Monographs on Statistics and Applied Probability 26

Density Estimation for Statistics and Data Analysis

B.W. Silverman

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Density Estimation for Statistics and Data Analysis

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CHAPMAN & HALL/CRC

Boca Raton London New York Washington, D.C.

Chapman & Hall/CRC Taylor & Francis Group 6000 Broken Sound Parkway NW, Suite 300 Boca Raton, FL 33487-2742

© 1998 by B. W. Silverman Originally published by Chapman & Hall Chapman & Hall/CRC is an imprint of Taylor & Francis Group, an Informa business

No claim to original U.S. Government works Printed in the United States of America on acid-free paper 20 19 18 17 16 15 14 13 12 11 10 9 International Standard Book Number-13: 978-0-412-24620-3 (Hardcover)

Library of Congress catalog number: 99-19608

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Library of Congress Cataloging-in-Publication Data	
Catalog record is available from the Library of Congress	

Visit the Taylor & Francis Web site at http://www.taylorandfrancis.com

and the CRC Press Web site at http://www.crcpress.com

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Preface

The recent surge of interest in the more technical aspects of density estimation has brought the subject into public view but has sadly created the impression, in some quarters, that density estimates are only of theoretical importance. I have aimed in this book to make the subject accessible to a wider audience of statisticians and others, hoping to encourage broader practical application and more relevant theoretical research. With these objects in mind, I have tried to concentrate on topics of methodological interest. Specialists in the field will, I am sure, notice omissions of the kind that are inevitable in a personal account; I hope in spite of these that they will find the treatment of the subject interesting and stimulating.

I would like to thank David Kendall for first kindling my interest in density estimation. For their useful suggestions and other help I am grateful to several people, including Adrian Baddeley, Christopher Chatfield, David Cox, Rowena Fowler and Anthony Robinson. Colleagues who have helped in various specific ways are acknowledged in the course of the text. I am also grateful to the University of Washington (Seattle) for the opportunity to present a course of lectures that formed the basis of the book.

Bernard Silverman Bath, May 1985



CHAPTER 1

Introduction

1.1 What is density estimation?

The probability density function is a fundamental concept in statistics. Consider any random quantity X that has probability density function f. Specifying the function f gives a natural description of the distribution of X, and allows probabilities associated with X to be found from the relation

$$P(a \le X \le b) = \int_a^b f(x) dx \quad \text{for all } a \le b.$$

Suppose, now, that we have a set of observed data points assumed to be a sample from an unknown probability density function. *Density estimation*, as discussed in this book, is the construction of an estimate of the density function from the observed data. The two main aims of the book are to explain how to estimate a density from a given data set and to explore how density estimates can be used, both in their own right and as an ingredient of other statistical procedures.

One approach to density estimation is parametric. Assume that the data are drawn from one of a known parametric family of distributions, for example the normal distribution with mean μ and variance σ^2 . The density f underlying the data could then be estimated by finding estimates of μ and σ^2 from the data and substituting these estimates into the formula for the normal density. In this book we shall not be considering parametric estimates of this kind; the approach will be more nonparametric in that less rigid assumptions will be made about the distribution of the observed data. Although it will be assumed that the distribution has a probability density f, the data will be allowed to speak for themselves in determining the estimate of f more than would be the case if f were constrained to fall in a given parametric family.

Density estimates of the kind discussed in this book were first

proposed by Fix and Hodges (1951) as a way of freeing discriminant analysis from rigid distributional assumptions. Since then, density estimation and related ideas have been used in a variety of contexts, some of which, including discriminant analysis, will be discussed in the final chapter of this book. The earlier chapters are mostly concerned with the question of how density estimates are constructed. In order to give a rapid feel for the idea and scope of density estimation, one of the most important applications, to the exploration and presentation of data, will be introduced in the next section and elaborated further by additional examples throughout the book. It must be stressed, however, that these valuable exploratory purposes are by no means the only setting in which density estimates can be used.

1.2 Density estimates in the exploration and presentation of data

A very natural use of density estimates is in the informal investigation of the properties of a given set of data. Density estimates can give valuable indication of such features as skewness and multimodality in the data. In some cases they will yield conclusions that may then be regarded as self-evidently true, while in others all they will do is to point the way to further analysis and/or data collection.

An example is given in Fig. 1.1. The curves shown in this figure were constructed by Emery and Carpenter (1974) in the course of a study of sudden infant death syndrome (also called 'cot death' or 'crib death'). The curve A is constructed from a particular observation, the degranulated mast cell count, made on each of 95 infants who died suddenly and apparently unaccountably, while the cases used to construct curve B were a control sample of 76 infants who died of known causes that would not affect the degranulated mast cell count. The investigators concluded tentatively from the density estimates that the density underlying the sudden infant death cases might be a mixture of the control density with a smaller proportion of a contaminating density of higher mean. Thus it appeared that in a minority (perhaps a quarter to a third) of the sudden deaths, the degranulated mast cell count was exceptionally high. In this example the conclusions could only be regarded as a cue for further clinical investigation.

Another example is given in Fig. 1.2. The data from which this figure was constructed were collected in an engineering experiment

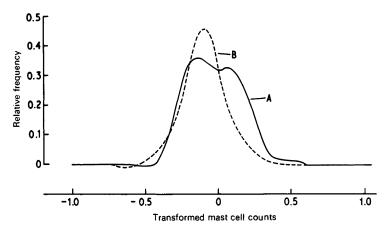


Fig. 1.1 Density estimates constructed from transformed and corrected degranulated mast cell counts observed in a cot death study. (A, Unexpected deaths; B, Hospital deaths.) After Emery and Carpenter (1974) with the permission of the Canadian Foundation for the Study of Infant Deaths. This version reproduced from Silverman (1981a) with the permission of John Wiley & Sons Ltd.

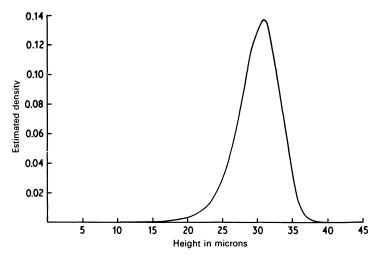


Fig. 1.2 Density estimate constructed from observations of the height of a steel surface. After Silverman (1980) with the permission of Academic Press, Inc. This version reproduced from Silverman (1981a) with the permission of John Wiley & Sons Ltd.

described by Bowyer (1980). The height of a steel surface above an arbitrary level was observed at about 15 000 points. The figure gives a density estimate constructed from the observed heights. It is clear from the figure that the distribution of height is skew and has a long lower tail. The tails of the distribution are particularly important to the engineer, because the upper tail represents the part of the surface which might come into contact with other surfaces, while the lower tail represents hollows where fatigue cracks can start and also where lubricant might gather. The non-normality of the density in Fig. 1.2 casts doubt on the Gaussian models typically used to model these surfaces, since these models would lead to a normal distribution of height. Models which allow a skew distribution of height would be more appropriate, and one such class of models was suggested for this data set by Adler and Firman (1981).

A third example is given in Fig. 1.3. The data used to construct this curve are a standard directional data set and consist of the directions in which each of 76 turtles was observed to swim when released. It is clear that most of the turtles show a preference for swimming approximately in the 60° direction, while a small proportion prefer exactly the opposite direction. Although further statistical model-

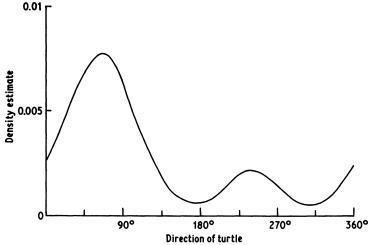


Fig. 1.3 Density estimate constructed from turtle data. After Silverman (1978a) with the permission of the Biometrika Trustees. This version reproduced from Silverman (1981a) with the permission of John Wiley & Sons Ltd.



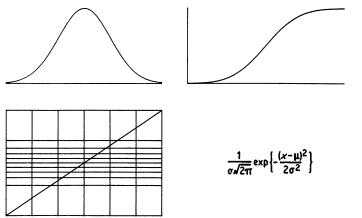


Fig. 1.4 Four ways of explaining the normal distribution: a graph of the density function; a graph of the cumulative distribution function; a straight line on probability paper; the formula for the density function.

ling of these data is possible (see Mardia, 1972) the density estimate really gives all the useful conclusions to be drawn from the data set.

An important aspect of statistics, often neglected nowadays, is the presentation of data back to the client in order to provide explanation and illustration of conclusions that may possibly have been obtained by other means. Density estimates are ideal for this purpose, for the simple reason that they are fairly easily comprehensible to non-mathematicians. Even those statisticians who are sceptical about estimating densities would no doubt explain a normal distribution by drawing a bell-shaped curve rather than by one of the other methods illustrated in Fig. 1.4. In all the examples given in this section, the density estimates are as valuable for explaining conclusions as for drawing these conclusions in the first place. More examples illustrating the use of density estimates for exploratory and presentational purposes, including the important case of bivariate data, will be given in later chapters.

1.3 Further reading

There is a vast literature on density estimation, much of it concerned with asymptotic results not covered in any detail in this book.

Prakasa Rao's (1983) book offers a comprehensive treatment of the theoretical aspects of the subject. Journal papers providing surveys and bibliography include Rosenblatt (1971), Fryer (1977), Wertz and Schneider (1979), and Bean and Tsokos (1980). Tapia and Thompson (1978) give an interesting perspective paying particular attention to their own version of the penalized likelihood approach described in Sections 2.8 and 5.4 below. A thorough treatment, rather technical in nature, of a particular question and its ramifications is given by Devroye and Györfi (1985). Other texts on the subject are Wertz (1978) and Delecroix (1983). Further references relevant to specific topics will be given, as they arise, later in this book.

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