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Extensions of Positive Definite Functions

Applications and Their Harmonic Analysis



Springer

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Dedicated to the memory of

*William B. Arveson*¹

(November 22, 1934–November 15, 2011)

*Edward Nelson*²

(May 4, 1932–September 10, 2014)

¹William Arveson (1934–2011) worked on operator algebras and harmonic analysis, and his results have been influential in our thinking and in our approach to the particular extension questions we consider here. In fact, Arveson's deep and pioneering work on completely positive maps may be thought of as a noncommutative variant of our present extension questions. We have chosen to give our results in the commutative setting, but readers with interests in noncommutative analysis will be able to make the connections. While the noncommutative theory was initially motivated by the more classical commutative theory, the tools involved are different, and there are not always direct links between theorems in one area and the other. One of Arveson's earlier results in operator algebras is an extension theorem for completely positive maps taking values in the algebra of all bounded operators on a Hilbert space. His theorem led naturally to the question of injectivity of von Neumann algebras in general, which culminated in the profound work by Alain Connes relating injectivity to hyperfiniteness. One feature of Arveson's work dating back to a series of papers in the 60s and 70s, is the study of noncommutative analogues of notions and results from classical harmonic analysis, including the Shilov and Choquet boundaries. The commutative analogues are visible in our present presentation.

²Edward Nelson (1932–2014) was known for his work on mathematical physics, on stochastic processes, on representation theory, and on mathematical logic. Especially his work on the first three areas has influenced our thinking, in more detail, infinite-dimensional group representations, the mathematical treatment of quantum field theory, the use of stochastic processes in quantum mechanics, and his reformulation of probability theory. Readers looking for beautiful expositions of the foundations in these areas are referred to the following two sets of very accessible lecture notes by Nelson, *Dynamical Theory of Brownian Motion*; and *Topics in Dynamics 1: Flows.*, both in Princeton University Press, the first 1967 and the second 1969.

Our formulation of the present extension problems in the form of type I and type II extensions (see Chap. 5 below) was especially influenced by independent ideas and results of both Bill Arveson and Ed Nelson. We use the two Nelson papers [Nel59, NS59] in our analysis of extensions of locally defined positive definite functions on Lie groups.

Foreword

We study two classes of extension problems and their interconnections:

- (1) Extension of positive definite (p.d.) continuous functions defined on subsets in locally compact groups G
- (2) In case of Lie groups, representations of the associated Lie algebras $La(G)$ by unbounded skew-Hermitian operators acting in a reproducing kernel Hilbert space (RKHS) \mathcal{H}_F

Our analysis is nontrivial even if $G = \mathbb{R}^n$ and even if $n = 1$. If $G = \mathbb{R}^n$, we are concerned in (2) with finding systems of strongly commuting self-adjoint operators $\{T_i\}$ extending a system of commuting Hermitian operators with common dense domain in \mathcal{H}_F .

Why extensions? In science, experimentalists frequently gather spectral data in cases when the observed data is limited, for example, limited by the precision of instruments or on account of a variety of other limiting external factors. (For instance, the human eye can only see a small portion of the electromagnetic spectrum.) Given this fact of life, it is both an art and a science to still produce solid conclusions from restricted or limited data. In a general sense, our monograph deals with the mathematics of extending some such given partial datasets obtained from experiments. More specifically, we are concerned with the problems of extending available partial information, obtained, for example, from sampling. In our case, the limited information is a restriction, and the extension in turn is the full positive definite function (in a dual variable); so an extension if available will be an everywhere defined generating function for the exact probability distribution which reflects the data, if it were fully available. Such extensions of local information (in the form of positive definite functions) will in turn furnish us with spectral information. In this form, the problem becomes an operator extension problem, referring to operators in a suitable reproducing kernel Hilbert spaces (RKHSs). In our presentation, we have stressed hands-on examples. Extensions are almost never unique, and so we deal with both the question of existence and, if there are extensions, how they relate back to the initial completion problem.

By a theorem of S. Bochner, the continuous p.d. functions are precisely the Fourier transforms of finite positive measures. In the case of locally compact Abelian groups G , the two sides in the Fourier duality are that of the group G itself vs. the dual character group \hat{G} to G . Of course, if $G = \mathbb{R}^n$, we may identify the two.

But in practical applications, a p.d. function will typically be given only as locally or, on some open subset, typically bounded, say an interval if $G = \mathbb{R}^1$ or a square or a disk in case $G = \mathbb{R}^2$. Hence four questions naturally arise:

- (a) Existence of extensions.
- (b) If there are extensions, find procedures for constructing them.
- (c) Moreover, what is the significance of choice of different extensions from available sets of p.d. extensions?
- (d) Finally, what are the generalizations and applications of the results in (a)–(c) to the case of an infinite number of dimensions?

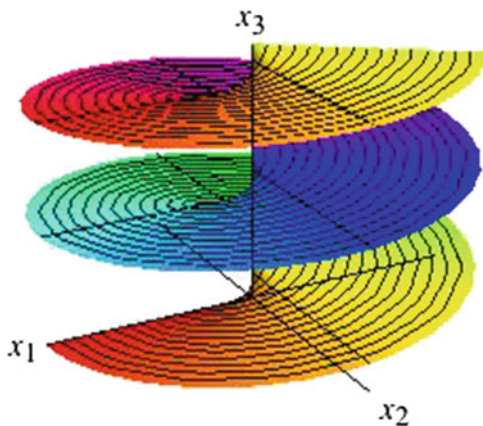
All four questions will be addressed, and the connections between (d) and probability theory will be stressed.

While the theory of p.d. functions is important in many areas of pure and applied mathematics, ranging from harmonic analysis, functional analysis, spectral theory, representations of Lie groups, and operator theory on the pure side to such applications as mathematical statistics, approximation theory, optimization (for more, see details below), and quantum physics, it is difficult for students and for the novice to the field to find accessible presentations in the literature which cover all these disparate points of view, as well as stressing common ideas and interconnections.

We have aimed at filling this gap and with a minimum number of prerequisites. We do expect that readers have some familiarity with measures and their Fourier transform, as well as with operators in Hilbert space, especially the theory of unbounded symmetric operators with dense domain. When needed, we have included brief tutorials. Further, in our cited references, we have included both research papers and books. To help with a historical perspective, we have included discussions of some landmark presentations, especially papers of S. Bochner, M.G. Krein, J. von Neumann, W. Rudin, and I.J. Schöenberg.

The significance to *stochastic processes* of the two questions, (1) and (2) above, is as follows. To simplify, consider first stochastic processes X_t indexed by time t but known only for “small” t . Then the corresponding covariance function $c_X(s, t)$ will also only be known for small values of s and t , or in the case of stationary processes, there is then a locally defined p.d. function F , known only in a bounded interval $J = (-a, a)$ and such that $F(s - t) = c_X(s, t)$. Hence, it is natural to ask how much can be said about extensions to values of t in the complement of J ? For example, what are the possible global extensions X_t , i.e., extension to all $t \in \mathbb{R}$? If there are extensions, then how does information about the locally defined covariance function influence the extended global process? What is the structure of the set of all extensions? The analogue questions are equally interesting for processes indexed by groups more general than \mathbb{R} .

Fig. 1 Riemann surface of $\log z$



Specifically, we consider partially defined p.d. continuous functions F on a fixed group. From F we then build an RKHS \mathcal{H}_F , and the operator extension problem is concerned with operators acting in \mathcal{H}_F and with unitary representations of G acting on \mathcal{H}_F . Our emphasis is on the interplay between the two problems and on the harmonic analysis of our RKHS \mathcal{H}_F .

In the cases of $G = \mathbb{R}^n$ and $G = \mathbb{R}^n/\mathbb{Z}^n$ and generally for locally compact Abelian groups, we establish a new Fourier duality theory, including for $G = \mathbb{R}^n$ a time/frequency duality, where the extension questions (1) are in time domain and extensions from (2) in frequency domain. Specializing to $n = 1$, we arrive of a spectral theoretic characterization of all skew-Hermitian operators with dense domain in a separable Hilbert space, having deficiency indices $(1, 1)$.

Our general results include non-compact and non-Abelian Lie groups, where the study of unitary representations in \mathcal{H}_F is subtle.

While, in the most general case, the obstructions to extendibility (of locally defined positive definite (p.d.) functions) are subtle, we point out that it has several explicit features: algebraic, analytic, and geometric. In Sect. 4.6, we give a continuous p.d. function F in a neighborhood of 0 in \mathbb{R}^2 for which $\text{Ext}(F)$ is empty. In this case, the obstruction for F is geometric in nature and involves properties of a certain Riemann surface. (See Fig. 1, Sect. 4.6, and Figs. 4.9 and 4.10 for details.)

Note on Presentation In presenting our results, we have aimed for a reader-friendly account. We have found it helpful to illustrate the ideas with worked examples. Each of our theorems holds in various degrees of generality, but when appropriate, we have not chosen to present details in their highest level of generality. Rather, we typically give the result in a setting where the idea is more transparent and easier to grasp. We then work the details systematically at this lower level of generality. But we also make comments about the more general versions, sketching these in rough outline. The more general versions of the respective theorems will typically be easy for readers to follow and to appreciate after the idea has already been fleshed out in a simpler context.

We have made a second choice in order to make it easier for students to grasp the ideas as well as the technical details: We have included a lot of worked examples. And at the end of each of these examples, we then outline how the specific details (from the example in question) serve to illustrate one or more features in the general theorems elsewhere in the monograph. Finally, we have made generous use of both tables and figures. These are listed with page references at the end of the book; see the last few items in the Table of Contents. And finally, we included a list of Symbols on page [xxv](#), after Table of Contents.

Preface

The art of doing mathematics consists in finding that special case which contains all the germs of generality.

— David Hilbert

On the one hand, the subject of positive definite (p.d.) functions has played an important role in standard graduate courses and in research papers, over decades, and yet when presenting the material for a particular purpose, the authors have found that there is not a single source which will help students and researchers to quickly form an overview of the essential ideas involved. Over the decades, new ideas have been incorporated into the study of p.d. functions and their more general cousin, p.d. kernels, from a host of diverse areas. An influence of more recent vintage is the theory of *operators in Hilbert space* and their *spectral theory*.

A novelty in our present approach is the use of diverse Hilbert spaces. In summary, to starting with a locally defined p.d. F , there is a natural associated Hilbert space, arising as a reproducing kernel Hilbert space (RKHS), \mathcal{H}_F . Then the question is as follows: When is it possible to realize globally defined p.d. extensions of F with the use of spectral theory for operators in the initial RKHS, \mathcal{H}_F ? And when will it be necessary to enlarge the Hilbert space, i.e., to pass to a *dilation Hilbert space*—a second Hilbert space \mathcal{K} containing an isometric copy of \mathcal{H}_F itself?

The theory of p.d. functions has a large number of applications in a host of areas, for example, in harmonic analysis, in representation theory (of both algebras and groups), in physics, and in the study of probability models, such as stochastic processes. One reason for this is the theorem of Bochner which links continuous p.d. functions on locally compact Abelian groups G to measures on the corresponding dual group. Analogous uses of p.d. functions exist for classes for non-Abelian groups. Even the seemingly modest case of $G = \mathbb{R}$ is of importance in the study of spectral theory for Schrödinger equations. And further, counting the study of Gaussian stochastic processes, there are even generalizations (Gelfand-Minlos) to the case of continuous p.d. functions on Fréchet spaces of test functions which make up part of a Gelfand triple.

These cases will be explored below but with the following important change in the starting point of the analysis—we focus on the case when the given p.d. function is only *partially defined*, i.e., is only known on a proper subset of the ambient group or space. How much of duality theory carries over when only partial information is available?

Applications In *machine learning*, extension problems for p.d. functions and RHKSs seem to be used in abundance. Of course, the functions are initially defined over finite sets which is different from the present setup, but the ideas from our continuous setting do carry over *mutatis mutandis*. Machine learning [PS03] is a field that has evolved from the study of pattern recognition and computational learning theory in artificial intelligence. It explores the construction and study of algorithms that can learn from and make predictions on limited data. Such algorithms operate by building models from “training data” inputs in order to make data-driven predictions or decisions. Contrast this with strictly static program instructions. Machine learning and pattern recognition can be viewed as two facets of the same field.

Another connection between extensions of p.d. functions and neighboring areas is *number theory*: the pair correlation of the zeros of the Riemann zeta function [GM87, HB10]. In the 1970s, Hugh Montgomery (assuming the Riemann hypothesis) determined the Fourier transform of the pair correlation function in number theory (it is a p.d. function). But the pair correlation function is specified only in a bounded interval centered at zero, again consistent with pair correlations of eigenvalues of large random Hermitian matrices (via Freeman Dyson). It is still not known what is the Fourier transform outside of this interval. Montgomery has conjectured that, on all of \mathbb{R} , it is equal to the Fourier transform of the pair correlation of the eigenvalues of large random Hermitian matrices; this is the “pair correlation conjecture.” And it is an important unsolved problem.

Yet another application of the tools for extending locally defined p.d. functions is that of the pioneering work of M.G. Krein, now called the *inverse spectral problem of the strings of Krein*; see [Kot13, Kei99, KW82]. This in turn is directly related to a host of the symmetric moment problems [Chi82]. In both cases, we arrive at the problem of extending a real p.d. function that is initially only known on an interval.

In summary, the purpose of the present monograph is to explore what can be said when a continuous p.d. function is only given on a subset of the ambient group (which is part of the application setting sketched above.) For this problem of partial information, even the case of p.d. functions defined only on bounded subsets of $G = \mathbb{R}$ (say an interval) or on bounded subsets of $G = \mathbb{R}^n$ is of substantial interest.

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We also are pleased to thank anonymous referees for careful reading, for lists of corrections, for constructive criticism, and for many extremely helpful suggestions, for example, pointing out to us more ways that the questions of extensions of fixed locally defined positive definite functions impact yet more areas of mathematics and are also part of important applications to neighboring areas. Remaining flaws are the responsibility of the coauthors.

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Symbols

$(\Omega, \mathcal{F}, \mathbb{P})$	Probability space: sample space Ω , sigma-algebra \mathcal{F} , probability measure \mathbb{P} (pp. 6, 159)
δ_x	Dirac measure, also called Dirac mass (pp. 19, 99)
$\int_J f(t) dX_t$	Ito-integral, defined for $f \in L^2(J)$ (pp. 9, 159)
$\langle \cdot, \cdot \rangle$ or $\langle \cdot, \cdot \rangle_H$	Inner product; we add a subscript (when necessary) in order to indicate which Hilbert space is responsible for the inner product in question. Caution: because of a physics tradition, all of our inner products are linear in the second variable. (This convention further has the advantage of giving simpler formulas in case of reproducing kernel Hilbert spaces (RKHSs).) (pp. 18, 197)
$\langle \lambda, x \rangle$	Duality pairing $\widehat{G} \leftrightarrow G$ of locally compact Abelian groups. (pp. 47, 53)
\mathbb{E}	Expectation, $\mathbb{E}(\cdots) = \int_{\Omega} \cdots d\mathbb{P}$ (pp. 9, 159)
\mathbb{R}	The real line
\mathbb{R}^n	The n -dimensional real Euclidean space
$\mathbb{T}^n = \mathbb{R}^n / \mathbb{Z}^n$	Tori (We identify \mathbb{T} with the circle group.)
\mathbb{Z}	The integers
$\mathfrak{M}_2(\Omega, F)$	Hilbert space of measures on Ω associated to a fixed kernel, or a p.d. function F (pp. 21)
$\mathcal{B}(G)$	The sigma-algebra of all Borel subsets of G (pp. 67, 209)
\mathcal{H}_F	The reproducing kernel Hilbert space (RKHS) of F (pp. 11, 18)
$\mathcal{M}(G)$	All Borel measures on G (pp. 39, 48)
\perp	Perpendicular w.r.t. a fixed Hilbert inner product (pp. 68, 121)
\widehat{G}	The dual character group, where G is a fixed locally compact Abelian group, i.e., $\lambda : G \rightarrow \mathbb{T}$, continuous, $\lambda(x+y) = \lambda(x)\lambda(y)$, $\forall x, y \in G$, $\lambda(-x) = \overline{\lambda(x)}$ (pp. 47, 53)
$\{B_t\}_{t \in \mathbb{R}}$	Standard Brownian motion (pp. 97, 157)
$\{X_g\}_{g \in G}$	Stochastic process indexed by G (pp. 6, 12)
$D^{(F)}$	The derivative operator $F_{\varphi} \mapsto F \frac{d\varphi}{dx}$ (pp. 23, 31)

D^*	Adjoint of a linear operator D (pp. 23, 44)
DEF	The deficiency space of $D^{(F)}$ acting in the Hilbert space \mathcal{H}_F (pp. 23, 127)
$dom(D)$	Domain of a linear operator D (pp. 23, 89)
$Ext(F)$	Set of unitary representations of G on a Hilbert space \mathcal{H} , i.e., the triples (U, \mathcal{H}, k_0) , that extend F (pp. 38, 93)
$Ext_1(F)$	The triples in $Ext(F)$, where the representation space is \mathcal{H}_F and so the extension of F is realized on \mathcal{H}_F (pp. 38, 93)
$Ext_2(F)$	$Ext(F) \setminus Ext_1(F)$, i.e., the extension is realized on an enlargement Hilbert space (pp. 38, 93)
F_φ	The convolution of F and φ , where $\varphi \in C_c(\Omega)$ (pp. 18, 48)
G	Group, with the group operation written $x \cdot y$, or $x + y$, depending on the context
J	Conjugation operator, acting in the Hilbert space \mathcal{H}_F for a fixed local p.d. function F . To say that J is a conjugation means that J is a conjugate linear operator which is also of period 2 (pp. 26, 28)
$La(G)$	The Lie algebra of a given Lie group G (pp. 55, 61)
$Rep(G, \mathcal{H})$	Set of unitary representations of a group G acting on some Hilbert space \mathcal{H} (pp. 91)
$S(= S_2)$	The isometry $S : \mathfrak{M}_2(\Omega, F) \rightarrow \mathcal{H}_F$ (onto) (pp. 21, 85)
T_F	Mercer operator associated to F (pp. 116, 152)
X	Random variable, $X : \Omega \rightarrow \mathbb{R}$ (pp. 9, 159)
ONB	Orthonormal basis (in a Hilbert space) (pp. 85, 115)
p.d.	Positive definite (pp. 1, 15)
RKHS	Reproducing kernel Hilbert space (pp. 18, 34)