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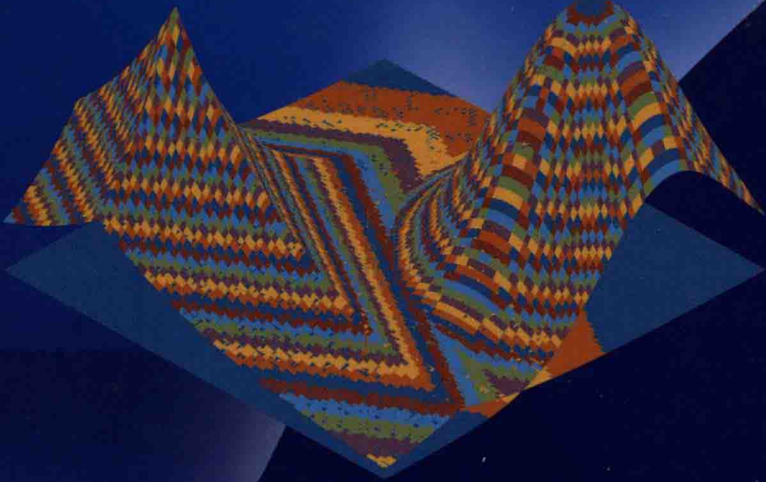

Kernel-based Approximation Methods using MATLAB

Gregory Fasshauer
Michael McCourt

Interdisciplinary Mathematical Sciences – Vol. 19

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In an attempt to introduce application scientists and graduate students to the exciting topic of positive definite kernels and radial basis functions, this book presents modern theoretical results on kernel-based approximation methods and demonstrates their implementation in various settings. The authors explore the historical context of this fascinating topic and explain recent advances as strategies to address long-standing problems.

Examples are drawn from fields as diverse as function approximation, spatial statistics, boundary value problems, machine learning, surrogate modeling and finance. Researchers from those and other fields can recreate the results within using the documented MATLAB code, also available through the online library. This combination of a strong theoretical foundation and accessible experimentation empowers readers to use positive definite kernels on their own problems of interest.

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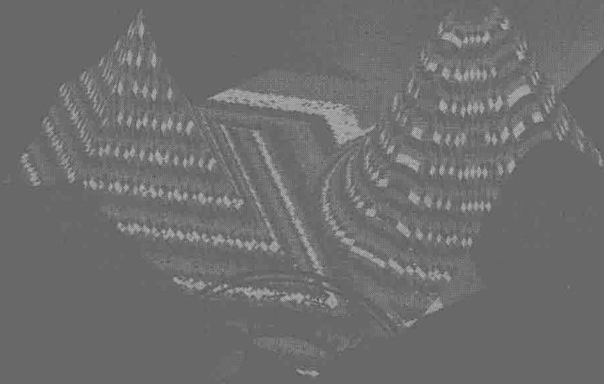

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This book is dedicated to
Inge, Conny, Marc and Pat

Jason, Laurie and Kevin

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and to Kaya, who kept us company
during some of the hardest work.

Preface

This book focuses on recent developments in the field of meshfree approximation using positive definite reproducing kernels, both from a theoretical and practical point of view. Since positive definite kernels play an important role in many different areas of mathematics, science and engineering, we hope to provide a broad view of this field of research. On the one hand, we aim to speak to graduate students and researchers in these diverse fields by providing each of them with at least some content they are familiar with. And on the other hand, we hope that our presentation of ideas from areas such as approximation theory, numerical analysis, spatial statistics, machine learning, finance, and computing with MATLAB[1] will enable our readers to take some of those ideas and apply them successfully to their own work which may be housed in only one of these areas, or even an entirely different area). Thus, we view this book as a hands-on guide for graduate students in applied mathematics and engineering interested in understanding and applying some of the most recent advances in kernel-based approximation.

Encouraged by the success of the format used for "Meshfree Approximation Methods with MATLAB" (Volume 6 in this book series [Fasshauer (2007)]), where a gentle introduction to the underlying theory of radial basis functions and moving least squares methods was combined with many — relatively short — MATLAB scripts that illustrated those concepts, we have decided on a similar format for this book. We need to emphasize that this book should in no way be considered a second (or revised and enlarged) edition of "Meshfree Approximation Methods with MATLAB". If anything, the present volume can be considered as a "Volume 2". There is very little theory overlap between the two books, and the use of MATLAB is considerably more sophisticated — due in part to some relatively recent additions to the MATLAB software such as `bsxfun`, `cellfun`, and other related functionality. Therefore, books developing the theoretical foundation for the use of kernels in approximation theory (such as, e.g., [Buhmann (2003); Wendland (2005)]), spatial

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statistics (e.g., [Stein (1999)]), statistical learning (e.g., [Steinwart and Christmann (2008)]) or statistics in general [Wahba (1990)] remain of great importance.

The book is divided into two parts: Part I focusses mostly on background information (and thus is probably a bit more theory-heavy), while Part II aims mainly to illustrate the basic concepts in the context of applications.

We begin the first part of the book with an chapter that puts positive definite kernels into perspective — both historically, as well as scientifically by pointing out connections to and important resources in related fields such as analysis, approximation theory, the theory of integral equations, mathematical physics, probability theory and statistics, geostatistics, statistical or machine learning, and various kinds of engineering or physics applications. Many of the fundamental concepts we develop to support our view of positive definite kernels should be familiar to beginning graduate students in applied mathematics and engineering: eigenvalues, eigenfunctions, orthogonality, change of basis, Sturm–Liouville theory, Green's kernels, maximum likelihood estimation, Bayesian statistics, convex optimization, etc. We do not aim to give any of these topics a thorough theoretical treatment — that is what we provide many pointers and references for. Instead, it is our goal to present these concepts as they relate to our work on positive definite kernels.

However, there are also new developments — or new interpretations of old ideas — that we believe to be important for the field of meshfree approximation. The first of these ideas is the use of different kinds of basis transformations to map the standard kernel basis to an alternate basis that is more advantageous for the application at hand. In particular, this leads to the so-called Hilbert–Schmidt SVD introduced in Chapter 13, a framework developed by the authors (motivated, however, by the ground-breaking work of Bengt Fornberg and his collaborators) which opens the door to stable computation with kernels in their often most accurate close-to-flat state. By stable computation we mean not only the solution and evaluation of interpolation problems, but also corresponding tasks for partial differential equations, as well as estimation of "optimal" kernel parametrizations via criteria such a maximum likelihood estimation, cross-validation and minimization of the kriging variance (or power function).

Another relatively new idea presented in this book is the notion of a designer kernel, i.e., the construction of a kernel that is ideally suited for a certain kind of application. We investigate several such approaches such as the use of the generalized Sobolev spaces of Chapter 8 (which are closely related to the Green's kernels of Chapter 6), or building a kernel from its eigenfunctions and eigenvalues (see, e.g., Section 3.9 and Chapter 7). This latter idea of working with a kernel in series form — rather than in closed form — ties in nicely with the Hilbert–Schmidt framework.

A third important topic is the implementation of various types of kernels in MATLAB. Chapter 4 lays the groundwork upon which later applications build upon. We go considerably beyond the use of basic radial kernels (RBFs) in this book. In particular, we consider the use of anisotropic kernels (both in radial and in tensor product form), zonal kernels, compactly supported kernels, space-time kernels, and kernels given only in series form.

In Part II we apply the fundamental concepts developed in the first part to applications in data fitting, machine learning, the numerical solution of partial differential equations, and finance. These concepts are illustrated in the context of kernel methods with examples based on accessible "textbook" versions of MATLAB code. However, our `GaussQR` library (discussed in Appendix D) contains "production" versions of the code which is also accessible to the interested reader. Discussion of context that deals with computational cost is spread throughout the book and can be found by looking up this topic in the index.

This book contains 72 MATLAB programs, 76 figures, 11 tables, and more than 650 references). Some code requires one or more of the following MATLAB toolboxes: Curve Fitting Toolbox™, Optimization Toolbox™, Statistics and Machine Learning Toolbox™. All MATLAB programs printed in the text are contained — in an extended version — in the `GaussQR` library. The code was developed and tested on MATLAB R2015a, the most recent update prior to publication; however, earlier versions of the code were also used on older MATLAB releases.

The manuscript for this book is based on the lecture notes for an evolving course on Meshfree Methods taught by the first author every two years at the Illinois Institute of Technology. Moreover, many of the ideas presented in this book emerged from discussions and research performed in IIT's Meshfree Methods seminar, a group co-organized by the first author together with Fred Hickernell. We thank all the participants of this group for their contributions, discussions, and willingness to be a sounding board for our ideas. However, special thanks are due to Qi Ye, whose Ph.D. research on generalized Sobolev spaces formed the basis for Chapter 8, and to Fred Hickernell, who inspired us with many insightful comments and ideas, some of which found their way into this book (such as the Chebyshev kernels of Section 3.9.2 and some of the fundamental insights on kernel parametrizations presented in Chapter 14).

Thanks are also due to Bengt Fornberg and Natasha Flyer for welcoming the second author to their research seminars at CU–Boulder, as well as his colleagues at UC–Denver, most notably Jan Mandel, Loren Cobb and Troy Butler. We thank MathWorks and Naomi Fernandes at their book program for providing us with a complimentary copy of their software and for helping us with some issues that arose during beta-testing of the latest release. Finally, many thanks are due to Rajesh Babu, Rok Ting Tan, and Elena Nash (as well as all the unnamed people working in the background) at World Scientific Publishing Co. who helped make this project a success.

Greg Fasshauer and Mike McCourt
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