Lecture 8:
Infinite-Dimensional Generalization continued

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Infinite-Dimensional Generalization: The K Operator and its Eigenbasis

Making the Derivative Operator Hermitian

We know that taking derivatives converts functions to other functions. Let's make this an operator D on our space by defining

$$D\,|f\,\rangle = |df/dx\,\rangle \tag{3.155}$$

We are implicitly making this definition in the $\{|x\,\rangle\}$ basis, but that is sensible since we have no other basis yet for our space! The matrix elements of D are easy to find. We recognize from our initial rules for the infinite extension that

$$\langle x\,|\,D\,|f\,\rangle = \left\langle x \,\middle|\, \frac{df}{dx} \right\rangle = \frac{df}{dx} \tag{3.156}$$

We also may write

$$\langle x\,|\,D\,|f\,\rangle = \int_a^b dx' \langle x\,|\,D\,|x'\,\rangle\langle x'\,|f\,\rangle = \int_a^b dx' \langle x\,|\,D\,|x'\,\rangle f(x') \tag{3.157}$$

Infinite-Dimensional Generalization: The K Operator and its Eigenbasis (cont.)

Putting the two together gives

$$\int_a^b dx' \langle x \,|\, D \,|x'\,\rangle f(x') = \frac{d}{dx} f(x) \tag{3.158}$$

That is, $\langle x \,|\, D \,|x'\,\rangle$ has the same behavior as $\left(\frac{d}{dx}\delta(x - x')\right) = \delta(x - x')\frac{d}{dx'}$; *i.e.*,

$$D_{xx'} \equiv \langle x \,|\, D \,|x'\,\rangle = \left(\frac{d}{dx}\delta(x - x')\right) = \delta(x - x')\frac{d}{dx'} \tag{3.159}$$

Unfortunately, D is not Hermitian. The conjugate transpose of the above matrix element is obtained by exchanging $x \leftrightarrow x'$; the conjugation does nothing because everything is real. So we have

$$D^*_{x'x} = \frac{d}{dx'}\delta(x' - x) = \frac{d}{dx'}\delta(x - x') = -\frac{d}{dx}\delta(x - x') = -D_{xx'} \tag{3.160}$$

where the first step is obtained by taking the conjugate transpose, the second by using the evenness of the delta function, and the third using Equations 3.138 and 3.141 together. So we have that D is in fact anti-Hermitian instead of Hermitian!

Infinite-Dimensional Generalization: The K Operator and its Eigenbasis (cont.)

The obvious solution is to consider a new operator K with

$$K = -iD \tag{3.161}$$

(The reason for the negative sign will become apparent later.) The Hermiticity requirement seems obviously met because the $-i$ provides the necessary sign flip. However, we must be careful about believing the above arithmetic – recall that these expressions only hold true when included in an integral. If we consider the expression $\langle g \,|\, K \,|f \,\rangle$, we see that this caveat becomes apparent. We first note that, if K is Hermitian, we have

$$\langle g \,|\, K \,|f \,\rangle = \langle g \,|K\, f \,\rangle = \langle K\, f \,|g \,\rangle^* = \langle f \,|\, K^\dagger |g \,\rangle^* = \langle f \,|\, K \,|g \,\rangle^* \tag{3.162}$$

Infinite-Dimensional Generalization: The K Operator and its Eigenbasis (cont.)

Let's calculate the expressions on the two ends explicitly by going through the matrix elements in the $\{|x\rangle\}$ basis:

$$\langle g\,|\,K\,|f\rangle = \int_a^b dx \int_a^b dx' \langle g\,|x\rangle\langle x\,|\,K\,|x'\rangle\langle x'\,|f\rangle \tag{3.163}$$

$$= \int_a^b dx\, g^*(x)\left[-i\frac{df}{dx}\right] = -i\int_a^b dx\, g^*(x)\left[\frac{df}{dx}\right]$$

$$\langle f\,|\,K\,|g\rangle^* = \left[\int_a^b dx \int_a^b dx' \langle f\,|x\rangle\langle x\,|\,K\,|x'\rangle\langle x'\,|g\rangle\right]^* \tag{3.164}$$

$$= \left[\int_a^b dx\, f^*(x)\left[-i\frac{dg}{dx}\right]\right]^* = i\int_a^b dx\,\left[\frac{dg^*}{dx}\right] f(x)$$

These two expressions are equal via integration by parts only if the surface term vanishes:

$$-i\, g^*(x)\, f(x)\big|_a^b \tag{3.165}$$

Infinite-Dimensional Generalization: The K Operator and its Eigenbasis (cont.)

Thus, **in order to make K a Hermitian operator, we must restrict our vector space to contain only functions that meet the condition that the above surface term vanishes for all members of the space.**

Shankar gives the example that this condition might be met by functions that vanish at the endpoints. Another example would be functions that take on equal values at the two endpoints. Shankar discusses a couple of other cases. It suffices here to say that conditions are frequently placed on the functions that can belong to the vector space of states in order to ensure that desired Hermitian operators are Hermitian.