) is

$$\hat{\boldsymbol{\beta}} = (T' \hat{\Sigma}^{-1} T)^{-1} T' \hat{\Sigma}^{-1} \mathbf{Y}, \quad (9.6.11)$$

whose variance matrix can be estimated by

$$\widehat{\text{var}}(\hat{\beta}) = (T' \hat{\Sigma}^{-1} T)^{-1}. \quad (9.6.12)$$

Consider the case where $K_0 = b(0, 1)$, the unit disk centered at the origin. Then, from (9.5.5),

$$\hat{\theta} \equiv \hat{E}(P(Z)) = \pi \hat{\beta}_1 / \hat{\beta}_2. \quad (9.6.13)$$

Using the δ -method (Kendall and Stuart, 1969, pp. 231, 244), it can be shown that

$$\begin{aligned} E(\hat{\theta}) &\simeq \frac{\pi \beta_1}{\beta_2} - \frac{\pi \text{cov}(\hat{\beta}_1, \hat{\beta}_2)}{\beta_2^2} + \frac{\pi \beta_1 \text{var}(\hat{\beta}_2)}{\beta_2^3} \\ &= E(P(Z)) + \text{bias}, \end{aligned} \quad (9.6.14)$$

where [using (9.6.11) and (9.6.12)] the bias can be estimated by

$$\widehat{\text{bias}} = \pi \left\{ -\frac{\widehat{\text{cov}}(\hat{\beta}_1, \hat{\beta}_2)}{\hat{\beta}_2^2} + \frac{\hat{\beta}_1 \widehat{\text{var}}(\hat{\beta}_2)}{\hat{\beta}_2^3} \right\}. \quad (9.6.15)$$

Furthermore,

$$\text{var}(\hat{\theta}) \simeq \pi^2 \left\{ \frac{\text{var}(\hat{\beta}_1)}{\beta_1^2} + \frac{\text{var}(\hat{\beta}_2)}{\beta_2^2} - \frac{2 \text{cov}(\hat{\beta}_1, \hat{\beta}_2)}{\beta_1 \beta_2} \right\} \frac{\beta_1^2}{\beta_2^2}, \quad (9.6.16)$$

which [using (9.6.11) and (9.6.12)] can be estimated by

$$\widehat{\text{var}}(\hat{\theta}) = \pi^2 \left\{ \frac{\widehat{\text{var}}(\hat{\beta}_1)}{\hat{\beta}_1^2} + \frac{\widehat{\text{var}}(\hat{\beta}_2)}{\hat{\beta}_2^2} - \frac{2 \widehat{\text{cov}}(\hat{\beta}_1, \hat{\beta}_2)}{\hat{\beta}_1 \hat{\beta}_2} \right\} \frac{\hat{\beta}_1^2}{\hat{\beta}_2^2}. \quad (9.6.17)$$

Similar expressions can be obtained for $\hat{E}(|Z|) = \pi \hat{\beta}_0 / \hat{\beta}_2$ and $\hat{\lambda} = \hat{\beta}_2 / \pi$.

The results (9.6.11) and (9.6.12) are general in that no assumption is made about K_0 beyond that it is a symmetric compact convex set in $\mathbb{R}^2$. Slight modifications to this method are made in Section 9.7 to allow inference on tumor-growth parameters.

Design and Diagnostics

A couple of issues arise that warrant further investigation. What are the optimal values of n and $t_1, \dots, t_n$, given the experimental constraints of pixel dimension? Because of the nontrivial correlation in Σ , the answer is not necessarily to make n as large as possible. The design space is limited to

$[0, t_{\max}]$, where $t_{\max}$ is the largest t for which $\hat{Q}_X(tK_0) > 0$. Specification of $0 \leq t_1 \leq t_2 \leq \dots \leq t_n \leq t_{\max}$ may be limited by the discreteness of the image data, but if a choice is possible, equally spaced explanatory variables gives a robust design.

Having fit the model by the method-of-moments, are there any diagnostic checks that can be carried out to assess the goodness-of-fit? One suggestion (Diggle, 1981b) is to compare the empirical covariance of X^ϵ [i.e., proportion of pixels in $(X^\epsilon \cap X^\epsilon \oplus \{-\mathbf{h}\})$], with the theoretical covariance $\chi(\mathbf{h})$, given in Section 9.4.1. For $Z = b(\mathbf{0}, R)$, where the random radius R has distribution function F , Hall (1988a, Section 5.2) proves that knowing $\chi(\mathbf{h})$ and porosity q , given in Section 9.4, is equivalent to knowing λ and F .

The error term δ in (9.6.8) is made up of two components, namely, lack of fit of the model and error caused by using an estimate $\hat{Q}_X$ of Q_X . Assuming the model is correct, what asymptotic results are available for Boolean model parameter estimation? A few results are given in the following text.

Asymptotics

Having worked out the biases and variances of estimators, a natural question to ask is whether they tend to zero as more information is accumulated. Sometimes it is not clear what “more information” means; here, the asymptotics are controlled by assuming the measure of the domain of observation $|A|$ tends to ∞ (increasing-domain asymptotics).

Baddeley (1980) proves a limit theorem for $\hat{Q}_X(tK_0)$, assuming $|A| \rightarrow \infty$. In his Theorem 2 applied to the Boolean model (9.4.1) (which recall has almost surely bounded grains), it can be seen that

$$\left\{ |A|^{1/2} (\hat{Q}_X(tK_0) - Q_X(tK_0)) : 0 \leq t \leq t_0 \right\}$$

converges weakly to a zero-mean Gaussian process on $[0, t_0]$, for any positive constant t_0 . [To invoke Baddeley's results, notice that $\Pr(\mathbf{0} \in X \oplus t\check{K}_0) = 1 - Q_X(tK_0)$.] Because $-\log(\cdot)$ is a continuous function,

$$\left\{ |A|^{1/2} (-\log \hat{Q}_X(tK_0) + \log Q_X(tK_0)) : 0 \leq t \leq t_0 \right\}$$

also converges weakly to a zero-mean Gaussian process. This justifies the model (9.6.8) and guarantees that the estimates (9.6.11) and (9.6.13) will be consistent and asymptotically Gaussian.

More generally, suppose that the random set X is given by (9.4.1), where D is now an almost surely locally finite random set. (For example, for the Boolean model, D is the Poisson process.) Then Mase's (1982b, Section 3) results can be invoked to prove that $\hat{Q}_X(tK_0)$ is consistent and asymptotically Gaussian, where t is fixed and nonnegative.

Another way to achieve the same asymptotic results for the Boolean model (9.4.1) is to keep $|A|$ fixed, but to let $\lambda \rightarrow \infty$ and $E(|Z|) \rightarrow 0$ in such a

way that $\lambda E(|Z|)$ remains constant. That is, define $Z = (\lambda^{-1/d})Z'$, where the standardized grain Z' satisfies $E(|Z'|) < \infty$, and let $\lambda \rightarrow \infty$.

9.7 MODELING GROWTH WITH RANDOM SETS

Growth of an entity can be observed and measured in a number of different ways; it is rarely one-dimensional, leading to ambiguity as to how the process can be summarized and analyzed. For example, cellular organization is known to be important in characterizing tumor growth (Rubin, 1982), but most of the mathematical models have used one-number summaries (e.g., volume, number of cells, leading front, mean radius) of the tumor in (sometimes stochastic) differential equations. These contributions (see, e.g., Laird, 1964; Burton, 1966; Saidel et al., 1976; Sawyer, 1977; Hanson and Tier, 1982; Bartoszynski et al., 1982; Le Cam, 1982; Miller et al., 1982; Adam, 1986; Swan, 1987; Norton, 1988) are typically answering different questions than are being asked in this section and are usually meant for applications where incidence data on many cancer patients are available.

The spatial component of growth models, although less prominent, has not been ignored completely (see, e.g., Shymko and Glass, 1976; Green, 1980; Goodall, 1985; Tautu, 1986; Adam, 1987). Furthermore, interacting-particle models, built at the cellular level (Section 9.7.1), allow simulations of and conjectures about the shape of tumors. Theoretical results have appeared that show the tumor to be asymptotically (i.e., as time tends to infinity) circular. Nevertheless, none of these results is relevant to the inference problems encountered when analyzing data like the sequence of images presented in Figure 9.13.

As has already been mentioned, one application of random-set growth models is to tumor growth. Although the data presented in Section 9.7.2 are of *in vitro* growth, one could imagine monitoring the changes in size and shape of a tumor in an individual via very precise, noninvasive imaging. Necessarily then, the data have to be good quality images sequenced at specified time intervals and taken under identical conditions. *In vivo* data of this type are unknown (to me), partly because tumors have been surgically removed as soon as possible after discovery, partly because the precision of x-ray pictures has been inadequate for detailing tumor *shape*, and partly because the importance of taking pictures under *identical* conditions, sequenced at specified intervals, has only recently been clinically appreciated. Apart from simply looking at the sequence of pictures, how can the clinician analyze such data? This section explores some possibilities in this regard. It is hoped that more theoretical research in image analysis, combined with higher-resolution sensing, will lead to a better description and understanding of tumor growth. Pictures of *in vitro* growth are analyzed in Sections 9.7.2 and 9.7.3 to demonstrate what can be done at present; the fits are remarkably good.

The general growth model is presented in Section 9.7.1 and various simulations illustrate its flexibility. Indeed, the contact processes (Eden, 1961; Williams and Bjerknes, 1972; Harris, 1974) are seen to be special cases of the model.

9.7.1 Random-Set Growth Models

Recall (9.4.1), the definition of the Boolean model. Think of the $\{s_1, s_2, \dots\}$ as *foci* (or germs) of growth; about each s_i an object (or grain) Z_i grows. With regard to the modeling of tumor growth, these foci are clinically verifiable (Chover and King, 1985). The same principle is now applied to the tumor itself as it grows, namely, within the tumor there are foci about which growth occurs. If this model is sensible, a much higher intensity of foci will occur in malignant tissue than in normal tissue. Let X_1 denote the tumor at time $t = 1$ and $F_1 \subset X_1$ denote the foci, countable in number. Then the tumor at time $t = 2$ is modeled to be

$$X_2 = \bigcup \{Z(s_i) : s_i \in F_1\}, \quad (9.7.1)$$

where $Z(s_i) \equiv Z_i \oplus s_i$, $i = 1, 2, \dots$, and $Z_1, Z_2, \dots$ are independent copies of a random set Z . This model was first proposed by Cressie (1984b), where F_1 consisted of Poisson points, homogeneous on X_1 ; it was extended by Cressie (1991) to the other cases presented in this section.

Poisson Foci

For Poisson foci in X_1 , the model (9.7.1) can be written as

$$X_2 = \bigcup \{Z(s_i) : s_i \in D\}, \quad (9.7.2)$$

where D is the *inhomogeneous* Poisson process with intensity function,

$$\lambda(s) = \begin{cases} \lambda, & s \in X_1, \\ 0, & \text{otherwise.} \end{cases} \quad (9.7.3)$$

That is, (9.7.2) is a conditional Boolean model. Then (9.4.8) yields the hitting function

$$T_{X_2}(K) = 1 - \exp\left\{-\lambda E\left(|(\check{Z} \oplus K) \cap X_1|\right)\right\}, \quad K \in \mathcal{K}, \quad (9.7.4)$$

which is used extensively in analyzing the tumor-growth data of Section 9.7.2.

Simulations of (9.7.2) yield pictures that evoke images of tumor growth. Figure 9.9 shows a progression from an initial disk in a through to an irregular set in d . Each set is generated from the previous one via the relations (9.7.2) and (9.7.3), with grain Z in each case being a disk centered at the origin of fixed radius. This circular growth is often seen in experiments

(Haji-Karim and Carlsson, 1978; Martinez and Griego, 1980) and has been proved mathematically for certain stochastic models of tumor growth (Richardson, 1973; Schurger, 1979; Bramson and Griffeath, 1980, 1981; Durrett and Liggett, 1981).

It is not expected that simulations such as Figure 9.9 are a realistic picture of *in vivo* tumor growth over long time periods. Initially, the growth is uninhibited, but before long lack of blood supply to parts of the tumor, as well as tissue barriers, result in a more complicated growth pattern. It is not my intention to model such patterns here, but I shall mention other researchers who have; without exception, they were only able to simulate and could not perform statistical inference (cf. Section 9.7.3) with their models. Notable is the work of Duchting (1980) and his co-workers (Duchting and Dehl, 1980; Duchting and Vogelsaenger, 1981, 1983). See also Ransom (1977), who models and then simulates the displacements that occur when interior tumor cells divide.

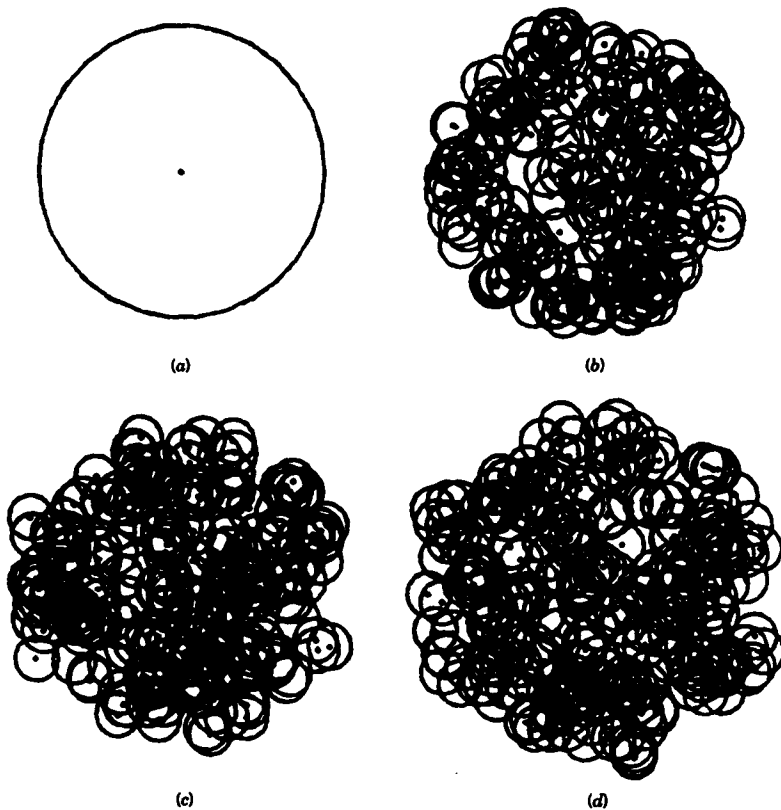


Figure 9.9 A realization of the tumor growth model (9.7.2). (a) X_1 , a disk centered at the origin. (b), (c), and (d) Realizations at successive times, obtained by iterating (9.7.2). [Source: Cressie, 1991]. Reprinted by permission of the Institute of Mathematical Statistics.

It is my hope that the model (9.7.2) and (9.7.3) provides a good description of a variety of growth processes; this will depend on the spatial scale of observations and the type of questions being asked. An important requirement is to be able to make statistical inferences about λ and the probability law of Z from data X_1 and X_2 . Section 9.7.3 discusses this important inferential aspect.

Nonrandom Foci

Suppose F_1 in (9.7.1) is an at-most-countable collection of foci, where the foci locations $\{s_1, s_2, \dots\}$ are fixed. Define

$$T_Z(K) \equiv \Pr(Z \cap K \neq \emptyset), \quad K \in \mathcal{K}, \quad (9.7.5)$$

the hitting function of the grain Z . Then, from (9.7.1) and (9.7.5),

$$T_{X_2}(K) = 1 - \prod_{i=1}^{\infty} \{1 - T_Z(K \oplus \{-s_i\})\}, \quad K \in \mathcal{K}. \quad (9.7.6)$$

A special case is when F_1 is a finite set of nodes of a regular grid; in $\mathbb{R}^2$,

$$F_1 = \{(i\Delta_1, j\Delta_2) : i, j \in \mathbb{Z}\} \cap X_1. \quad (9.7.7)$$

It is easy to simulate

$$X_2 = \bigcup \{Z(s_i) : s_i \in F_1\}, \quad (9.7.8)$$

where F_1 is given by (9.7.7). Figure 9.10 shows an analogous simulation to Figure 9.9, where now foci are nonrandom and belong to a square grid in X_1 . For illustrative purposes, the grains are once again disks of fixed radius.

Grains need not be disks, and if one is modeling tumor growth at the cellular level, it may make more sense to choose them as rectangular blocks (dominoes) of dimension $2\Delta \times \Delta$, where Δ is the square-grid spacing. A growth process can then be generated by (9.7.8), where Z is a north-pointing domino with probability (w.p.) p_1 , a south-pointing domino w.p. p_2 , an east-pointing domino w.p. p_3 , a west-pointing domino w.p. p_4 , and a $\Delta \times \Delta$ square w.p. $1 - p_1 - p_2 - p_3 - p_4$. Figure 9.11 shows an analogous simulation to Figure 9.10 (i.e., regular foci), with these dominoes and square as realizations of the random grain.

Contact Processes

A natural question to ask is whether models of the type presented in Figure 9.11 have anything in common with interacting-particle systems (see, e.g., Liggett, 1985; Durrett, 1988). Although the latter are typically continuous-time models, they can be discretized in time by considering small time intervals. That is, they are Markov processes whose state ξ_t at time t is a subset of $\mathbb{Z}^2$

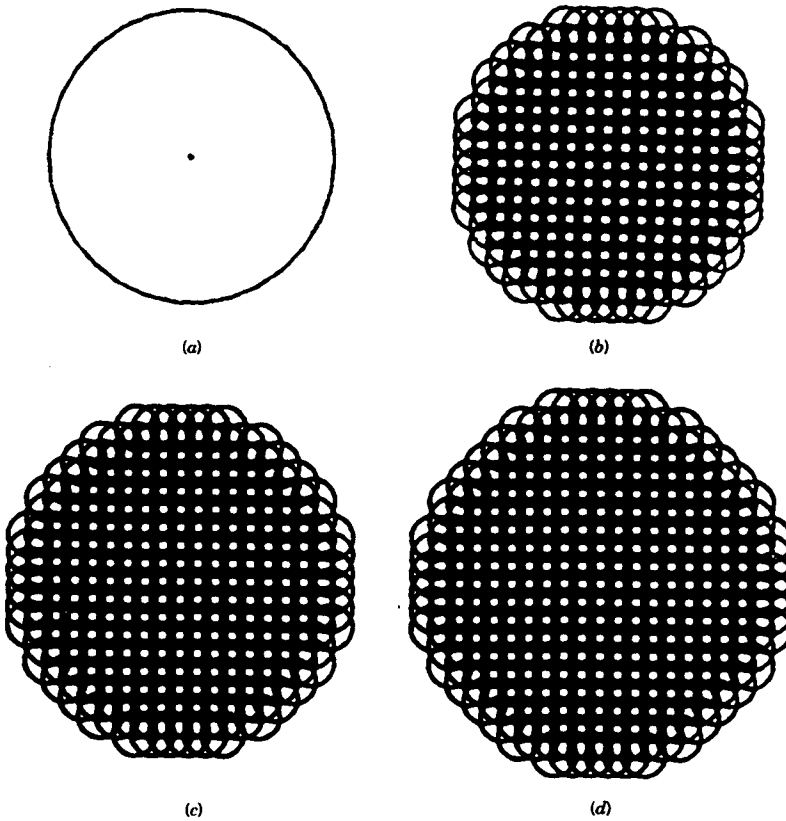


Figure 9.10 Same as in Figure 9.9 except that now growth is simulated by iterating the model (9.7.8). [Source: Cressie, 1991]. Reprinted by permission of the Institute of Mathematical Statistics.

(more generally, a subset of $\mathbb{Z}^d$, the set of d -dimensional vectors with integer coordinates). For u small, (1) tumor cells die at rate δ ; that is,

$$\Pr(s \notin \xi_{t+u} | s \in \xi_t) \approx \delta \cdot u; \quad (9.7.9)$$

(2) tumor cells are born at rate $r_s(\xi_t)$; that is,

$$\Pr(s \in \xi_{t+u} | s \notin \xi_t) \approx r_s(\xi_t) \cdot u. \quad (9.7.10)$$

Contact processes occur when $r_s(\xi_t) = 0$ if s is not a nearest neighbor of any point in ξ_t (Harris, 1974).

Suppose ξ_1 is given and ξ_{1+u} is the random set obtained from the Markov process (9.7.9) and (9.7.10); u is a small positive number. Let $F_1 = \xi_1$ in (9.7.8). Does there exist a random grain Z in (9.7.8) that yields the random

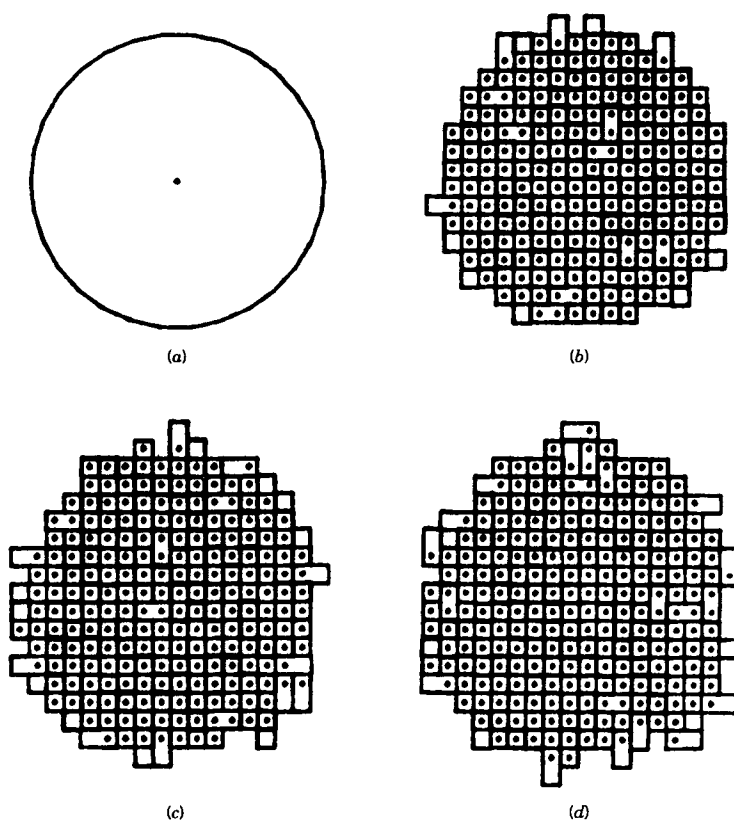


Figure 9.11 Same as in Figure 9.10, except that now the random grain Z is a square w.p. $1/5$ or dominoes in each of the four directions, each w.p. $1/5$. [Source: Cressie, 1991]. Reprinted by permission of the Institute of Mathematical Statistics.

set X_2 , identical in distribution to ξ_{1+u} ? Consider the contact process; here, $r_s(\xi) = \text{number of points in } (\xi \cap N_s)$, where $N_s \equiv \{v: \|v - s\| = 1\}$. Then clearly such a random grain *does* exist (Fig. 9.11 gives an example where $\delta = 0$; when $\delta > 0$, then $Z = \emptyset$ with positive probability). But the contact process just described is simply the Williams–Bjerknes (1972) tumor growth model (which was built in two dimensions because they restricted attention to the basal layer of an epithelium). Eden’s (1961) model is the special case $\delta = 0$. Thus, the process defined by repeated application of (9.7.1) is flexible enough to include various contact processes as special cases.

Much research has been devoted to contact processes, usually with the aim of obtaining asymptotic ($t \rightarrow \infty$) properties, such as an asymptotically circular shape in some metric (Richardson, 1973; Schurger, 1979; Bramson and Griffeath, 1980, 1981; Durrett and Liggett, 1981), the critical value of δ above which the tumor eventually dies out (Harris, 1974; Griffeath, 1981; Andjel, 1988), and rates of convergence (Griffeath, 1981).

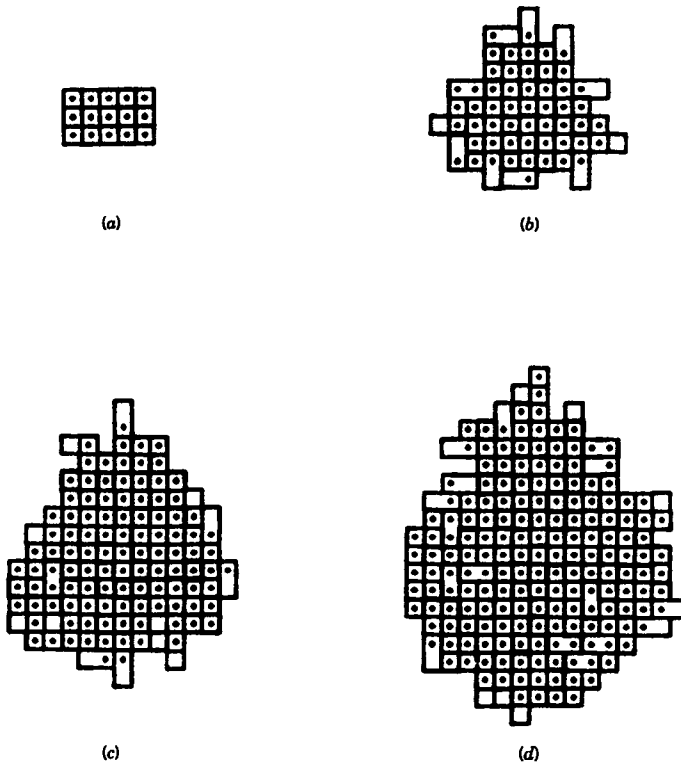


Figure 9.12 Same as in Figure 9.11, except that now (a) X_1 is a rectangle; (b) the set is X_6 ; (c) the set is X_{11} ; (d) the set is X_{16} . [Source: Cressie, 1991]. Reprinted by permission of the Institute of Mathematical Statistics.

To demonstrate the asymptotically circular shape previously mentioned, I used the same parameters as in Figure 9.11, but now with a rectangular initial set X_1 . Shown in Figure 9.12a–d are generations of the tumor at times $t = 1$, $t = 6$, $t = 11$, and $t = 16$, respectively.

Some Final Remarks

One could now return to the Poisson-foci case and ask the same questions regarding asymptotics that were asked for the contact process. Most notably, is there an asymptotically circular shape in some metric? I conjecture that there is; see Figure 9.9.

One could also combine the two cases and build a random-set model based on *random regular* foci. Suppose F_1 is defined by (9.7.7). Define the thinned set F_1^* as follows. For each $s_i \in F_1$, $s_i \in F_1^*$ w.p. p_i , independently of whether $s_j \in F_1^*$, for any $j \neq i$. Finally, define

$$X_2 = \bigcup \{Z(s_i) : s_i \in F_1^*\}, \quad (9.7.11)$$

where $Z_1, Z_2, \dots$ are independent copies of the random set Z (with hitting function T_Z). The hitting function of X_2 is

$$T_{X_2}(K) = 1 - \prod_{i=1}^{\infty} [1 - p_i + p_i \{1 - T_Z(K \oplus \{-s_i\})\}], \quad K \in \mathcal{X}. \quad (9.7.12)$$

If $\Delta_1 = \Delta_2 = \Delta$ in (9.7.7) and $p_i = \lambda \cdot \Delta^2$, then for Δ small,

$$\begin{aligned} T_{X_2}(K) &\approx 1 - \exp \left\{ -\lambda \int_{X_1} T_Z(K \oplus \{-s\}) \nu(ds) \right\} \\ &= 1 - \exp \left\{ -\lambda E(|(\check{Z} \oplus K) \cap X_1|) \right\}. \end{aligned}$$

Thus $\lim_{\Delta \rightarrow 0} T_{X_2}(K)$ is precisely (9.7.4), the hitting function of the random-set model based on Poisson foci (as it should be).

9.7.2 Tumor-Growth Data

Cancer is a disease involving disordered cell growth and is characterized by the presence of one or more malignant tumors (International Union Against Cancer, 1978). A *tumor* is any abnormal swelling, including those due to passing inflammation. However, the term is usually used to mean *neoplasm* (meaning new growth). Neoplasms are often categorized into two main types. Benign tumors are almost always enclosed in a capsule of fibrous tissue and do not invade surrounding tissue; the cells resemble their tissue of origin and reproduce in a relatively orderly, controlled manner. Malignant tumors directly invade surrounding tissue; their cells usually reproduce in a rapid, disorderly manner and can spread through the body via the lymphatic or blood system to develop secondary tumors (metastases) elsewhere.

A good review of the mathematical theories of carcinogenesis can be found in the papers by Whittemore (1978), Whittemore and Keller (1978), Forbes and Gibberd (1984), and Murdoch et al. (1987). The process of carcinogenesis is generally considered to follow the degeneration of a normal cell to a malignant state through a finite number of intermediate stages; heritable alterations to the cell are accumulated at each stage. What causes this degeneration? It is generally thought to start at the level of DNA, the genetic material of the cell. Normal cells contain DNA segments called protooncogenes that appear to be responsible for regulation of cell growth. A *carcinogen* alters the DNA by transforming protooncogenes to oncogenes (DNA segments that produce cancer when transferred to normal cells). The effects of exposure to a carcinogen are often not seen for many years after the exposure occurred.

Other factors, such as hormones, dietary components, asbestos, and so on (called *promoters*) then modify cells or body defense mechanisms to allow for more rapid growth once the cellular DNA has been altered. Cell organization is also important, but it seems that this spatial component has not been given

the attention it deserves (Rubin, 1982, 1985; Takahashi et al., 1986). The implication is that to understand tumor growth in humans, it is necessary to understand the growth process at the supracellular as well as the cellular level. The spatial statistical analyses that follow attempt to do this; they are based largely on Cressie and Hulting (1992).

In Vitro Growth of Cell Islands

Cells from the human breast cancer cell line MCF-7 (Soule et al., 1973) were grown in a flat dish covered with a nutrient medium. This cell line typically grows in compact cell islands, as is seen from the sequence of three images (photographed 72 hours apart) presented in Figure 9.13. These data were

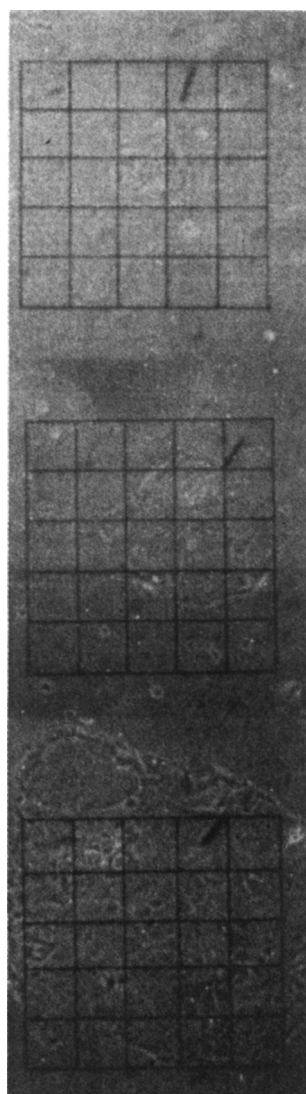


Figure 9.13 *In vitro* growth of human breast cancer cell line MCF-7. The sequence of cell islands X_1 , X_2 , X_3 were photographed 72 hours apart. Each of the 25 squares on the photographs are 1 mm^2 at $40\times$ magnification. [Source: Dr. G. C. Buehring, University of California, Berkeley]

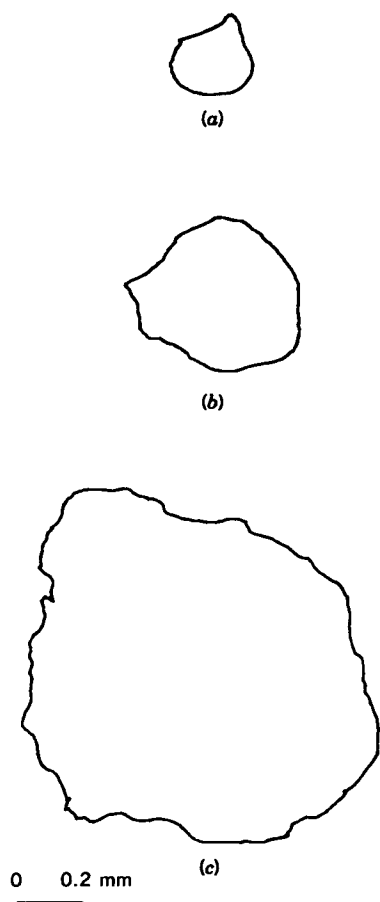


Figure 9.14 Digitized boundary of the cell islands shown in Figure 9.13. (a), (b), and (c) The boundaries of X_1 , X_2 , and X_3 , respectively. [Source: Cressie, 1991]. Reprinted by permission of the Institute of Mathematical Statistics.

supplied by Dr. G. C. Buehring (School of Public Health, University of California, Berkeley) and come from experiments similar to those described in Buehring and Williams (1976).

Shown in Figure 9.14 are digitized boundaries of the cell islands of Figure 9.13; details of the digitization are given later in this section. Let $X_i \subset \mathbb{R}^2$ denote the cell-island boundary and its interior, taken at the i th time point, $i = 1, 2, 3$. Recall that time points are 72 hours apart.

The model I shall fit to these data is given by (9.7.2) and (9.7.3), after a transformation to isotropy. My reasons for choosing this model are based on observations made in Section 9.7.1. Because Poisson foci are seen in normal tissue, I assume that the same occurs in malignant tissue, only at very, very much higher intensities λ . Because at the cellular level asymptotic growth is circular, assume that at the supracellular level (after 72 hours of growth) the grains are disks with random radius R .

After transformation to spaces where the model is likely to hold, data of Figure 9.14 are analyzed by matching theoretical hitting functions, given by

(9.7.4), with empirical hitting functions calculated from the images. This yields estimates and standard deviations of parameters λ , $E(R)$, and $\text{var}(R)$. Full details can be found in Cressie and Hulting (1992); I shall present a number of their results in succeeding text.

Stochastic Geometric Model of Tumor Growth

The *basic* model describes how X_{t+1} , the time- $(t+1)$ tumor, evolves from X_t , the time- t tumor, and was first suggested by Cressie (1984b). An important modification transforms the plane to ensure isotropy of the growth process, but for the moment consider the untransformed version of the model. Let X_1 denote the initial tumor and D_2 denote a homogeneous Poisson process of intensity λ_2 . Then, define the time-2 tumor to be

$$X_2 \equiv \bigcup \{Z_2(s_i) : s_i \in D_2 \cap X_1\}, \quad (9.7.13)$$

where $Z_2(s_i) \equiv Z_{i,2} \oplus s_i$, $i = 1, 2, \dots$, and $\{Z_{i,2} : i = 1, 2, \dots\}$ are independent copies of the RACS Z_2 . In general,

$$X_{t+1} \equiv \bigcup \{Z_{t+1}(s_i) : s_i \in D_{t+1} \cap X_t\}, \quad t = 1, 2, \dots, \quad (9.7.14)$$

where $Z_{t+1}(s_i) \equiv Z_{i,t+1} \oplus s_i$ ($i = 1, 2, \dots$); $Z_{1,t+1}, Z_{2,t+1}, \dots$ are independent copies of the RACS Z_{t+1} ; and D_{t+1} is a homogeneous Poisson process of intensity λ_{t+1} , independent from $Z_{1,t+1}, Z_{2,t+1}, \dots$. Notice that X_{t+1} does not necessarily include all of X_t .

Conditional on observing X_t , the hitting function of X_{t+1} is the complement of

$$Q_{X_{t+1}}(K) = \exp\left\{-\lambda_{t+1}E\left(\left|\left(\check{Z}_{t+1} \oplus K\right) \cap X_t\right|\right)\right\}, \quad K \in \mathcal{K}, \quad (9.7.15)$$

which is a general version of (9.7.4).

Set-Growth Parameters

The parameters of the set-growth process (9.7.14) are those from the probability law of the RACS Z_{t+1} and the probability law of the point process D_{t+1} , having conditioned on the time- t tumor X_t . Suppose that the source of randomness in $\{Z_{i,t+1} : i = 1, 2, \dots\}$ is a scaling random variable R_{t+1} ; that is, Z_{t+1} is distributed as $R_{t+1} \cdot B$, where B is a fixed closed set in $\mathbb{R}^d$ and scalar multiplication is defined by (9.3.5). Then the goal is to carry out statistical inference on λ_{t+1} , $E(R_{t+1})$, $\text{var}(R_{t+1})$, and possibly higher-order moments, for each $t = 1, 2, \dots$. This means not only estimating the parameters, but also providing standard deviations for the estimators. It is natural to make B a disk, and indeed there is some clinical evidence (e.g., Haji-Karim and Carlsson, 1978; Martinez and Griego, 1980) that growth of tumors is spheroidal.

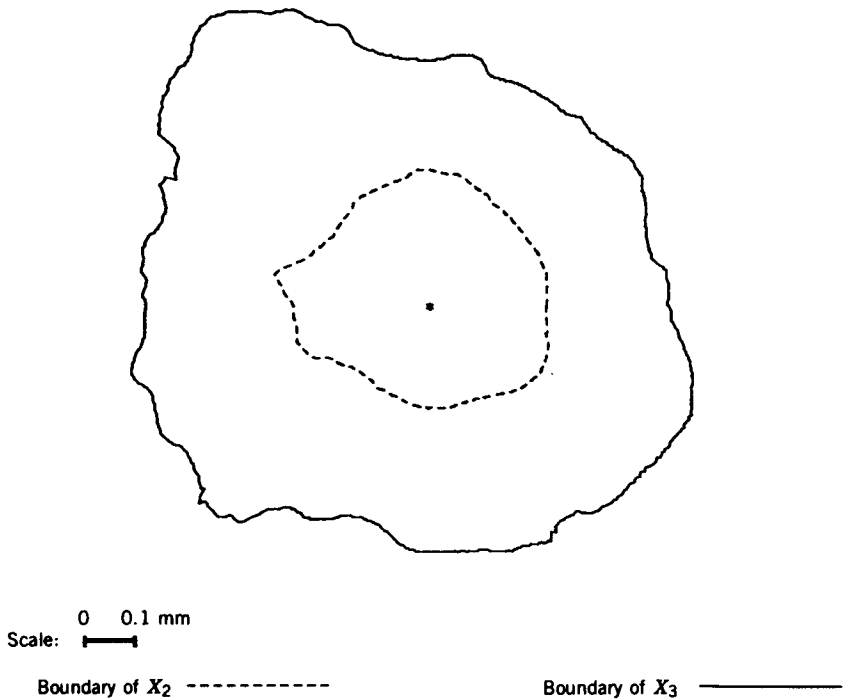


Figure 9.15 Evolution of X_3 from X_2 , where the data are the (digitized) cell islands at times 2 and 3.

For the data of Figure 9.14, results will be presented for X_2 growing from X_1 and for X_3 growing from X_2 . To illustrate the technique, I shall give full details for the evolution of X_3 from X_2 . Figure 9.15 shows X_2 centered at the origin, which is its center of gravity. The outer curve is the boundary of X_3 , which evolved from X_2 in a period of 72 hours.

Isotropic Growth on the Transformed Scale

It is natural to analyze these data rotationally rather than translationally, which leads to the question of whether the growth process is isotropic (i.e., no direction of growth is preferred). If the mechanism of growth is something like a contact process (e.g., Harris, 1974), parts of the boundary of X_2 that exhibit higher curvature may grow at a faster rate. However, a transformation of $\mathbb{R}^2$ that transforms X_2 into a set whose boundary has constant curvature (i.e., a disk) would make an isotropy assumption reasonable. This transformation is also important for *comparison* of the two growth periods; in both cases, one starts from the same initial set (i.e., a disk) in the transformed spaces. Finally, but least importantly, the hitting functions are easier to calculate for this isotropic process.

Define $b(\mathbf{s}, r) \equiv \{\mathbf{u}: \|\mathbf{u} - \mathbf{s}\| \leq r\}$ to be the closed ball of radius r whose center is at $\mathbf{s} \in \mathbb{R}^d$. Notice that $\lambda \cdot b(\mathbf{s}, r) = b(\lambda\mathbf{s}, |\lambda|r)$ and $b(\mathbf{s}_1, r_1) \oplus b(\mathbf{s}_2, r_2) = b(\mathbf{s}_1 + \mathbf{s}_2, r_1 + r_2)$.

After transformation, it will be assumed in (9.7.14) that

$$Z_{t+1} = b(\mathbf{0}, R_{t+1}), \quad (9.7.16)$$

a disk of random radius R_{t+1} , and that D_{t+1} is a *homogeneous* Poisson process. Then the goal is to estimate λ_{t+1} , $E(R_{t+1})$, $\text{var}(R_{t+1})$, $\dots$.

The appropriate transformation that converts X_2 into a disk is not hard to perform. Let the boundary of X_2 be described by the polar coordinates $\{(r_2(\theta), \theta): 0 \leq \theta < 2\pi\}$, where the radius $r_2(\theta)$ is a function of the angle θ ; that is, assume X_2 is star-shaped. If it is not and there are several boundary points $r_{2,1}^0, \dots, r_{2,k}^0$ at $\theta = \theta_0$, then choose $r_2(\theta_0) = \max\{r_{2,1}^0, \dots, r_{2,k}^0\}$. The *geometric-signature transformation* from $\mathbb{R}^2$ onto $\mathbb{R}^2$ is defined in polar coordinates as

$$S_2(\mathbf{u}) \equiv (\mathbf{u} \cdot \{r_2/r_2(\theta)\}, \theta), \quad \mathbf{u} = (u, \theta)' \in \mathbb{R}^2, \quad (9.7.17)$$

where

$$r_2 \equiv (1/2)[\sup\{r_2(\theta): 0 \leq \theta < 2\pi\} + \inf\{r_2(\theta): 0 \leq \theta < 2\pi\}]. \quad (9.7.18)$$

Zahn and Roskies (1972) also take this boundary-description approach to analyzing the size and shape of objects.

The quantity r_2 in (9.7.18) is the average radius of the largest inscribed circle and the smallest circumscribed circle centered at $\mathbf{0}$; $2r_2$ has a clinical interpretation as the mean caliper width of the tumor X_2 . Along with the area $|X_2|$ (or its square root), r_2 is a measure of the *size* of the tumor.

In any fixed direction, (9.7.17) preserves ratios of distances from the origin. Figure 9.16 shows a plot of the multiplicative ratio $r_2/r_2(\theta)$, as a function of $\theta \in [0, 2\pi)$. When this transformation is applied to the boundaries of X_2 and X_3 , presented in Figure 9.15, the result is Figure 9.17. Notice that X_2 is transformed to the disk of radius r_2 . The outer curve shows the boundary of Y_3 , the transformation of X_3 .

After the transformation, it is reasonable to assume that the stochastic mechanism resulting in Y_3 does not depend on direction. When analyzing spatial data, stationarity is usually an important assumption because it allows subregions of the spatial process to serve as replicates and hence to provide estimates of spatial parameters. Here isotropy is important for the same reason.

Stochastic-Geometric Model on the Transformed Scale

Now assume that the conditional Boolean model given by (9.7.14) and (9.7.16) applies on the *transformed* scale. Specifically, because X_2 is trans-

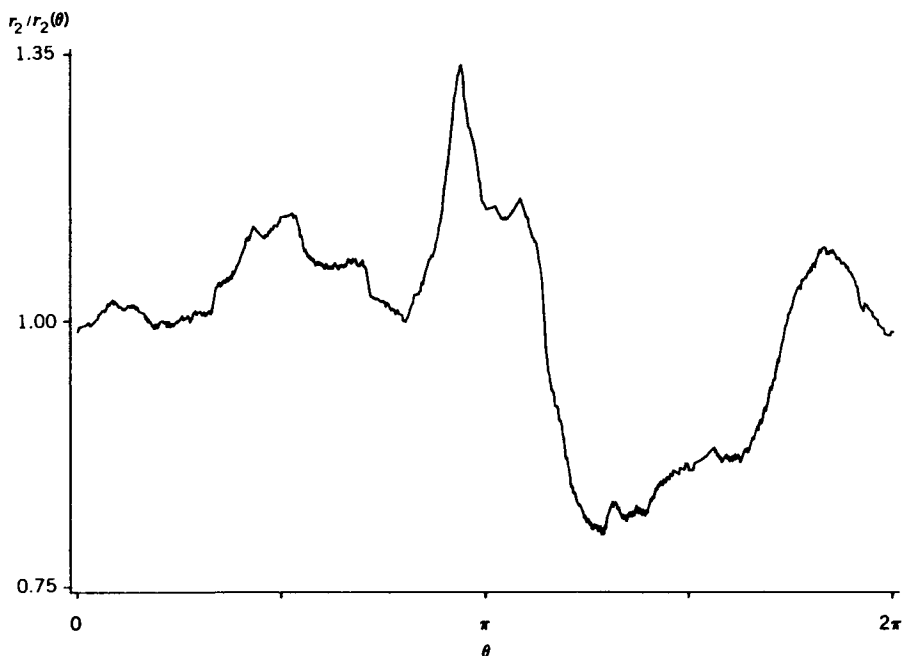


Figure 9.16 Plot shows the geometric signature transformation of the boundary of X_2 (the inner set in Figure 9.15).

formed to $b(\mathbf{0}, r_2)$ (the disk of radius r_2) and because $Z_3 = b(\mathbf{0}, R_3)$, the model for Y_3 is

$$Y_3 = \bigcup \{b(s_i, R_{3,i}) : s_i \in D_3 \cap b(\mathbf{0}, r_2)\}, \quad (9.7.19)$$

which is an isotropic RACS. It can be characterized by its hitting function, which from (9.7.15) is the complement of

$$\begin{aligned} \Pr(Y_3 \cap K = \emptyset | \text{time-2 tumor is } b(\mathbf{0}, r_2)) \\ = \exp\{-\lambda_3 E(|b(\mathbf{0}, R_3) \oplus K| \cap b(\mathbf{0}, r_2))\}, \quad K \in \mathcal{K}. \end{aligned}$$

Denote this function by Q_{Y_3} . Then for $K = b(s, l)$, a disk of radius l centered at s ,

$$Q_{Y_3}(b(s, l)) = \exp\{-\lambda_3 E(|b(s, R_3 + l) \cap b(\mathbf{0}, r_2)|)\}. \quad (9.7.20)$$

Define

$$q(u, h; \lambda, R) \equiv \exp\{-\lambda E(|b(u, R + h) \cap b(\mathbf{0}, 1)|)\}, \quad (9.7.21)$$

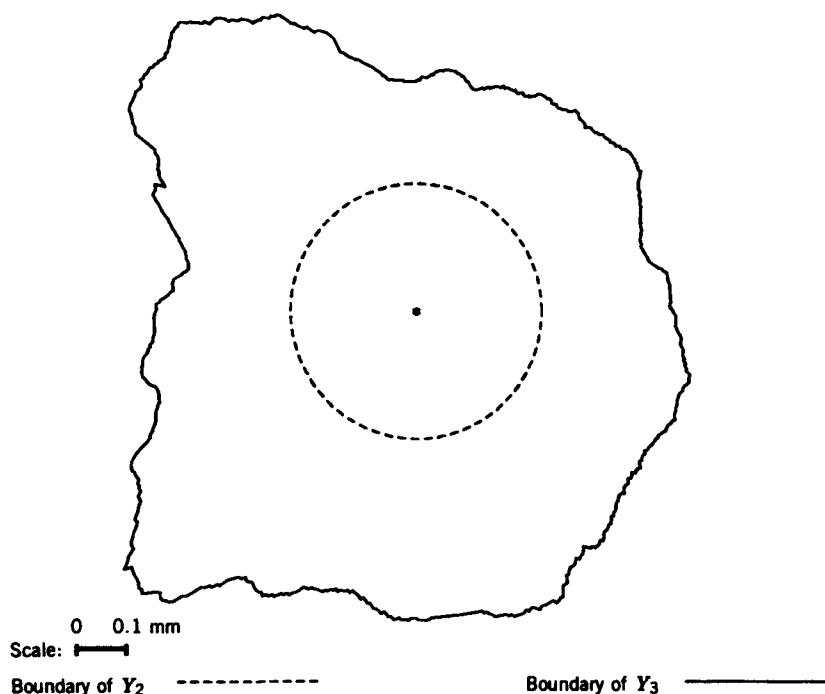


Figure 9.17 Evolution of Y_3 from Y_2 , where Y_2 is a unit disk on the transformed scale. These data represent the geometric-signature transformation of the boundaries of X_3 and X_2 presented in Figure 9.15.

where $u \equiv \|u\|$, $h > 0$, $\lambda > 0$, and $R > 0$. It is easily seen from (9.7.20) that

$$Q_{Y_3}(b(s, l)) = q(s/r_2, l/r_2; \lambda_3 r_2^2, R_3/r_2), \quad (9.7.22)$$

where $s \equiv \|s\|$. Notice that Q_{Y_3} depends on s only through s because the RACS is isotropic.

By working in units of r_2 (the size of the tumor X_2), one can concentrate on the shape characteristics and transform back to the original units later. Thus, for the moment, assume $r_2 = 1$.

From the exponent of (9.7.20), write

$$A_l(R_3) \equiv |b(s, R_3 + l) \cap b(0, 1)|, \quad (9.7.23)$$

the area of intersection of two disks distance s apart, one of radius $(R_3 + l)$ and the other of radius 1. Figure 9.18 shows the geometrical configuration.

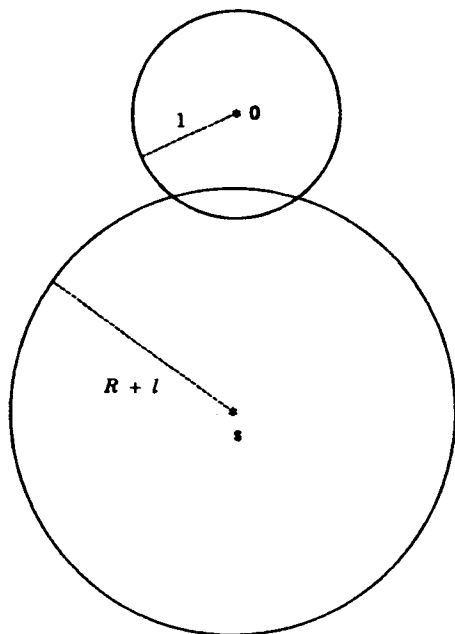


Figure 9.18 Two disks distance s apart, one with radius $R + l$, the other with radius 1. The expected area of intersection is used to define $q(u, h; \lambda, R)$ given by (9.7.21).

Theoretical Investigation of the Hitting Function

From (9.7.20), (9.7.22), and (9.7.23),

$$-\log q(s, l; \lambda_3, R_3) = \lambda_3 E(A_l(R_3)), \quad (9.7.24)$$

and, provided $R_3 + l \geq 1$ and $|R_3 + l - s| < 1$,

$$\begin{aligned} A_l(R_3) \equiv & (\pi/2) \{ (R_3 + l)^2 + 1 \} - y(l) \{ (R_3 + l)^2 - y(l)^2 \}^{1/2} \\ & - (R_3 + l)^2 \sin^{-1}(y(l)/(R_3 + l)) - \sin^{-1}(s - y(l)) \\ & - (s - y(l)) \{ 1 - (s - y(l))^2 \}^{1/2}, \end{aligned} \quad (9.7.25)$$

where $y(l) \equiv (s^2 + (R_3 + l)^2 - 1)/(2s)$. Expand (9.7.25) in a Taylor series about some fixed value R_3^0 to obtain

$$\begin{aligned} -\log q(s, l; \lambda_3, R_3) \\ = & \lambda_3 \{ A_l(R_3^0) + E(R_3 - R_3^0) A_l'(R_3^0) + E(R_3 - R_3^0)^2 A_l''(R_3^0)/2! + \cdots \} \\ \equiv & \beta_1 x_1(l) + \beta_2 x_2(l) + \beta_3 x_3(l) + \cdots, \end{aligned} \quad (9.7.26)$$

where $x_{j+1}(l) \equiv A_l^{(j)}(R_3^0)/j!$, $j = 0, 1, 2, \dots$, and

$$\lambda_3 = \beta_1, \quad (9.7.27)$$

$$E(R_3) = (\beta_2/\beta_1) + R_3^0, \quad (9.7.28)$$

$$\text{var}(R_3) = (\beta_3/\beta_1) - (\beta_2/\beta_1)^2. \quad (9.7.29)$$

Notice that (9.7.26) is a linear combination of explanatory variables $\{x_j(\cdot)\}$, whose coefficients are functions of the parameters to be estimated. Formulas for the independent variables are straightforward to evaluate because they are just derivatives of $A_l(\cdot)$ given by (9.7.25).

Empirical Investigation of the Hitting Function

In order to estimate parameters β_1 , β_2 , and β_3 , the theoretical function (9.7.24) will be matched to its empirical version. This is very much in the spirit of the classical method-of-moments technique of parameter estimation.

Isotropy of the RACS (9.7.19) ensures that

$$\begin{aligned} Q_{Y_3}(b(s, l)) &= (2\pi)^{-1} \left| \left\{ \theta: \theta \in [0, 2\pi); Y_3 \cap b(s, l) = \emptyset, \text{ where } s = (s, \theta)' \right\} \right|_1 \\ &= (2\pi)^{-1} \left| \left\{ \theta: \theta \in [0, 2\pi); s > \frac{r_3(\theta)}{r_2(\theta)} + l \right\} \right|_1 \\ &\equiv \hat{q}(s, l; \lambda_3, R_3), \end{aligned} \quad (9.7.30)$$

where $|\cdot|_1$ denotes one-dimensional Lebesgue measure. Recall that $r_2 = 1$, and so $\{(r_3(\theta)/r_2(\theta), \theta): \theta \in [0, 2\pi)\}$ in (9.7.30) is the boundary of Y_3 . That is, $\hat{q}(s, l; \lambda_3, R_3)$ is the proportion of angles θ for which $r_3(\theta)/r_2(\theta) < s - l$. Notice that $\{(r_3(\theta), \theta): \theta \in [0, 2\pi)\}$ is the boundary of X_3 , the untransformed time-3 tumor.

The values of the parameters β_1 , β_2 , and β_3 that bring $\beta_1 x_1(l) + \beta_2 x_2(l) + \beta_3 x_3(l)$ closest to $-\log \hat{q}(s, l; \lambda_3, R_3)$ will be used to obtain estimates of λ_3 , $E(R_3)$, and $\text{var}(R_3)$. Before I describe how to do this, some of the computational aspects involved in obtaining $\hat{q}(s, l; \lambda_3, R_3)$ will be presented briefly.

Computational Aspects

The original data came as photographic images, so they were not initially in a suitable form for computing $\hat{q}(s, l; \lambda_3, R_3)$. The information in the photographs had to be converted to numerical data by digitizing the relevant features of each picture. In this case, it is sufficient to quantify the boundaries of the cell islands. The method used consisted of tracing the outline of the cell islands using a pointer on a graphics tablet. The software interface to the device generated a sequence of Cartesian coordinates that define a

polygonal approximation to each of the boundaries. (A common reference point on each picture allowed the cell islands to be aligned.) Denote the sampled coordinates as (x_{ik}^0, y_{ik}^0) where $k = 1, 2, 3$ indexes the time and $i = 1, \dots, n_k$ indexes the coordinate pairs of the boundary at time k . (Digitization of the boundaries represented in Figure 9.14 yielded $n_1 = 213$, $n_2 = 510$, and $n_3 = 704$.) For the computational aspects of this study, X_k refers not to the cell-island image, but to the approximating polygon.

From the boundary description, it is possible to determine the cell island's center of gravity $(\bar{x}_k, \bar{y}_k)$ and its area. Henceforth, assume that the origin of the plane is moved to $(\bar{x}_1, \bar{y}_1)$ when studying the evolution of X_2 from X_1 and to $(\bar{x}_2, \bar{y}_2)$ when studying the evolution of X_3 from X_2 . For the data of Figure 9.14, $|X_1| = 0.00465 \text{ mm}^2$, $|X_2| = 0.01932 \text{ mm}^2$, and $|X_3| = 0.0969 \text{ mm}^2$, leading to areal growth factors of 4.155 and 5.016, respectively.

Computation and application of the geometric signature transformation S_2 requires a polar-coordinate representation for the boundaries of X_2 and X_3 . Using

$$\theta_{ik}^0 = \begin{cases} \arctan(y_{ik}^0/x_{ik}^0), & \text{if } x_{ik}^0 \geq 0, \\ \pi + \arctan(y_{ik}^0/x_{ik}^0), & \text{if } x_{ik}^0 < 0, \end{cases}$$

and $r_k(\theta_{ik}^0) = \{(x_{ik}^0)^2 + (y_{ik}^0)^2\}^{1/2}$, each of the sample boundary points (x_{ik}^0, y_{ik}^0) can be converted to polar coordinates $(r_k(\theta_{ik}^0), \theta_{ik}^0)$. For any given $\theta^* \in (0, 2\pi]$, not necessarily a sample boundary point, Cressie and Hulting (1992) give the linear-interpolation formula used to compute $r_k(\theta^*)$. Hence S_2 may be calculated using (9.7.18).

The necessary elements to compute $\hat{q}(s, l; \lambda_3, R_3)$ are now in place. Let $\{\theta_0^*, \dots, \theta_J^*\}$ be the sequence $\theta_j^* = 2\pi(j/J)$, $j = 0, \dots, J$, of equispaced angles. For fixed s and l , define

$$\delta(s, l, \theta_j^*) = \begin{cases} 1, & \text{if } s > \frac{r_3(\theta_j^*)}{r_2(\theta_j^*)} + l, \\ 0, & \text{else.} \end{cases}$$

Then $\hat{q}$, defined by (9.7.30), is evaluated by

$$\hat{q}(s, l; \lambda_3, R_3) = \frac{1}{J} \sum_{j=1}^J \delta(s, l, \theta_j^*);$$

a choice of $J = 750$ was made here.

9.7.3 Fitting the Tumor-Growth Parameters

Define

$$W(l) \equiv -\log \hat{q}(s, l; \lambda_3, R_3) \quad (9.7.31)$$

to be the dependent variable in the linear model

$$W(l) = (x_1(l), x_2(l), x_3(l))(\beta_1, \beta_2, \beta_3)' + \epsilon(l), \quad (9.7.32)$$

obtained by matching (9.7.26) with (9.7.30). Here, $\epsilon(\cdot)$ is an error term that represents a combination of higher-order Taylor series terms in (9.7.26), lack of model fit, and sampling fluctuations; it is assumed to have mean zero and homoskedastic variance σ^2 , assumptions that will be checked by analyses of the residuals.

Choosing the Design Constants

In order to implement estimation through (9.7.32), design constants R_3^0 , s , n , and $l_1, \dots, l_n$ must be chosen. In analyzing the growth from time 2 to time 3, $R_3^0 = 1.2$, $s = 3.2$, $n = 13$, and $l_1, \dots, l_n = 1.05(0.02)1.29$ were chosen.

The choice of R_3^0 is based on the rate of growth as measured by the areas of the cell islands. Define C_k to be the areal growth factors; that is, $|X_{k+1}| = C_k |X_k|$, $k = 1, 2$. Assuming that X_2 is a disk of radius 1 and X_3 is a disk of radius $1 + R_3$, C_2 is obtained from $\pi(1 + R_3)^2 = C_2\pi$. Substituting in the observed value for C_2 (5.016) and solving for R_3 yields the value $R_3^0 = 1.2$.

It is possible to vary *both* s and l in selecting the remaining design points. I chose to fix s and vary l because numerical evidence demonstrated that $A_l(R_3^0)$ varies approximately as a function of the difference $s - l$. Now if $l \geq 1$, then $R_3 + l$ is always ≥ 1 , satisfying one of the conditions of (9.7.25). The other condition can be expressed as $s - R_3 - 1 \leq l \leq s - R_3 + 1$, which suggests taking s so that $s - R_3^0 - 1 \approx 1$; that is, choose $s = 3.2$. Substituting $s = 3.2$ and $R_3^0 = 1.2$ into the preceding inequality gives an approximate range for l to be $(1.0, 3.0]$. However, for these data, zero estimates for $\hat{q}(s, l; \lambda_3, R_3)$ were obtained for $l > 1.4$, effectively reducing the range to the interval $(1.0, 1.4]$. Because observations are inexpensive, any number of l values may be selected. However, it is wise to avoid taking values of l close to 1.0 and 1.4, as well as values that are too close together. In these two instances, one can expect either imprecise or highly correlated observations, respectively. Moreover, the Taylor series approximation in (9.7.26) gets worse as l gets further from $R_3^0 = 1.2$. Diagnostic plots (see following text) were made for various choices of $l_1, \dots, l_n$, and the final choice was made on the basis that the linear model (9.7.32) should provide an adequate description of the data.

Table 9.3 Design Constants $l_1, \dots, l_{13}$, Dependent Variable $W(l)$, and Independent Variables $x_1(l)$, $x_2(l)$, and $x_3(l)$; Time 3 from Time 2

l	$W(l)$	$x_1(l)$	$x_2(l)$	$x_3(l)$
1.05	0.83011	0.030741	0.53380	2.61583
1.07	0.90965	0.042402	0.62957	2.20634
1.09	0.96758	0.055837	0.71218	1.94088
1.11	1.05173	0.070830	0.78582	1.75022
1.13	1.10262	0.087225	0.85279	1.60419
1.15	1.17334	0.104907	0.91454	1.48727
1.17	1.24479	0.123779	0.97204	1.39054
1.19	1.38897	0.143764	1.02598	1.30847
1.21	1.50208	0.164798	1.07686	1.23744
1.23	1.57022	0.186821	1.12509	1.17493
1.25	1.72224	0.209785	1.17095	1.11917
1.27	1.83258	0.233645	1.21469	1.06885
1.29	1.92873	0.258360	1.25652	1.02297

Estimating the Growth Parameters

The data for estimating β_1 , β_2 , and β_3 in the linear model (9.7.32) are given in Table 9.3. For reasons already given, the error term $\epsilon(\cdot)$ will not necessarily be uncorrelated; however, the choice of the design constants were to make $\epsilon(l_1), \dots, \epsilon(l_n)$ look as much as possible like white noise. We therefore proceed with ordinary-least-squares estimation of the parameters; more efficient estimation procedures would try to model the serial correlation in the errors, such as in Section 9.5.1.

Estimates of β_1 , β_2 , and β_3 , denoted by b_1 , b_2 , and b_3 , respectively, are given in Table 9.4, along with estimates of the estimators' standard deviations, an estimate of $\sigma^2 \equiv \text{var}(\epsilon(l_i))$, and t -statistics to assess the significance of each coefficient. Writing (9.7.32) as

$$W = X\beta + \epsilon, \tag{9.7.33}$$

Table 9.4 Estimates of Linear Regression Parameters, their Standard Deviations, and their t -Statistics^a; Time 3 from Time 2

β_i	b_i	$(\widehat{\text{sd}}(b_i))$	$t \ (\hat{\sigma}^2 = 5.52 \times 10^{-4})$
β_1	4.04668	(0.31894)	12.688
β_2	0.57624	(0.06949)	8.293
β_3	0.16165	(0.01660)	9.740

^a $\hat{\sigma}^2$ denotes the estimated error variance.

where $\text{var}(\epsilon) = \sigma^2 I$, standard results give

$$\mathbf{b} \equiv (b_1, b_2, b_3)' = (X'X)^{-1}X'W, \quad (9.7.34)$$

$$\widehat{\text{var}}(\mathbf{b}) = (X'X)^{-1}\hat{\sigma}^2, \quad (9.7.35)$$

$$\hat{\sigma}^2 = W'(I - X(X'X)^{-1}X')W/(n - 3). \quad (9.7.36)$$

To obtain estimates of the growth parameters, sample versions of (9.7.27), (9.7.28), and (9.7.29) are invoked:

$$\hat{\lambda}_3 \equiv b_1, \quad (9.7.37)$$

$$\hat{E}(R_3) \equiv (b_2/b_1) + R_3^0, \quad (9.7.38)$$

$$\widehat{\text{var}}(R_3) \equiv (b_3/b_1) - (b_2/b_1)^2. \quad (9.7.39)$$

Because these are obtained from a nonlinear transformation of the original estimators, a δ -method calculation is needed to obtain their approximate biases and variances. Specifically,

$$\widehat{\text{bias}}(\hat{\lambda}_3) = 0,$$

$$\widehat{\text{var}}(\hat{\lambda}_3) = \widehat{\text{var}}(b_1);$$

$$\widehat{\text{bias}}(\hat{E}(R_3)) = -\frac{\widehat{\text{cov}}(b_1, b_2)}{b_1^2} + \frac{b_2 \widehat{\text{var}}(b_1)}{b_1^3},$$

$$\widehat{\text{var}}(\hat{E}(R_3)) = \left\{ \frac{\widehat{\text{var}}(b_2)}{b_2^2} + \frac{\widehat{\text{var}}(b_1)}{b_1^2} - \frac{2\widehat{\text{cov}}(b_1, b_2)}{b_1 b_2} \right\} \frac{b_2^2}{b_1^2};$$

$$\widehat{\text{bias}}(\widehat{\text{var}}(R_3)) = -\frac{\widehat{\text{cov}}(b_3, b_1)}{b_1^2} + \frac{b_3 \widehat{\text{var}}(b_1)}{b_1^3} - \frac{3b_2^2 \widehat{\text{var}}(b_1)}{b_1^4}$$

$$+ \frac{4b_2 \widehat{\text{cov}}(b_1, b_2)}{b_1^3} - \frac{\widehat{\text{var}}(b_2)}{b_1^2},$$

$$\begin{aligned} \widehat{\text{var}}(\widehat{\text{var}}(R_3)) = & \frac{b_3 \widehat{\text{var}}(b_1)}{b_1^4} + \frac{\widehat{\text{var}}(b_3)}{b_1^2} + \frac{4b_2^4 \widehat{\text{var}}(b_1)}{b_1^6} + \frac{4b_2^2 \widehat{\text{var}}(b_2)}{b_1^4} \\ & - \frac{2b_3 \widehat{\text{cov}}(b_1, b_3)}{b_1^3} - \frac{4b_3 b_2^2 \widehat{\text{var}}(b_1)}{b_1^5} + \frac{4b_2 b_3 \widehat{\text{cov}}(b_1, b_2)}{b_1^4} \\ & + \frac{4b_2^2 \widehat{\text{cov}}(b_3, b_1)}{b_1^4} - \frac{4b_2 \widehat{\text{cov}}(b_2, b_3)}{b_1^3} - \frac{8b_2^3 \widehat{\text{cov}}(b_1, b_2)}{b_1^5}, \end{aligned}$$

Table 9.5 Estimates of Growth Parameters, their Standard Deviations, and their Biases; Time 3 from Time 2

Parameter	Estimator	Estimate	(sd)	[bias]
<i>Standardized</i>				
λ_3	b_1	4.04668	(0.3189)	[0.0]
$E(R_3)$	$(b_2/b_1) + R_3^0$	1.34240	(0.0283)	[0.0022]
$\text{var}(R_3)$	$(b_3/b_1) - (b_2/b_1)^2$	0.01967	(0.0114)	[-0.0015]
<i>Actual ($r_2 = 0.2604$ mm)</i>				
λ_3	b_1/r_2^2	59.685 mm ⁻²	(4.7035)	[0.0]
$E(R_3)$	$\{(b_2/b_1) + R_3^0\}r_2$	0.3496 mm	(0.00737)	[0.00057]
$\text{var}(R_3)$	$\{(b_3/b_1) - (b_2/b_1)^2\}r_2^2$	0.00133 mm ²	(0.00077)	[-0.00010]

where the values given by (9.7.34) and (9.7.35) are used in the computations. The estimated biases and standard deviations are given in Table 9.5.

Recall it was assumed that $r_2 = 1$. In fact r_2 is not 1, but the simple relationships

$$\lambda_3^{(a)} = \lambda_3^{(s)}/r_2^2, \quad R_3^{(a)} = R_3^{(s)}r_2 \tag{9.7.40}$$

(where the superscripts (a) and (s) stand for actual and standardized, respectively), allow reconstruction of *actual* parameter estimates from *standardized* parameter estimates (obtained assuming $r_2 = 1$). The size variable $r_2 = 0.2604$ allows the latter half of Table 9.5 to be constructed.

Regression Diagnostics

The error variance σ^2 is estimated by $\hat{\sigma}^2 = 5.52 \times 10^{-4}$ (on the standardized scale), which is very small when compared to the regression mean-squared error of 8.1303. The adjusted $R^2 = 0.9997$.

The model is a remarkably good fit to the data, as seen by the small estimated standard deviations in Table 9.4. Figure 9.19*a* shows a plot of the data $W(\cdot)$ versus the fitted relation $b_1x_1(\cdot) + b_2x_2(\cdot) + b_3x_3(\cdot)$, and Figure 9.19*b* shows the residuals

$$\hat{\epsilon}(l_i) \equiv W(l_i) - b_1x_1(l_i) - b_2x_2(l_i) - b_3x_3(l_i), \quad i = 1, \dots, n, \tag{9.7.41}$$

versus the fitted relation. There is no obvious lack of fit.

The simple residual plot of Figure 9.19*b* can sometimes miss important features unexplained by the fitted regression line. Part of the reason for its failure is that it is only a single two-dimensional summary of a model in four-dimensional space. A series of added variable (AV) and detrended added variable (DAV) plots, designed to assess the role of the explanatory

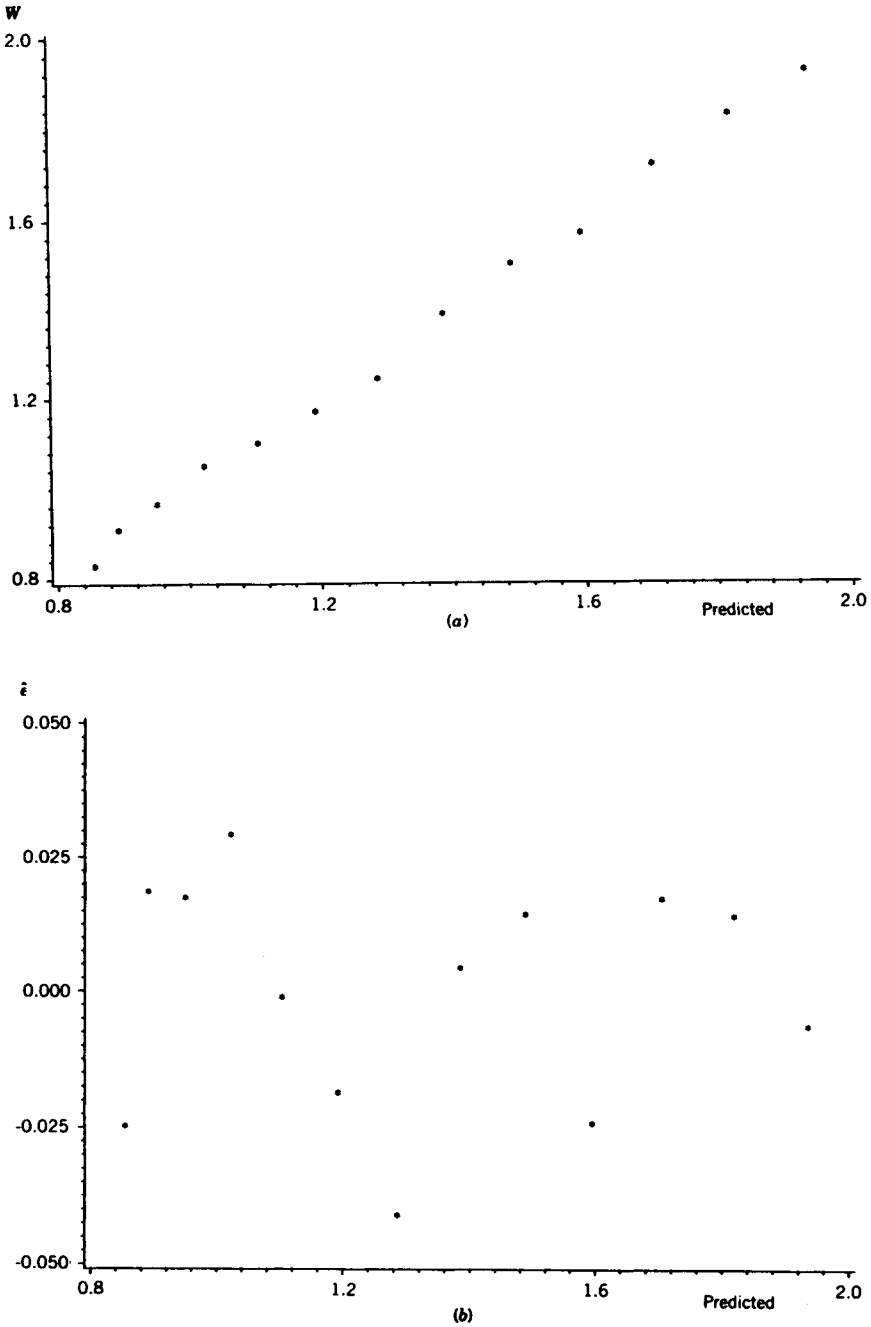


Figure 9.19 (a) Plot of data $\{W(l_i)\}$ versus predicted values $\{b_1x_1(l_i) + b_2x_2(l_i) + b_3x_3(l_i)\}$. (b) Plot of residuals $\{\hat{e}(l_i)\}$ versus predicted values $\{b_1x_1(l_i) + b_2x_2(l_i) + b_3x_3(l_i)\}$.

variables x_1, x_2, x_3 in the regression, provides additional visual summaries of the model. The AV plot for x_i shows $\hat{\epsilon}_{W \cdot [i]}$ versus $\hat{\epsilon}_{i \cdot [i]}$, where $\hat{\epsilon}_{W \cdot [i]}$ is the residual from the regression of W on $\{x_j: j \neq i\}$ and $\hat{\epsilon}_{i \cdot [i]}$ is the residual from the regression of x_i on $\{x_j: j \neq i\}$, $i = 1, 2, 3$. The DAV plot shows $\hat{\epsilon}$ versus $\hat{\epsilon}_{i \cdot [i]}$, $i = 1, 2, 3$.

To understand the purpose of these plots, note that $\hat{\epsilon}_{W \cdot [i]} = \hat{\epsilon} + b_i \hat{\epsilon}_{i \cdot [i]}$. Thus, a least-squares line fitted to the AV plot will have slope b_i . Then the DAV plot can be obtained from the AV plot by removing the systematic component. Therefore, the AV plot gives an indication of the consistency and strength of the functional relationship between x_i and W , whereas the associated DAV plot highlights model deficiencies (Cook and Weisberg, 1982; Cook, 1986). Figure 9.20a and b displays the AV/DAV pair for $i = 1$ (i.e., for the variable x_1). The AV plot suggests a strong linear relationship and the DAV plot of the residuals shows no serious model deficiencies. Similar conclusions may be drawn for x_2 and x_3 . The AV/DAV plots were found to be useful in choosing l values during the early stages of modeling. The displays helped to identify nonlinear relationships for extreme l values by clearly depicting the effects of suspected failures in the model assumptions.

Evolution of the Cell Island at Time 2 from the Cell Island at Time 1

Having modeled and fitted the cell island at time 3 from that at time 2, we now consider fitting time 2 from time 1. The sequence of steps was repeated. The multiplicative ratios $\{r_1/r_1(\theta): \theta \in [0, 2\pi)\}$ were determined and $\mathbb{R}^2$ was transformed using the geometric-signature transformation $S_1(\cdot)$ defined analogously to (9.7.17). Again, without loss of generality, assume $r_1 = 1$, and transform X_1 to a unit disk and the boundary of X_2 to $\{(r_2(\theta)/r_1(\theta), \theta): \theta \in [0, 2\pi)\}$, which defines the set Y_2 . An analogous stochastic model to (9.7.19) is posited and the function $q(s, l; \lambda_2, R_2)$ now represents the complement of the (conditional) hitting function of Y_2 . Matching $-\log q_2(s, l; \lambda_2, R_2)$ with its empirical version $-\log \hat{q}_2(s, l; \lambda_2, R_2)$ yields parameter estimates, standard deviations, and biases for λ_2 , $E(R_2)$, and $\text{var}(R_2)$, which are given in standardized form in the first half of Table 9.6. The cell-island size is $r_1 = 0.1097$ mm, from which actual estimates were computed; they are presented in the latter half of Table 9.6. Design constants chosen were $R_2^0 = 1.0$, $s = 3.0$, $n = 22$, and $l_i = 1.05(0.02)1.47$. Diagnostic checking again showed an excellent fit ($\hat{\sigma}^2 = 0.0047$, regression mean-squared error = 26.4464, and adjusted $R^2 = 0.9987$).

Interpretation of the Results

Comparison of Tables 9.5 and 9.6 shows that the character of the tumor has changed significantly (in a statistical sense) from one time interval to the next, in a way that is not obvious from inspection of Figure 9.14. Comparison of standardized estimates for each table avoids a confounding of the size variable. In the first 72 hours (between time 1 and time 2), foci of growth

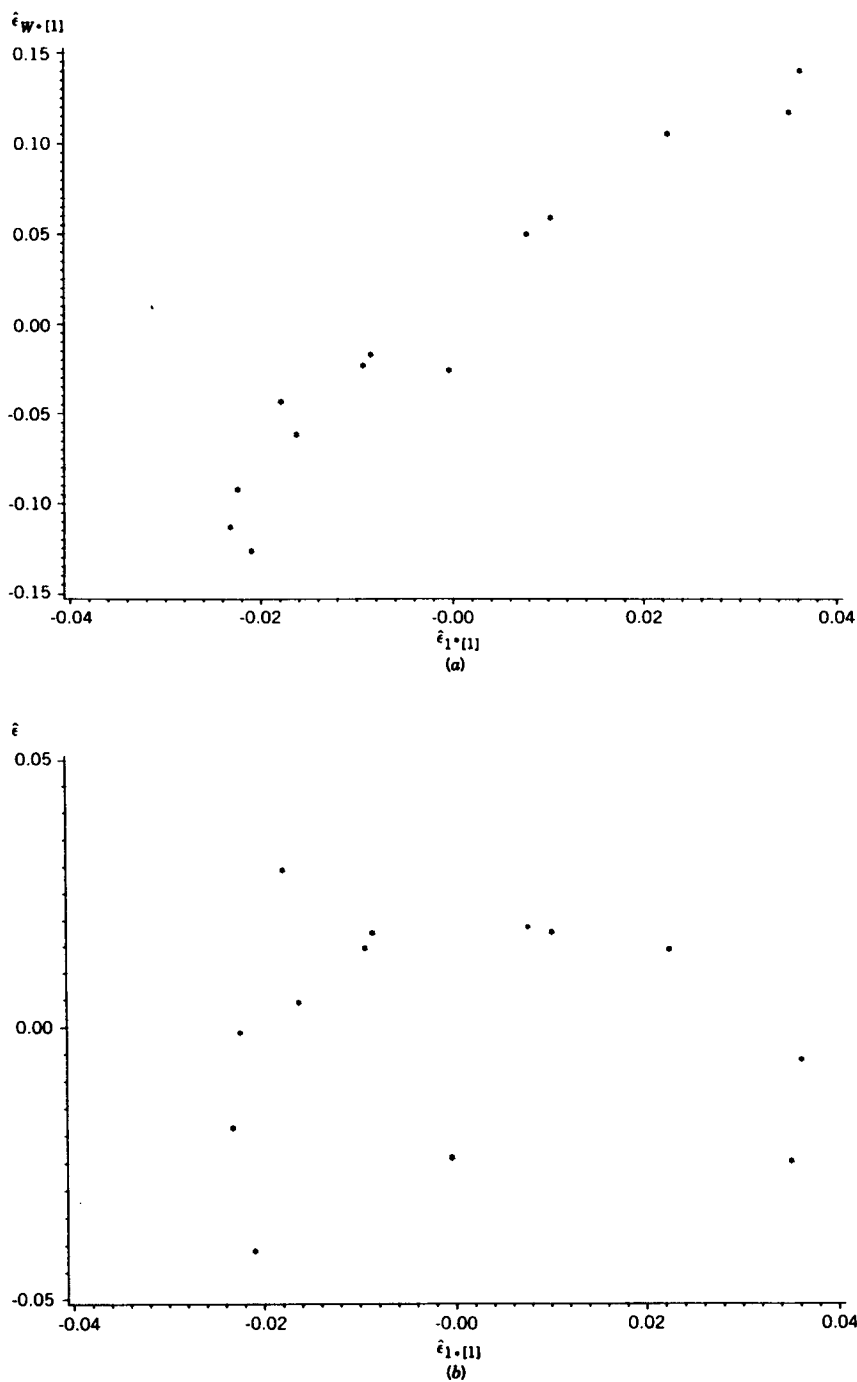


Figure 9.20 (a) Added variable (AV) plot of $\{\hat{\epsilon}_{W \cdot [1]}(l_i)\}$ versus $\{\hat{\epsilon}_{1 \cdot [1]}(l_i)\}$. (b) Detrended added variable (DAV) plot of residuals $\{\hat{\epsilon}(l_i)\}$ versus $\{\hat{\epsilon}_{1 \cdot [1]}(l_i)\}$.

Table 9.6 Estimates of Growth Parameters, their Standard Deviations, and their Biases; Time 2 from Time 1

Parameter	Estimate	($\widehat{\text{sd}}$)	($\widehat{\text{bias}}$)
<i>Standardized</i>			
λ_2	5.26194	(0.2968)	[0.0]
$E(R_2)$	1.04758	(0.0205)	[0.0011]
$\text{var}(R_2)$	0.02978	(0.0076)	[−0.00071]
<i>Actual ($r_1 = 0.1097 \text{ mm}$)</i>			
λ_2	438.495 mm^{-2}	(24.733)	[0.0]
$E(R_2)$	0.11492 mm	(0.00225)	[0.00012]
$\text{var}(R_2)$	0.00036 mm^{-2}	(0.00009)	[−0.00001]

occur at a higher intensity, but the average radius of growth is smaller, as compared to the next 72 hours (between time 2 and time 3). Simulation of the model (Section 9.7.1) indicates that greater growth potential occurs when the growth radii are larger, in spite of a drop in the intensity of growth foci. Whereas $|X_2| = 4.15|X_1|$, it is seen that in the later period $|X_3| = 5.01|X_2|$.

The analysis demonstrates that the model (9.7.19) provides an *excellent description* of the image data. Although the growth process does not occur according to a time scale of 72 hours, the dynamic conditional Boolean model may provide conjectures about how the cell island is growing. It appears that foci of growth occur randomly and the growth is isotropic with approximately constant radius of growth (on the transformed scale).

The model allows a tumor to *regress* as well as *grow*. It would be interesting to see if parameter estimates $\hat{\lambda}$, $\hat{E}(R)$, and $\widehat{\text{var}}(R)$ could be used to monitor the effect of a treatment regime on tumor shape and size.

Some Final Remarks

I see the flexibility of growth or regression within the same model as an advantage. However, if strong growth is expected, it might be seen as a disadvantage of the model that a point in X_t may not necessarily be contained in X_{t+1} . D. Stoyan has suggested the following modification of (9.7.14):

$$X_{t+1}^* = \bigcup \{Z_{t+1}(s_i) : s_i \in D_{t+1} \cap X_t^*\} \cup X_t^*. \quad (9.7.42)$$

Notice that $X_t^* \subset X_{t+1}^*$. The complement of the hitting function (conditional on X_t^*) is easily seen to be

$$Q_{X_{t+1}^*}(K) = \begin{cases} 0, & \text{if } K \cap X_t^* \neq \emptyset, \\ Q_{X_{t+1}}(K), & \text{if } K \cap X_t^* = \emptyset, \end{cases}$$

where $Q_{X_{i+1}}(K)$ is given by (9.7.15) with X_i^* substituted for X_i . Thus, from a practical point of view, inference on X_{i+1}^* conditional on X_i^* is *identical* with inference on X_{i+1} conditional on X_i . Moreover, the analysis and interpretation of the tumor-growth data remain the same regardless of whether (9.7.14) or (9.7.42) is chosen.

If the mechanism of growth of an object is something like a contact process (Harris, 1974), then growth will be concentrated on or near its boundary. Thus, the model (9.7.19) might be more realistic if Y_2 were an annulus rather than the disk $b(\mathbf{0}, r_2)$. A little thought reveals that, in a certain region of s and l values, (9.7.20) is unaffected by this change.

Suppose $1 - \rho$ is the radius of the interior boundary of the annulus (centered at $\mathbf{0}$) and 1 is the radius of the exterior boundary. Then, for this annulus to replace the unit disk $b(\mathbf{0}, 1)$ in (9.7.23) without change of $A_l(R_3)$, the inequality, $R_3 + l + 1 - s < \rho$ is required. For the choice of design constants given for time 3 from time 2, this implies $\rho > 0.29$; that is, $1 - \rho < 0.71$ (in units of r_2). For the choice of design constants given for time 2 from time 1, this implies $\rho > 0.47$; that is, $1 - \rho < 0.53$ (in units of r_1).

The two preceding remarks could now be combined to yield, on the transformed scale, a modification to the model (9.7.19), namely,

$$Y_3^{**} = \bigcup \{b(s_i, R_{3,i}) : s_i \in D_3 \cap (b(\mathbf{0}, r_2) \setminus b(\mathbf{0}, \rho r_2))\} \cup b(\mathbf{0}, r_2),$$

$$0 < \rho < 1.$$

Here the foci of growth are restricted to the annulus $b(\mathbf{0}, r_2) \setminus b(\mathbf{0}, \rho r_2)$ and $Y_2^{**} = b(\mathbf{0}, r_2)$ is always contained in Y_3^{**} .

In conclusion, the accurate description achieved by these conditional Boolean models is encouraging. Although no claim can be made that an explanation for tumor growth at the supracellular level has been found, the stochastic model has raised interesting questions that warrant translation into biological terms.

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