

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.

ABHISHEK BHATTACHARYA is Assistant Professor in the Theoretical Statistics and Mathematics Unit (SMU) at the Indian Statistical Institute, Kolkata.

RABI BHATTACHARYA is Professor in the Department of Mathematics at The University of Arizona, Tucson.

INSTITUTE OF MATHEMATICAL STATISTICS
MONOGRAPHS

Editorial Board

D. R. Cox (University of Oxford)
B. Hambly (University of Oxford)
S. Holmes (Stanford University)
X.-L. Meng (Harvard University)

IMS Monographs are concise research monographs of high quality on any branch of statistics or probability of sufficient interest to warrant publication as books. Some concern relatively traditional topics in need of up-to-date assessment. Others are on emerging themes. In all cases the objective is to provide a balanced view of the field.

Cambridge University Press

978-1-107-01958-4 — Nonparametric Inference on Manifolds: With Applications to Shape Spaces

Abhishek Bhattacharya , Rabi Bhattacharya

Frontmatter

[More Information](#)

Nonparametric Inference
on Manifolds
With Applications to Shape Spaces

ABHISHEK BHATTACHARYA

Indian Statistical Institute, Kolkata

RABI BHATTACHARYA

University of Arizona



CAMBRIDGE
UNIVERSITY PRESS

Cambridge University Press
978-1-107-01958-4 — Nonparametric Inference on Manifolds: With Applications to Shape Spaces
Abhishek Bhattacharya , Rabi Bhattacharya
Frontmatter
[More Information](#)

CAMBRIDGE
UNIVERSITY PRESS

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

Cambridge University Press is part of the University of Cambridge.
It furthers the University's mission by disseminating knowledge in the pursuit of
education, learning and research at the highest international levels of excellence.

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

© A. Bhattacharya and R. Bhattacharya 2012

This publication is in copyright. Subject to statutory exception
and to the provisions of relevant collective licensing agreements,
no reproduction of any part may take place without the written
permission of Cambridge University Press.

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

Cambridge University Press has no responsibility for the persistence or
accuracy of URLs for external or third-party internet websites referred to in
this publication, and does not guarantee that any content on such websites is,
or will remain, accurate or appropriate.

Contents

<i>Commonly used notation</i>	<i>page</i> ix
<i>Preface</i>	xi
1 Introduction	1
2 Examples	8
2.1 Data example on S^1 : wind and ozone	8
2.2 Data examples on S^2 : paleomagnetism	8
2.3 Data example on Σ_2^k : shapes of gorilla skulls	12
2.4 Data example on Σ_2^k : brain scan shapes of schizophrenic and normal patients	15
2.5 Data example on affine shape space $A\Sigma_2^k$: application to handwritten digit recognition	17
2.6 Data example on reflection similarity shape space $R\Sigma_3^k$: glaucoma detection	18
2.7 References	20
3 Location and spread on metric spaces	21
3.1 Introduction	21
3.2 Location on metric spaces	22
3.3 Variation on metric spaces	27
3.4 Asymptotic distribution of the sample mean	28
3.5 Asymptotic distribution of the sample variation	30
3.6 An example: the unit circle	31
3.7 Data example on S^1	34
3.8 References	35
4 Extrinsic analysis on manifolds	36
4.1 Extrinsic mean and variation	36
4.2 Asymptotic distribution of the sample extrinsic mean	37
4.3 Asymptotic distribution of the sample extrinsic variation	39
4.4 Asymptotic joint distribution of the sample extrinsic mean and variation	41

vi	<i>Contents</i>	
4.5	Two-sample extrinsic tests	42
4.6	Hypothesis testing using extrinsic mean and variation	46
4.7	Equivariant embedding	48
4.8	Extrinsic analysis on the unit sphere S^d	49
4.9	Applications on the sphere	51
4.10	References	55
5	Intrinsic analysis on manifolds	57
5.1	Intrinsic mean and variation	57
5.2	Asymptotic distribution of the sample intrinsic mean	59
5.3	Intrinsic analysis on S^d	64
5.4	Two-sample intrinsic tests	65
5.5	Data example on S^2	69
5.6	Some remarks	71
5.7	References	75
6	Landmark-based shape spaces	77
6.1	Introduction	77
6.2	Geometry of shape manifolds	78
6.3	References	80
7	Kendall's similarity shape spaces Σ_m^k	82
7.1	Introduction	82
7.2	Geometry of similarity shape spaces	83
7.3	References	86
8	The planar shape space Σ_2^k	87
8.1	Introduction	87
8.2	Geometry of the planar shape space	88
8.3	Examples	89
8.4	Intrinsic analysis on the planar shape space	90
8.5	Other Fréchet functions	96
8.6	Extrinsic analysis on the planar shape space	97
8.7	Extrinsic mean and variation	98
8.8	Asymptotic distribution of the sample extrinsic mean	99
8.9	Two-sample extrinsic tests on the planar shape space	101
8.10	Planar size-and-shape manifold	103
8.11	Applications	105
8.12	References	109
9	Reflection similarity shape spaces $R\Sigma_m^k$	110
9.1	Introduction	110
9.2	Extrinsic analysis on the reflection shape space	111
9.3	Asymptotic distribution of the sample extrinsic mean	117

<i>Contents</i>		vii
9.4	Two-sample tests on the reflection shape spaces	122
9.5	Other distances on the reflection shape spaces	123
9.6	Application: glaucoma detection	125
9.7	References	128
10	Stiefel manifolds $V_{k,m}$	130
10.1	Introduction	130
10.2	Extrinsic analysis on $V_{k,m}$	130
10.3	References	134
11	Affine shape spaces $A\Sigma_m^k$	135
11.1	Introduction	135
11.2	Geometry of affine shape spaces	137
11.3	Extrinsic analysis on affine shape spaces	139
11.4	Asymptotic distribution of the sample extrinsic mean	141
11.5	Application to handwritten digit recognition	144
11.6	References	146
12	Real projective spaces and projective shape spaces	147
12.1	Introduction	147
12.2	Geometry of the real projective space $\mathbb{R}P^m$	148
12.3	Geometry of the projective shape space $P_0\Sigma_m^k$	149
12.4	Intrinsic analysis on $\mathbb{R}P^m$	150
12.5	Extrinsic analysis on $\mathbb{R}P^m$	151
12.6	Asymptotic distribution of the sample extrinsic mean	153
12.7	References	155
13	Nonparametric Bayes inference on manifolds	156
13.1	Introduction	156
13.2	Density estimation on metric spaces	157
13.3	Full support and posterior consistency	158
13.4	Posterior computations	163
13.5	Application to unit sphere S^d	165
13.6	Application to the planar shape space Σ_2^k	166
13.7	Application to morphometrics: classification of gorilla skulls	168
13.8	Proofs of theorems	170
13.9	References	181
14	Nonparametric Bayes regression, classification and hypothesis testing on manifolds	182
14.1	Introduction	182
14.2	Regression using mixtures of product kernels	183
14.3	Classification	185

viii	<i>Contents</i>	
14.4	Nonparametric Bayes testing	192
14.5	Examples	196
14.6	Proofs	202
Appendix A	Differentiable manifolds	209
Appendix B	Riemannian manifolds	214
Appendix C	Dirichlet processes	218
Appendix D	Parametric models on S^d and Σ_2^k	225
<i>References</i>		229
<i>Index</i>		235

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 $St_k(m)$; 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
 $j: M \rightarrow E$: 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
 $d_xP: T_xE \rightarrow T_{P(x)}\tilde{M}$: differential of the projection map $P: U \rightarrow \tilde{M}$, for U a neighborhood of nonfocal point μ ; see §4.2
 D_r, D : partial derivative with respect to r th 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 matricesSkew(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 χ_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.