Reproducing kernel Hilbert spaces

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Lecture given on March 8, 2017 at the
Mathematical Junior Kolloquium of the University of Vienna

For the slides and for more details on the mathematics see
`http://www.mat.univie.ac.at/~neum/cohSpaces.html`

Abstract

This lecture gives an introduction to reproducing kernel Hilbert spaces and their basic properties.

Reproducing kernel Hilbert spaces and the associated coherent states have applications in complex analysis and group theory, but also many other fields of mathematics, statistics, and physics.

To illustrate their power it is shown how to derive simple error estimates for numerical integration.

Then the most relevant theorems about reproducing kernel Hilbert spaces are presented.

Reproducing kernels

We write $\phi^*\psi$ or $\langle\phi,\psi\rangle$ for the inner product of two vectors ϕ,ψ in a complex Hilbert space. The inner product is taken to be antilinear in the first argument.

A **reproducing kernel Hilbert space** is a Hilbert space $\mathbb{K}$ of complex-valued functions on a set Z with an involution $^-$ together with a **reproducing kernel** $K : Z \times Z \to \mathbb{C}$ such that the functions k_z $(z \in Z)$ defined by

$$k_z(x) := K(\overline{x}, z) \tag{1}$$

span a space dense in $\mathbb{K}$ and satisfy

$$\psi(z) = k_{\overline{z}}^*\psi \quad \text{for all } \psi \in \mathbb{K},\ z \in Z. \tag{2}$$

(The involution can be trivial. If Z is a complex manifold it is complex conjugation.)

Examples of reproducing kernels were first discussed
by ZAREMBA 1907 in the context of boundary value problems and
by MERCER 1909 in the context of integral equations.

The theory was systematically developed by ARONSZAJN 1950,
KREIN 1963, and others, based on the notion of **functions of positive type**.

The content of this lecture is based on very old mathematics, all discovered before 1980.

The news are in the companion lecture today at 16:15.

I learnt about reproducing kernels about 30 years ago from a paper by DAVIS & RABINOWITZ 1954 about errors in numerical quadrature.

With time I learnt about many other applications in many fields of mathematics, statistics, and physics.

Now I recognize that the concept of a **coherent space**, the algebraic structure underlying reproducing kernel Hilbert spaces, is one of the basic unifying concepts of large parts of mathematics and its applications.

Illustrative application:

Error bounds for numerical integration

The **Hardy space** (Hardy 1915) is the space of complex-valued functions analytic in the open complex unit disk and square integrable on its boundary. An equivalent description is as the space of power series

$$f(x) = \sum_{k=0}^{\infty} f_k x^k$$

with complex f_k and finite $\sum |f_k|^2$, with inner product

$$f^* g := \sum_{k=0}^{\infty} \overline{f}_k g_k.$$

The **Szegö kernel** $K(z, z') := (1 - \overline{z} z')^{-1}$ (Szegö 1911) is a reproducing kernel for the Hardy space. (This is essentially the Cauchy integral formula.)

The resulting functions k_z are given by $k_z(x) := (1 - xz)^{-1}$.

An N-point **quadrature formula** of order $p \geq 0$ for approximating the integral

$$I(f) := \int_a^b f(x)dx$$

over an interval $[a,b] \subset]-1,1[$ is a linear functional of the form

$$Q(f) = \sum_{j=1}^{N} \alpha_j f(x_j), \quad x_j \in [a,b]$$

such that $Q(f) = I(f)$ for all polynomials of degree $\leq p$.

Because of the reproducing kernel property, the integration error $E(f) := I(f) - Q(f)$ is a continuous linear functional with $E(1) = 0$.

Define $Ek(z) := Ek_z$. Then, if C_Q is a bound on $\|Ek\|$ and the range of f is contained in a disk with center c_f and radius r_f,

$$|Ef| = |E(f - c_f)| = |Ek^*(f - c_f)| \leq \|Ek\| \; \|f - c_f\| \leq C_Q r_f.$$

Linear transformations produce error bounds for quadrature rules over arbitrary intervals $[a.b]$, using range enclosures for arguments ranging over open disks whose union covers $[a, b]$.

Given an expression for $f(x)$, such disks can be computed using a generalized interval arithmetic for complex disks (Henrici 1971).

The constants C_Q can be precalculated for all integration formulas of interest. Using outward rounding, this gives mathematically rigorous and efficiently computable error bounds even with floating-point computations (Eiermann 1989).

Functions of positive type

A complex $n \times n$ matrix G is **Hermitian** if $\overline{G}_{jk} = G_{kj}$ for $j, k = 1, \ldots, n$, **positive semidefinite** if $u^* G u \geq 0$ for all $u \in \mathbb{C}^n$, and **conditionally semidefinite** if $u^* G u \geq 0$ for all $u \in \mathbb{C}^n$ with $\sum_k u_k = 0$.

Let Z be a nonempty set. We call a function $F : Z \times Z \to \mathbb{C}$ **of positive type** (resp. **conditionally positive**) over Z if, for every finite sequence $z_1, \ldots, z_n$ in Z, the **Gram matrix** of $z_1, \ldots, z_n$, i.e., the $n \times n$-matrix G with entries

$$G_{jk} = F(z_j, z_k), \tag{3}$$

is Hermitian and positive semidefinite (resp. conditionally semidefinite).

In particular, every function of positive type is conditionally positive.

Three almost trivial results have quite nontrivial converses.

Proposition 1. Let Z be a subset of a Hilbert space $\mathbb{H}$. Then the functions $F, F', F'' : Z \times Z \to \mathbb{C}$ defined by

$$F(z, z') := z^* z', \quad F'(z, z') := z'^* z, \quad F''(z, z') := \mathrm{Re}\ z^* z'$$

are of positive type.

The converse is a famous theorem by Aronszajn (or Moore) discussed later.

Proposition 2. If $F : Z \times Z \to \mathbb{C}$ is conditionally positive then, for any function $f : Z \to \mathbb{C}$ and any $\gamma \geq 0$, the function $\widetilde{F} : Z \times Z \to \mathbb{C}$ defined by

$$\widetilde{F}(z, z') := \overline{f(z)} + f(z') + \gamma F(z, z') \quad \text{for } z, z' \in Z \tag{4}$$

is conditionally positive.

A converse is given by a theorem by SCHOENBERG discussed later.

Proposition 3. Let Z be a subset of a Euclidean space $\mathbb{H}$. Then for any function $g : Z \to \mathbb{C}$, the function $\widetilde{F} : Z \times Z \to \mathbb{C}$ defined by

$$\widetilde{F}(z, z') := \overline{g(z)} + g(z') - \|\overline{z} - z'\|^2 \quad \text{for } z, z' \in Z \tag{5}$$

is conditionally positive.

A converse is given by a theorem by MENGER discussed later.

Less trivial but important are the following two constructions:

Theorem 4.
(i) The pointwise product of functions of positive type on the same set is of positive type.
(ii) The composition of a function of positive type with values in a domain $D \subset \mathbb{C}$ with a completely positive function $\phi : D \to \mathbb{C}$ is of positive type.

Here $\phi : D \to \mathbb{C}$ is called **completely positive** if $\phi(x)$ has a convergent expansion in powers of x with real, nonnegative coefficients.

Many other constructions are known.

Hilbert spaces from kernels

Theorem 5. (Moore, Aronszajn)
Let $K : Z \times Z \to \mathbb{C}$ be of positive type. Then there is a unique Hilbert space $\overline{\mathbb{Q}}$ of complex-valued functions on Z with the Hermitian inner product $\langle \cdot, \cdot \rangle$ (antilinear in the first component) such that the following properties hold.

(i) $\overline{\mathbb{Q}}$ contains the functions $q_z : Z \to \mathbb{C}$ defined for $z \in Z$ by

$$q_z(x) := K(x, z) = \overline{K(z, x)}. \quad \textbf{(coherent states)} \tag{6}$$

(ii) The space $\mathbb{Q}$ of finite linear combinations of the q_z is dense in $\overline{\mathbb{Q}}$.

(iii) The following relations hold:

$$\langle q_z, q_x \rangle = K(z, x), \tag{7}$$

$$\psi(z) = \langle q_z, \psi \rangle \quad \text{for all } \psi \in \overline{\mathbb{Q}}. \quad \textbf{(reproducing kernel)} \tag{8}$$

(iv) For each $z \in Z$, the linear functional ι_z defined by

$$\iota_z \psi := \psi(z) \tag{9}$$

is continuous.

If we define, with an arbitrary choice of an involution on Z, for $\psi \in \overline{\mathbb{Q}}$ the function $\widetilde{\psi} : Z \to \mathbb{C}$ by

$$\widetilde{\psi}(z) := \psi(\widetilde{z}),$$

(8) says that $\mathbb{H} := \{\psi \mid \widetilde{\psi} \in \overline{\mathbb{Q}}\}$ is a reproducing kernel Hilbert space with reproducing kernel K and $k_z = \widetilde{q}_z$.

A paper by KOLMOGOROV 1941 contains the result for the special case where Z is countable.

ARONSZAJN 1943 states the theorem in full generality and gives a detailed proof in French. His later English paper from 1950 states the theorem on p.344 and attributes it to MOORE.

ARONSZAJN 1950 cites on p.338 a 1935 book by MOORE and a very short notice from 1916, but the theorem does not seem to be in one of these references.

MOORE's book discusses in Chapter III near p.182 functions of positive type under the name *positive Hermitian matrices* but does not construct a Hilbert space from them.

A book by FARAUT & KORÁNYI 1994 ascribes the theorem to a paper by BERGMAN 1933, but the theorem does not seem to be there either.

The reproducing kernel has the following orthogonal resolution:

Proposition 6. Let ψ_α $(\alpha \in I)$ be an orthonormal basis for $\overline{\mathbb{Q}}$. Then

$$K(z,w) = \sum_{\alpha \in I} \psi_\alpha(z)\overline{\psi_\alpha(w)}. \tag{10}$$

The coherent states can be characterized as follows:

Theorem 7. (Bochner 1922)
Let $K : Z \times Z \to \mathbb{C}$ be of positive type, and let $\mathbb{Q}$ be the space constructed in Theorem 5. If $x \in Z$ satisfies $K(x,x) \neq 0$ then

$$\min\{\psi^*\psi \mid \psi \in \mathbb{Q},\ \psi(x) = \alpha\} = \frac{|\alpha|^2}{K(x,x)}.$$

If $\alpha = K(x,x)$, the minimum is attained precisely at q_x.

The functions belonging to the Hilbert space have the following characterization:

Theorem 8. (Kreĭn 1963)
Let $K : Z \times Z \to \mathbb{C}$ be of positive type and $\psi : Z \to \mathbb{C}$. Define the function $K_\varepsilon : Z \times Z \to \mathbb{C}$ by

$$K_\varepsilon(z, z') := K(z, z') - \varepsilon\psi(z)\overline{\psi(z')}.$$

(i) If $\psi \in \overline{\mathbb{Q}}$ and $0 < \varepsilon \leq \|\psi\|^{-2}$ then K_ε is of positive type.
(ii) If K_ε is of positive type for some $\varepsilon > 0$ then $\psi \in \overline{\mathbb{Q}}$.

Conditionally positive functions

Conditionally positive functions have the following characterizations:

Theorem 9. (Schoenberg 1942)
If F is conditionally positive then the function P_a, defined for any $a \in Z$ by

$$P_a(z, z') := F(z, z') - F(z, a) - F(a, z') + F(a, a), \qquad (11)$$

is of positive type. Conversely, if a map $F : Z \times Z \to \mathbb{C}$ is such that if P_a is of positive type for *some* $a \in Z$ then F is conditionally positive.

Theorem 10. (i) A map $F : Z \times Z \to \mathbb{C}$ is conditionally positive iff there is an embedding $z \to q_z$ of Z into a Euclidean space $\mathbb{H}$ such that

$$F(z, z') = \overline{f(z)} + f(z') + q_z^* q_{z'} \tag{12}$$

holds for some $f : Z \to \mathbb{C}$.

(ii) (Menger 1928)

A map $F : Z \times Z \to \mathbb{C}$ satisfying $F(z, z') = F(z', z)$ for $z, z' \in Z$ is conditionally positive iff there is an embedding $z \to q_z$ of Z into a real Euclidean space such that

$$F(z, z') = g(z) + g(z') - \|q_z - q_{z'}\|^2 \tag{13}$$

holds for some $g : Z \to \mathbb{R}$.

The Berezin–Wallach set

Many reproducing kernels of interest have the exponential form discussed in the following theorem.

Theorem 11. (SCHOENBERG 1942, HERZ 1962, HORN 1969)
(i) If $F : Z \times Z \to \mathbb{C} \cup \{-\infty\}$ is conditionally positive then, for all $\beta > 0$,

$$K(z, z') := e^{\beta F(z,z')} \tag{14}$$

(where $e^{-\infty} := 0$) is of positive type.
(ii) Let $F : Z \times Z \to \mathbb{C} \cup \{-\infty\}$. If there is a sequence of positive numbers β_k converging to 0 such that

$$K_k(z, z') := e^{\beta_k F(z,z')}$$

is of positive type for all k then F is conditionally positive.

Here a function $F : Z \times Z \to \mathbb{C} \cup \{-\infty\}$ is called **conditionally positive** if
(i) either F takes only infinite values,
(ii) or there is an equivalence relation $\equiv$ on Z such that F is conditionally positive on each equivalence class, and $F(z, z') = -\infty$ whenever $z \not\equiv z'$.

The **Berezin–Wallach set** of a mapping $F : Z \times Z \to \mathbb{C} \cup \{\infty\}$ is the set $W(F)$ of nonnegative real numbers β for which

$$K(z, z') := e^{\beta F(z,z')} \tag{15}$$

is of positive type.

This set was introduced by Wallach 1979 in the context of representations of Lie groups. But already earlier, Berezin 1975 computed the Berezin–Wallach set for the case when $-F$ is the Kähler potential of a Siegel domain.

Theorem 12. (i) The Berezin–Wallach set $W(F)$ is a closed set containing 0.
(ii) $W(F)$ contains with β and β' their sum and hence all linear combinations with nonnegative integral coefficients.
(iii) If $W(F)$ contains an open set it contains all sufficiently large positive real numbers.
(iv) If F is conditionally positive then $W(F)$ contains all nonnegative real numbers.
(v) If 0 is a limit point of $W(F)$ then F is conditionally positive.

Coherent spaces and coherent manifolds

Coherent spaces and coherent manifolds

are the subject of the following Mathematical Kolloquium lecture.

A **coherent space** is a nonempty set Z with a distinguished function $K : Z \times Z \to \mathbb{C}$ of positive type called the **coherent product**.

A **coherent manifold** is a smooth ($= C^\infty$) real manifold Z with a smooth coherent product $K : Z \times Z \to \mathbb{C}$ with which Z is a coherent space.

Thus coherent spaces abstract the essential algebra needed to define a reproducing kernel Hilbert space.

On the other hand, coherent manifolds have the additional structure needed to be able to interpret objects related to reproducing kernel Hilbert space in a geometric way.

Coherent spaces are closely related to

(i) Christoffel–Darboux kernels for orthogonal polynomials,
(ii) Euclidean representations of finite geometries,
(iii) zonal spherical functions on symmetric spaces,
(iv) coherent states for Lie groups acting on homogeneous spaces,
(v) unitary representations of groups,
(vi) abstract harmonic analysis,
(vii) states of C^*-algebras in functional analysis,
(viii) reproducing kernel Hilbert spaces in complex analysis,
(ix) Pick–Nevanlinna interpolation theory,
(x) transfer functions in control theory,
(xi) positive definite kernels for radial basis functions,
(xii) positive definite kernels in data mining,

and

(xiii) positive definite functions in probability theory,
(xvi) exponential families in probability theory and statistics,
(xv) the theory of random matrices,
(xvi) Hida distributions for white noise analysis,
(xvii) Kähler manifolds and geometric quantization,
(xviii) coherent states in quantum mechanics,
(xix) squeezed states in quantum optics,
(xx) inverse scattering in quantum mechanics,
(xxi) Hartree–Fock equations in quantum chemistry,
(xxii) mean field calculations in statistical mechanics,
(xxiii) path integrals in quantum mechanics,
(xxiv) functional integrals in quantum field theory,
(xxv) integrable quantum systems.

Thank you for your attention!

For the slides and for more details on the mathematics see
`http://www.mat.univie.ac.at/~neum/cohSpaces.html`