Nonparametric Inference on Manifolds

This book introduces in a systematic manner a general nonparametric theory of statistics on manifolds, with emphasis on manifolds of shapes. The theory has important and varied applications in medical diagnostics, image analysis, and machine vision. An early chapter of examples establishes the effectiveness of the new methods and demonstrates how they outperform their parametric counterparts.

Inference is developed for both intrinsic and extrinsic Fréchet means of probability distributions on manifolds, and then applied to spaces of shapes defined as orbits of landmarks under a Lie group of transformations – in particular, similarity, reflection similarity, affine, and projective transformations. In addition, nonparametric Bayesian theory is adapted and extended to manifolds for the purposes of density estimation, regression, and classification. Ideal for statisticians who analyze manifold data and wish to develop their own methodology, this book is also of interest to probabilists, mathematicians, computer scientists, and morphometricians with mathematical training.

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INSTITUTE OF MATHEMATICAL STATISTICS
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With Applications to Shape Spaces

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CAMBRIDGE
UNIVERSITY PRESS

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University Printing House, Cambridge CB2 8BS, United Kingdom

One Liberty Plaza, 20th Floor, New York, NY 10006, USA

477 Williamstown Road, Port Melbourne, VIC 3207, Australia

314-321, 3rd Floor, Plot 3, Splendor Forum, Jasola District Centre, New Delhi - 110025, India

103 Penang Road, #05-06/07, Visioncrest Commercial, Singapore 238467

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www.cambridge.org
Information on this title: www.cambridge.org/9781107019584

First published 2012
First paperback edition 2015

A catalogue record for this publication is available from the British Library

ISBN 978-1-107-01958-4 Hardback
ISBN 978-1-107-48431-3 Paperback

Contents

Commonly used notation

Manifolds

S^d: d-dimensional sphere

$\mathbb{R}P^k$, $\mathbb{C}P^k$: k-dimensional real, resp. complex, projective space; all lines in $\mathbb{R}^{k+1}$, resp. $\mathbb{C}^{k+1}$, passing through the origin

$V_{k,m}$: Stiefel manifold $\mathrm{St}_k(m)$; all k-frames (k mutually orthogonal directions) in $\mathbb{R}^m$; see §10.1

d_E, d_g: extrinsic distance, geodesic distance; see §4.1, §5.1

d_F, d_P: Procrustes distance: full, partial; see §9.5

$j\colon M \to E$: embedding of the manifold M into the Euclidean space E; $\tilde{M} = j(M)$; see §4.1

$T_u(M)$ or T_uM: tangent space of the manifold M at $u \in M$; see §4.2

$d_xP\colon T_xE \to T_{P(x)}\tilde{M}$: differential of the projection map $P\colon U \to \tilde{M}$, for U a neighborhood of nonfocal point μ; see §4.2

D_r, D: partial derivative with respect to rth coordinate, resp. vector of partial derivatives; see §3.4

$L = L_{\mu_E}$: orthogonal linear projection of vectors in $T_{\mu_E}E \equiv E$ onto $T_{\mu_E}\tilde{M}$; see §4.5.1

r_*: exponential map at p is injective on $\{v \in T_p(M) : |v| < r_*\}$; see §5.1

Shape spaces

Σ_m^k: similarity shape space of k-ads in m dimensions; see §7.1

Σ_{0m}^k: similarity shape space of "nonsingular" k-ads in $m > 2$ dimensions; see §7.2

S_m^k: preshape sphere of k-ads in m dimensions; see§7.1

S_m^k/G: preshape sphere of k-ads in m dimensions modulo transformation group G; see §7.1

$A\Sigma_m^k$: affine shape space of k-ads in m dimensions; see §11.1

$P\Sigma_m^k$: projective shape space of k-ads in m dimensions; see §12.3

$R\Sigma_m^k$: reflection shape space of k-ads in m dimensions; see §9.1

$S\Sigma_2^k$: planar size-and-shape space of k-ads; see §8.10

$SA\Sigma_2^k$: special affine shape space of k-ads in m dimensions; see §11.2

Transformation groups

A': transpose of the matrix A

U^*: conjugate transpose of the complex matrix U

GL(m): general linear group; $m \times m$ nonsingular matrices

$M(m, k)$: $m \times k$ real matrices

O(m): $m \times m$ orthogonal matrices

$S(k)$: $k \times k$ symmetric matrices

Skew(k): $k \times k$ skew-symmetric matrices

SO(m): special orthogonal group; $m \times m$ orthogonal matrices with determinant +1

SU(k): special unitary group; $k \times k$ unitary matrices with determinant +1

Statistics

$\xrightarrow{\mathcal{L}}$: convergence in distribution

$\mathcal{X}_d^2$: chi-squared distribution with d degrees of freedom

$N_d(0, \Sigma)$: mean zero d-dimensional Normal distribution

$Z_{1-\frac{\alpha}{2}}$: upper $(1 - \frac{\alpha}{2})$-quantile of $N(0, 1)$ distribution; see §5.4.1

μ_E, μ_{nE} (μ_I, μ_{nI}): extrinsic (intrinsic) mean of the distribution Q, resp. sample extrinsic (intrinsic) mean of the empirical distribution Q_n; see §4.1 (§5.1)

μ_F, μ_{nF}: (local) Fréchet mean of the distribution Q, resp. sample Fréchet mean of the empirical distribution Q_n; see §8.5

V, V_n: variation of the distribution Q, resp. sample variation of the empirical distribution Q_n; see §3.3

$K(m; \mu, \kappa)$: probability density (kernel) on a metric space M with variable $m \in M$ and parameters $\mu \in M$ and $\kappa \in N$, a Polish space; see §13.2

Preface

This book presents in a systematic manner a general nonparametric theory of statistics on manifolds with emphasis on manifolds of shapes, and with applications to diverse fields of science and engineering. There are many areas of significant application of statistics on manifolds. For example, directional statistics (statistics on the sphere S^2) are used to study shifts in the Earth's magnetic poles over geological time, which have an important bearing on the subject of tectonics. Applications in morphometrics involve classification of biological species and subspecies. There are many important applications to medical diagnostics, image analysis (including scene recognition), and machine vision (e.g., robotics). We take a fresh look here in analyzing existing data pertaining to a number of such applications. It is our goal to lay the groundwork for other future applications of this exciting emerging field of nonparametric statistics.

Landmark-based shape spaces were first introduced by D. G. Kendall more than three decades ago, and pioneering statistical work on shapes with applications to morphometrics was carried out by F. Bookstein around the same time. Statistics on spheres, or directional statistics, arose even earlier, and a very substantial statistical literature on directional statistics exists, including a seminal 1953 paper by R. A. Fisher and books by Watson (1983), Mardia and Jupp (2000), Fisher et al. (1987), and others. For statistics on shape spaces, important parametric models have been developed by Kent, Dryden, Mardia, and others, and a comprehensive treatment of the literature may be found in the book by Dryden and Mardia (1998). In contrast, the present book concerns nonparametric statistical inference, much of which is of recent origin.

Although the past literature on manifolds, especially that on shape spaces, has generally focused on parametric models, there were a number of instances of the use of model-independent procedures in the 1990s and earlier. In particular, Hendriks and Landsman (1996, 1998) provided nonparametric procedures for statistics on submanifolds of Euclidean spaces, which are special cases of what is described as extrinsic analysis in this book. Independently of this, Vic Patrangenaru, in his 1998 dissertation, arrived at nonparametric extrinsic methods for statistics on general manifolds. Intrinsic statistical inference, as well as further development of general extrinsic inference, with particular emphasis on Kendall's shape spaces, appeared in two papers in the *Annals of Statistics* (2003, 2005) by Patrangenaru and the second author of this monograph. Our aim here is to present the current state of this general theory and advances, including many new results that provide adequate tools of inference on shape spaces.

A first draft of the book submitted to the IMS was the Ph.D. dissertation of the first author at the University of Arizona. The present monograph under joint authorship came about at the suggestion of the IMS editors. It has substantially more material and greater emphasis on exposition than the first draft.

For the greater part of the book (Chapters 1–12) we focus on the *Fréchet mean* of a probability distribution Q on a manifold, namely, the minimizer, if unique, of the expected squared distance from a point of a manifold-valued random variable having the distribution Q. If the distance chosen is the geodesic distance with respect to a natural Riemannian structure, such a mean is called *intrinsic*. If, on the other hand, the manifold is embedded in a Euclidean space, or a vector space, then the distance induced on the manifold by the Euclidean distance is called *extrinsic*, and the corresponding Fréchet mean is termed an extrinsic mean. One would generally prefer an equivariant embedding that preserves a substantial amount of the geometry of the manifold. An advantage of extrinsic means is that they are generally unique. By contrast, sufficiently broad conditions for uniqueness of the intrinsic mean are not known, thus impeding its use somewhat.

The last two chapters of the book represent a point of departure from the earlier part. Based on recent joint work of the first author and David Dunson, nonparametric Bayes procedures are derived for functional inference on shape spaces – nonparametric density estimation, classification, and regression.

The manifolds of shapes arising in applications are of fairly high dimension, and the Fréchet means capture important and distinguishing features of the distributions on them. In analyzing real data, the nonparametric methods developed in the monograph often seem to provide sharper inferences than do their parametric counterparts. The parametric models do, however, play a significant role in the construction of nonparametric Bayes priors for density estimation and shape classification in the last two chapters.

Readership This monograph is suitable for graduate students in mathematics, statistics, science, engineering, and computer science who have taken (1) a graduate course in asymptotic statistics and (2) a graduate course in differential geometry. For such students special topics courses may be based on it. The book is also meant to serve as a reference for researchers in the areas mentioned. For the benefit of readers, extrinsic analysis, whose geometric component does not involve much more than introductory differentiable manifolds, is separated from intrinsic inference for the most part. Appendix A, on differentiable manifolds, provides some background. Some basic notions from Riemannian geometry are collected in Appendix B.

For background in statistics, one may refer to Bickel and Doksum (2001, Chaps. 1–5), Bhattacharya and Patrangenaru (2012, Pt. II), Casella and Berger (2001, Chaps. 5–10), or Ferguson (1996). For geometry, Do Carmo (1992) and Gallot et al. (1990) are good references that contain more than what is needed. Other good references are Boothby (1986) (especially for differentiable manifolds) and Lee (1997) (for Riemannian geometry). A very readable upper division introduction to geometry is given in Millman and Parker (1977), especially Chapters 4 and 7.

For a basic course on the subject matter of the monograph, we suggest Chapters 1–4, 6, 8 (Sections 8.1–8.3, 8.6, 8.11), and 9, as well as Appendices A, B, and C. A more specialized course on the application of nonparametric Bayes theory to density estimation, regression, and classification on manifolds may be based on Chapters 1, 5, 13, and 14 and Appendices A–D. Chapters 10–12, in addition to the basics, would be of special interest to students and researchers in computer science.

MATLAB code and data sets MATLAB was used for computation in the examples presented in the book. The MATLAB code, with all data sets embedded, can be downloaded from http://www.isical.ac.in/~abhishek.

Acknowledgments The authors are indebted to the series editors Xiao-Li Meng and David Cox for their kind suggestions for improving the substance of the book as well as its presentation, and thank Lizhen Lin for her invaluable help with corrections and editing. Also appreciated are helpful suggestions from a reviewer and from the Cambridge University Press editor Diana Gillooly. The authors gratefully acknowledge support from National Science Foundation grants DMS 0806011 and 1107053, and National Institute of Environmental Health Sciences grant R01ES017240.